



Full wwPDB EM Validation Report ⓘ

Aug 8, 2026 – 08:21 am BST

PDB ID : 30FF / pdb_000030ff
EMDB ID : EMD-57691
Title : TFIID-containing RNA polymerase II pre-initiation complex in the presence of the +1 nucleosome
Authors : Zhan, Y.; Abril-Garrido, J.; Grabbe, F.; Seweryn, P.; Neef, U.; Dienemann, C.; Cramer, P.
Deposited on : 2026-04-22
Resolution : 8.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

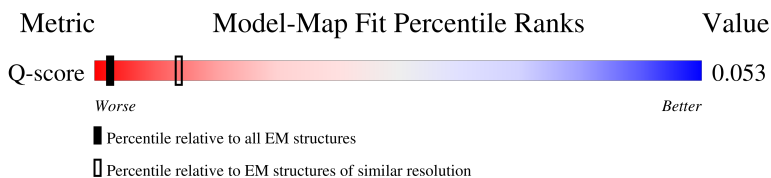
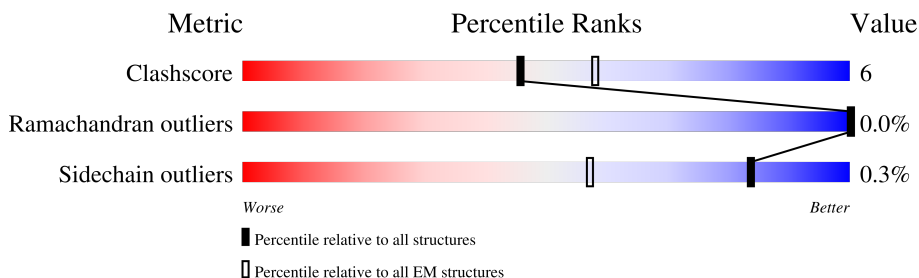
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



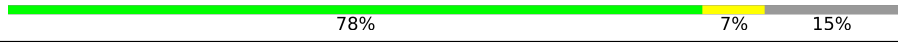
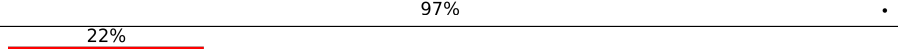
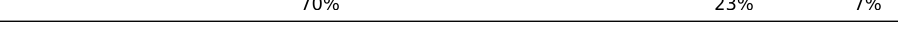
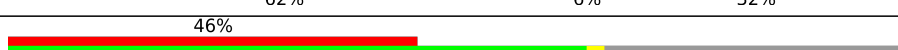
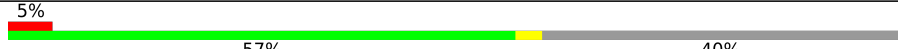
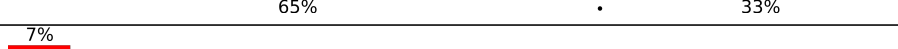
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	328 (8.00 - 9.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	782	
2	1	760	
3	2	548	
4	3	462	

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Mol	Chain	Length	Quality of chain
5	4	395	
6	5	308	
7	6	71	
8	7	309	
9	8	346	
10	9	323	
11	A	1984	
12	B	1300	
13	C	275	
14	D	184	
15	DA	1893	
16	DB	1199	
17	DD	1085	
17	Dd	1085	
18	DE	800	
18	De	800	
19	DF	677	
19	Df	677	
20	DG	349	
21	DH	310	
22	DI	264	
22	Di	264	
23	DJ	218	
23	Dj	218	
24	DL	161	

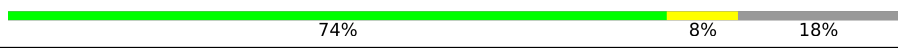
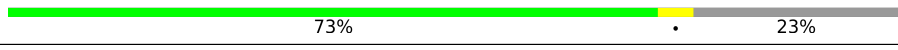
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Mol	Chain	Length	Quality of chain
24	Dl	161	
25	Dc	929	
26	Dk	211	
27	Dm	124	
28	E	210	
29	F	127	
30	G	172	
31	H	150	
32	I	125	
33	J	67	
34	K	117	
35	L	58	
36	M	316	
37	N	227	
38	O	339	
39	Q	517	
40	R	249	
41	T	227	
42	U	376	
43	V	109	
44	W	439	
45	X	291	
46	a	136	
46	e	136	
47	b	103	

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Mol	Chain	Length	Quality of chain
47	f	103	
48	c	130	
48	g	130	
49	d	126	
49	h	126	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	2A1	0	801	-	X	-	-
50	2A1	0	804	-	X	-	-
50	2A1	0	807	-	X	-	-
50	2A1	0	812	-	X	-	-
50	2A1	0	815	-	X	-	-
50	2A1	2	603	-	X	-	-
50	2A1	2	604	-	X	-	-
50	2A1	N	301	-	X	-	-
50	2A1	N	303	-	X	-	-
50	2A1	N	304	-	X	-	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 125749 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

- Molecule 2 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	714	Total	C	N	O	S	0	0
			5751	3683	999	1040	29		

- Molecule 3 is a protein called General transcription factor IIIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	265	Total	C	N	O	S	0	0
			2167	1382	378	395	12		

- Molecule 4 is a protein called General transcription factor IIIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	421	Total	C	N	O	S	0	0
			3338	2154	584	587	13		

- Molecule 5 is a protein called General transcription factor IIIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	347	Total	C	N	O	S	0	0
			2732	1726	471	508	27		

- Molecule 6 is a protein called General transcription factor IIIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	263	Total	C	N	O	S	0	0
			2066	1323	344	380	19		

- Molecule 7 is a protein called General transcription factor IIIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	69	Total	C	N	O	S	0	0
			549	352	88	106	3		

- Molecule 8 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	212	Total	C	N	O	S	0	0
			1724	1083	297	332	12		

- Molecule 9 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	299	Total	C	N	O	S	0	0
			2378	1535	406	426	11		

- Molecule 10 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	287	Total	C	N	O	S	0	0
			2334	1493	402	422	17		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1423	Total	C	N	O	S	0	0
			11274	7092	2016	2094	72		

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	1136	Total	C	N	O	S	0	0
			9076	5739	1597	1676	64		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 15 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	DA	558	Total	C	N	O	S	0	0
			4563	2913	791	832	27		

- Molecule 16 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	DB	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 17 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	DD	159	Total	C	N	O	S	0	0
			1331	830	248	250	3		
17	Dd	158	Total	C	N	O	S	0	0
			1308	814	238	253	3		

- Molecule 18 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	DE	546	Total	C	N	O	S	0	0
			4364	2766	757	820	21		
18	De	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DE	40	THR	PRO	conflict	UNP Q8C092
DE	?	-	GLY	deletion	UNP Q8C092
DE	53	ALA	VAL	conflict	UNP Q8C092
DE	54	SER	ALA	conflict	UNP Q8C092
DE	55	SER	ALA	conflict	UNP Q8C092
DE	56	SER	ALA	conflict	UNP Q8C092
DE	57	THR	ALA	conflict	UNP Q8C092
DE	67	THR	GLY	conflict	UNP Q8C092

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Chain	Residue	Modelled	Actual	Comment	Reference
DE	85	ALA	PRO	conflict	UNP Q8C092
DE	86	PRO	ALA	conflict	UNP Q8C092
DE	87	ASP	GLU	conflict	UNP Q8C092
DE	108	LYS	ASN	conflict	UNP Q8C092
DE	121	GLY	ARG	conflict	UNP Q8C092
DE	136	VAL	LEU	conflict	UNP Q8C092
DE	138	SER	GLY	conflict	UNP Q8C092
DE	143	VAL	ALA	conflict	UNP Q8C092
DE	144	THR	ALA	conflict	UNP Q8C092
DE	155	ALA	VAL	conflict	UNP Q8C092
DE	158	PRO	SER	conflict	UNP Q8C092
DE	162	ASP	GLU	conflict	UNP Q8C092
DE	170	GLY	VAL	conflict	UNP Q8C092
DE	171	ALA	THR	conflict	UNP Q8C092
DE	172	THR	SER	conflict	UNP Q8C092
DE	174	VAL	PHE	conflict	UNP Q8C092
DE	188	GLY	ALA	conflict	UNP Q8C092
DE	310	SER	TYR	conflict	UNP Q8C092
DE	635	PHE	TYR	conflict	UNP Q8C092
DE	741	ILE	VAL	conflict	UNP Q8C092
De	40	THR	PRO	conflict	UNP Q8C092
De	?	-	GLY	deletion	UNP Q8C092
De	53	ALA	VAL	conflict	UNP Q8C092
De	54	SER	ALA	conflict	UNP Q8C092
De	55	SER	ALA	conflict	UNP Q8C092
De	56	SER	ALA	conflict	UNP Q8C092
De	57	THR	ALA	conflict	UNP Q8C092
De	67	THR	GLY	conflict	UNP Q8C092
De	85	ALA	PRO	conflict	UNP Q8C092
De	86	PRO	ALA	conflict	UNP Q8C092
De	87	ASP	GLU	conflict	UNP Q8C092
De	108	LYS	ASN	conflict	UNP Q8C092
De	121	GLY	ARG	conflict	UNP Q8C092
De	136	VAL	LEU	conflict	UNP Q8C092
De	138	SER	GLY	conflict	UNP Q8C092
De	143	VAL	ALA	conflict	UNP Q8C092
De	144	THR	ALA	conflict	UNP Q8C092
De	155	ALA	VAL	conflict	UNP Q8C092
De	158	PRO	SER	conflict	UNP Q8C092
De	162	ASP	GLU	conflict	UNP Q8C092
De	170	GLY	VAL	conflict	UNP Q8C092
De	171	ALA	THR	conflict	UNP Q8C092

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Chain	Residue	Modelled	Actual	Comment	Reference
De	172	THR	SER	conflict	UNP Q8C092
De	174	VAL	PHE	conflict	UNP Q8C092
De	188	GLY	ALA	conflict	UNP Q8C092
De	310	SER	TYR	conflict	UNP Q8C092
De	635	PHE	TYR	conflict	UNP Q8C092
De	741	ILE	VAL	conflict	UNP Q8C092

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	DF	408	Total	C	N	O	S	0	0
			3109	1970	542	579	18		
19	Df	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DG	145	Total	C	N	O	S	0	0
			1180	748	217	211	4		

- Molecule 21 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	DH	209	Total	C	N	O	S	0	0
			1633	1034	283	311	5		

- Molecule 22 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	DI	120	Total	C	N	O	S	0	0
			959	610	166	177	6		
22	Di	121	Total	C	N	O	S	0	0
			967	615	167	178	7		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	6	THR	MET	conflict	UNP Q17QQ4
DI	138	THR	ALA	conflict	UNP Q17QQ4
DI	168	GLN	PRO	conflict	UNP Q17QQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
DI	169	THR	ALA	conflict	UNP Q17QQ4
DI	180	MET	VAL	conflict	UNP Q17QQ4
DI	231	MET	VAL	conflict	UNP Q17QQ4
DI	240	SER	ALA	conflict	UNP Q17QQ4
DI	248	ARG	HIS	conflict	UNP Q17QQ4
DI	249	GLU	ASP	conflict	UNP Q17QQ4
Di	6	THR	MET	conflict	UNP Q17QQ4
Di	138	THR	ALA	conflict	UNP Q17QQ4
Di	168	GLN	PRO	conflict	UNP Q17QQ4
Di	169	THR	ALA	conflict	UNP Q17QQ4
Di	180	MET	VAL	conflict	UNP Q17QQ4
Di	231	MET	VAL	conflict	UNP Q17QQ4
Di	240	SER	ALA	conflict	UNP Q17QQ4
Di	248	ARG	HIS	conflict	UNP Q17QQ4
Di	249	GLU	ASP	conflict	UNP Q17QQ4

- Molecule 23 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	DJ	90	Total	C	N	O	S	0	0
			720	466	115	135	4		
23	Dj	95	Total	C	N	O	S	0	0
			760	488	124	144	4		

- Molecule 24 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	DL	74	Total	C	N	O	S	0	0
			605	379	105	118	3		
24	DI	107	Total	C	N	O	S	0	0
			877	547	158	167	5		

- Molecule 25 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Dc	127	Total	C	N	O	S	0	0
			1011	638	174	193	6		

- Molecule 26 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Dk	98	Total	C	N	O	S	0	0
			786	499	142	140	5		

- Molecule 27 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Dm	87	Total	C	N	O	S	0	0
			724	456	131	131	6		

- Molecule 28 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 29 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- Molecule 30 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 31 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 32 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	I	114	Total	C	N	O	S	0	0
			928	571	166	180	11		

- Molecule 33 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 34 is a protein called RNA polymerase II subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 35 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 36 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M	252	Total	C	N	O	S	0	0
			1954	1224	346	367	17		

- Molecule 37 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	227	Total	C	N	O	P	0	0
			4645	2201	862	1356	226		

- Molecule 38 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 39 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 40 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	R	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 41 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	T	227	Total	C	N	O	P	0	0
			4656	2206	860	1364	226		

- Molecule 42 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	U	113	Total	C	N	O	S	0	0
			931	585	152	190	4		

- Molecule 43 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	V	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 44 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W	202	Total	C	N	O	S	0	0
			1659	1042	299	307	11		

- Molecule 45 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	X	171	Total	C	N	O	S	0	0
			1403	895	243	261	4		

- Molecule 46 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	a	97	Total	C	N	O	S	0	0
			801	505	155	138	3		
46	e	98	Total	C	N	O	S	0	0
			810	511	157	139	3		

- Molecule 47 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	b	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
47	f	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

- Molecule 48 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	c	109	Total	C	N	O		0	0
			843	531	167	145			
48	g	106	Total	C	N	O		0	0
			818	516	160	142			

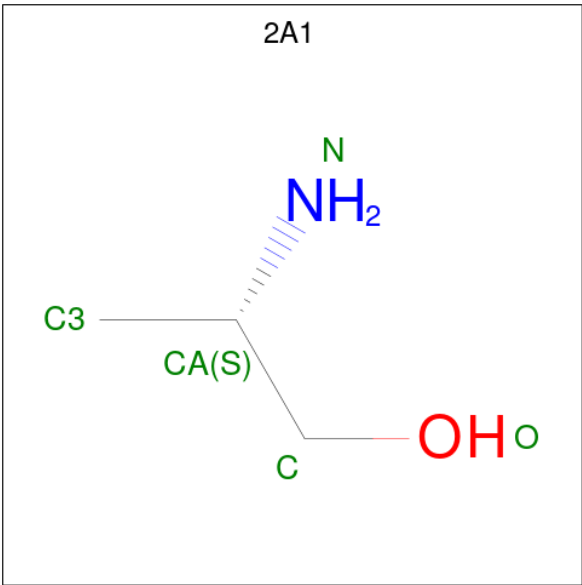
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	100	ARG	GLY	engineered mutation	UNP P06897
g	100	ARG	GLY	engineered mutation	UNP P06897

- Molecule 49 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	d	97	Total	C	N	O	S	0	0
			766	480	142	142	2		
49	h	95	Total	C	N	O	S	0	0
			744	468	134	140	2		

- Molecule 50 is (2S)-2-aminopropan-1-ol (CCD ID: 2A1) (formula: C₃H₉NO) (labeled as "Ligand of Interest" by depositor).



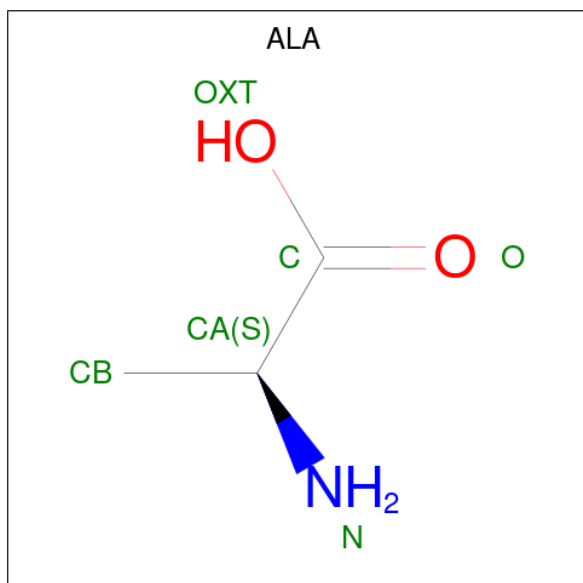
Mol	Chain	Residues	Atoms				AltConf
50	0	1	Total	C	N	O	0
			5	3	1	1	
50	0	1	Total	C	N	O	0
			5	3	1	1	
50	0	1	Total	C	N	O	0
			5	3	1	1	
50	0	1	Total	C	N	O	0
			5	3	1	1	
50	0	1	Total	C	N	O	0
			5	3	1	1	
50	0	1	Total	C	N	O	0
			5	3	1	1	
50	0	1	Total	C	N	O	0
			5	3	1	1	
50	0	1	Total	C	N	O	0
			5	3	1	1	
50	0	1	Total	C	N	O	0
			5	3	1	1	
50	0	1	Total	C	N	O	0
			5	3	1	1	

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Mol	Chain	Residues	Atoms				AltConf
50	2	1	Total	C	N	O	0
			5	3	1	1	
50	2	1	Total	C	N	O	0
			5	3	1	1	
50	2	1	Total	C	N	O	0
			5	3	1	1	
50	2	1	Total	C	N	O	0
			5	3	1	1	
50	N	1	Total	C	N	O	0
			5	3	1	1	
50	N	1	Total	C	N	O	0
			5	3	1	1	
50	N	1	Total	C	N	O	0
			5	3	1	1	
50	N	1	Total	C	N	O	0
			5	3	1	1	
50	N	1	Total	C	N	O	0
			5	3	1	1	

- Molecule 51 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



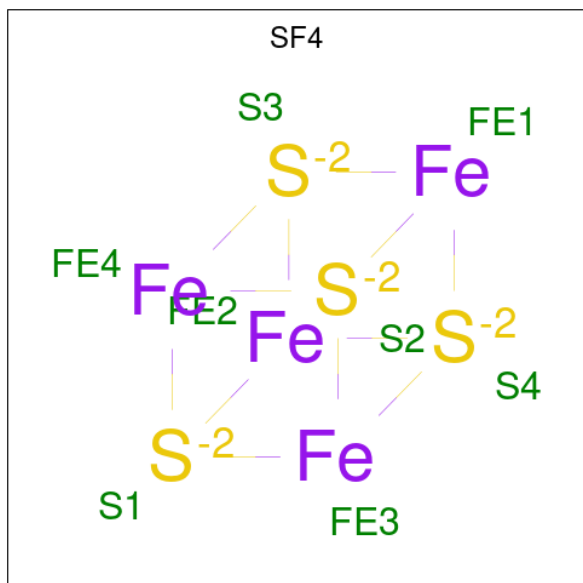
Mol	Chain	Residues	Atoms				AltConf
51	0	1	Total	C	N	O	0
			6	3	1	2	

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Mol	Chain	Residues	Atoms				AltConf
51	2	1	Total	C	N	O	0
			5	3	1	1	
51	2	1	Total	C	N	O	0
			6	3	1	2	

- Molecule 52 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
52	1	1	Total	Fe	S	0
			8	4	4	

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
53	4	3	Total	Zn	0
			3	3	
53	5	2	Total	Zn	0
			2	2	
53	7	2	Total	Zn	0
			2	2	
53	A	2	Total	Zn	0
			2	2	
53	B	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
53	C	1	Total 1	Zn 1	0
53	I	2	Total 2	Zn 2	0
53	J	1	Total 1	Zn 1	0
53	L	1	Total 1	Zn 1	0
53	M	1	Total 1	Zn 1	0
53	W	1	Total 1	Zn 1	0

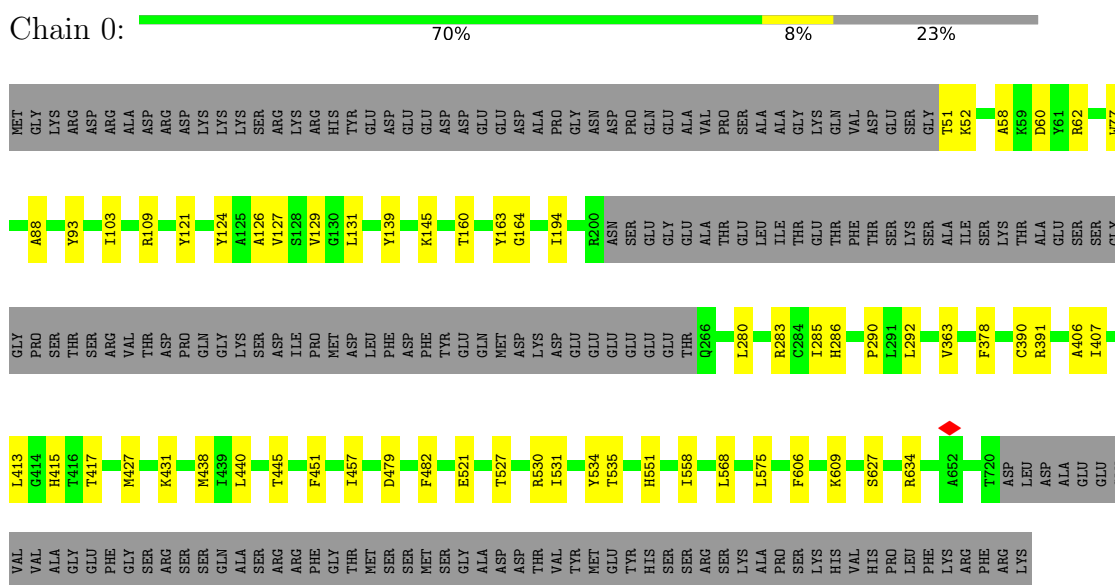
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
54	A	1	Total 1	Mg 1	0

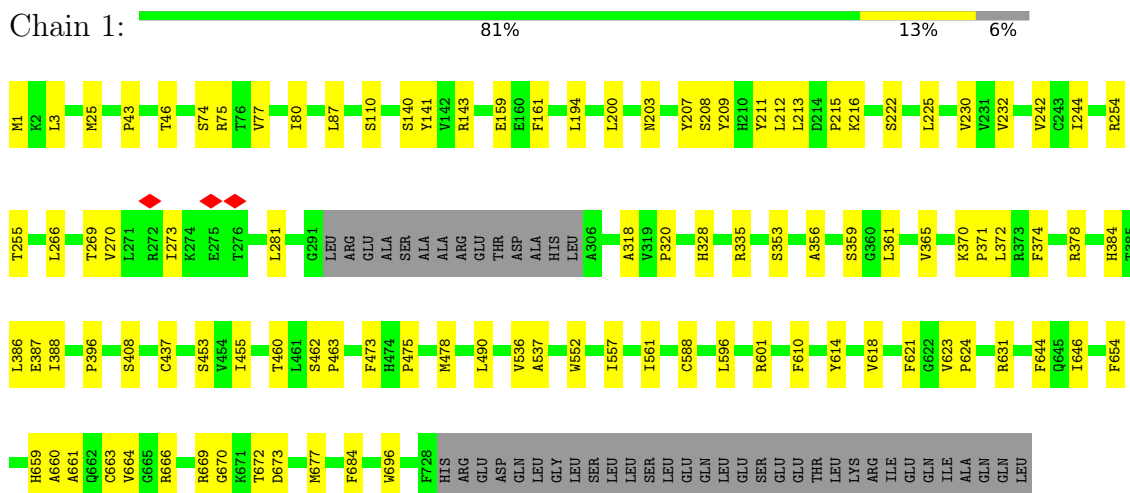
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPB

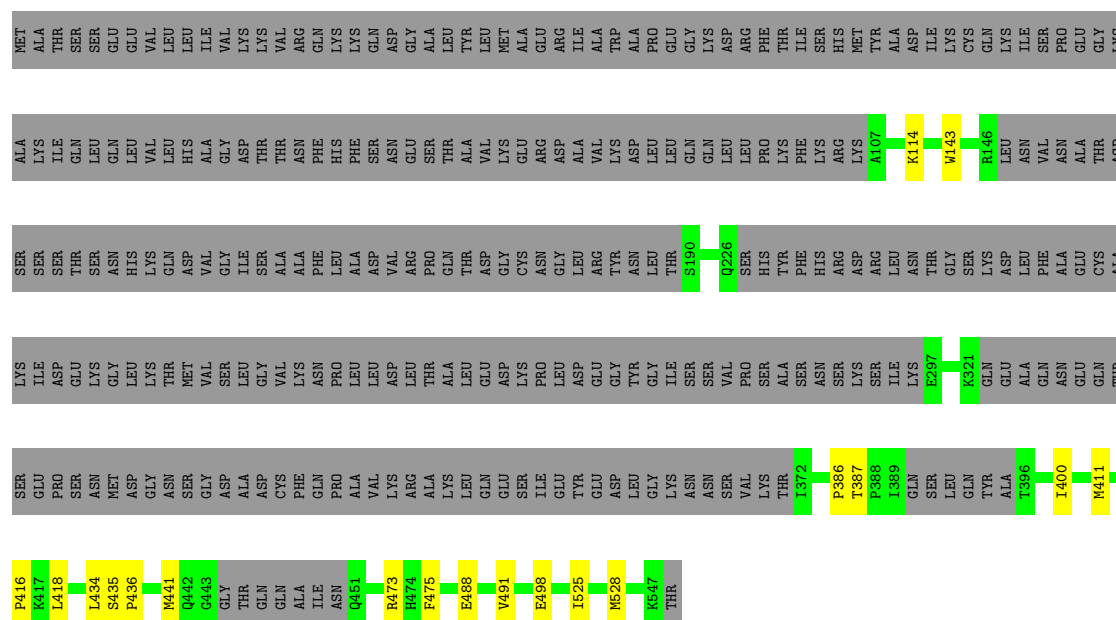


- Molecule 2: TFIIH basal transcription factor complex helicase XPD subunit



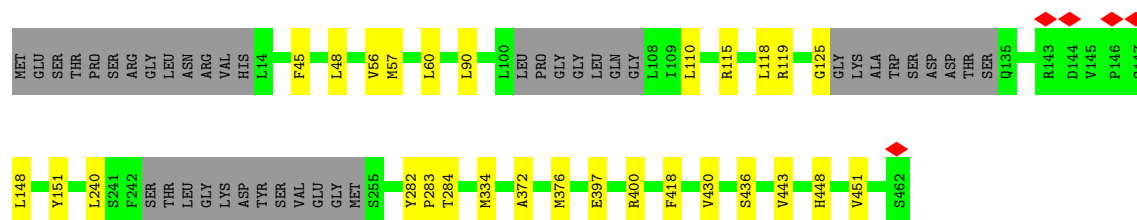
- Molecule 3: General transcription factor IIH subunit 1

Chain 2:  45% 52%



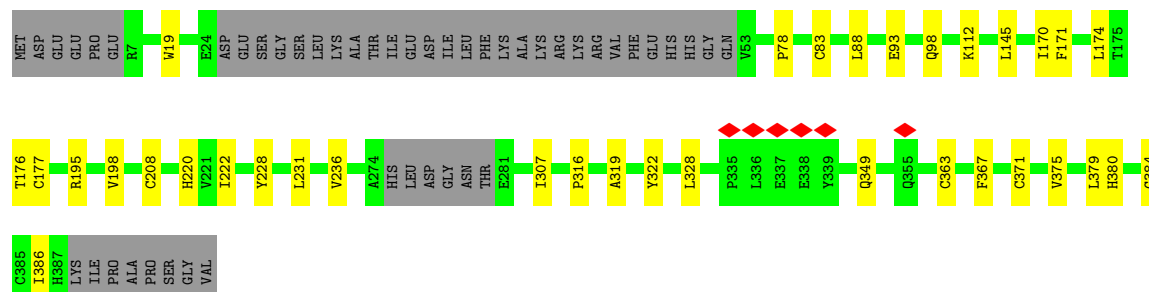
- Molecule 4: General transcription factor IIH subunit 4

Chain 3:  85% 6% 9%



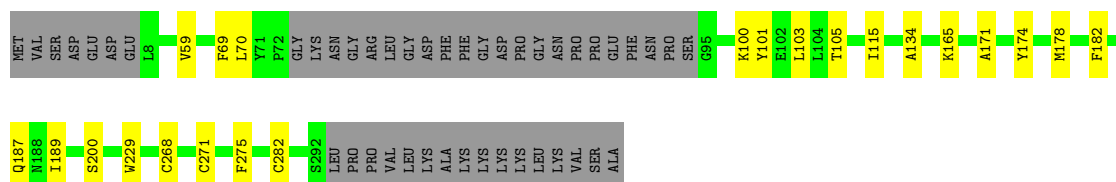
- Molecule 5: General transcription factor IIH subunit 2

Chain 4:  79% 9% 12%



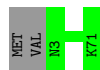
- Molecule 6: General transcription factor IIH subunit 3

Chain 5:  78% 7% 15%



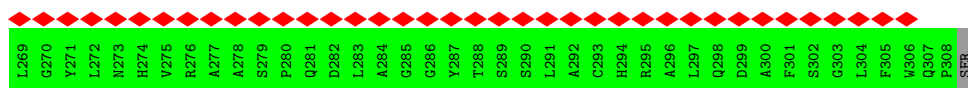
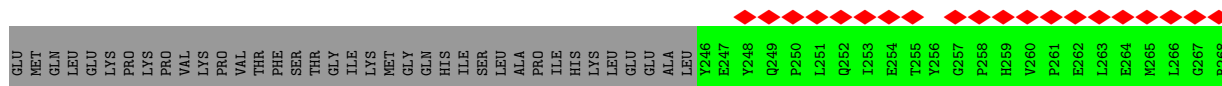
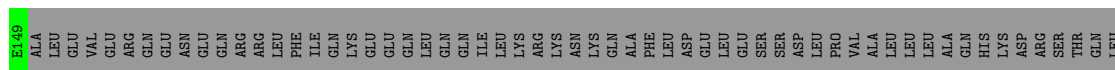
- Molecule 7: General transcription factor IIH subunit 5

Chain 6: 97%



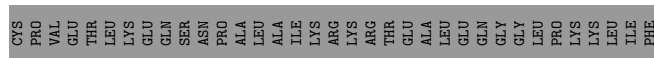
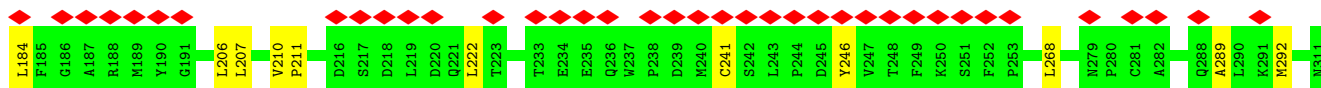
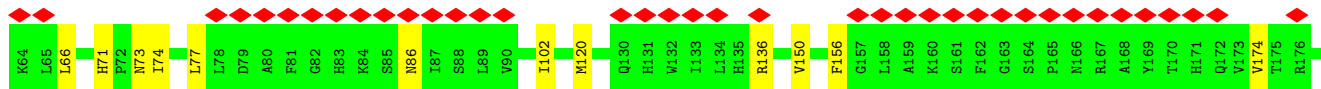
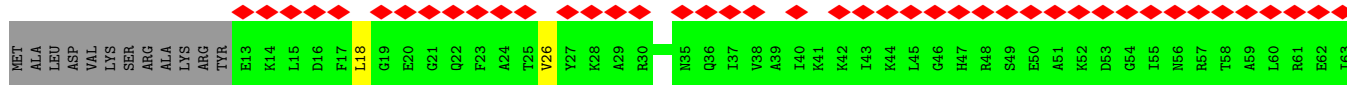
- Molecule 8: CDK-activating kinase assembly factor MAT1

Chain 7: 22%

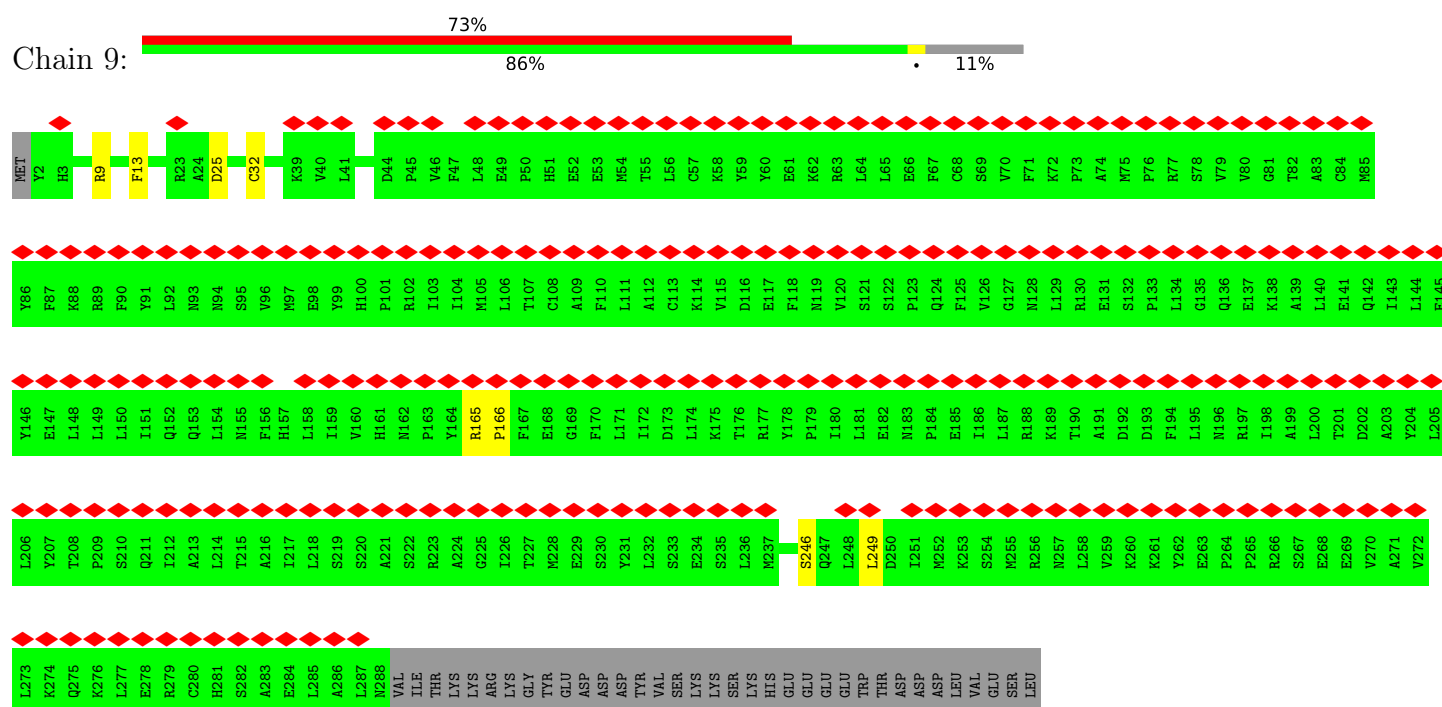


- Molecule 9: Cyclin-dependent kinase 7

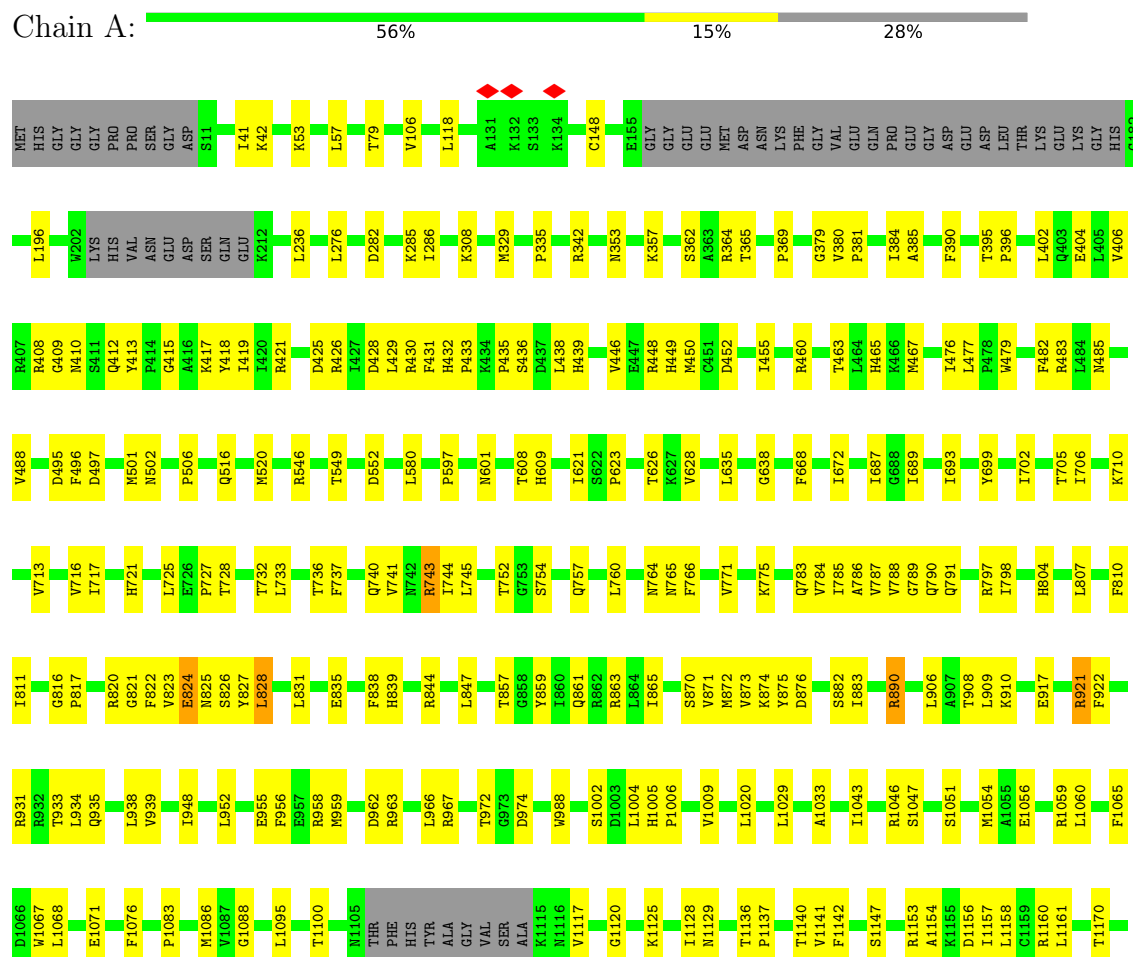
Chain 8: 34%



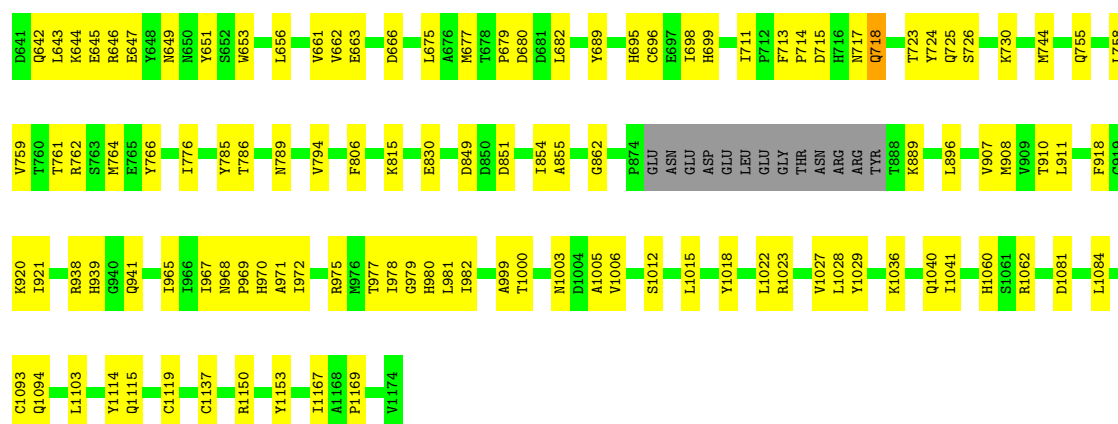
- Molecule 10: Cyclin-H



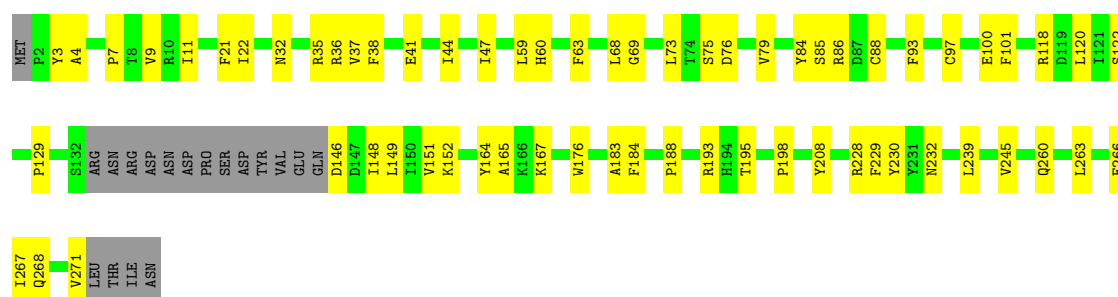
• Molecule 11: DNA-directed RNA polymerase subunit



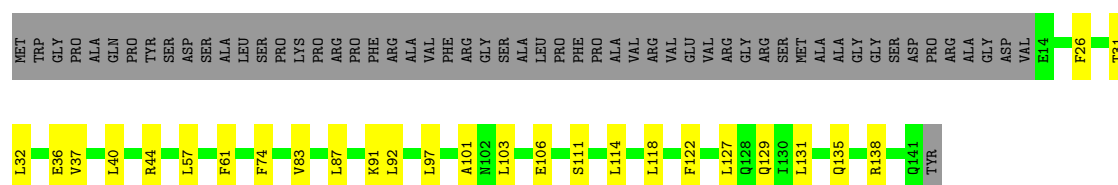




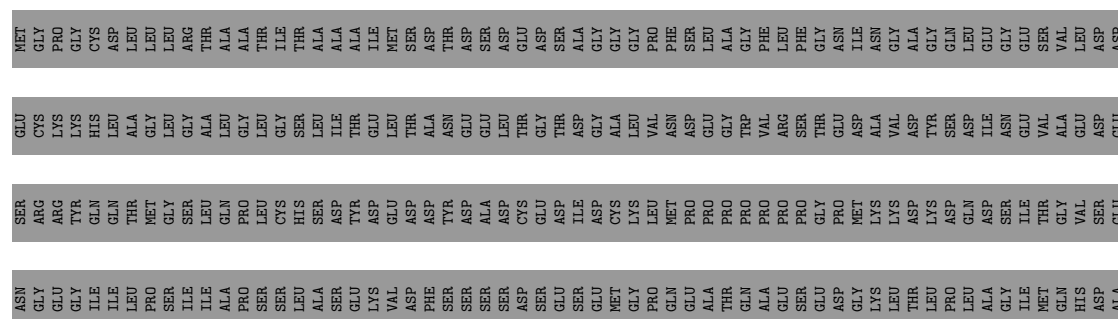
• Molecule 13: DNA-directed RNA polymerase II subunit RPB3



• Molecule 14: DNA-directed RNA polymerase II subunit RPB4



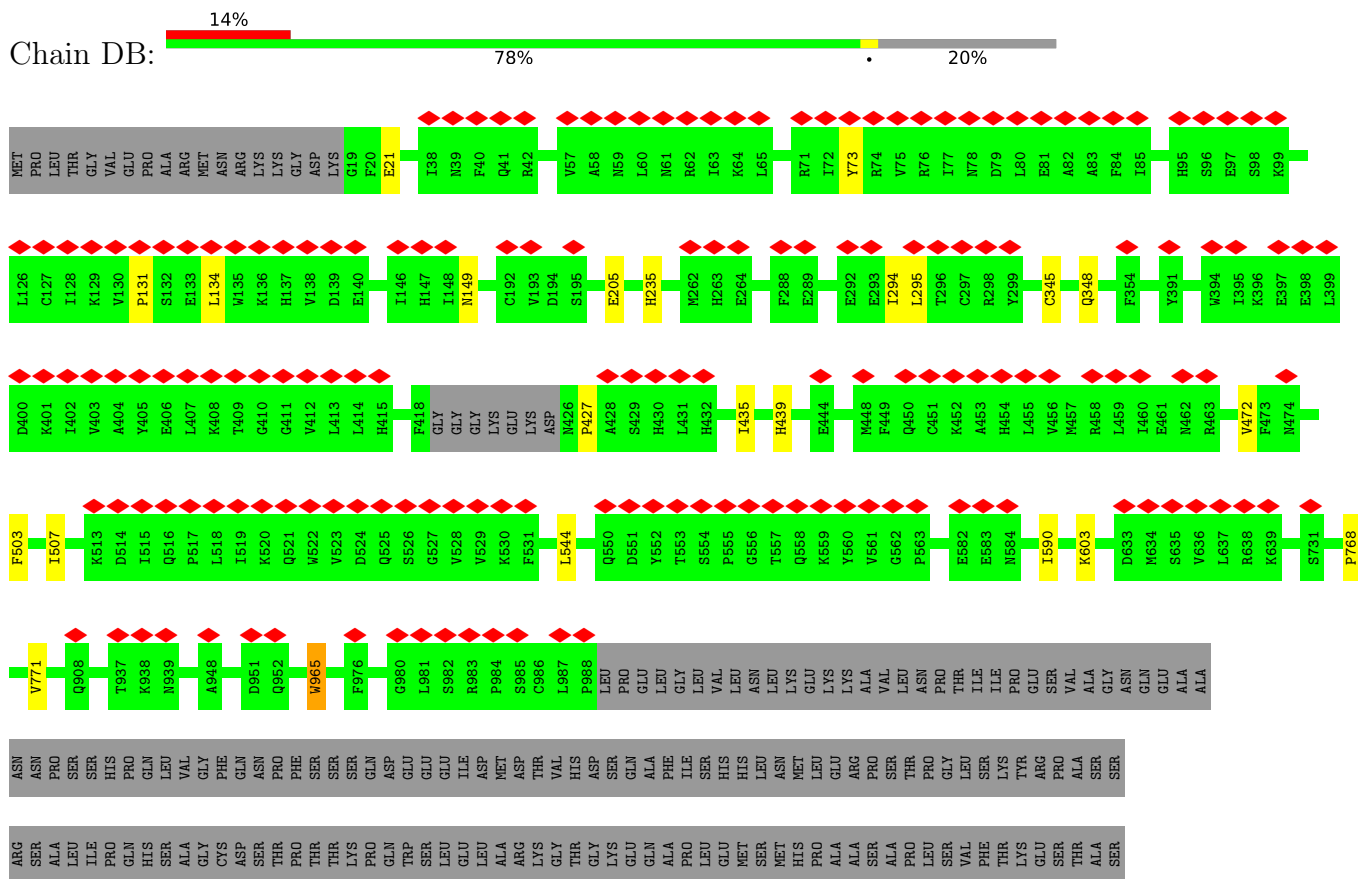
• Molecule 15: Transcription initiation factor TFIID subunit 1





[illegible]

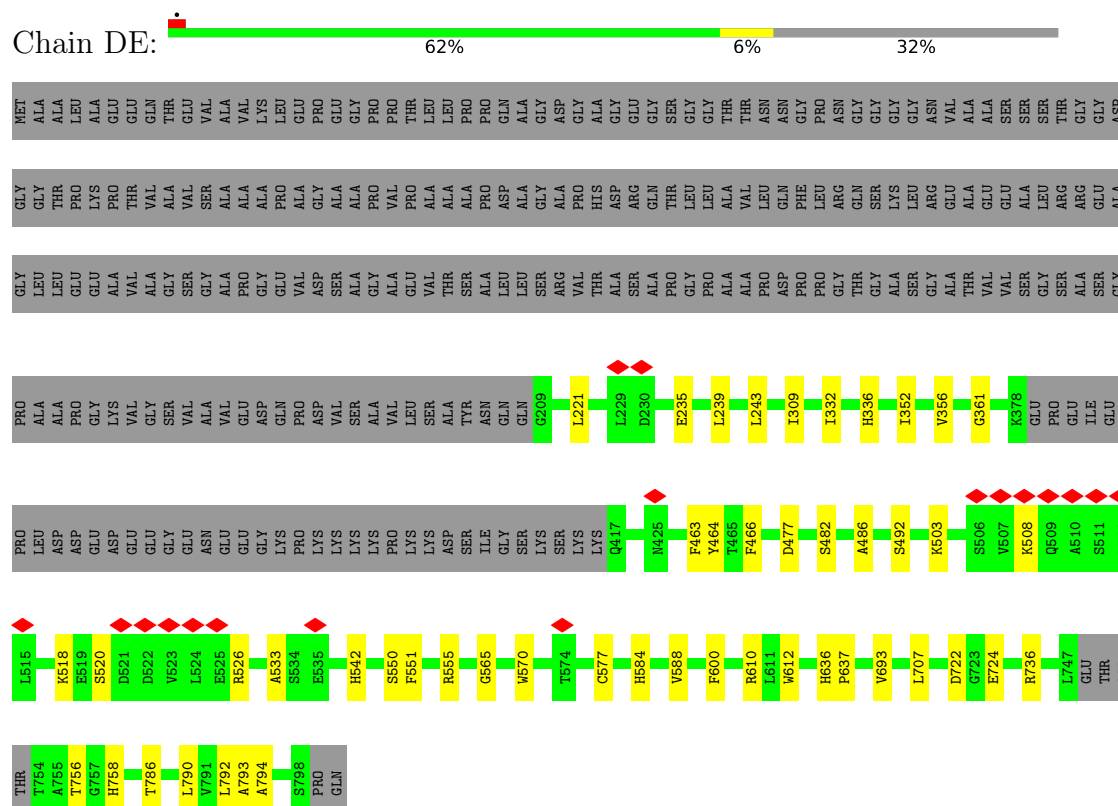
- Molecule 16: Transcription initiation factor TFIID subunit 2



- Molecule 17: Transcription initiation factor TFIID subunit 4

L910	Q911	N912	L913	V914	E915	K916	S918	E919	Q922	N925	F926	S927	V928	K929	D930	D931	D932	E933	Y934	E935	Q936	A937	S938	D939	V940	R941	A942	Q943	L944	K945	F946	F947	E948	Q949	L950	D951	L966	NET	ARG	ALA	ALA	LYS	SER	ARG	SER	ARG	GLN	GLU	ASP	PRO	GLU	Q981	D1003
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-------

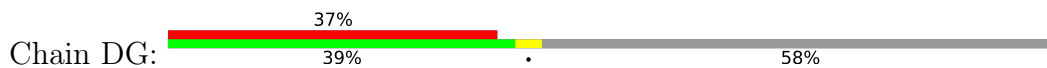
- Molecule 18: Transcription initiation factor TFIID subunit 5

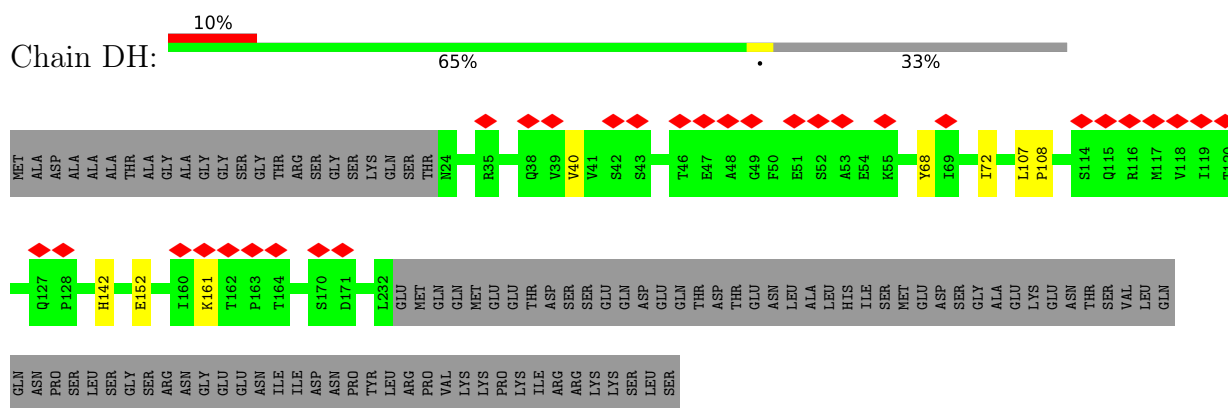


- Molecule 18: Transcription initiation factor TFIID subunit 5

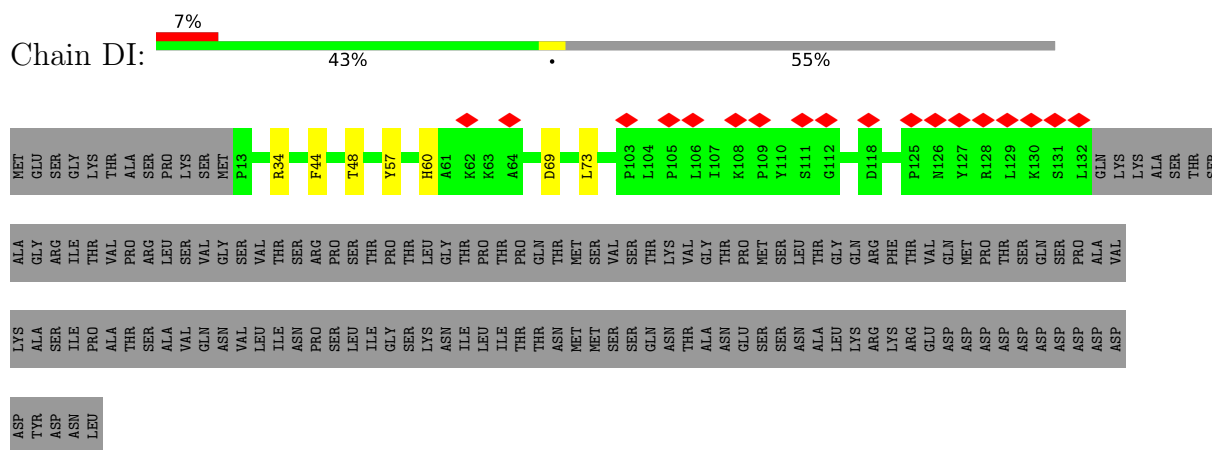


Chain Df:

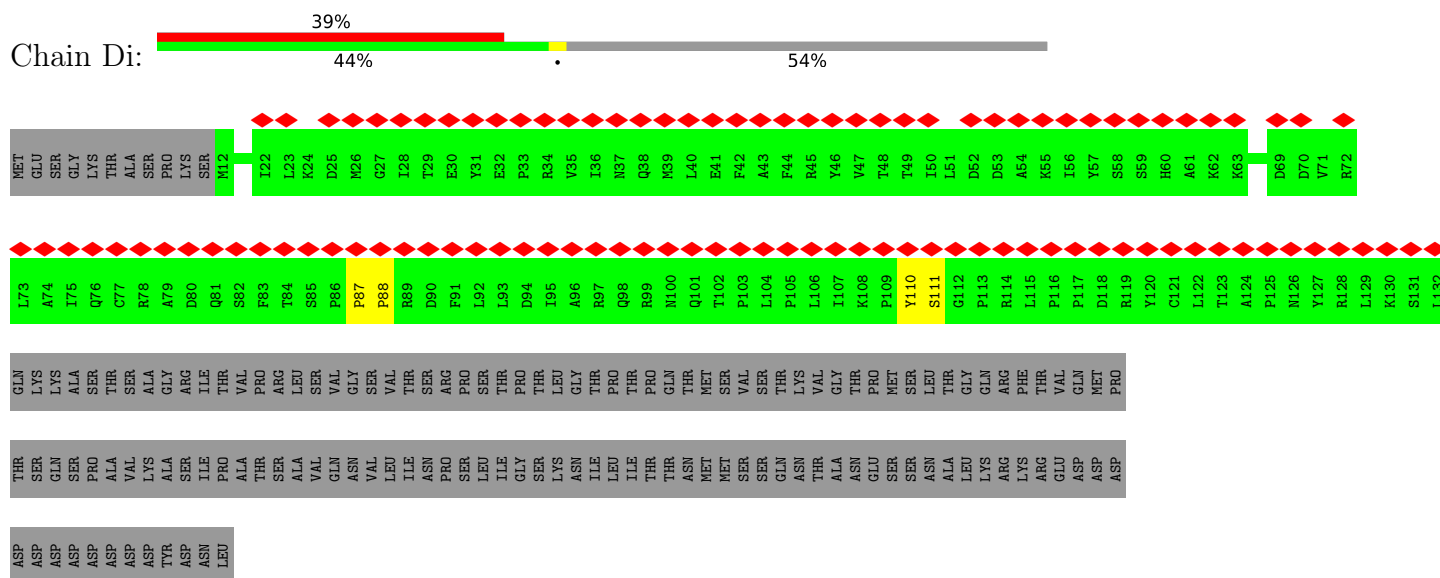




• Molecule 22: Transcription initiation factor TFIID subunit 9



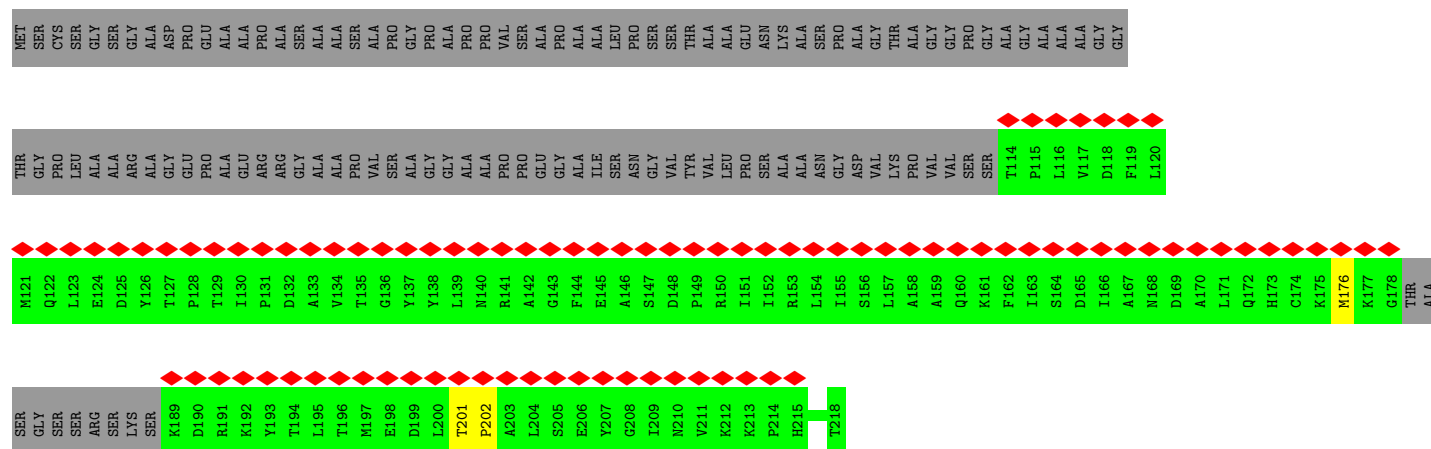
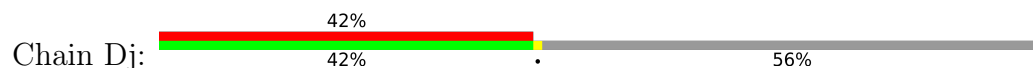
• Molecule 22: Transcription initiation factor TFIID subunit 9



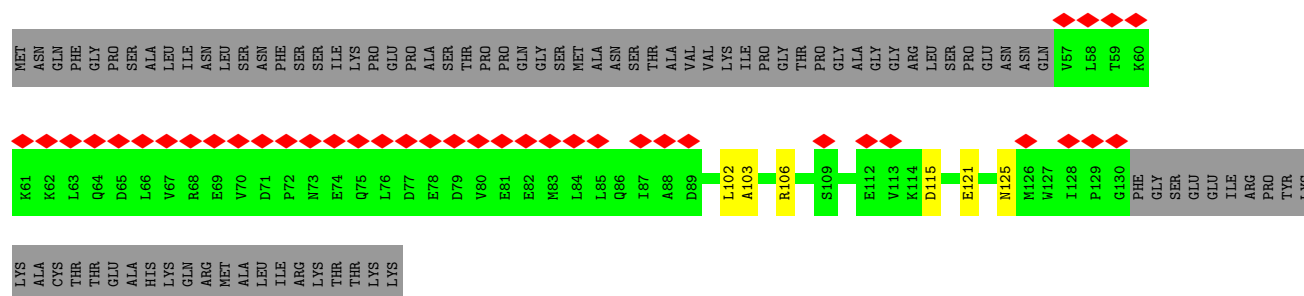
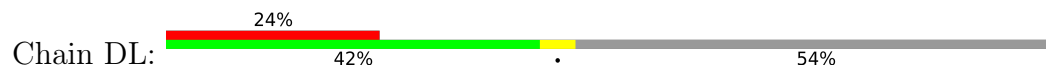
• Molecule 23: Transcription initiation factor TFIID subunit 10



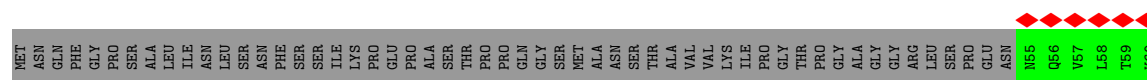
- Molecule 23: Transcription initiation factor TFIID subunit 10

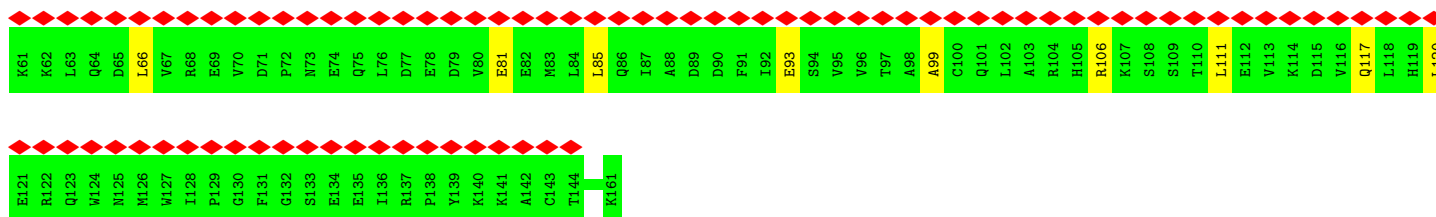


- Molecule 24: Transcription initiation factor TFIID subunit 12

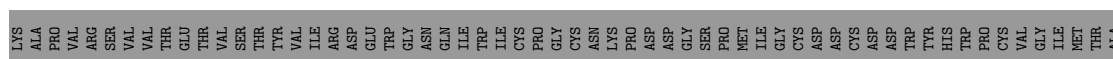
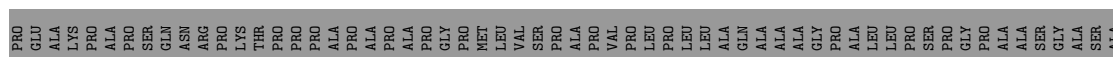
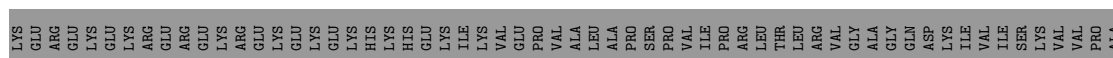
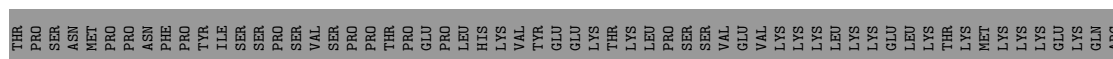
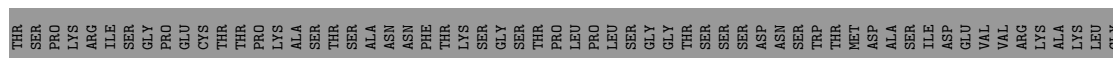
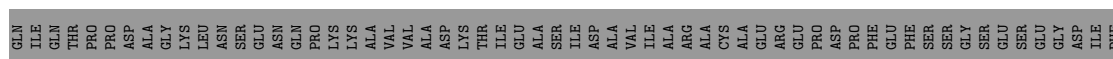
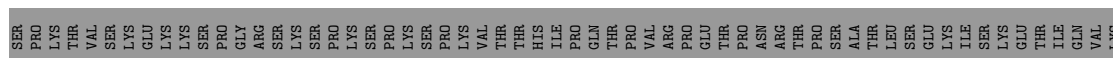
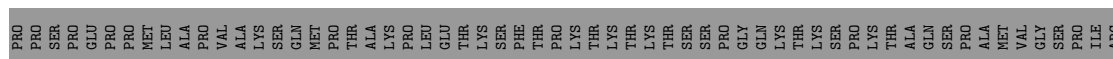
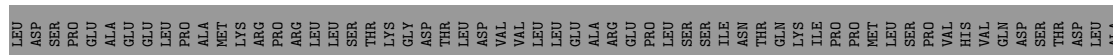
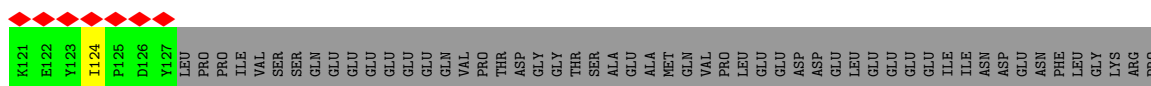
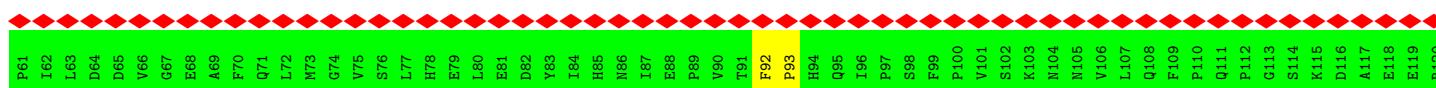
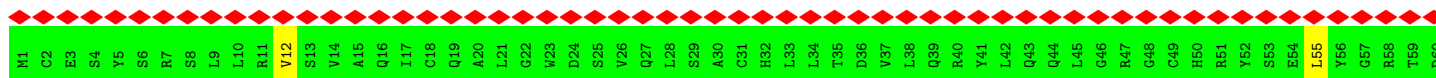


- Molecule 24: Transcription initiation factor TFIID subunit 12





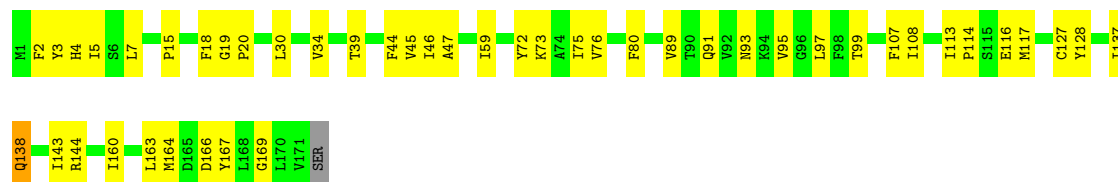
• Molecule 25: Transcription initiation factor TFIID subunit 3





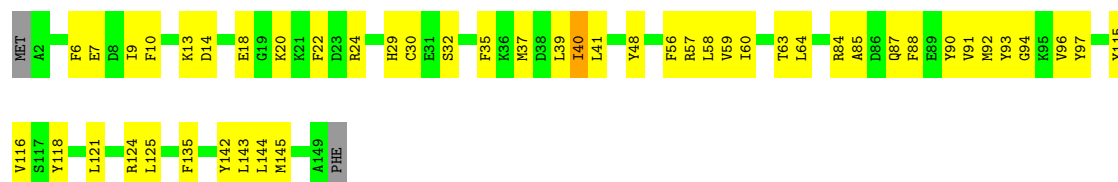
- Molecule 30: DNA-directed RNA polymerase II subunit RPB7

Chain G: 73% 26% ..



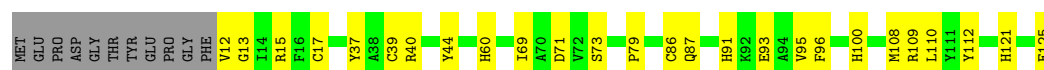
- Molecule 31: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 67% 31% ..



- Molecule 32: DNA-directed RNA polymerase II subunit RPB9

Chain I: 70% 21% 9%



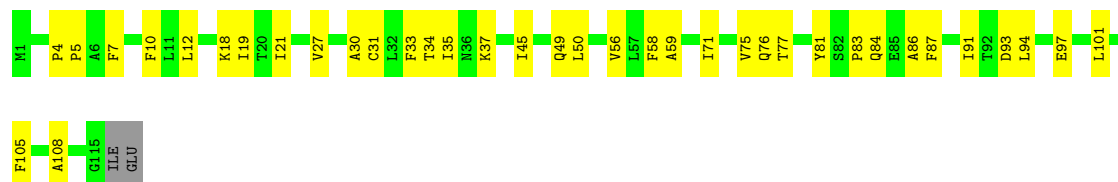
- Molecule 33: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 76% 19%



- Molecule 34: RNA polymerase II subunit J

Chain K: 67% 32%



- Molecule 35: RNA polymerase II subunit K

MET	ASP	THR	GLN	LYS	ASP	VAL	GLN	PRO	PRO	LYS	GLN	GLN	PRO	M15	M16	Y17	I28	K29	S30	R31	D32	R42	I43	M44	Y45	A57	R58
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Chain M: 65% 15% 20%

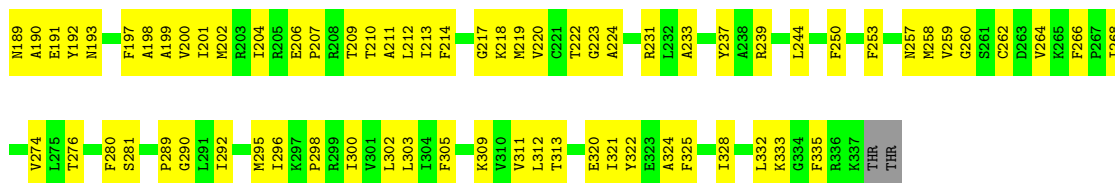
A261	A262	Q263	Q264	A264	S265	K288	Y289	L292	Y293	L299	F300	P301	F304	G305	F306	D307	P308	P309	V310	D311	K312	L313	P314	G315	L316																					
ALA	SER	PHE	ASP	GLU	PHE	GLY	ASN	SER	LYS	TYR	GLN	ASN	ARG	T106	A125	D126	R127	L130	P131	I134	V183	F195	L199	F214	F218	C219	P225	V228	Q229	G230	A231	A232	I235	L242	D243	L244	V245	P246	G247	R248	A256	A257	L258	Y259		
MET	ALA	SER	THR	SER	ARG	LEU	ASP	ALA	LEU	PRO	ARG	VAL	T114	D26	I33	C37	G38	L39	T34	PHE	SER	ASN	ASP	LYS	ALA	THR	LYS	ASP	PRO	SER	ARG	VAL	GLY	ASP	GLN	ASN	LEU	SER	THR	MET	ILE	GLY	LYS	GLY	THR	GLY

Chain N: 22% 34% 63%

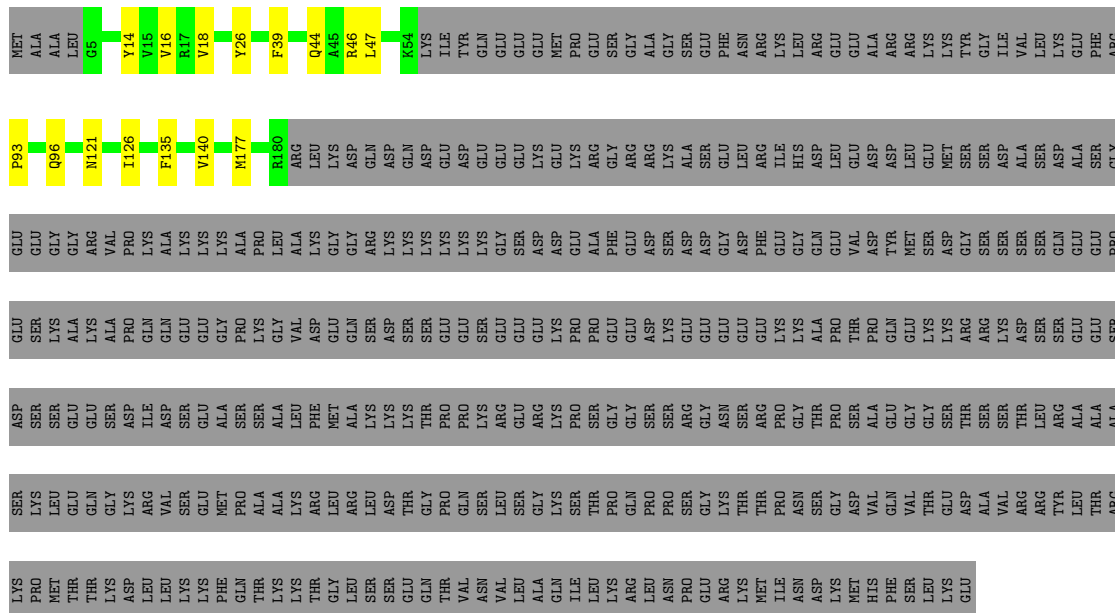
The diagram illustrates a network structure with nodes and connections. The nodes are labeled with codes such as C194, T198, G199, T200, C201, A204, T205, A206, T207, A208, T209, A210, C211, A212, T213, C214, C215, G216, A217, A123, C124, C125, G126, C127, A130, A131, A132, C133, G142, C143, G144, C145, T146, G147, T148, C149, C150, C151, C152, C153, G154, C155, G156, T157, T158, T159, T160, A161, A162, C163, C164, G165, C166, C167, A168, A169, G170, G171, G172, G173, A177, C178, T179, C180, C181, C182, T183, A184, G185, T186, C187, C190, A191, G192, C193, G57, A61, G62, G63, T64, G65, C67, T68, A69, C70, A71, T72, T73, G74, G75, A76, G77, C82, C83, G84, G85, T86, G87, C88, C89, G90, A91, G92, G93, C94, C95, G96, C97, T98, C99, A100, A101, T102, T103, G104, G105, T106, C107, G108, T109, A110, G111, A114, G115, C116, T117, C118, T119, A120, C122, G19, A8, A7, G6, G5, G4, G3, G2, A2, T3, T4, A5, A6, A7, G8, G9, G10, G11, G12, T13, G14, G15, G16, G17, G18, C19, G20, C21, G22, T23, T24, C25, G26, T27, C28, C29, T30, C31, A32, C33, A34, C40, C41, T42, T43, G44, A45, A46, C47, T48, C49, G50, A51, G52, C53, C54, G55, A56, G57, A61, G62, G63, T64, G65, C67, T68, A69, C70, A71, T72, T73, G74, G75, A76, G77, C82, C83, G84, G85, T86, G87, C88, C89, G90, A91, G92, G93, C94, C95, G96, C97, T98, C99, A100, A101, T102, T103, G104, G105, T106, C107, G108, T109, A110, G111, A114, G115, C116, T117, C118, T119, A120, C122, G19, A8, A7, G6, G5, G4, G3, G2, A2, T3, T4, A5, A6, A7, G8, G9, G10, G11, G12, T13, G14, G15, G16, G17, G18, C19, G20, C21, G22, T23, T24, C25, G26, T27, C28, C29, T30, C31, A32, C33, A34, C40, C41, T42, T43, G44, A45, A46, C47, T48, C49, G50, A51, G52, C53, C54, G55, A56, G57, A61, G62, G63, T64, G65, C67, T68, A69, C70, A71, T72, T73, G74, G75, A76, G77, C82, C83, G84, G85, T86, G87, C88, C89, G90, A91, G92, G93, C94, C95, G96, C97, T98, C99, A100, A101, T102, T103, G104, G105, T106, C107, G108, T109, A110, G111, A114, G115, C116, T117, C118, T119, A120, C122, G19, A8, A7, G6, G5, G4, G3, G2, A2, T3, T4, A5, A6, A7, G8, G9, G10, G11, G12, T13, G14, G15, G16, G17, G18, C19, G20, C21, G22, T23, T24, C25, G26, T27, C28, C29, T30, C31, A32, C33, A34, C40, C41, T42, T43, G44, A45, A46, C47, T48, C49, G50, A51, G52, C53, C54, G55, A56, G57, A61, G62, G63, T64, G65, C67, T68, A69, C70, A71, T72, T73, G74, G75, A76, G77, C82, C83, G84, G85, T86, G87, C88, C89, G90, A91, G92, G93, C94, C95, G96, C97, T98, C99, A100, A101, T102, T103, G104, G105, T106, C107, G108, T109, A110, G111, A114, G115, C116, T117, C118, T119, A120, C122, G19, A8, A7, G6, G5, G4, G3, G2, A2, T3, T4, A5, A6, A7, G8, G9, G10, G11, G12, T13, G14, G15, G16, G17, G18, C19, G20, C21, G22, T23, T24, C25, G26, T27, C28, C29, T30, C31, A32, C33, A34, C40, C41, T42, T43, G44, A45, A46, C47, T48, C49, G50, A51, G52, C53, C54, G55, A56, G57, A61, G62, G63, T64, G65, C67, T68, A69, C70, A71, T72, T73, G74, G75, A76, G77, C82, C83, G84, G85, T86, G87, C88, C89, G90, A91, G92, G93, C94, C95, G96, C97, T98, C99, A100, A101, T102, T103, G104, G105, T106, C107, G108, T109, A110, G111, A114, G115, C116, T117, C118, T119, A120, C122, G19, A8, A7, G6, G5, G4, G3, G2, A2, T3, T4, A5, A6, A7, G8, G9, G10, G11, G12, T13, G14, G15, G16, G17, G18, C19, G20, C21, G22, T23, T24, C25, G26, T27, C28, C29, T30, C31, A32, C33, A34, C40, C41, T42, T43, G44, A45, A46, C47, T48, C49, G50, A51, G52, C53, C54, G55, A56, G57, A61, G62, G63, T64, G65, C67, T68, A69, C70, A71, T72, T73, G74, G75, A76, G77, C82, C83, G84, G85, T86, G87, C88, C89, G90, A91, G92, G93, C94, C95, G96, C97, T98, C99, A100, A101, T102, T103, G104, G105, T106, C107, G108, T109, A110, G111, A114, G115, C116, T117, C118, T119, A120, C122, G19, A8, A7, G6, G5, G4, G3, G2, A2, T3, T4, A5, A6, A7, G8, G9, G10, G11, G12, T13, G14, G15, G16, G17, G18, C19, G20, C21, G22, T23, T24, C25, G26, T27, C28, C29, T30, C31, A32, C33, A34, C40, C41, T42, T43, G44, A45, A46, C47, T48, C49, G50, A51, G52, C53, C54, G55, A56, G57, A61, G62, G63, T64, G65, C67, T68, A69, C70, A71, T72, T73, G74, G75, A76, G77, C82, C83, G84, G85, T86, G87, C88, C89, G90, A91, G92, G93, C94, C95, G96, C97, T98, C99, A100, A101, T102, T103, G104, G105, T106, C107, G108, T109, A110, G111, A114, G115, C116, T117, C118, T119, A120, C122, G19, A8, A7, G6, G5, G4, G3, G2, A2, T3, T4, A5, A6, A7, G8, G9, G10, G11, G12, T13, G14, G15, G16, G17, G18, C19, G20, C21, G22, T23, T24, C25, G26, T27, C28, C29, T30, C31, A32, C33, A34, C40, C41, T42, T43, G44, A45, A46, C47, T48, C49, G50, A51, G52, C53, C54, G55, A56, G57, A61, G62, G63, T64, G65, C67, T68, A69, C70, A71, T72, T73, G74, G75, A76, G77, C82, C83, G84, G85, T86, G87, C88, C89, G90, A91, G92, G93, C94, C95, G96, C97, T98, C99, A100, A101, T102, T103, G104, G105, T106, C107, G108, T109, A110, G111, A114, G115, C116, T117, C118, T119, A120, C122, G19, A8, A7, G6, G5, G4, G3, G2, A2, T3, T4, A5, A6, A7, G8, G9, G10, G11, G12, T13, G14, G15, G16, G17, G18, C19, G20, C21, G22, T23, T24, C25, G26, T27, C28, C29, T30, C31, A32, C33, A34, C40, C41, T42, T4

Chain 0: 29% 24% 47%

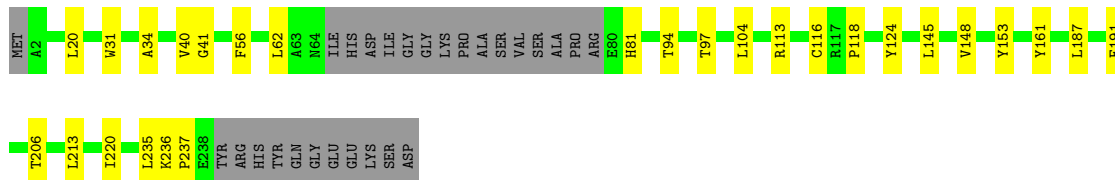
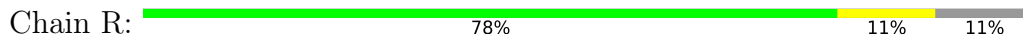
[illegible]



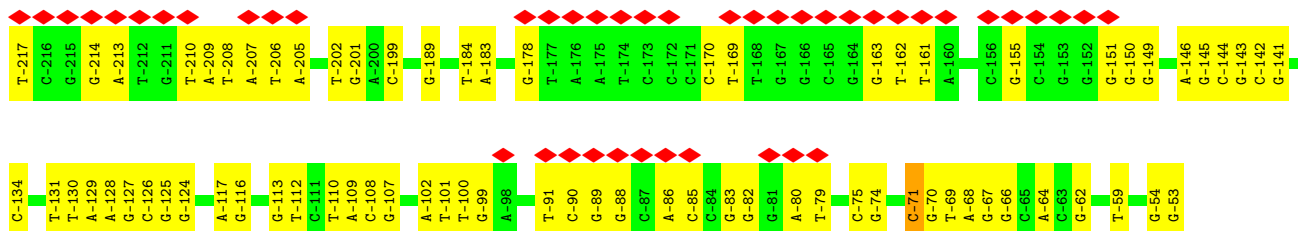
- Molecule 39: General transcription factor IIF subunit 1

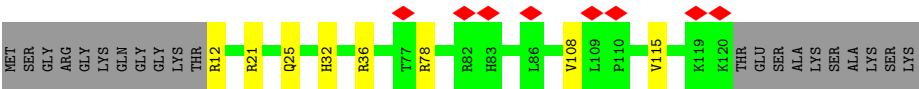


- Molecule 40: General transcription factor IIF subunit 2



- Molecule 41: Template DNA

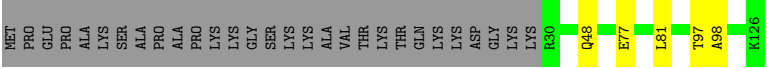




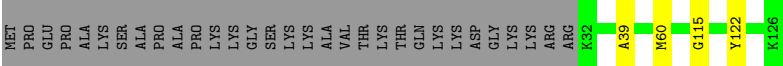
● Molecule 48: Histone H2A type 1



● Molecule 49: Histone H2B 1.1



● Molecule 49: Histone H2B 1.1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30253	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.00	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.014	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0012	Depositor
Map size (Å)	537.6, 537.6, 537.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, 2A1, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.24	0/4994	0.69	0/6745
2	1	0.25	0/5875	0.76	1/7955 (0.0%)
3	2	0.27	0/2210	0.73	0/2975
4	3	0.24	0/3412	0.68	0/4622
5	4	0.25	0/2793	0.68	0/3780
6	5	0.24	0/2103	0.66	0/2846
7	6	0.24	0/555	0.71	0/747
8	7	0.31	0/1756	0.83	4/2367 (0.2%)
9	8	0.25	0/2437	0.70	0/3306
10	9	0.31	0/2384	0.80	0/3220
11	A	0.39	0/11479	0.82	5/15496 (0.0%)
12	B	0.41	0/9257	0.83	5/12493 (0.0%)
13	C	0.41	0/2102	0.76	0/2857
14	D	0.27	0/1064	0.70	0/1428
15	DA	0.27	0/4679	0.72	2/6320 (0.0%)
16	DB	0.25	0/7993	0.66	2/10836 (0.0%)
17	DD	0.27	0/1344	0.76	0/1795
17	Dd	0.22	0/1322	0.66	0/1772
18	DE	0.24	0/4469	0.70	1/6050 (0.0%)
18	De	0.25	0/4433	0.71	0/6004
19	DF	0.27	0/3167	0.77	4/4303 (0.1%)
19	Df	0.25	0/3140	0.68	0/4268
20	DG	0.30	0/1199	0.74	0/1612
21	DH	0.31	0/1673	0.81	0/2285
22	DI	0.31	0/981	0.76	0/1332
22	Di	0.30	0/989	0.72	0/1343
23	DJ	0.23	0/736	0.64	0/998
23	Dj	0.28	0/776	0.68	0/1049
24	DL	0.22	0/613	0.67	0/829
24	Di	0.19	0/889	0.61	0/1194
25	Dc	0.26	0/1035	0.69	0/1406
26	Dk	0.19	0/800	0.60	0/1070

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
27	Dm	0.18	0/733	0.57	0/977
28	E	0.42	0/1752	0.73	0/2366
29	F	0.48	0/646	0.73	0/871
30	G	0.37	0/1382	0.73	0/1874
31	H	0.55	0/1207	0.76	1/1628 (0.1%)
32	I	0.39	0/949	0.73	0/1284
33	J	0.32	0/516	0.70	0/696
34	K	0.49	0/939	0.78	0/1271
35	L	0.30	0/378	0.72	0/500
36	M	0.35	0/1984	0.70	1/2679 (0.0%)
37	N	0.45	0/5211	0.94	9/8039 (0.1%)
38	O	0.48	0/1448	0.73	0/1948
39	Q	0.30	0/1167	0.74	0/1576
40	R	0.27	0/1817	0.69	0/2445
41	T	0.43	0/5223	0.85	2/8062 (0.0%)
42	U	0.27	0/946	0.76	1/1274 (0.1%)
43	V	0.31	0/816	0.71	1/1105 (0.1%)
44	W	0.32	0/1686	0.71	0/2266
45	X	0.31	0/1427	0.78	0/1916
46	a	0.29	0/813	0.78	0/1090
46	e	0.32	0/822	0.75	0/1102
47	b	0.26	0/660	0.79	0/883
47	f	0.26	0/645	0.77	0/862
48	c	0.28	0/853	0.84	0/1149
48	g	0.27	0/828	0.79	0/1117
49	d	0.29	0/777	0.78	0/1041
49	h	0.26	0/755	0.65	0/1013
All	All	0.33	0/129039	0.76	39/176337 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	2
2	1	0	5
4	3	0	1
5	4	0	1
10	9	0	1
11	A	0	3
13	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	DE	0	2
19	DF	0	1
22	DI	0	1
28	E	0	1
36	M	0	1
46	a	0	1
47	b	0	1
48	c	0	1
48	g	0	1
All	All	0	24

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	71	DG	O4'-C1'-N9	11.01	124.92	108.40
11	A	824	GLU	N-CA-CB	-9.08	96.31	110.30
37	N	71	DG	C1'-O4'-C4'	-8.42	97.06	109.70
16	DB	965	TRP	CA-CB-CG	7.32	127.51	113.60
42	U	32	ASP	N-CA-C	6.65	124.96	110.80
16	DB	965	TRP	CB-CA-C	6.41	124.25	110.21
8	7	93	ARG	N-CA-C	6.32	117.97	111.14
19	DF	92	ILE	N-CA-C	6.15	122.16	108.88
12	B	715	ASP	CB-CA-C	-5.94	98.05	110.17
19	DF	91	PHE	CA-C-N	5.90	133.04	122.13
19	DF	91	PHE	C-N-CA	5.90	133.04	122.13
37	N	108	DG	N9-C1'-C2'	5.79	122.18	113.50
12	B	718	GLN	CB-CA-C	5.76	119.28	109.72
37	N	72	DA	C4'-C3'-O3'	5.75	118.62	110.00
2	1	75	ARG	N-CA-C	5.69	117.94	111.11
37	N	180	DC	N1-C1'-C2'	5.56	121.83	113.50
12	B	972	ILE	N-CA-C	5.55	120.87	108.88
41	T	-71	DC	N1-C1'-C2'	5.54	121.81	113.50
8	7	95	TYR	CA-CB-CG	-5.52	103.97	113.90
37	N	72	DA	O4'-C1'-N9	5.50	116.65	108.40
8	7	94	GLU	N-CA-C	5.47	118.07	111.40
18	DE	361	GLY	N-CA-C	5.45	122.20	112.22
15	DA	826	ARG	CA-C-N	5.38	127.49	120.28
15	DA	826	ARG	C-N-CA	5.38	127.49	120.28
11	A	1435	THR	N-CA-C	5.36	122.22	110.80
12	B	22	TRP	CA-CB-CG	-5.36	103.41	113.60
31	H	40	ILE	N-CA-C	-5.28	100.71	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	95	TYR	N-CA-C	5.20	118.88	112.54
11	A	775	LYS	CB-CG-CD	5.18	123.22	111.30
41	T	-71	DC	O3'-P-O5'	5.18	111.76	104.00
37	N	56	DA	C4'-C3'-O3'	5.16	117.74	110.00
11	A	828	LEU	N-CA-C	-5.14	105.58	111.14
36	M	307	ASP	N-CA-C	-5.14	105.75	112.23
12	B	698	ILE	N-CA-C	-5.08	105.65	110.42
11	A	910	LYS	N-CA-C	5.06	120.99	109.81
37	N	75	DG	N9-C1'-C2'	5.03	121.04	113.50
37	N	34	DA	C4'-C3'-O3'	5.03	117.54	110.00
19	DF	90	GLU	N-CA-C	5.02	119.41	113.28
43	V	6	TYR	CA-CB-CG	-5.00	104.89	113.90

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	109	ARG	Sidechain
1	0	391	ARG	Sidechain
2	1	254	ARG	Sidechain
2	1	378	ARG	Sidechain
2	1	631	ARG	Sidechain
2	1	666	ARG	Sidechain
2	1	669	ARG	Sidechain
4	3	115	ARG	Sidechain
5	4	195	ARG	Sidechain
10	9	9	ARG	Sidechain
11	A	743	ARG	Sidechain
11	A	890	ARG	Sidechain
11	A	921	ARG	Sidechain
13	C	118	ARG	Sidechain
18	DE	555	ARG	Sidechain
18	DE	736	ARG	Sidechain
19	DF	320	ARG	Sidechain
22	DI	34	ARG	Sidechain
28	E	162	ARG	Sidechain
36	M	248	ARG	Sidechain
46	a	43	ARG	Sidechain
47	b	24	ARG	Sidechain
48	c	21	ARG	Sidechain
48	g	33	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4890	0	4949	38	0
2	1	5751	0	5794	61	0
3	2	2167	0	2175	13	0
4	3	3338	0	3343	16	0
5	4	2732	0	2703	20	0
6	5	2066	0	2100	16	0
7	6	549	0	558	0	0
8	7	1724	0	1697	22	0
9	8	2378	0	2397	13	0
10	9	2334	0	2357	6	0
11	A	11274	0	11408	259	0
12	B	9076	0	9116	178	0
13	C	2059	0	2008	55	0
14	D	1050	0	1033	23	0
15	DA	4563	0	4485	24	0
16	DB	7796	0	7751	13	0
17	DD	1331	0	1351	5	0
17	Dd	1308	0	1318	13	0
18	DE	4364	0	4244	24	0
18	De	4327	0	4197	9	0
19	DF	3109	0	3045	7	0
19	Df	3081	0	3012	10	0
20	DG	1180	0	1235	6	0
21	DH	1633	0	1621	4	0
22	DI	959	0	969	8	0
22	Di	967	0	977	2	0
23	DJ	720	0	719	3	0
23	Dj	760	0	759	2	0
24	DL	605	0	606	7	0
24	Di	877	0	893	7	0
25	Dc	1011	0	975	5	0
26	Dk	786	0	818	3	0
27	Dm	724	0	744	2	0
28	E	1721	0	1737	52	0
29	F	636	0	665	39	0
30	G	1351	0	1358	41	0
31	H	1186	0	1147	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	I	928	0	859	22	0
33	J	507	0	523	13	0
34	K	920	0	942	37	0
35	L	373	0	381	9	0
36	M	1954	0	1990	38	0
37	N	4645	0	2544	159	0
38	O	1422	0	1514	83	0
39	Q	1138	0	1103	11	0
40	R	1788	0	1819	26	0
41	T	4656	0	2548	102	0
42	U	931	0	888	22	0
43	V	806	0	818	25	0
44	W	1659	0	1665	51	0
45	X	1403	0	1428	45	0
46	a	801	0	839	3	0
46	e	810	0	851	4	0
47	b	653	0	696	4	0
47	f	638	0	676	1	0
48	c	843	0	908	6	0
48	g	818	0	877	7	0
49	d	766	0	797	3	0
49	h	744	0	771	3	0
50	0	70	0	0	3	0
50	2	20	0	0	0	0
50	N	30	0	0	0	0
51	0	6	0	5	1	0
51	2	11	0	10	0	0
52	1	8	0	0	0	0
53	4	3	0	0	0	0
53	5	2	0	0	0	0
53	7	2	0	0	0	0
53	A	2	0	0	0	0
53	B	1	0	0	0	0
53	C	1	0	0	0	0
53	I	2	0	0	0	0
53	J	1	0	0	0	0
53	L	1	0	0	0	0
53	M	1	0	0	0	0
53	W	1	0	0	0	0
54	A	1	0	0	0	0
All	All	125749	0	121716	1502	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1502) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:N:178:DC:O2	41:T:-178:DG:N2	1.89	1.03
11:A:608:THR:HG21	11:A:771:VAL:HG13	1.55	0.88
41:T:-207:DA:H2'	41:T:-206:DT:H71	1.62	0.82
11:A:706:ILE:HG22	11:A:710:LYS:HE3	1.62	0.81
12:B:849:ASP:HB3	35:L:15:MET:HE1	1.63	0.79
29:F:108:ARG:HD2	29:F:118:TRP:CD1	2.17	0.78
11:A:962:ASP:HB3	11:A:1043:ILE:HG23	1.65	0.77
2:1:200:LEU:HD23	2:1:225:LEU:HD12	1.66	0.77
11:A:874:LYS:HB3	29:F:111:PRO:HG3	1.64	0.77
12:B:270:ILE:HB	12:B:308:ALA:HB3	1.65	0.76
28:E:17:ILE:HG21	28:E:74:VAL:HG11	1.68	0.76
12:B:23:GLN:NE2	12:B:27:TRP:HE1	1.84	0.75
12:B:968:ASN:HD21	12:B:970:HIS:HB2	1.52	0.75
11:A:847:LEU:HD21	12:B:723:THR:HG21	1.67	0.74
38:O:199:ALA:HB2	38:O:214:PHE:CD2	2.23	0.74
14:D:91:LYS:H	14:D:122:PHE:HZ	1.34	0.73
31:H:64:LEU:HD13	31:H:85:ALA:HB2	1.70	0.73
19:Df:390:THR:HG23	19:Df:391:LEU:HD22	1.70	0.72
41:T:-131:DT:H2''	41:T:-130:DT:C5	2.25	0.72
37:N:11:DG:H2''	37:N:12:DG:C8	2.25	0.72
12:B:975:ARG:HB3	12:B:977:THR:HG23	1.70	0.72
15:DA:1055:VAL:HG13	15:DA:1056:ALA:H	1.55	0.71
14:D:87:LEU:HB3	14:D:97:LEU:HD22	1.73	0.71
8:7:20:LYS:HE3	8:7:62:LEU:HD13	1.73	0.70
11:A:727:PRO:HA	11:A:736:THR:HG21	1.73	0.70
22:DI:44:PHE:O	22:DI:48:THR:HG23	1.91	0.70
41:T:-86:DA:H2''	41:T:-85:DC:C6	2.27	0.70
37:N:148:DT:H2''	37:N:149:DC:C6	2.26	0.70
12:B:1027:VAL:HG22	13:C:195:THR:HG21	1.74	0.70
50:O:812:2A1:O	50:O:813:2A1:C3	2.40	0.70
40:R:187:LEU:HD23	40:R:220:ILE:HD11	1.74	0.69
38:O:174:LEU:HD12	38:O:178:LEU:HD11	1.74	0.69
18:DE:636:HIS:CD2	18:DE:637:PRO:HD2	2.27	0.69
11:A:917:GLU:HA	11:A:956:PHE:CZ	2.28	0.68
37:N:200:DT:H2''	37:N:201:DC:C5	2.28	0.68
10:9:32:CYS:SG	30:G:20:PRO:HD3	2.34	0.68
1:0:58:ALA:HB2	4:3:334:MET:HB3	1.76	0.68
12:B:635:LEU:HD21	12:B:640:ILE:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:787:VAL:HG13	11:A:824:GLU:HA	1.77	0.67
2:1:3:LEU:HD13	2:1:25:MET:HE1	1.76	0.67
12:B:27:TRP:CH2	12:B:762:ARG:HB2	2.31	0.66
23:Dj:176:MET:HE1	27:Dm:75:ILE:HD11	1.78	0.66
19:DF:347:THR:HG22	19:DF:348:THR:H	1.60	0.66
12:B:505:LEU:HD22	12:B:509:VAL:HB	1.78	0.66
33:J:21:TYR:HB2	33:J:38:LEU:HD11	1.77	0.66
38:O:192:TYR:HB2	38:O:200:VAL:HG22	1.77	0.66
38:O:302:LEU:HA	38:O:311:VAL:O	1.95	0.66
45:X:120:MET:HE3	45:X:124:LEU:HD21	1.76	0.66
12:B:910:THR:HG22	35:L:43:ILE:HA	1.77	0.66
37:N:7:DA:H1'	38:O:214:PHE:CZ	2.31	0.66
11:A:687:ILE:HD11	11:A:766:PHE:CD2	2.31	0.66
37:N:87:DG:H2''	37:N:88:DC:C5	2.30	0.65
41:T:-163:DG:H2''	41:T:-162:DT:C5	2.31	0.65
2:1:386:LEU:HB3	2:1:388:ILE:HG23	1.77	0.65
3:2:436:PRO:HA	3:2:441:MET:HG2	1.78	0.65
11:A:706:ILE:O	11:A:710:LYS:HG3	1.96	0.65
44:W:183:GLN:HG2	45:X:216:PHE:CE2	2.31	0.65
45:X:146:ARG:HA	45:X:175:LEU:HB2	1.78	0.65
11:A:784:VAL:C	11:A:826:SER:HB2	2.22	0.65
28:E:13:ILE:HD13	28:E:132:GLN:HG3	1.79	0.65
29:F:74:ALA:HB2	29:F:89:PRO:HG3	1.79	0.64
2:1:664:VAL:HG12	2:1:677:MET:HB3	1.78	0.64
12:B:270:ILE:HB	12:B:308:ALA:CB	2.26	0.64
37:N:47:DC:H5'	37:N:47:DC:C6	2.33	0.64
11:A:433:PRO:HA	11:A:438:LEU:HD11	1.79	0.64
11:A:1158:LEU:HG	11:A:1307:VAL:HB	1.79	0.64
22:DI:60:HIS:CE1	24:DL:115:ASP:HB3	2.31	0.64
37:N:109:DT:H2''	37:N:110:DA:C8	2.32	0.64
37:N:181:DC:H2''	37:N:182:DC:C5	2.32	0.64
29:F:57:MET:HE1	29:F:120:VAL:HG13	1.78	0.64
30:G:97:LEU:HD21	30:G:128:TYR:CD1	2.33	0.64
11:A:1480:CYS:O	30:G:19:GLY:HA2	1.97	0.64
37:N:24:DT:H2'	37:N:25:DC:C6	2.32	0.64
45:X:99:LEU:HD13	45:X:120:MET:SD	2.37	0.64
32:I:73:SER:HA	32:I:95:VAL:HG21	1.79	0.64
37:N:31:DC:H2''	37:N:32:DA:C8	2.33	0.64
1:0:438:MET:HE2	1:0:440:LEU:HD21	1.79	0.64
12:B:509:VAL:HG11	12:B:524:LYS:HB3	1.80	0.64
28:E:18:MET:HE3	28:E:60:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:N:148:DT:H2''	37:N:149:DC:C5	2.33	0.63
42:U:357:ILE:HG21	43:V:9:THR:HG21	1.79	0.63
11:A:713:VAL:HG13	11:A:741:VAL:HG13	1.78	0.63
37:N:22:DG:H2''	37:N:23:DT:C6	2.33	0.63
12:B:1012:SER:HB3	12:B:1022:LEU:HD12	1.80	0.63
34:K:31:CYS:HB2	34:K:83:PRO:HB2	1.81	0.63
8:7:90:PRO:HG2	8:7:95:TYR:CE2	2.34	0.63
12:B:643:LEU:HD11	12:B:656:LEU:HD21	1.81	0.62
1:0:164:GLY:H	1:0:292:LEU:HD21	1.64	0.62
36:M:231:ALA:HB2	36:M:304:PHE:CD1	2.33	0.62
39:Q:26:TYR:HA	40:R:97:THR:HG22	1.81	0.62
2:1:557:ILE:HD13	2:1:561:ILE:HD12	1.81	0.62
41:T:-89:DG:H1'	41:T:-88:DG:C5	2.34	0.62
42:U:366:ILE:HD11	43:V:48:LEU:HD21	1.81	0.62
44:W:113:ARG:HD2	45:X:219:LEU:HD12	1.80	0.62
2:1:462:SER:OG	2:1:463:PRO:HD2	1.99	0.62
2:1:372:LEU:HD23	2:1:408:SER:HB3	1.81	0.62
12:B:646:ARG:HG3	12:B:651:TYR:O	1.99	0.62
12:B:677:MET:H	12:B:682:LEU:HG	1.65	0.62
30:G:4:HIS:CE1	30:G:73:LYS:HD2	2.35	0.62
37:N:7:DA:H1'	38:O:214:PHE:CE1	2.35	0.62
37:N:110:DA:H2''	37:N:111:DG:C8	2.35	0.62
41:T:-208:DT:H2''	41:T:-207:DA:C8	2.34	0.62
11:A:790:GLN:HA	11:A:822:PHE:HA	1.82	0.61
11:A:1468:THR:HA	29:F:60:TYR:HB3	1.83	0.61
28:E:91:CYS:HB2	28:E:121:MET:HE1	1.82	0.61
11:A:745:LEU:CD1	11:A:817:PRO:HB3	2.30	0.61
11:A:827:TYR:OH	12:B:718:GLN:HG3	2.00	0.61
36:M:260:MET:HG2	36:M:300:PHE:CE1	2.35	0.61
4:3:125:GLY:HA2	6:5:105:THR:HG23	1.82	0.61
11:A:956:PHE:HA	11:A:959:MET:HE3	1.82	0.61
37:N:210:DA:H2''	37:N:211:DC:C6	2.35	0.61
37:N:211:DC:H2''	37:N:212:DA:N7	2.15	0.61
31:H:40:ILE:HD12	31:H:124:ARG:HD2	1.83	0.61
2:1:77:VAL:HA	2:1:80:ILE:HD12	1.81	0.61
11:A:452:ASP:OD1	11:A:476:ILE:HG12	1.99	0.61
37:N:29:DC:H2'	37:N:30:DT:H72	1.82	0.61
11:A:717:ILE:HA	11:A:737:PHE:CE1	2.36	0.61
12:B:553:LEU:HA	12:B:556:ILE:HD12	1.83	0.61
37:N:98:DT:H2''	37:N:99:DC:C5	2.35	0.61
8:7:8:ARG:NH1	44:W:178:ALA:HA	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:18:LEU:HB2	9:8:26:VAL:HG13	1.83	0.61
30:G:114:PRO:HG2	30:G:164:MET:HG3	1.82	0.61
28:E:44:PHE:CG	28:E:52:ARG:HG3	2.36	0.61
12:B:633:LEU:HD12	12:B:679:PRO:HG3	1.82	0.60
11:A:760:LEU:HD22	11:A:764:ASN:ND2	2.15	0.60
30:G:30:LEU:HD21	30:G:72:TYR:CG	2.36	0.60
31:H:7:GLU:HG3	31:H:59:VAL:HG22	1.83	0.60
37:N:10:DG:H2''	37:N:11:DG:C8	2.36	0.60
12:B:85:LEU:HB2	12:B:131:THR:OG1	2.00	0.60
40:R:237:PRO:HG3	45:X:75:PHE:HB3	1.83	0.60
44:W:110:MET:CE	45:X:220:TRP:HA	2.31	0.60
13:C:268:GLN:HA	13:C:271:VAL:HG12	1.81	0.60
37:N:198:DT:H2''	37:N:199:DG:C8	2.36	0.60
41:T:-90:DC:H2''	41:T:-89:DG:C8	2.36	0.60
45:X:89:HIS:HB2	45:X:139:PHE:CD1	2.36	0.60
8:7:9:CYS:SG	8:7:33:SER:HB3	2.41	0.60
1:0:531:ILE:HA	1:0:534:TYR:CE2	2.37	0.60
12:B:387:HIS:CD2	12:B:504:THR:HG21	2.37	0.59
1:0:283:ARG:HA	1:0:286:HIS:CD2	2.37	0.59
11:A:874:LYS:CB	29:F:111:PRO:HG3	2.32	0.59
37:N:193:DG:H2''	37:N:194:DC:C6	2.37	0.59
41:T:-54:DG:H2''	41:T:-53:DG:C8	2.36	0.59
38:O:169:VAL:HG13	38:O:222:THR:HG22	1.85	0.59
30:G:127:CYS:HB3	30:G:138:GLN:HB3	1.84	0.59
44:W:33:ALA:HA	44:W:52:LEU:HD11	1.84	0.59
10:9:25:ASP:HB3	11:A:1482:TYR:CE2	2.38	0.59
13:C:88:CYS:HB2	13:C:97:CYS:HB3	1.83	0.59
42:U:333:ASN:HB2	43:V:93:VAL:HG22	1.85	0.59
11:A:455:ILE:O	11:A:506:PRO:HD2	2.02	0.59
12:B:65:ILE:O	12:B:85:LEU:HA	2.02	0.59
31:H:88:PHE:CG	31:H:144:LEU:HB3	2.37	0.59
11:A:1005:HIS:HD2	11:A:1006:PRO:HD2	1.68	0.59
11:A:1479:LYS:HB3	29:F:103:PRO:HA	1.84	0.59
29:F:80:MET:HG3	29:F:103:PRO:HD3	1.85	0.59
37:N:213:DT:H2''	37:N:214:DC:C6	2.38	0.59
40:R:191:PHE:CE2	40:R:236:LYS:HD3	2.37	0.59
37:N:183:DT:H2''	37:N:184:DA:C8	2.38	0.59
15:DA:409:HIS:CE1	15:DA:411:GLU:HB2	2.38	0.58
37:N:204:DA:H2'	37:N:205:DT:H71	1.84	0.58
38:O:187:ALA:HB3	38:O:190:ALA:HB2	1.85	0.58
45:X:89:HIS:HB2	45:X:139:PHE:CE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:163:PRO:HA	38:O:262:CYS:HB3	1.84	0.58
37:N:88:DC:H2''	37:N:89:DC:C4	2.39	0.58
37:N:104:DG:H2'	37:N:105:DG:C8	2.38	0.58
45:X:151:LEU:HD13	45:X:171:ILE:HG21	1.84	0.58
48:g:50:VAL:HG21	49:h:122:TYR:CG	2.38	0.58
41:T:-83:DG:H2''	41:T:-82:DG:C8	2.39	0.58
44:W:144:LEU:HD13	44:W:161:VAL:HG11	1.86	0.58
12:B:815:LYS:HB2	12:B:918:PHE:CE1	2.38	0.58
11:A:1471:PHE:CZ	29:F:61:GLU:HA	2.39	0.58
12:B:285:LEU:HD23	12:B:298:MET:HE1	1.84	0.58
41:T:-202:DT:H2''	41:T:-201:DG:C5	2.38	0.58
28:E:55:ARG:HH22	28:E:132:GLN:HE22	1.52	0.57
37:N:142:DG:C2	41:T:-141:DG:N2	2.72	0.57
41:T:-110:DT:H4'	41:T:-109:DA:H5'	1.85	0.57
11:A:948:ILE:HD13	11:A:1005:HIS:CE1	2.39	0.57
28:E:13:ILE:HG23	28:E:135:LEU:HD23	1.85	0.57
37:N:2:DA:H2	41:T:-2:DT:O2	1.87	0.57
38:O:163:PRO:HD2	38:O:322:TYR:HA	1.86	0.57
43:V:48:LEU:HA	43:V:52:VAL:CG2	2.34	0.57
36:M:214:PHE:HB3	36:M:218:PHE:CE2	2.38	0.57
44:W:36:ILE:HG21	44:W:48:MET:HG2	1.85	0.57
2:1:232:VAL:HG22	2:1:455:ILE:HD13	1.85	0.57
41:T:-206:DT:H2'	41:T:-205:DA:C8	2.38	0.57
12:B:717:ASN:OD1	12:B:979:GLY:N	2.31	0.57
20:DG:134:HIS:CE1	20:DG:141:LYS:HE2	2.40	0.57
2:1:161:PHE:CZ	2:1:194:LEU:HA	2.39	0.57
13:C:76:ASP:HA	13:C:239:LEU:CD2	2.34	0.57
38:O:223:GLY:HA3	41:T:-5:DT:H4'	1.87	0.57
11:A:1243:LEU:HB3	11:A:1259:ILE:HG23	1.86	0.57
31:H:35:PHE:HB2	31:H:37:MET:HG2	1.86	0.57
37:N:17:DG:N1	41:T:-17:DC:O2	2.37	0.57
11:A:419:ILE:HG13	11:A:429:LEU:HD21	1.86	0.57
12:B:1094:GLN:HB2	12:B:1103:LEU:HD13	1.87	0.57
13:C:7:PRO:HB2	34:K:101:LEU:HD13	1.87	0.57
13:C:267:ILE:HG12	34:K:84:GLN:HB3	1.87	0.57
38:O:197:PHE:CE2	38:O:199:ALA:HB3	2.40	0.57
6:5:275:PHE:CZ	6:5:282:CYS:HB2	2.40	0.56
29:F:70:ALA:O	29:F:89:PRO:HB2	2.05	0.56
37:N:149:DC:H2''	37:N:150:DC:C5	2.39	0.56
37:N:180:DC:H2''	37:N:181:DC:C5	2.40	0.56
4:3:148:LEU:HA	4:3:151:TYR:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:705:THR:HG21	11:A:752:THR:HG23	1.86	0.56
12:B:625:LEU:HD13	12:B:675:LEU:HD13	1.87	0.56
13:C:84:TYR:CZ	13:C:167:LYS:HE2	2.41	0.56
44:W:34:LEU:HD13	44:W:66:LEU:HD12	1.87	0.56
47:b:32:LYS:HG3	47:b:52:TYR:CZ	2.41	0.56
12:B:94:SER:O	12:B:122:ALA:HB1	2.05	0.56
12:B:640:ILE:O	12:B:644:LYS:HG3	2.06	0.56
11:A:921:ARG:HA	11:A:956:PHE:HB2	1.88	0.56
12:B:502:HIS:CE1	12:B:504:THR:HG23	2.40	0.56
13:C:47:ILE:HA	13:C:165:ALA:HA	1.88	0.56
11:A:728:THR:H	11:A:736:THR:HG21	1.71	0.56
11:A:917:GLU:HA	11:A:956:PHE:CE1	2.41	0.56
28:E:44:PHE:HB2	28:E:52:ARG:HG3	1.86	0.56
37:N:160:DT:H2"	37:N:161:DA:C8	2.41	0.56
38:O:199:ALA:HB2	38:O:214:PHE:CE2	2.40	0.56
19:DF:327:TRP:CZ2	19:DF:371:THR:HB	2.40	0.56
38:O:264:VAL:HG21	38:O:268:ILE:HD11	1.88	0.56
44:W:104:LYS:HG3	44:W:191:LEU:HD22	1.88	0.56
37:N:22:DG:H2"	37:N:23:DT:C5	2.41	0.56
44:W:144:LEU:HD22	44:W:161:VAL:HG21	1.88	0.56
38:O:300:ILE:HG21	38:O:312:LEU:HB3	1.86	0.56
11:A:479:TRP:HB2	11:A:483:ARG:NH2	2.21	0.56
11:A:1147:SER:O	11:A:1154:ALA:HB2	2.05	0.56
37:N:180:DC:H2"	37:N:181:DC:C4	2.41	0.56
12:B:256:ILE:HD11	12:B:373:LEU:HD21	1.89	0.55
17:DD:1003:ASP:HB3	43:V:3:TYR:CD1	2.41	0.55
34:K:50:LEU:HD13	34:K:75:VAL:HG22	1.86	0.55
43:V:3:TYR:CD2	43:V:98:CYS:HB3	2.41	0.55
44:W:126:SER:HA	44:W:166:SER:HB3	1.88	0.55
34:K:81:TYR:CE2	34:K:86:ALA:HB2	2.41	0.55
50:O:801:2A1:O	50:O:802:2A1:C3	2.55	0.55
31:H:58:LEU:HD11	31:H:143:LEU:HD11	1.87	0.55
2:1:255:THR:HG23	2:1:396:PRO:HB3	1.88	0.55
11:A:804:HIS:NE2	32:I:100:HIS:CD2	2.74	0.55
37:N:150:DC:H2"	37:N:151:DC:C5	2.42	0.55
2:1:141:TYR:CZ	2:1:387:GLU:HA	2.42	0.55
36:M:235:ILE:HA	36:M:299:LEU:HB3	1.89	0.55
45:X:88:ARG:HG2	45:X:97:LEU:HD11	1.87	0.55
18:De:221:LEU:HD13	18:De:321:LEU:HD21	1.87	0.55
28:E:44:PHE:CB	28:E:52:ARG:HG3	2.37	0.55
11:A:369:PRO:HD3	11:A:496:PHE:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1215:GLU:HG2	11:A:1256:VAL:HG22	1.87	0.55
42:U:357:ILE:CG2	43:V:9:THR:HG21	2.37	0.55
6:5:178:MET:HG3	6:5:182:PHE:CE2	2.42	0.54
11:A:495:ASP:OD2	11:A:497:ASP:CG	2.49	0.54
12:B:794:VAL:HG13	12:B:965:ILE:HG23	1.89	0.54
26:Dk:144:THR:HG23	26:Dk:145:SER:H	1.71	0.54
8:7:78:VAL:HG21	8:7:106:VAL:HG22	1.89	0.54
12:B:59:VAL:HG21	12:B:91:ILE:HD11	1.90	0.54
12:B:794:VAL:HG22	12:B:967:ILE:HG22	1.90	0.54
13:C:37:VAL:HG13	13:C:41:GLU:HB2	1.89	0.54
18:DE:565:GLY:HA2	18:DE:588:VAL:HG23	1.89	0.54
31:H:57:ARG:O	31:H:145:MET:HA	2.08	0.54
1:0:535:THR:HG23	1:0:627:SER:HB2	1.89	0.54
28:E:90:TYR:C	28:E:94:MET:HE3	2.33	0.54
37:N:27:DT:H2'	37:N:28:DC:C5	2.42	0.54
38:O:212:LEU:O	38:O:219:MET:HA	2.06	0.54
38:O:280:PHE:CE1	38:O:296:ILE:HD11	2.43	0.54
22:DI:60:HIS:HE1	24:DL:115:ASP:HB3	1.72	0.54
19:Df:318:CYS:SG	19:Df:326:HIS:HB3	2.48	0.54
28:E:17:ILE:CG2	28:E:74:VAL:HG11	2.37	0.54
11:A:687:ILE:HD11	11:A:766:PHE:CE2	2.42	0.54
12:B:604:ILE:O	12:B:612:ILE:HA	2.08	0.54
29:F:77:ALA:HB2	30:G:15:PRO:HB3	1.90	0.54
31:H:59:VAL:HG21	31:H:88:PHE:CZ	2.43	0.54
41:T:-22:DC:H2''	41:T:-21:DG:C5'	2.38	0.54
48:c:25:GLN:NE2	49:d:48:GLN:HE22	2.05	0.54
12:B:446:TYR:CZ	12:B:456:GLN:HA	2.43	0.54
11:A:502:ASN:HB3	12:B:1084:LEU:HD13	1.90	0.54
13:C:84:TYR:CE1	13:C:167:LYS:HG2	2.42	0.54
28:E:55:ARG:NH2	28:E:132:GLN:HE22	2.06	0.54
37:N:72:DA:H2''	37:N:73:DT:H72	1.89	0.54
38:O:239:ARG:HG3	38:O:239:ARG:HH11	1.73	0.54
38:O:250:PHE:CE2	38:O:253:PHE:HB2	2.43	0.54
41:T:-134:DC:OP1	46:a:39:PRO:HD2	2.07	0.54
41:T:-131:DT:H2''	41:T:-130:DT:C6	2.43	0.54
42:U:18:ILE:HD11	42:U:46:TRP:CZ3	2.43	0.54
9:8:120:MET:HE1	9:8:150:VAL:HA	1.89	0.53
13:C:44:ILE:HD11	13:C:176:TRP:HA	1.88	0.53
37:N:17:DG:C2	41:T:-16:DC:C2	2.96	0.53
40:R:206:THR:HG21	40:R:213:LEU:HD13	1.90	0.53
44:W:148:MET:HG3	44:W:149:THR:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:353:SER:HB2	2:1:356:ALA:HB3	1.90	0.53
11:A:597:PRO:HD3	11:A:668:PHE:CD1	2.43	0.53
12:B:613:ARG:HB3	12:B:615:TYR:HE2	1.73	0.53
28:E:8:TYR:HA	28:E:37:LEU:HD13	1.90	0.53
29:F:70:ALA:HB2	29:F:90:LEU:HA	1.90	0.53
34:K:56:VAL:HG22	34:K:77:THR:HG22	1.90	0.53
28:E:20:LEU:HA	28:E:182:TYR:CZ	2.44	0.53
41:T:-202:DT:H2''	41:T:-201:DG:C4	2.43	0.53
15:DA:744:GLU:HG3	15:DA:749:ARG:HE	1.73	0.53
30:G:5:ILE:HD11	30:G:76:VAL:HG11	1.90	0.53
31:H:84:ARG:HA	31:H:87:GLN:OE1	2.08	0.53
8:7:40:VAL:CG2	44:W:122:THR:HA	2.38	0.53
11:A:196:LEU:HD12	11:A:308:LYS:HE2	1.90	0.53
11:A:702:ILE:HD13	11:A:786:ALA:HA	1.91	0.53
11:A:1029:LEU:HD22	28:E:159:LEU:HA	1.91	0.53
31:H:60:ILE:HG13	31:H:135:PHE:CZ	2.44	0.53
37:N:50:DG:C6	37:N:51:DA:C6	2.95	0.53
37:N:150:DC:H2''	37:N:151:DC:C6	2.43	0.53
41:T:-75:DC:H2''	41:T:-74:DG:C8	2.44	0.53
45:X:133:ILE:HD12	45:X:138:ALA:HB3	1.89	0.53
12:B:26:CYS:SG	12:B:699:HIS:HD2	2.32	0.53
12:B:907:VAL:HG13	12:B:921:ILE:HG12	1.91	0.53
15:DA:616:HIS:CD2	15:DA:691:MET:HG2	2.44	0.53
44:W:110:MET:SD	45:X:219:LEU:HG	2.49	0.53
38:O:204:ILE:HD12	38:O:207:PRO:HG2	1.91	0.53
38:O:311:VAL:HG22	41:T:-3:DA:H2''	1.90	0.53
11:A:717:ILE:HA	11:A:737:PHE:HE1	1.73	0.53
12:B:99:TRP:CZ2	40:R:148:VAL:HG21	2.43	0.53
12:B:1119:CYS:HB2	12:B:1137:CYS:SG	2.48	0.53
28:E:20:LEU:HD22	28:E:103:LEU:CD2	2.39	0.53
31:H:60:ILE:HG13	31:H:135:PHE:HZ	1.73	0.53
37:N:76:DA:H2''	37:N:77:DG:C6	2.44	0.53
33:J:35:LEU:HD22	33:J:46:ARG:HA	1.91	0.53
2:1:537:ALA:HB1	2:1:621:PHE:CE2	2.44	0.52
11:A:409:GLY:O	11:A:415:GLY:HA3	2.09	0.52
18:DE:486:ALA:HB2	18:DE:551:PHE:CZ	2.44	0.52
30:G:117:MET:HG2	30:G:164:MET:HE2	1.91	0.52
37:N:118:DC:H1'	37:N:119:DT:C5	2.43	0.52
38:O:325:PHE:HA	38:O:328:ILE:HG22	1.90	0.52
2:1:536:VAL:HG21	2:1:610:PHE:CE2	2.45	0.52
9:8:66:LEU:HD23	9:8:77:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:745:LEU:HD13	11:A:817:PRO:HB3	1.90	0.52
36:M:225:PRO:HD2	36:M:228:VAL:HG21	1.92	0.52
37:N:11:DG:H2"	37:N:12:DG:N7	2.24	0.52
44:W:107:LEU:HD11	44:W:187:ILE:HG21	1.90	0.52
12:B:939:HIS:NE2	12:B:980:HIS:HA	2.24	0.52
37:N:51:DA:C2	37:N:52:DG:C6	2.97	0.52
44:W:110:MET:HE3	45:X:220:TRP:HA	1.92	0.52
19:Df:334:ALA:HB1	19:Df:379:GLY:HA2	1.91	0.52
37:N:199:DG:H2"	37:N:200:DT:C5	2.45	0.52
38:O:172:VAL:HG21	38:O:250:PHE:CE1	2.45	0.52
41:T:-162:DT:H2"	41:T:-161:DT:C6	2.45	0.52
37:N:102:DT:H2'	37:N:103:DT:C6	2.44	0.52
42:U:29:PHE:HB3	42:U:35:ASP:HA	1.91	0.52
12:B:30:ILE:HG22	12:B:766:TYR:CE2	2.45	0.52
12:B:42:GLN:H	12:B:42:GLN:CD	2.17	0.52
28:E:48:PRO:HA	28:E:52:ARG:NH1	2.25	0.52
37:N:160:DT:H2"	37:N:161:DA:N7	2.24	0.52
1:0:129:VAL:HG23	1:0:131:LEU:HG	1.90	0.52
1:0:445:THR:HB	1:0:451:PHE:HD2	1.75	0.52
19:Df:224:TYR:HB2	19:Df:255:MET:HE3	1.91	0.52
28:E:20:LEU:HD22	28:E:103:LEU:HD21	1.92	0.52
31:H:64:LEU:HG	31:H:142:TYR:CD2	2.45	0.52
31:H:118:TYR:CZ	31:H:143:LEU:HB2	2.44	0.52
41:T:-99:DG:N2	48:c:12:ARG:HH12	2.07	0.52
41:T:-69:DT:H2"	41:T:-68:DA:C8	2.44	0.52
2:1:335:ARG:HE	2:1:365:VAL:CG2	2.22	0.52
11:A:406:VAL:HG11	11:A:419:ILE:HD11	1.91	0.52
11:A:784:VAL:O	11:A:826:SER:HB2	2.09	0.52
30:G:143:ILE:HA	30:G:169:GLY:O	2.10	0.52
38:O:266:PHE:CZ	38:O:333:LYS:HA	2.45	0.52
42:U:356:GLY:HA3	42:U:367:PHE:CZ	2.45	0.52
44:W:106:LYS:O	44:W:110:MET:HG2	2.10	0.52
1:0:285:ILE:HD13	1:0:290:PRO:HB3	1.91	0.52
11:A:608:THR:CG2	11:A:771:VAL:HG13	2.32	0.52
11:A:1120:GLY:H	11:A:1385:VAL:HG23	1.74	0.52
12:B:296:GLU:O	12:B:300:MET:HG2	2.10	0.52
12:B:446:TYR:CE2	12:B:456:GLN:HA	2.45	0.52
37:N:26:DG:N2	41:T:-25:DG:C2	2.78	0.52
38:O:172:VAL:HG21	38:O:250:PHE:CD1	2.45	0.52
45:X:158:HIS:CG	45:X:166:ILE:HD11	2.45	0.52
11:A:958:ARG:HD3	11:A:1046:ARG:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:19:PRO:HB3	12:B:680:ASP:HB3	1.92	0.52
12:B:237:VAL:HG11	12:B:369:VAL:HG22	1.92	0.52
13:C:21:PHE:CD2	34:K:105:PHE:HE2	2.28	0.52
14:D:87:LEU:HD11	14:D:101:ALA:HB2	1.91	0.52
37:N:67:DC:H2''	37:N:68:DT:C2	2.45	0.52
11:A:1005:HIS:CD2	11:A:1006:PRO:HD2	2.44	0.51
11:A:1208:SER:HA	11:A:1266:GLU:HG3	1.91	0.51
12:B:156:LEU:HA	12:B:161:CYS:SG	2.50	0.51
12:B:908:MET:HB3	35:L:45:TYR:CE1	2.45	0.51
37:N:154:DG:H3'	46:e:47:VAL:HG21	1.91	0.51
1:O:121:TYR:CE1	1:O:285:ILE:HG21	2.46	0.51
11:A:693:ILE:HD13	11:A:828:LEU:HD21	1.91	0.51
12:B:911:LEU:HD12	35:L:42:ARG:HD3	1.91	0.51
14:D:32:LEU:HD11	30:G:4:HIS:HB2	1.91	0.51
16:DB:131:PRO:HD2	16:DB:134:LEU:HD12	1.91	0.51
32:I:87:GLN:HB2	32:I:121:HIS:CE1	2.44	0.51
42:U:14:TYR:CZ	43:V:11:LEU:HD13	2.45	0.51
11:A:408:ARG:HH12	11:A:413:TYR:C	2.17	0.51
12:B:388:TYR:CZ	12:B:505:LEU:HD21	2.45	0.51
17:Dd:911:GLN:HG3	24:Dl:66:LEU:HD21	1.91	0.51
11:A:41:ILE:HG21	11:A:57:LEU:HD23	1.92	0.51
11:A:329:MET:HA	11:A:335:PRO:HA	1.91	0.51
11:A:831:LEU:HD23	11:A:835:GLU:C	2.35	0.51
11:A:1346:VAL:HG12	11:A:1352:VAL:HG11	1.91	0.51
12:B:273:PHE:HB3	12:B:284:ILE:HG12	1.92	0.51
35:L:17:TYR:CD1	35:L:28:ILE:HB	2.46	0.51
37:N:120:DA:H1'	37:N:121:DG:N7	2.25	0.51
41:T:-12:DC:OP2	41:T:-12:DC:H3'	2.10	0.51
42:U:370:ALA:HA	43:V:56:VAL:O	2.09	0.51
1:O:479:ASP:HA	1:O:482:PHE:CE2	2.46	0.51
11:A:713:VAL:CG1	11:A:741:VAL:HG13	2.40	0.51
12:B:939:HIS:CE1	12:B:980:HIS:HA	2.46	0.51
13:C:44:ILE:HG13	13:C:176:TRP:HD1	1.74	0.51
28:E:44:PHE:CD1	28:E:52:ARG:HG3	2.46	0.51
31:H:41:LEU:HD11	31:H:143:LEU:HD22	1.92	0.51
9:8:136:ARG:O	9:8:174:VAL:HG22	2.11	0.51
29:F:90:LEU:HG	29:F:94:MET:HE2	1.93	0.51
1:O:124:TYR:HB3	1:O:163:TYR:CE2	2.46	0.51
11:A:435:PRO:HA	11:A:438:LEU:HB2	1.91	0.51
11:A:609:HIS:HA	11:A:626:THR:HB	1.93	0.51
12:B:565:THR:O	12:B:576:ILE:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:165:LYS:HE2	6:5:200:SER:HB2	1.93	0.51
11:A:465:HIS:CE1	11:A:467:MET:HE2	2.46	0.51
11:A:628:VAL:HA	11:A:638:GLY:HA3	1.92	0.51
11:A:859:TYR:O	11:A:863:ARG:HG2	2.11	0.51
12:B:744:MET:SD	12:B:908:MET:HG2	2.50	0.51
33:J:47:ARG:HD2	33:J:47:ARG:C	2.36	0.51
11:A:1308:TYR:HB2	11:A:1337:GLU:CD	2.36	0.51
16:DB:205:GLU:HG2	16:DB:235:HIS:CD2	2.46	0.51
25:Dc:55:LEU:HD21	17:Dd:920:THR:HG23	1.91	0.51
4:3:430:VAL:HG12	4:3:443:VAL:HB	1.93	0.51
12:B:215:TYR:CG	12:B:238:SER:HB3	2.46	0.51
32:I:87:GLN:HB2	32:I:121:HIS:HE1	1.76	0.51
4:3:448:HIS:HA	4:3:451:VAL:HG12	1.93	0.50
11:A:859:TYR:CE2	11:A:1125:LYS:HE3	2.46	0.50
37:N:212:DA:H2''	37:N:213:DT:C6	2.45	0.50
42:U:366:ILE:HG12	43:V:48:LEU:HD11	1.92	0.50
25:Dc:12:VAL:HG23	19:Df:118:ILE:HA	1.93	0.50
37:N:95:DC:H2''	37:N:96:DG:C8	2.46	0.50
11:A:580:LEU:HD22	31:H:64:LEU:HD12	1.94	0.50
11:A:745:LEU:HD11	11:A:817:PRO:HB3	1.92	0.50
11:A:1009:VAL:HG11	11:A:1051:SER:HA	1.94	0.50
12:B:1062:ARG:HD3	12:B:1081:ASP:O	2.11	0.50
13:C:75:SER:HB2	13:C:79:VAL:HB	1.93	0.50
15:DA:611:LYS:HE3	20:DG:10:HIS:O	2.11	0.50
37:N:29:DC:H2'	37:N:30:DT:C7	2.42	0.50
38:O:210:THR:HG21	41:T:-6:DT:H4'	1.93	0.50
2:1:232:VAL:HG13	2:1:455:ILE:HB	1.92	0.50
11:A:811:ILE:HG12	12:B:689:TYR:OH	2.10	0.50
12:B:1029:TYR:CE2	12:B:1036:LYS:HG2	2.46	0.50
16:DB:345:CYS:HA	16:DB:348:GLN:HE21	1.77	0.50
36:M:263:GLN:HB3	36:M:314:PRO:HD2	1.94	0.50
43:V:67:PHE:HB2	43:V:72:TRP:CE3	2.46	0.50
11:A:406:VAL:CG1	11:A:419:ILE:HD11	2.42	0.50
11:A:931:ARG:HD2	11:A:939:VAL:HG11	1.94	0.50
12:B:613:ARG:HB3	12:B:615:TYR:CE2	2.46	0.50
12:B:1028:LEU:HD13	12:B:1041:ILE:HB	1.94	0.50
13:C:245:VAL:HG11	34:K:105:PHE:CE2	2.45	0.50
13:C:263:LEU:HD12	34:K:21:ILE:HD11	1.93	0.50
14:D:92:LEU:HG	14:D:122:PHE:CE2	2.46	0.50
32:I:69:ILE:HG22	32:I:71:ASP:H	1.75	0.50
36:M:131:PRO:HD2	36:M:134:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:190:ALA:HB1	38:O:200:VAL:CG1	2.41	0.50
2:1:209:TYR:HB3	2:1:242:VAL:HG13	1.92	0.50
11:A:699:TYR:HA	11:A:702:ILE:HD12	1.94	0.50
11:A:1347:LEU:HD22	11:A:1354:PRO:O	2.12	0.50
28:E:76:PHE:CE2	28:E:105:VAL:HG21	2.47	0.50
34:K:21:ILE:HG12	34:K:33:PHE:CD2	2.47	0.50
2:1:359:SER:HB2	8:7:147:LEU:HB3	1.92	0.50
13:C:4:ALA:HB2	34:K:93:ASP:O	2.11	0.50
13:C:35:ARG:HA	13:C:38:PHE:CD2	2.46	0.50
21:DH:40:VAL:HG21	23:DJ:130:ILE:HG12	1.93	0.50
45:X:172:GLU:OE2	45:X:178:SER:HB3	2.12	0.50
28:E:59:THR:HG22	28:E:76:PHE:H	1.76	0.50
34:K:19:ILE:HA	34:K:34:THR:O	2.11	0.50
37:N:97:DC:H2"	37:N:98:DT:C5	2.46	0.50
42:U:337:CYS:SG	42:U:353:LEU:HD13	2.52	0.50
45:X:129:LYS:HE2	45:X:173:GLU:OE1	2.12	0.50
11:A:798:ILE:HG21	11:A:838:PHE:CE1	2.47	0.50
11:A:1192:TRP:HZ3	11:A:1246:ILE:HG22	1.77	0.50
15:DA:802:HIS:CD2	15:DA:884:GLN:HB3	2.46	0.50
28:E:73:PHE:CE2	28:E:99:ILE:HG13	2.47	0.50
38:O:231:ARG:HA	38:O:253:PHE:CE1	2.46	0.50
11:A:1181:PRO:HB2	11:A:1197:TYR:CD1	2.47	0.49
25:Dc:124:ILE:HD12	25:Dc:124:ILE:H	1.77	0.49
32:I:39:CYS:HB3	32:I:44:TYR:HB3	1.93	0.49
1:0:413:LEU:HA	1:0:427:MET:HE2	1.93	0.49
11:A:875:TYR:HB3	29:F:53:THR:HG22	1.93	0.49
12:B:285:LEU:HD11	12:B:305:LEU:HD21	1.93	0.49
28:E:18:MET:HA	28:E:18:MET:HE2	1.94	0.49
28:E:59:THR:HG22	28:E:75:PHE:HA	1.94	0.49
30:G:114:PRO:HB2	30:G:164:MET:HE3	1.93	0.49
41:T:-22:DC:H2"	41:T:-21:DG:H5"	1.94	0.49
42:U:372:GLY:HA3	43:V:58:PHE:CZ	2.47	0.49
11:A:687:ILE:HG22	12:B:969:PRO:HB3	1.95	0.49
11:A:1344:MET:HE1	28:E:137:ILE:HG22	1.94	0.49
12:B:1012:SER:HB3	12:B:1022:LEU:HB2	1.94	0.49
18:DE:235:GLU:HB3	18:DE:309:ILE:HG22	1.93	0.49
29:F:91:LEU:HD23	29:F:94:MET:HE3	1.94	0.49
2:1:460:THR:HB	2:1:661:ALA:HB1	1.93	0.49
5:4:171:PHE:CE2	5:4:174:LEU:HA	2.47	0.49
5:4:363:CYS:SG	5:4:384:GLY:HA3	2.52	0.49
12:B:1015:LEU:HA	12:B:1018:TYR:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:E:52:ARG:HD3	28:E:53:PRO:HD3	1.95	0.49
33:J:8:PHE:CD2	33:J:48:MET:HE1	2.47	0.49
38:O:260:GLY:HA3	38:O:321:ILE:HG21	1.94	0.49
38:O:280:PHE:CZ	38:O:296:ILE:HD11	2.47	0.49
38:O:298:PRO:HG2	38:O:324:ALA:HB2	1.94	0.49
4:3:148:LEU:HD23	4:3:284:THR:HG22	1.94	0.49
5:4:349:GLN:HB2	6:5:69:PHE:CD2	2.47	0.49
11:A:1210:TRP:CZ2	11:A:1282:ASP:HB3	2.48	0.49
19:Df:276:LEU:HD13	19:Df:324:ASP:HB3	1.94	0.49
29:F:51:ARG:HD3	29:F:118:TRP:CZ2	2.47	0.49
33:J:40:LEU:HD22	33:J:45:CYS:HB3	1.95	0.49
34:K:27:VAL:HG11	34:K:76:GLN:NE2	2.27	0.49
34:K:35:ILE:HD11	34:K:87:PHE:HZ	1.77	0.49
38:O:174:LEU:HG	38:O:217:GLY:O	2.12	0.49
38:O:289:PRO:HG3	41:T:-1:DA:H1'	1.94	0.49
11:A:106:VAL:HG13	11:A:236:LEU:HD13	1.95	0.49
11:A:408:ARG:HB3	11:A:412:GLN:HB2	1.95	0.49
14:D:44:ARG:HG3	14:D:57:LEU:HD21	1.94	0.49
15:DA:1164:CYS:HB2	20:DG:184:ILE:HG13	1.94	0.49
37:N:87:DG:H2''	37:N:88:DC:C6	2.48	0.49
37:N:190:DC:H2''	37:N:191:DA:C5	2.48	0.49
45:X:158:HIS:CD2	45:X:166:ILE:HD11	2.48	0.49
11:A:362:SER:HB2	12:B:1084:LEU:HD12	1.94	0.49
12:B:968:ASN:ND2	12:B:970:HIS:HB2	2.23	0.49
22:DI:73:LEU:HD21	24:DL:102:LEU:HD23	1.95	0.49
31:H:92:MET:HE3	31:H:118:TYR:CD2	2.48	0.49
41:T:-129:DA:H1'	41:T:-128:DA:C5	2.48	0.49
11:A:381:PRO:HD2	11:A:384:ILE:HD12	1.95	0.49
11:A:410:ASN:HA	11:A:449:HIS:CE1	2.48	0.49
11:A:972:THR:HG23	11:A:974:ASP:H	1.76	0.49
11:A:1366:PHE:HB2	11:A:1374:VAL:HG21	1.95	0.49
12:B:759:VAL:CG1	12:B:999:ALA:HB2	2.43	0.49
16:DB:472:VAL:HG21	16:DB:507:ILE:HG12	1.95	0.49
18:De:486:ALA:HB2	18:De:551:PHE:CE1	2.48	0.49
31:H:10:PHE:CE2	31:H:32:SER:HB3	2.48	0.49
34:K:30:ALA:HA	34:K:76:GLN:HA	1.95	0.49
41:T:-214:DG:H2''	41:T:-213:DA:C8	2.48	0.49
6:5:268:CYS:SG	6:5:271:CYS:HB2	2.53	0.49
11:A:425:ASP:HB2	36:M:39:LEU:CD1	2.42	0.49
11:A:1029:LEU:CD2	28:E:159:LEU:HA	2.43	0.49
11:A:1137:PRO:HB2	11:A:1341:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:44:ARG:HG2	30:G:47:ALA:HB1	1.94	0.49
34:K:56:VAL:HG11	34:K:59:ALA:HB2	1.95	0.49
36:M:231:ALA:HA	36:M:301:PRO:CG	2.43	0.49
2:1:141:TYR:CE1	2:1:387:GLU:HA	2.48	0.48
2:1:618:VAL:HG11	2:1:663:CYS:O	2.12	0.48
12:B:50:PHE:HB2	12:B:397:GLY:HA2	1.95	0.48
18:De:600:PHE:CZ	18:De:612:TRP:HB2	2.48	0.48
18:De:707:LEU:HD13	18:De:738:TRP:CG	2.48	0.48
32:I:91:HIS:CE1	32:I:93:GLU:HB3	2.47	0.48
32:I:109:ARG:HH21	32:I:125:GLU:C	2.20	0.48
37:N:211:DC:H2''	37:N:212:DA:C5	2.47	0.48
3:2:411:MET:HE1	6:5:115:ILE:HG13	1.94	0.48
11:A:1189:ASP:HB3	11:A:1193:VAL:CG2	2.43	0.48
13:C:228:ARG:HD2	13:C:230:TYR:OH	2.12	0.48
38:O:219:MET:SD	38:O:237:TYR:HB3	2.53	0.48
41:T:-127:DG:C5	41:T:-126:DC:C4	3.01	0.48
12:B:789:ASN:O	12:B:968:ASN:HB2	2.13	0.48
37:N:98:DT:H2''	37:N:99:DC:C6	2.48	0.48
37:N:199:DG:H2''	37:N:200:DT:C4	2.48	0.48
38:O:305:PHE:CD2	41:T:-1:DA:H5'	2.48	0.48
3:2:114:LYS:HE2	3:2:143:TRP:CZ3	2.49	0.48
11:A:906:LEU:HD13	11:A:966:LEU:HD22	1.93	0.48
12:B:285:LEU:HD21	12:B:305:LEU:HD11	1.95	0.48
17:DD:892:THR:HG23	24:DL:103:ALA:HB1	1.95	0.48
22:DI:57:TYR:HA	22:DI:60:HIS:HB3	1.94	0.48
41:T:-21:DG:H5'	41:T:-21:DG:C8	2.49	0.48
11:A:952:LEU:HD11	11:A:1006:PRO:HB2	1.96	0.48
12:B:506:TRP:CD1	12:B:506:TRP:C	2.92	0.48
12:B:546:GLU:OE1	39:Q:121:ASN:HB3	2.13	0.48
12:B:1040:GLN:OE1	13:C:198:PRO:HD3	2.13	0.48
13:C:68:LEU:HD22	13:C:120:LEU:HD21	1.94	0.48
29:F:106:ILE:HD12	29:F:123:LEU:HD12	1.95	0.48
36:M:306:PHE:CE1	36:M:310:VAL:HB	2.49	0.48
37:N:8:DG:N3	38:O:198:ALA:HB3	2.28	0.48
38:O:290:GLY:HA3	38:O:305:PHE:CE2	2.48	0.48
2:1:624:PRO:HD2	2:1:660:ALA:HB2	1.96	0.48
11:A:702:ILE:HA	11:A:752:THR:HG22	1.96	0.48
11:A:716:VAL:HG12	11:A:737:PHE:CD1	2.49	0.48
11:A:811:ILE:HG23	12:B:689:TYR:CE2	2.49	0.48
11:A:1009:VAL:HA	11:A:1065:PHE:CZ	2.48	0.48
12:B:53:MET:HB3	12:B:57:ARG:CZ	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:642:GLN:HB3	12:B:651:TYR:CE2	2.48	0.48
30:G:137:ILE:HG12	30:G:163:LEU:HD23	1.95	0.48
31:H:10:PHE:HB3	31:H:30:CYS:HB3	1.95	0.48
37:N:69:DA:H1'	37:N:70:DC:C5	2.48	0.48
37:N:99:DC:H2''	37:N:100:DA:C8	2.48	0.48
5:4:198:VAL:HG11	5:4:208:CYS:SG	2.53	0.48
11:A:689:ILE:HD11	12:B:981:LEU:HB3	1.95	0.48
12:B:27:TRP:CZ2	12:B:762:ARG:HB2	2.47	0.48
12:B:132:VAL:CG1	12:B:140:LEU:HB3	2.44	0.48
37:N:30:DT:C2	41:T:-29:DG:N2	2.82	0.48
41:T:-142:DC:H2''	41:T:-141:DG:N7	2.29	0.48
5:4:319:ALA:HA	5:4:322:TYR:CD2	2.48	0.48
11:A:844:ARG:HA	11:A:847:LEU:HD12	1.95	0.48
11:A:959:MET:SD	11:A:1047:SER:HA	2.54	0.48
13:C:9:VAL:HG11	34:K:105:PHE:CD2	2.49	0.48
13:C:146:ASP:HB3	33:J:16:ASN:HB2	1.94	0.48
19:DF:83:LEU:HD23	19:DF:86:PHE:CZ	2.49	0.48
31:H:10:PHE:CE2	31:H:39:LEU:HB2	2.49	0.48
37:N:3:DT:H5'	38:O:292:ILE:HG12	1.94	0.48
37:N:178:DC:N3	41:T:-178:DG:N1	2.48	0.48
38:O:300:ILE:HD11	38:O:320:GLU:HB3	1.94	0.48
49:d:77:GLU:HB3	49:d:98:ALA:HB1	1.96	0.48
4:3:60:LEU:HD13	4:3:118:LEU:HD23	1.95	0.48
11:A:465:HIS:CE1	11:A:467:MET:HB2	2.49	0.48
11:A:1140:THR:O	11:A:1357:THR:HA	2.13	0.48
13:C:59:LEU:HD12	13:C:151:VAL:HG23	1.96	0.48
18:DE:492:SER:HB2	18:DE:542:HIS:HB2	1.95	0.48
18:DE:508:LYS:HE3	18:DE:526:ARG:HD3	1.96	0.48
30:G:15:PRO:HA	30:G:18:PHE:CE1	2.48	0.48
11:A:962:ASP:O	11:A:966:LEU:HG	2.14	0.48
14:D:131:LEU:O	14:D:135:GLN:HG2	2.14	0.48
32:I:40:ARG:HD3	39:Q:177:MET:CB	2.44	0.48
32:I:91:HIS:HE1	32:I:93:GLU:HB3	1.79	0.48
33:J:21:TYR:CZ	33:J:25:LEU:HD11	2.49	0.48
36:M:260:MET:CE	36:M:293:TYR:HA	2.44	0.48
37:N:7:DA:H2''	38:O:214:PHE:CG	2.49	0.48
37:N:63:DG:C2	41:T:-62:DG:C2	3.02	0.48
41:T:-162:DT:H2''	41:T:-161:DT:C5	2.47	0.48
18:De:747:LEU:HD23	18:De:747:LEU:H	1.79	0.47
8:7:11:THR:HG21	44:W:111:ARG:HD3	1.95	0.47
11:A:430:ARG:HH22	36:M:26:ASP:CG	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:745:LEU:HD23	11:A:745:LEU:HA	1.59	0.47
12:B:761:THR:H	12:B:764:MET:HE3	1.79	0.47
15:DA:842:ILE:HG23	15:DA:846:LEU:HD12	1.97	0.47
18:DE:463:PHE:CD2	18:DE:793:ALA:HB3	2.49	0.47
28:E:74:VAL:HA	28:E:103:LEU:O	2.14	0.47
31:H:41:LEU:HD21	31:H:143:LEU:HD21	1.96	0.47
31:H:118:TYR:CE1	31:H:143:LEU:HB2	2.49	0.47
37:N:99:DC:H2''	37:N:100:DA:N7	2.29	0.47
41:T:-28:DG:H2''	41:T:-27:DA:C8	2.48	0.47
44:W:106:LYS:HG2	45:X:220:TRP:CZ2	2.48	0.47
1:0:575:LEU:HD22	1:0:606:PHE:HZ	1.79	0.47
9:8:74:ILE:HG23	9:8:156:PHE:CZ	2.49	0.47
11:A:601:ASN:HB3	11:A:988:TRP:CZ3	2.49	0.47
11:A:1004:LEU:HD22	11:A:1060:LEU:HB2	1.95	0.47
18:DE:584:HIS:CE1	18:DE:610:ARG:HH11	2.32	0.47
37:N:5:DA:O4'	38:O:257:ASN:HB2	2.13	0.47
37:N:142:DG:C5	37:N:143:DC:C4	3.02	0.47
38:O:274:VAL:HA	38:O:281:SER:HB2	1.97	0.47
44:W:52:LEU:HD12	44:W:59:LEU:HD13	1.95	0.47
45:X:77:VAL:O	45:X:81:ILE:HG12	2.15	0.47
13:C:22:ILE:HA	13:C:229:PHE:O	2.15	0.47
13:C:32:ASN:O	13:C:36:ARG:HG3	2.15	0.47
13:C:69:GLY:HA3	35:L:57:ALA:HB1	1.95	0.47
14:D:61:PHE:HA	30:G:46:ILE:HG22	1.97	0.47
36:M:235:ILE:HG23	36:M:299:LEU:HB3	1.96	0.47
37:N:200:DT:H2''	37:N:201:DC:C4	2.49	0.47
45:X:144:ASN:HB3	45:X:174:ALA:HB1	1.95	0.47
17:Dd:878:LEU:HD23	17:Dd:899:VAL:HG13	1.97	0.47
43:V:19:LEU:HD22	43:V:33:ALA:HA	1.96	0.47
1:0:77:TRP:CZ2	1:0:145:LYS:HE3	2.50	0.47
8:7:63:PHE:HB2	8:7:69:ASP:OD1	2.14	0.47
11:A:365:THR:HG22	11:A:482:PHE:CD2	2.50	0.47
11:A:410:ASN:HD21	11:A:417:LYS:HA	1.80	0.47
11:A:857:THR:HG21	11:A:1100:THR:HG22	1.97	0.47
12:B:31:SER:HA	12:B:766:TYR:CE1	2.49	0.47
12:B:643:LEU:HG	12:B:651:TYR:HE1	1.80	0.47
12:B:851:ASP:O	35:L:30:SER:HB3	2.14	0.47
13:C:149:LEU:HD21	13:C:152:LYS:HE3	1.97	0.47
13:C:183:ALA:HB3	13:C:232:ASN:HB3	1.96	0.47
18:DE:332:ILE:HG23	18:DE:336:HIS:HD2	1.80	0.47
28:E:10:LEU:HD21	28:E:55:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:H:48:TYR:CG	31:H:90:TYR:HB2	2.49	0.47
31:H:91:VAL:HA	31:H:143:LEU:O	2.14	0.47
38:O:204:ILE:HG13	38:O:207:PRO:HD2	1.96	0.47
38:O:295:MET:HE3	38:O:324:ALA:O	2.13	0.47
45:X:111:ILE:HG12	45:X:115:GLN:HB2	1.96	0.47
11:A:668:PHE:CE1	11:A:672:ILE:HD11	2.49	0.47
11:A:1009:VAL:HA	11:A:1065:PHE:CE2	2.49	0.47
12:B:214:LYS:HE2	12:B:215:TYR:CE1	2.50	0.47
12:B:1003:ASN:ND2	12:B:1006:VAL:HG23	2.30	0.47
21:DH:142:HIS:NE2	21:DH:152:GLU:HA	2.30	0.47
31:H:94:GLY:HA3	31:H:118:TYR:HA	1.96	0.47
37:N:155:DC:H2''	37:N:156:DG:C8	2.50	0.47
37:N:171:DG:H2''	37:N:172:DG:N7	2.30	0.47
2:1:110:SER:HA	2:1:211:TYR:OH	2.15	0.47
11:A:623:PRO:CG	31:H:18:GLU:HG3	2.44	0.47
23:Dj:201:THR:HB	23:Dj:202:PRO:HD3	1.97	0.47
30:G:89:VAL:HG21	30:G:137:ILE:HG23	1.96	0.47
31:H:58:LEU:CD1	31:H:143:LEU:HD11	2.44	0.47
37:N:48:DT:C4	37:N:49:DC:N4	2.83	0.47
37:N:170:DG:H2''	37:N:171:DG:N7	2.29	0.47
38:O:206:GLU:HB3	38:O:207:PRO:HD3	1.96	0.47
44:W:22:ILE:HA	44:W:26:TYR:CD1	2.50	0.47
44:W:145:PHE:HA	44:W:152:PHE:HA	1.96	0.47
1:0:60:ASP:OD1	1:0:62:ARG:HG2	2.14	0.47
1:0:609:LYS:HE2	41:T:-46:DT:H4'	1.97	0.47
11:A:827:TYR:CZ	12:B:718:GLN:HG3	2.50	0.47
30:G:89:VAL:HG21	30:G:137:ILE:CG2	2.45	0.47
37:N:23:DT:H2'	37:N:24:DT:C6	2.50	0.47
37:N:71:DG:H1'	37:N:72:DA:OP1	2.15	0.47
37:N:108:DG:O6	41:T:-109:DA:N6	2.48	0.47
44:W:77:ARG:HD3	44:W:91:TYR:CD1	2.49	0.47
48:c:115:VAL:HG11	46:e:113:ILE:HG12	1.97	0.47
2:1:80:ILE:HD11	2:1:208:SER:N	2.30	0.47
15:DA:1055:VAL:HG13	15:DA:1056:ALA:N	2.27	0.47
15:DA:1170:THR:HB	20:DG:178:SER:HB3	1.96	0.47
31:H:63:THR:HA	31:H:142:TYR:CE1	2.50	0.47
34:K:18:LYS:NZ	34:K:37:LYS:HB2	2.30	0.47
41:T:-71:DC:H1'	41:T:-70:DG:O4'	2.15	0.47
42:U:22:ILE:HA	42:U:39:LEU:HD21	1.96	0.47
1:0:88:ALA:HA	1:0:93:TYR:CD1	2.50	0.46
2:1:140:SER:HB2	2:1:384:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:41:ARG:NH2	8:7:47:PRO:HA	2.30	0.46
11:A:717:ILE:HG12	11:A:737:PHE:HZ	1.79	0.46
11:A:1141:VAL:HA	11:A:1357:THR:HG23	1.98	0.46
13:C:188:PRO:HB3	13:C:208:TYR:HB2	1.97	0.46
16:DB:294:ILE:HG13	16:DB:295:LEU:H	1.80	0.46
28:E:104:ILE:O	28:E:129:GLN:HA	2.15	0.46
29:F:57:MET:HB2	29:F:123:LEU:HB3	1.96	0.46
29:F:68:THR:CG2	30:G:59:ILE:HG21	2.46	0.46
31:H:39:LEU:HD22	31:H:58:LEU:HD22	1.96	0.46
37:N:3:DT:H1'	38:O:303:LEU:HD11	1.97	0.46
37:N:3:DT:C4	37:N:4:DA:N6	2.83	0.46
37:N:88:DC:H5'	48:c:78:ARG:CZ	2.45	0.46
11:A:402:LEU:HB3	11:A:446:VAL:HG21	1.97	0.46
12:B:638:ARG:HG3	12:B:639:HIS:N	2.31	0.46
12:B:653:TRP:CH2	12:B:662:VAL:HG21	2.50	0.46
12:B:1115:GLN:HB3	12:B:1150:ARG:HD2	1.97	0.46
13:C:85:SER:HA	13:C:97:CYS:SG	2.55	0.46
18:De:497:TRP:HB3	19:Df:131:LEU:HD22	1.97	0.46
28:E:24:ARG:HH12	28:E:128:GLU:CD	2.23	0.46
43:V:62:LEU:HD21	43:V:65:TYR:HB3	1.97	0.46
1:O:51:THR:HG23	1:O:52:LYS:H	1.80	0.46
11:A:1142:PHE:HE2	11:A:1317:LYS:O	1.99	0.46
12:B:726:SER:O	12:B:730:LYS:HE2	2.15	0.46
30:G:30:LEU:O	30:G:34:VAL:HG22	2.16	0.46
30:G:89:VAL:HG22	30:G:99:THR:HG22	1.97	0.46
30:G:114:PRO:CG	30:G:164:MET:HG3	2.45	0.46
36:M:232:ALA:HB2	36:M:258:ILE:HA	1.98	0.46
36:M:256:ALA:HB1	36:M:289:TYR:HA	1.96	0.46
37:N:5:DA:H2	41:T:-5:DT:O2	1.99	0.46
37:N:65:DG:C2	41:T:-64:DA:C2	3.04	0.46
2:1:320:PRO:HA	2:1:374:PHE:CG	2.50	0.46
4:3:397:GLU:HA	4:3:400:ARG:HG2	1.98	0.46
12:B:638:ARG:O	12:B:642:GLN:HG3	2.15	0.46
14:D:103:LEU:HD13	14:D:114:LEU:HB3	1.98	0.46
17:Dd:902:VAL:O	17:Dd:906:THR:HG23	2.15	0.46
28:E:55:ARG:O	28:E:76:PHE:HB2	2.16	0.46
34:K:7:PHE:HA	34:K:10:PHE:CE2	2.50	0.46
41:T:-125:DG:C6	41:T:-124:DG:C6	3.03	0.46
41:T:-108:DC:H2''	41:T:-107:DG:C8	2.50	0.46
45:X:99:LEU:HD22	45:X:120:MET:HB2	1.98	0.46
2:1:46:THR:HG21	2:1:672:THR:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:143:ARG:HD2	2:1:159:GLU:OE1	2.16	0.46
8:7:8:ARG:HH22	44:W:114:ILE:CG2	2.28	0.46
11:A:717:ILE:HG12	11:A:737:PHE:CZ	2.50	0.46
11:A:797:ARG:NH1	11:A:820:ARG:HB2	2.31	0.46
37:N:-6:DG:C2	41:T:7:DT:O2	2.69	0.46
37:N:5:DA:N3	38:O:169:VAL:HG21	2.30	0.46
37:N:88:DC:H2''	37:N:89:DC:C5	2.51	0.46
41:T:-146:DA:C6	41:T:-145:DG:C6	3.04	0.46
41:T:-59:DT:H6	41:T:-59:DT:H2'	1.55	0.46
6:5:59:VAL:HG12	6:5:70:LEU:HD23	1.96	0.46
9:8:102:ILE:HD11	9:8:206:LEU:HD23	1.98	0.46
11:A:909:LEU:O	11:A:967:ARG:NE	2.48	0.46
11:A:1211:LEU:HA	11:A:1259:ILE:O	2.15	0.46
13:C:184:PHE:CE1	13:C:229:PHE:HB3	2.51	0.46
29:F:62:ARG:HD3	29:F:127:ASP:HB3	1.98	0.46
44:W:132:CYS:HB3	44:W:157:CYS:SG	2.56	0.46
45:X:194:ARG:HD2	45:X:200:ILE:HD11	1.98	0.46
2:1:46:THR:HB	2:1:670:GLY:HA2	1.97	0.46
3:2:387:THR:HG21	6:5:171:ALA:HA	1.98	0.46
5:4:386:ILE:HD11	6:5:134:ALA:HB3	1.98	0.46
11:A:908:THR:O	11:A:963:ARG:HG3	2.16	0.46
31:H:10:PHE:HB3	31:H:30:CYS:CB	2.46	0.46
44:W:107:LEU:HD22	44:W:184:ILE:HG12	1.97	0.46
49:d:81:LEU:HD13	49:d:97:THR:HB	1.97	0.46
2:1:269:THR:HG21	2:1:386:LEU:HG	1.97	0.46
3:2:434:LEU:CD1	6:5:229:TRP:HE1	2.29	0.46
4:3:372:ALA:HB1	4:3:376:MET:SD	2.55	0.46
19:DF:22:VAL:HG13	22:DI:44:PHE:CE2	2.51	0.46
30:G:95:VAL:HG11	44:W:152:PHE:CZ	2.51	0.46
32:I:96:PHE:HB3	32:I:112:TYR:CE2	2.50	0.46
36:M:219:CYS:SG	36:M:229:GLN:HA	2.56	0.46
36:M:246:PRO:C	36:M:248:ARG:H	2.23	0.46
40:R:191:PHE:HB2	40:R:235:LEU:HB3	1.98	0.46
2:1:140:SER:HB2	2:1:384:HIS:NE2	2.31	0.46
11:A:395:THR:CG2	11:A:396:PRO:HD2	2.45	0.46
11:A:410:ASN:HA	11:A:449:HIS:HE1	1.81	0.46
11:A:798:ILE:HD11	11:A:838:PHE:HB3	1.97	0.46
12:B:27:TRP:HZ2	12:B:1000:THR:HG21	1.81	0.46
16:DB:294:ILE:HG13	16:DB:295:LEU:N	2.31	0.46
28:E:13:ILE:CD1	28:E:132:GLN:HG3	2.44	0.46
38:O:305:PHE:CE2	41:T:-2:DT:H2''	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:W:145:PHE:HB2	44:W:152:PHE:CE2	2.51	0.46
48:g:80:ILE:HG12	48:g:83:HIS:CE1	2.51	0.46
1:0:445:THR:HB	1:0:451:PHE:CD2	2.51	0.46
11:A:1004:LEU:HB2	11:A:1060:LEU:O	2.16	0.46
11:A:1054:MET:HE3	11:A:1065:PHE:HE1	1.80	0.46
11:A:1483:GLY:CA	29:F:80:MET:HA	2.46	0.46
12:B:759:VAL:HG12	12:B:999:ALA:HB2	1.96	0.46
16:DB:439:HIS:CD2	16:DB:965:TRP:CH2	3.03	0.46
17:DD:1003:ASP:OD2	43:V:1:MET:HA	2.16	0.46
18:DE:352:ILE:O	18:DE:356:VAL:HG22	2.16	0.46
30:G:45:VAL:HA	30:G:76:VAL:HG12	1.97	0.46
37:N:9:DG:H2''	37:N:10:DG:C8	2.51	0.46
37:N:40:DC:H2''	37:N:41:DC:H5	1.79	0.46
38:O:309:LYS:HB3	41:T:-2:DT:H5''	1.97	0.46
39:Q:44:GLN:HE22	39:Q:46:ARG:HG3	1.80	0.46
11:A:385:ALA:HB1	11:A:450:MET:O	2.16	0.45
11:A:390:PHE:HB3	11:A:448:ARG:CZ	2.46	0.45
12:B:1003:ASN:OD1	12:B:1005:ALA:HB3	2.17	0.45
16:DB:427:PRO:HG2	16:DB:435:ILE:HD11	1.98	0.45
20:DG:79:THR:HB	20:DG:85:PHE:CD2	2.50	0.45
32:I:12:VAL:HG23	32:I:13:GLY:H	1.79	0.45
37:N:109:DT:H1'	37:N:110:DA:C4	2.50	0.45
40:R:191:PHE:CE2	40:R:236:LYS:HA	2.51	0.45
44:W:66:LEU:HB3	44:W:72:ILE:HG23	1.98	0.45
11:A:811:ILE:HD12	32:I:79:PRO:HB3	1.97	0.45
11:A:857:THR:CG2	11:A:1100:THR:HG22	2.46	0.45
11:A:955:GLU:CD	11:A:1051:SER:H	2.23	0.45
12:B:19:PRO:HA	12:B:680:ASP:OD2	2.17	0.45
28:E:162:ARG:HD2	28:E:163:TYR:CE2	2.51	0.45
37:N:22:DG:C2	41:T:-21:DG:C2	3.04	0.45
37:N:130:DA:H2''	37:N:131:DA:C8	2.52	0.45
41:T:-69:DT:H2''	41:T:-68:DA:C5	2.50	0.45
1:0:551:HIS:HB2	1:0:558:ILE:HD11	1.97	0.45
2:1:460:THR:HB	2:1:661:ALA:CB	2.46	0.45
13:C:93:PHE:HB3	13:C:164:TYR:CD1	2.52	0.45
37:N:125:DC:H2''	37:N:126:DG:C8	2.51	0.45
40:R:187:LEU:CD2	40:R:220:ILE:HD11	2.44	0.45
44:W:30:HIS:HB3	44:W:66:LEU:HD21	1.97	0.45
44:W:42:CYS:SG	44:W:91:TYR:HB3	2.57	0.45
44:W:100:VAL:HA	44:W:103:VAL:HG22	1.98	0.45
1:0:51:THR:HG23	1:0:52:LYS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:273:ILE:HD13	2:1:281:LEU:HD11	1.99	0.45
2:1:328:HIS:CD2	8:7:103:GLU:HG2	2.51	0.45
3:2:386:PRO:HD2	6:5:174:TYR:CZ	2.51	0.45
5:4:328:LEU:HD21	5:4:375:VAL:HG12	1.97	0.45
11:A:421:ARG:HB2	11:A:425:ASP:OD1	2.16	0.45
11:A:621:ILE:HD12	31:H:124:ARG:HB2	1.99	0.45
11:A:717:ILE:HD11	11:A:816:GLY:HA2	1.98	0.45
11:A:1161:LEU:HB2	11:A:1307:VAL:HG21	1.97	0.45
14:D:26:PHE:HZ	30:G:80:PHE:CZ	2.34	0.45
30:G:7:LEU:HB2	30:G:72:TYR:CZ	2.52	0.45
36:M:130:LEU:HD22	36:M:134:ILE:HD13	1.98	0.45
37:N:25:DC:H2'	37:N:26:DG:C8	2.51	0.45
37:N:82:DC:H2''	37:N:83:DC:C6	2.52	0.45
39:Q:126:ILE:HD11	39:Q:140:VAL:HG22	1.98	0.45
2:1:244:ILE:HG23	2:1:437:CYS:HB3	1.97	0.45
5:4:316:PRO:HB3	6:5:178:MET:SD	2.57	0.45
8:7:40:VAL:HG23	44:W:122:THR:HA	1.99	0.45
11:A:118:LEU:HD12	11:A:148:CYS:HB3	1.99	0.45
11:A:827:TYR:OH	11:A:839:HIS:CE1	2.69	0.45
13:C:93:PHE:HB3	13:C:164:TYR:CG	2.52	0.45
14:D:44:ARG:HB3	14:D:61:PHE:HE2	1.81	0.45
29:F:69:ARG:NH2	29:F:80:MET:HG2	2.32	0.45
36:M:260:MET:HG2	36:M:300:PHE:CZ	2.51	0.45
37:N:15:DG:C6	37:N:16:DG:C6	3.04	0.45
11:A:552:ASP:HB2	31:H:24:ARG:HB2	1.98	0.45
12:B:274:ARG:NH2	12:B:312:GLN:HE22	2.15	0.45
12:B:711:ILE:O	12:B:714:PRO:HD3	2.17	0.45
12:B:941:GLN:OE1	12:B:971:ALA:HB1	2.16	0.45
15:DA:816:TRP:CD2	15:DA:870:LEU:HD23	2.52	0.45
22:DI:73:LEU:HD11	24:DL:102:LEU:HD23	1.97	0.45
30:G:116:GLU:HG2	30:G:164:MET:HE1	1.99	0.45
38:O:167:ASN:HB2	41:T:-4:DT:O4'	2.16	0.45
38:O:180:LEU:HB3	38:O:200:VAL:HG23	1.99	0.45
39:Q:18:VAL:HG21	40:R:31:TRP:HB3	1.98	0.45
41:T:-150:DG:H2''	41:T:-149:DG:C8	2.52	0.45
41:T:-32:DT:H2''	41:T:-31:DG:C8	2.52	0.45
1:0:103:ILE:HA	1:0:126:ALA:HB2	1.99	0.45
2:1:200:LEU:HD21	2:1:222:SER:HA	1.97	0.45
9:8:210:VAL:HG13	9:8:211:PRO:HD2	1.99	0.45
11:A:485:ASN:O	11:A:488:VAL:HG22	2.16	0.45
11:A:934:LEU:HD22	11:A:938:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1117:VAL:HA	11:A:1136:THR:HG21	1.98	0.45
12:B:18:THR:HG1	12:B:21:LEU:HD13	1.81	0.45
12:B:18:THR:OG1	12:B:21:LEU:HD13	2.17	0.45
12:B:136:GLY:O	12:B:137:GLU:HG3	2.17	0.45
12:B:570:ASN:HA	12:B:615:TYR:CD1	2.51	0.45
13:C:11:ILE:HG12	13:C:21:PHE:HB3	1.99	0.45
28:E:11:TRP:CE3	28:E:37:LEU:HB2	2.52	0.45
28:E:46:ASP:HB3	28:E:52:ARG:HB3	1.97	0.45
30:G:137:ILE:HG12	30:G:163:LEU:CD2	2.46	0.45
31:H:96:VAL:HG22	31:H:116:VAL:HG22	1.99	0.45
32:I:86:CYS:SG	32:I:121:HIS:HB3	2.56	0.45
37:N:2:DA:C2	41:T:-2:DT:O2	2.67	0.45
11:A:404:GLU:O	11:A:408:ARG:HG3	2.17	0.45
11:A:713:VAL:HG21	11:A:745:LEU:CG	2.46	0.45
12:B:1167:ILE:O	12:B:1169:PRO:HD3	2.16	0.45
13:C:148:ILE:HD11	33:J:13:ILE:HD12	1.99	0.45
17:Dd:901:TYR:CE2	24:Dl:117:GLN:HG2	2.52	0.45
37:N:107:DC:O3'	37:N:108:DG:C8	2.70	0.45
37:N:144:DG:C2	41:T:-143:DG:N2	2.85	0.45
44:W:25:PHE:HB3	45:X:220:TRP:CD1	2.52	0.45
11:A:963:ARG:O	11:A:967:ARG:HG2	2.17	0.45
12:B:331:THR:HG23	12:B:334:LYS:H	1.81	0.45
12:B:509:VAL:CG1	12:B:524:LYS:HB3	2.46	0.45
12:B:602:SER:O	12:B:614:ILE:HA	2.17	0.45
13:C:84:TYR:HB3	13:C:86:ARG:HG2	1.99	0.45
16:DB:768:PRO:HB2	16:DB:771:VAL:HG23	1.98	0.45
37:N:4:DA:H2	41:T:-4:DT:O2	1.99	0.45
37:N:16:DG:C4	37:N:17:DG:C8	3.05	0.45
39:Q:47:LEU:HD23	40:R:104:LEU:HD22	1.98	0.45
41:T:-17:DC:H2'	41:T:-16:DC:C6	2.52	0.45
45:X:78:LEU:HB2	45:X:119:LEU:HD22	1.98	0.45
1:0:131:LEU:HD11	5:4:19:TRP:CZ2	2.52	0.45
11:A:379:GLY:HA3	11:A:477:LEU:HD12	1.99	0.45
11:A:705:THR:CG2	11:A:752:THR:HG23	2.47	0.45
17:Dd:885:ILE:HD13	24:Dl:93:GLU:HA	1.98	0.45
37:N:4:DA:H1'	38:O:257:ASN:ND2	2.33	0.45
45:X:148:LYS:HG3	45:X:185:LEU:HG	1.98	0.45
11:A:549:THR:CG2	11:A:635:LEU:HD21	2.47	0.44
11:A:737:PHE:O	11:A:741:VAL:HG23	2.18	0.44
11:A:922:PHE:CE1	11:A:952:LEU:HD13	2.51	0.44
12:B:725:GLN:OE1	12:B:938:ARG:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:111:SER:OG	14:D:127:LEU:HD21	2.18	0.44
18:DE:600:PHE:CZ	18:DE:612:TRP:HB2	2.51	0.44
18:DE:693:VAL:HB	18:DE:707:LEU:HB2	1.97	0.44
19:DF:138:ILE:O	19:DF:139:GLU:HG3	2.17	0.44
28:E:26:TYR:HA	28:E:64:HIS:HA	1.99	0.44
37:N:42:DT:H3'	37:N:43:DT:H72	1.98	0.44
41:T:-189:DG:H3'	48:g:29:GLY:HA3	1.98	0.44
11:A:1476:ASP:CG	11:A:1479:LYS:HB2	2.42	0.44
22:Di:87:PRO:HA	22:Di:88:PRO:HD3	1.87	0.44
34:K:35:ILE:HB	34:K:71:ILE:CG1	2.47	0.44
39:Q:39:PHE:CZ	40:R:94:THR:HG21	2.52	0.44
42:U:14:TYR:CE2	42:U:50:LEU:HD13	2.52	0.44
11:A:725:LEU:HB3	11:A:733:LEU:HD11	1.99	0.44
11:A:745:LEU:HB3	11:A:822:PHE:CE1	2.53	0.44
12:B:776:ILE:HB	12:B:806:PHE:CZ	2.52	0.44
16:DB:544:LEU:HD23	16:DB:590:ILE:HD11	2.00	0.44
31:H:97:TYR:CZ	31:H:115:TYR:HB3	2.52	0.44
37:N:8:DG:H5'	38:O:214:PHE:HB3	1.99	0.44
37:N:152:DC:H2''	37:N:153:DC:C6	2.51	0.44
40:R:34:ALA:HB3	40:R:40:VAL:HG12	1.98	0.44
41:T:-151:DG:H2''	41:T:-150:DG:N7	2.33	0.44
42:U:46:TRP:HD1	43:V:15:LEU:HB2	1.82	0.44
42:U:353:LEU:HD12	42:U:370:ALA:HB3	1.98	0.44
44:W:34:LEU:HD13	44:W:66:LEU:CD1	2.47	0.44
4:3:240:LEU:O	4:3:283:PRO:HB3	2.18	0.44
6:5:100:LYS:HG3	6:5:101:TYR:H	1.82	0.44
10:9:32:CYS:HB2	11:A:1483:GLY:O	2.18	0.44
11:A:460:ARG:HB2	11:A:501:MET:HE3	2.00	0.44
11:A:760:LEU:HD13	11:A:764:ASN:OD1	2.18	0.44
11:A:890:ARG:NH2	11:A:1033:ALA:HB1	2.32	0.44
12:B:624:PRO:HA	12:B:663:GLU:O	2.18	0.44
13:C:4:ALA:HB1	34:K:97:GLU:HB2	1.98	0.44
14:D:31:THR:HG22	30:G:3:TYR:CE2	2.52	0.44
18:DE:722:ASP:HB2	18:DE:724:GLU:OE1	2.17	0.44
36:M:264:ALA:N	36:M:313:LEU:HD21	2.32	0.44
36:M:300:PHE:CE1	36:M:313:LEU:HD11	2.52	0.44
37:N:92:DG:H1'	37:N:93:DG:O4'	2.17	0.44
38:O:211:ALA:HA	38:O:220:VAL:O	2.18	0.44
41:T:-210:DT:H2''	41:T:-209:DA:C8	2.53	0.44
44:W:106:LYS:HE3	45:X:223:VAL:O	2.16	0.44
45:X:109:LEU:H	45:X:109:LEU:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:361:LEU:O	2:1:365:VAL:HG12	2.18	0.44
11:A:431:PHE:CD1	36:M:33:ILE:HG21	2.53	0.44
11:A:705:THR:HB	11:A:752:THR:HG22	1.99	0.44
11:A:789:GLY:N	11:A:823:VAL:O	2.39	0.44
11:A:791:GLN:HG2	11:A:823:VAL:HG23	2.00	0.44
22:DI:60:HIS:CD2	24:DL:106:ARG:HH21	2.34	0.44
17:Dd:912:ASN:ND2	26:Dk:192:ARG:HH11	2.15	0.44
28:E:151:MET:HG2	28:E:192:LYS:HB2	1.99	0.44
37:N:14:DG:C4	37:N:15:DG:C8	3.06	0.44
41:T:-68:DA:H1'	41:T:-67:DG:N7	2.33	0.44
44:W:180:PHE:CD1	45:X:219:LEU:HD23	2.52	0.44
1:0:363:VAL:O	1:0:407:ILE:HA	2.18	0.44
2:1:557:ILE:HD13	2:1:561:ILE:CD1	2.47	0.44
2:1:588:CYS:HB2	2:1:614:TYR:HE1	1.83	0.44
5:4:145:LEU:HD12	5:4:176:THR:HG21	1.99	0.44
9:8:241:CYS:HA	9:8:246:TYR:CD2	2.52	0.44
11:A:1192:TRP:CZ3	11:A:1246:ILE:HG22	2.52	0.44
12:B:713:PHE:CZ	12:B:982:ILE:HG22	2.53	0.44
33:J:35:LEU:HD13	33:J:46:ARG:HB3	1.99	0.44
37:N:40:DC:H2''	37:N:41:DC:C5	2.52	0.44
41:T:-142:DC:H2''	41:T:-141:DG:C8	2.53	0.44
48:g:71:ALA:HA	48:g:83:HIS:CD2	2.53	0.44
11:A:516:GLN:HA	11:A:520:MET:CG	2.48	0.44
11:A:732:THR:O	11:A:736:THR:HG23	2.17	0.44
13:C:3:TYR:C	34:K:49:GLN:HE22	2.26	0.44
13:C:266:GLU:HG2	34:K:21:ILE:HG13	1.99	0.44
14:D:118:LEU:HD22	14:D:127:LEU:HD22	1.99	0.44
18:De:722:ASP:HB2	18:De:724:GLU:CD	2.41	0.44
31:H:118:TYR:HB2	31:H:121:LEU:HB2	2.00	0.44
37:N:76:DA:H1'	37:N:77:DG:N1	2.32	0.44
37:N:88:DC:H2''	37:N:89:DC:C2	2.52	0.44
38:O:191:GLU:CG	38:O:201:ILE:HB	2.48	0.44
40:R:20:LEU:O	40:R:113:ARG:HA	2.18	0.44
41:T:-170:DC:H2''	41:T:-169:DT:C5	2.52	0.44
43:V:35:GLN:O	43:V:39:GLN:HG2	2.17	0.44
45:X:78:LEU:CB	45:X:119:LEU:HD22	2.48	0.44
11:A:419:ILE:HD12	11:A:438:LEU:HD22	1.99	0.44
11:A:952:LEU:HD22	11:A:1051:SER:CB	2.48	0.44
11:A:1067:TRP:CH2	11:A:1071:GLU:HG3	2.52	0.44
15:DA:826:ARG:HD2	15:DA:828:GLU:OE2	2.18	0.44
30:G:97:LEU:HB2	30:G:108:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:H:56:PHE:CE1	31:H:58:LEU:HD13	2.52	0.44
37:N:46:DA:C6	41:T:-45:DA:C2	3.06	0.44
37:N:116:DC:H2''	37:N:117:DT:C6	2.52	0.44
37:N:126:DG:C5	37:N:127:DC:C4	3.06	0.44
38:O:163:PRO:CG	38:O:312:LEU:HD13	2.47	0.44
38:O:259:VAL:HG22	38:O:313:THR:OG1	2.18	0.44
44:W:36:ILE:HG22	44:W:43:VAL:HG21	1.99	0.44
45:X:81:ILE:HD11	45:X:103:LEU:HD23	2.00	0.44
47:b:24:ARG:O	47:b:24:ARG:HG2	2.18	0.44
11:A:436:SER:HA	11:A:439:HIS:NE2	2.33	0.44
11:A:876:ASP:CG	29:F:111:PRO:HG2	2.43	0.44
11:A:933:THR:HG22	11:A:1056:GLU:HA	1.99	0.44
11:A:1128:ILE:HG13	11:A:1129:ASN:N	2.33	0.44
12:B:40:VAL:HG22	12:B:43:GLN:HB2	2.00	0.44
12:B:96:PRO:HG2	12:B:120:TYR:CZ	2.53	0.44
12:B:268:PRO:HB2	12:B:308:ALA:HB2	1.99	0.44
12:B:517:GLY:O	12:B:520:VAL:HG13	2.18	0.44
12:B:679:PRO:HD3	12:B:696:CYS:SG	2.58	0.44
12:B:758:LEU:HA	12:B:758:LEU:HD23	1.83	0.44
13:C:263:LEU:CD1	34:K:21:ILE:HD11	2.48	0.44
34:K:45:ILE:HG12	34:K:94:LEU:HD22	2.00	0.44
44:W:21:VAL:HG21	44:W:103:VAL:HG11	2.00	0.44
11:A:410:ASN:OD1	11:A:417:LYS:HG2	2.18	0.43
18:DE:570:TRP:CZ3	18:DE:577:CYS:HB2	2.53	0.43
33:J:21:TYR:CB	33:J:38:LEU:HD11	2.46	0.43
36:M:235:ILE:HD11	36:M:300:PHE:CE2	2.53	0.43
37:N:-8:DA:C2	41:T:9:DC:O2	2.71	0.43
37:N:56:DA:H1'	37:N:57:DG:C8	2.53	0.43
37:N:199:DG:OP2	37:N:199:DG:H2'	2.17	0.43
40:R:34:ALA:HB2	40:R:62:LEU:HD23	2.00	0.43
2:1:207:TYR:HB2	2:1:211:TYR:CD2	2.53	0.43
11:A:364:ARG:HB3	12:B:1060:HIS:NE2	2.33	0.43
14:D:106:GLU:CD	14:D:138:ARG:HH12	2.26	0.43
21:DH:107:LEU:HB3	21:DH:108:PRO:HD3	2.00	0.43
30:G:44:PHE:O	30:G:76:VAL:HA	2.19	0.43
31:H:64:LEU:HG	31:H:142:TYR:CG	2.53	0.43
41:T:-129:DA:H2''	41:T:-128:DA:N7	2.34	0.43
43:V:80:GLU:OE2	43:V:89:LYS:HE2	2.18	0.43
44:W:54:PHE:CE1	45:X:192:VAL:HG11	2.53	0.43
11:A:549:THR:HG23	11:A:635:LEU:HD21	1.99	0.43
12:B:274:ARG:NH1	12:B:311:ILE:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:521:GLY:O	12:B:524:LYS:HE2	2.18	0.43
12:B:622:CYS:HA	12:B:666:ASP:HA	2.00	0.43
15:DA:824:ARG:HB2	15:DA:861:TRP:HB3	2.00	0.43
29:F:61:GLU:HG2	29:F:106:ILE:HG21	2.00	0.43
30:G:91:GLN:NE2	30:G:93:ASN:HD21	2.16	0.43
34:K:19:ILE:HD12	34:K:35:ILE:HG12	2.00	0.43
36:M:228:VAL:HG22	36:M:265:SER:HB3	1.99	0.43
38:O:193:ASN:HB2	43:V:67:PHE:CE2	2.54	0.43
6:5:187:GLN:HB3	6:5:189:ILE:HD12	2.01	0.43
11:A:890:ARG:HH21	11:A:1033:ALA:HB1	1.84	0.43
12:B:453:TRP:NE1	12:B:466:VAL:HB	2.34	0.43
13:C:60:HIS:CD2	13:C:63:PHE:HB2	2.52	0.43
30:G:114:PRO:CD	30:G:164:MET:HG3	2.48	0.43
32:I:60:HIS:CD2	32:I:60:HIS:O	2.71	0.43
34:K:87:PHE:CE2	34:K:91:ILE:HD11	2.53	0.43
36:M:289:TYR:HA	36:M:292:ILE:HG12	2.00	0.43
37:N:32:DA:H2"	37:N:33:DC:C6	2.53	0.43
40:R:81:HIS:HB3	40:R:116:CYS:SG	2.57	0.43
42:U:368:SER:HB2	43:V:52:VAL:HG12	2.00	0.43
2:1:601:ARG:HD2	2:1:659:HIS:NE2	2.34	0.43
11:A:875:TYR:HA	11:A:1083:PRO:HG3	2.01	0.43
11:A:1189:ASP:HB3	11:A:1193:VAL:HG23	2.00	0.43
11:A:1433:GLU:H	11:A:1433:GLU:CD	2.26	0.43
12:B:91:ILE:HG23	12:B:124:LEU:HD11	2.00	0.43
12:B:725:GLN:CD	12:B:938:ARG:HA	2.44	0.43
17:DD:916:LYS:O	17:DD:919:GLU:HG3	2.18	0.43
29:F:57:MET:HE2	29:F:106:ILE:HD11	2.00	0.43
36:M:195:PHE:CZ	36:M:199:LEU:HD11	2.53	0.43
37:N:32:DA:C4	37:N:33:DC:C4	3.06	0.43
37:N:114:DA:C6	37:N:115:DG:C6	3.06	0.43
41:T:-89:DG:C4	41:T:-88:DG:C6	3.06	0.43
44:W:106:LYS:O	44:W:110:MET:HE2	2.19	0.43
48:g:66:LEU:HB3	48:g:87:ALA:HB1	1.99	0.43
2:1:596:LEU:HD22	2:1:610:PHE:HZ	1.83	0.43
3:2:488:GLU:O	3:2:491:VAL:HG22	2.18	0.43
10:9:165:ARG:HB3	10:9:166:PRO:HD3	2.00	0.43
11:A:872:MET:HG2	11:A:873:VAL:N	2.34	0.43
11:A:1189:ASP:CG	11:A:1213:ARG:HE	2.26	0.43
12:B:785:TYR:O	12:B:786:THR:HG22	2.18	0.43
18:DE:243:LEU:HD23	18:DE:243:LEU:HA	1.88	0.43
21:DH:68:TYR:CE2	21:DH:72:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:E:171:PRO:O	28:E:207:ARG:HA	2.19	0.43
31:H:92:MET:O	31:H:142:TYR:HA	2.19	0.43
32:I:79:PRO:HB2	32:I:96:PHE:CZ	2.54	0.43
34:K:49:GLN:HG2	34:K:93:ASP:HB2	2.00	0.43
36:M:125:ALA:HB1	36:M:130:LEU:HB2	2.01	0.43
38:O:162:VAL:HB	38:O:322:TYR:CG	2.54	0.43
38:O:180:LEU:HD13	38:O:199:ALA:HA	2.00	0.43
38:O:183:ILE:HA	38:O:244:LEU:CD2	2.47	0.43
45:X:146:ARG:O	45:X:175:LEU:HD13	2.19	0.43
2:1:43:PRO:HG3	2:1:696:TRP:CG	2.54	0.43
8:7:37:LEU:HD22	8:7:47:PRO:HB3	2.00	0.43
11:A:282:ASP:HA	11:A:285:LYS:HE3	2.01	0.43
11:A:1221:MET:HE3	11:A:1227:THR:HA	2.01	0.43
12:B:67:LEU:HB2	12:B:84:TYR:HB2	2.00	0.43
12:B:82:PRO:HA	12:B:133:ILE:O	2.18	0.43
12:B:422:PHE:HE2	40:R:161:TYR:CE1	2.36	0.43
36:M:127:ARG:HD3	40:R:153:TYR:CE1	2.54	0.43
1:0:77:TRP:CE2	1:0:145:LYS:HE3	2.54	0.43
1:0:127:VAL:HG21	1:0:160:THR:HA	2.00	0.43
2:1:213:LEU:O	2:1:216:LYS:HE3	2.18	0.43
2:1:552:TRP:HB3	2:1:557:ILE:CG1	2.48	0.43
3:2:473:ARG:HG2	5:4:307:ILE:HD13	2.01	0.43
10:9:13:PHE:CD1	29:F:55:PRO:HB2	2.54	0.43
11:A:380:VAL:HG13	11:A:482:PHE:HE1	1.84	0.43
11:A:861:GLN:O	11:A:865:ILE:HG22	2.19	0.43
11:A:1142:PHE:HB2	11:A:1353:ASP:HB3	2.01	0.43
12:B:94:SER:HA	40:R:145:LEU:O	2.18	0.43
12:B:415:VAL:HA	12:B:434:ALA:HB1	2.00	0.43
12:B:508:MET:HB3	12:B:621:ILE:HD13	2.00	0.43
12:B:862:GLY:HA2	12:B:896:LEU:O	2.18	0.43
28:E:46:ASP:HB3	28:E:52:ARG:H	1.84	0.43
33:J:21:TYR:CE2	33:J:25:LEU:HD11	2.54	0.43
37:N:7:DA:H5"	38:O:218:LYS:HD3	2.00	0.43
38:O:312:LEU:HB2	38:O:321:ILE:HG23	1.99	0.43
41:T:-151:DG:H2"	41:T:-150:DG:C8	2.54	0.43
41:T:-91:DT:H6	41:T:-91:DT:H2'	1.65	0.43
45:X:85:MET:HE1	45:X:137:TYR:CB	2.49	0.43
45:X:99:LEU:HB2	45:X:120:MET:HE2	2.00	0.43
48:g:51:TYR:CE1	49:h:115:GLY:HA3	2.53	0.43
1:0:390:CYS:SG	1:0:406:ALA:HA	2.59	0.43
2:1:266:LEU:O	2:1:270:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:400:ILE:HD12	3:2:400:ILE:H	1.83	0.43
13:C:101:PHE:CE2	13:C:122:SER:HB3	2.54	0.43
14:D:40:LEU:HD23	30:G:75:ILE:CG2	2.49	0.43
15:DA:481:GLU:H	15:DA:481:GLU:CD	2.26	0.43
28:E:101:ARG:HA	28:E:126:ILE:O	2.19	0.43
32:I:17:CYS:HB2	32:I:39:CYS:SG	2.58	0.43
37:N:22:DG:H2''	37:N:23:DT:H71	2.01	0.43
38:O:168:ILE:N	38:O:224:ALA:O	2.52	0.43
40:R:41:GLY:HA3	40:R:56:PHE:CZ	2.54	0.43
1:0:634:ARG:HE	37:N:48:DT:P	2.42	0.43
11:A:713:VAL:HG21	11:A:745:LEU:HG	2.01	0.43
11:A:1002:SER:HB3	11:A:1059:ARG:HA	2.00	0.43
12:B:273:PHE:CG	12:B:284:ILE:HG23	2.54	0.43
12:B:675:LEU:HD12	12:B:695:HIS:C	2.44	0.43
15:DA:1200:THR:O	15:DA:1204:GLU:HG2	2.19	0.43
18:DE:477:ASP:OD2	18:DE:550:SER:HA	2.18	0.43
18:DE:482:SER:HB3	18:DE:792:LEU:HD11	2.00	0.43
32:I:96:PHE:CD2	32:I:110:LEU:HD13	2.54	0.43
36:M:260:MET:HE2	36:M:293:TYR:HA	2.01	0.43
39:Q:93:PRO:HA	39:Q:96:GLN:CD	2.44	0.43
42:U:34:VAL:HG12	42:U:36:GLU:H	1.84	0.43
1:0:551:HIS:CB	1:0:558:ILE:HD11	2.49	0.42
50:O:807:2A1:N	51:O:808:ALA:HB3	2.34	0.42
2:1:475:PRO:HG3	2:1:478:MET:HE2	2.01	0.42
3:2:416:PRO:HG2	3:2:418:LEU:HG	2.00	0.42
9:8:207:LEU:HD11	9:8:268:LEU:HD21	2.01	0.42
11:A:428:ASP:OD2	11:A:430:ARG:NH1	2.51	0.42
11:A:783:GLN:O	11:A:826:SER:HA	2.18	0.42
12:B:27:TRP:CE2	12:B:762:ARG:HG3	2.54	0.42
12:B:755:GLN:CD	12:B:776:ILE:HG23	2.44	0.42
19:DF:95:ARG:HG2	19:DF:96:PHE:H	1.84	0.42
37:N:53:DC:H2'	37:N:54:DC:C5	2.54	0.42
37:N:171:DG:H2''	37:N:172:DG:C8	2.53	0.42
40:R:118:PRO:HG3	40:R:124:TYR:CD1	2.54	0.42
41:T:-184:DT:H2'	41:T:-183:DA:C5	2.54	0.42
2:1:318:ALA:HB3	2:1:374:PHE:CE1	2.53	0.42
9:8:289:ALA:HA	9:8:292:MET:HG3	2.01	0.42
11:A:668:PHE:CZ	11:A:672:ILE:HD11	2.54	0.42
11:A:736:THR:O	11:A:740:GLN:HG3	2.19	0.42
12:B:565:THR:HG22	12:B:610:ARG:HB3	2.00	0.42
13:C:260:GLN:HB2	34:K:91:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:H:7:GLU:CG	31:H:59:VAL:HG22	2.48	0.42
37:N:33:DC:H2'	37:N:34:DA:C8	2.54	0.42
37:N:211:DC:H2''	37:N:212:DA:C8	2.54	0.42
38:O:187:ALA:HB3	38:O:190:ALA:CB	2.47	0.42
38:O:204:ILE:HG12	38:O:237:TYR:CZ	2.53	0.42
1:O:415:HIS:CE1	1:O:417:THR:HG1	2.37	0.42
2:1:490:LEU:HB2	2:1:677:MET:HE1	2.01	0.42
5:4:98:GLN:HB3	5:4:236:VAL:HG12	2.01	0.42
11:A:909:LEU:HD12	11:A:967:ARG:HD3	2.01	0.42
28:E:17:ILE:HD11	28:E:135:LEU:HD21	2.01	0.42
29:F:73:ILE:HD13	29:F:92:ILE:HG22	2.01	0.42
30:G:34:VAL:HG21	30:G:72:TYR:CE2	2.54	0.42
31:H:92:MET:HE3	31:H:118:TYR:CG	2.55	0.42
34:K:12:LEU:HD23	34:K:37:LYS:HG2	2.02	0.42
35:L:32:ASP:OD1	35:L:32:ASP:N	2.51	0.42
37:N:27:DT:H2'	37:N:28:DC:C6	2.54	0.42
41:T:-102:DA:C8	41:T:-101:DT:C4	3.07	0.42
48:c:108:VAL:HG11	46:e:102:VAL:HG11	2.00	0.42
1:O:139:TYR:CZ	5:4:19:TRP:HB2	2.54	0.42
5:4:78:PRO:HG2	5:4:83:CYS:HB2	2.01	0.42
5:4:222:ILE:HD12	5:4:228:TYR:HA	2.00	0.42
11:A:788:VAL:HG23	11:A:825:ASN:O	2.19	0.42
11:A:883:ILE:H	11:A:883:ILE:HG13	1.69	0.42
12:B:849:ASP:OD2	12:B:855:ALA:HB2	2.18	0.42
13:C:193:ARG:HA	13:C:193:ARG:HD3	1.91	0.42
13:C:208:TYR:CD1	13:C:230:TYR:CD2	3.07	0.42
17:DD:1011:ALA:HB2	43:V:96:VAL:HG21	2.01	0.42
18:De:594:SER:HB3	18:De:598:TYR:O	2.20	0.42
18:De:636:HIS:CG	18:De:637:PRO:HD2	2.54	0.42
30:G:113:ILE:CG2	30:G:117:MET:HB2	2.49	0.42
36:M:309:PRO:HG2	36:M:312:LYS:CG	2.49	0.42
37:N:41:DC:C6	37:N:42:DT:H72	2.55	0.42
41:T:-145:DG:C5	41:T:-144:DC:C4	3.07	0.42
1:O:363:VAL:HG21	1:O:378:PHE:CE1	2.54	0.42
12:B:285:LEU:HB3	12:B:292:PHE:HE1	1.84	0.42
18:DE:503:LYS:HB2	18:DE:533:ALA:HB1	2.02	0.42
36:M:231:ALA:HA	36:M:301:PRO:CD	2.49	0.42
41:T:-67:DG:C5	41:T:-66:DG:C6	3.08	0.42
44:W:25:PHE:CE1	45:X:212:VAL:HG11	2.53	0.42
45:X:89:HIS:HE1	45:X:94:THR:HG23	1.84	0.42
8:7:79:LEU:O	8:7:83:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:86:LEU:HD23	12:B:130:LYS:HA	2.01	0.42
12:B:830:GLU:OE2	12:B:889:LYS:HE3	2.20	0.42
12:B:1012:SER:OG	12:B:1023:ARG:NH1	2.53	0.42
28:E:20:LEU:C	28:E:20:LEU:HD23	2.44	0.42
31:H:59:VAL:HB	31:H:144:LEU:HB2	2.01	0.42
34:K:58:PHE:HB3	34:K:76:GLN:HB3	2.01	0.42
37:N:18:DG:C2	41:T:-17:DC:O2	2.72	0.42
44:W:14:LEU:HB3	44:W:96:TYR:CD1	2.54	0.42
11:A:53:LYS:HE3	11:A:53:LYS:HB2	1.89	0.42
11:A:379:GLY:O	11:A:482:PHE:HA	2.20	0.42
11:A:811:ILE:HG23	12:B:689:TYR:CZ	2.55	0.42
11:A:931:ARG:HA	11:A:939:VAL:HG21	2.02	0.42
11:A:1430:CYS:HA	11:A:1435:THR:HA	2.02	0.42
12:B:131:THR:HA	12:B:140:LEU:O	2.20	0.42
12:B:223:SER:HG	12:B:350:HIS:CE1	2.38	0.42
12:B:666:ASP:OD1	12:B:666:ASP:C	2.63	0.42
18:DE:756:THR:HB	18:DE:758:HIS:CE1	2.54	0.42
23:DJ:128:PRO:HB2	23:DJ:160:GLN:HE22	1.84	0.42
29:F:66:LEU:HD23	29:F:66:LEU:HA	1.84	0.42
29:F:95:LYS:HB3	29:F:95:LYS:HE3	1.86	0.42
32:I:100:HIS:CD2	32:I:100:HIS:O	2.72	0.42
37:N:11:DG:H2'	37:N:12:DG:C5	2.55	0.42
37:N:61:DA:H2'	37:N:62:DC:C5	2.54	0.42
38:O:193:ASN:HB2	43:V:67:PHE:HE2	1.85	0.42
2:1:230:VAL:HG13	2:1:453:SER:HB3	2.02	0.42
11:A:875:TYR:HA	11:A:1083:PRO:CG	2.50	0.42
11:A:1147:SER:HB2	11:A:1154:ALA:HA	2.02	0.42
11:A:1173:THR:HA	11:A:1213:ARG:O	2.20	0.42
11:A:1479:LYS:HB3	29:F:103:PRO:CA	2.50	0.42
12:B:603:MET:HE2	12:B:603:MET:HB2	1.88	0.42
12:B:1114:TYR:CG	12:B:1153:TYR:HD2	2.37	0.42
28:E:103:LEU:HD11	28:E:130:PHE:CD2	2.55	0.42
34:K:35:ILE:HB	34:K:71:ILE:HG13	2.02	0.42
41:T:-126:DC:C2'	41:T:-125:DG:C8	3.03	0.42
42:U:32:ASP:OD1	42:U:33:GLY:N	2.50	0.42
1:0:127:VAL:HG22	1:0:160:THR:HG23	2.01	0.42
4:3:119:ARG:HG3	4:3:119:ARG:HH11	1.84	0.42
5:4:112:LYS:HG3	5:4:177:CYS:SG	2.59	0.42
11:A:282:ASP:O	11:A:286:ILE:HG12	2.20	0.42
11:A:721:HIS:HA	32:I:108:MET:O	2.20	0.42
11:A:1403:ASP:O	11:A:1407:CYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:204:THR:HB	12:B:206:TYR:CE2	2.54	0.42
12:B:645:GLU:O	12:B:649:ASN:HB3	2.19	0.42
13:C:208:TYR:CE1	13:C:230:TYR:HB3	2.55	0.42
13:C:245:VAL:HG11	34:K:105:PHE:CZ	2.55	0.42
14:D:32:LEU:HA	14:D:36:GLU:OE1	2.20	0.42
14:D:74:PHE:CZ	14:D:83:VAL:HG21	2.55	0.42
18:DE:518:LYS:HE3	18:DE:520:SER:OG	2.20	0.42
24:DL:121:GLU:O	24:DL:125:ASN:HA	2.20	0.42
34:K:45:ILE:HG23	34:K:94:LEU:HD13	2.02	0.42
37:N:8:DG:C5'	38:O:214:PHE:HB3	2.49	0.42
37:N:50:DG:C2	41:T:-49:DG:C2	3.08	0.42
37:N:99:DC:H2''	37:N:100:DA:C5	2.55	0.42
39:Q:14:TYR:HB2	39:Q:135:PHE:CD2	2.54	0.42
42:U:25:VAL:HB	42:U:29:PHE:CE1	2.55	0.42
42:U:46:TRP:CD1	43:V:15:LEU:HB2	2.54	0.42
2:1:473:PHE:HE2	2:1:475:PRO:HB3	1.83	0.42
11:A:432:HIS:CE1	36:M:37:CYS:N	2.87	0.42
11:A:743:ARG:HG3	11:A:744:ILE:N	2.35	0.42
11:A:1483:GLY:HA2	29:F:80:MET:HA	2.02	0.42
12:B:225:LEU:HB3	12:B:228:SER:O	2.19	0.42
14:D:61:PHE:HD2	30:G:47:ALA:HB2	1.82	0.42
29:F:105:ILE:HA	29:F:119:GLY:HA2	2.02	0.42
37:N:69:DA:N3	37:N:70:DC:C4	2.88	0.42
37:N:216:DG:OP2	37:N:216:DG:C8	2.73	0.42
44:W:127:PHE:CE1	44:W:138:ASP:HA	2.54	0.42
48:c:32:HIS:CE1	48:c:36:ARG:HE	2.37	0.42
9:8:74:ILE:HD12	9:8:156:PHE:HZ	1.85	0.41
11:A:196:LEU:HD12	11:A:308:LYS:CE	2.50	0.41
15:DA:404:MET:HE2	15:DA:404:MET:HA	2.02	0.41
18:DE:221:LEU:HD21	18:DE:239:LEU:HD13	2.01	0.41
17:Dd:901:TYR:CE1	24:DI:120:LEU:HD22	2.55	0.41
37:N:-4:DG:C2	41:T:5:DC:O2	2.73	0.41
37:N:20:DG:C2	37:N:21:DC:C2	3.07	0.41
37:N:52:DG:C8	37:N:53:DC:C5	3.08	0.41
37:N:144:DG:C2	41:T:-143:DG:C2	3.08	0.41
38:O:189:ASN:O	38:O:202:MET:HA	2.20	0.41
38:O:209:THR:OG1	38:O:233:ALA:HB1	2.20	0.41
44:W:127:PHE:CE2	44:W:163:GLU:HB2	2.54	0.41
5:4:367:PHE:HB3	5:4:371:CYS:HB2	2.01	0.41
8:7:8:ARG:HD2	8:7:8:ARG:C	2.45	0.41
11:A:764:ASN:OD1	11:A:766:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:639:HIS:O	12:B:643:LEU:HG	2.19	0.41
12:B:776:ILE:HD12	12:B:806:PHE:CD1	2.55	0.41
12:B:1040:GLN:HE21	13:C:195:THR:HG23	1.85	0.41
17:Dd:901:TYR:HE1	24:Dl:120:LEU:HD22	1.85	0.41
24:Dl:99:ALA:HB1	24:Dl:111:LEU:HD11	2.02	0.41
29:F:65:VAL:HG21	29:F:106:ILE:HD11	2.02	0.41
37:N:51:DA:C6	37:N:52:DG:O6	2.72	0.41
39:Q:16:VAL:O	40:R:40:VAL:HG22	2.20	0.41
41:T:-113:DG:C5	41:T:-112:DT:C4	3.08	0.41
44:W:183:GLN:NE2	44:W:184:ILE:HB	2.36	0.41
46:a:76:ALA:HB1	46:a:83:LEU:HD12	2.02	0.41
47:f:91:LEU:HB3	47:f:96:ARG:O	2.20	0.41
2:1:1:MET:HG3	2:1:3:LEU:HD21	2.02	0.41
4:3:56:VAL:HG13	4:3:110:LEU:HD11	2.03	0.41
11:A:418:TYR:CD1	11:A:426:ARG:NH1	2.88	0.41
11:A:705:THR:HB	11:A:752:THR:CG2	2.50	0.41
11:A:934:LEU:HD11	11:A:1006:PRO:HG2	2.01	0.41
18:DE:466:PHE:CE1	19:DF:131:LEU:HD13	2.54	0.41
19:Df:249:ASP:HA	19:Df:250:PRO:HD3	1.90	0.41
37:N:186:DT:C4	37:N:187:DC:N4	2.89	0.41
38:O:289:PRO:CG	41:T:-1:DA:H1'	2.50	0.41
41:T:-208:DT:H2''	41:T:-207:DA:H8	1.83	0.41
45:X:165:GLY:N	45:X:202:PHE:CE2	2.89	0.41
5:4:220:HIS:CG	5:4:231:LEU:HD22	2.55	0.41
11:A:807:LEU:HB2	11:A:810:PHE:CE2	2.55	0.41
11:A:1065:PHE:O	11:A:1068:LEU:HB3	2.21	0.41
19:Df:403:ILE:HG12	19:Df:407:LEU:HG	2.01	0.41
29:F:118:TRP:CE3	29:F:123:LEU:HD21	2.55	0.41
31:H:40:ILE:HB	31:H:124:ARG:HB3	2.02	0.41
36:M:261:ALA:HA	36:M:300:PHE:CE2	2.55	0.41
37:N:107:DC:H1'	37:N:108:DG:C5	2.56	0.41
9:8:71:HIS:HE1	9:8:73:ASN:OD1	2.04	0.41
11:A:687:ILE:HD12	11:A:765:ASN:HB2	2.02	0.41
11:A:1170:THR:HA	11:A:1216:LEU:HA	2.02	0.41
13:C:88:CYS:CB	13:C:97:CYS:HB3	2.48	0.41
15:DA:825:ILE:HG13	15:DA:862:TRP:CD1	2.55	0.41
28:E:9:ARG:HG3	28:E:136:LEU:HD21	2.01	0.41
28:E:20:LEU:HD21	28:E:24:ARG:NE	2.36	0.41
29:F:83:LEU:HA	29:F:95:LYS:HE2	2.01	0.41
36:M:231:ALA:HB3	36:M:261:ALA:HB1	2.03	0.41
37:N:-7:DA:C2	41:T:8:DT:N3	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:N:100:DA:H2''	37:N:101:DA:C8	2.56	0.41
37:N:120:DA:H1'	37:N:121:DG:C5	2.54	0.41
37:N:133:DC:P	47:b:31:THR:HG21	2.60	0.41
41:T:-199:DC:H5''	48:g:78:ARG:HD3	2.03	0.41
41:T:-100:DT:H2''	41:T:-99:DG:C8	2.56	0.41
45:X:120:MET:HG3	45:X:124:LEU:CD1	2.51	0.41
2:1:462:SER:HB3	2:1:654:PHE:CE1	2.56	0.41
8:7:85:ARG:O	8:7:88:ASP:HB2	2.20	0.41
8:7:89:PHE:HD1	8:7:95:TYR:HB3	1.85	0.41
11:A:425:ASP:HB2	36:M:39:LEU:HD13	2.03	0.41
11:A:463:THR:HG22	12:B:1093:CYS:HB2	2.01	0.41
25:Dc:55:LEU:HD22	17:Dd:1065:PHE:CD2	2.55	0.41
28:E:17:ILE:HD12	28:E:74:VAL:HG13	2.03	0.41
28:E:26:TYR:OH	28:E:101:ARG:HD2	2.20	0.41
29:F:65:VAL:HG11	29:F:120:VAL:HG11	2.01	0.41
31:H:20:LYS:HE2	31:H:22:PHE:O	2.20	0.41
31:H:93:TYR:CD1	31:H:142:TYR:CZ	3.08	0.41
34:K:75:VAL:HB	34:K:83:PRO:HB3	2.03	0.41
36:M:263:GLN:O	36:M:268:LYS:HE3	2.20	0.41
37:N:44:DT:C6	37:N:45:DT:H72	2.55	0.41
38:O:211:ALA:HB2	38:O:237:TYR:CE2	2.56	0.41
44:W:128:LYS:HE3	44:W:128:LYS:HB3	1.93	0.41
45:X:168:LEU:HB2	45:X:201:LEU:HD21	2.02	0.41
2:1:212:LEU:C	2:1:215:PRO:HD2	2.46	0.41
8:7:40:VAL:HG21	44:W:122:THR:HA	2.01	0.41
11:A:1192:TRP:CH2	11:A:1258:ARG:HD2	2.55	0.41
12:B:333:GLU:OE2	12:B:337:LYS:HE3	2.20	0.41
12:B:388:TYR:CE2	12:B:505:LEU:HD21	2.56	0.41
12:B:502:HIS:HE1	12:B:504:THR:HG23	1.85	0.41
13:C:73:LEU:HD23	13:C:129:PRO:HA	2.03	0.41
16:DB:503:PHE:CZ	16:DB:507:ILE:HD11	2.55	0.41
24:Dl:81:GLU:O	24:Dl:85:LEU:HG	2.21	0.41
37:N:123:DA:C5	37:N:124:DC:C4	3.08	0.41
37:N:179:DT:H2''	37:N:180:DC:C6	2.56	0.41
40:R:34:ALA:CA	40:R:62:LEU:HD23	2.50	0.41
45:X:103:LEU:HD13	45:X:116:LYS:HE3	2.02	0.41
2:1:207:TYR:HB2	2:1:211:TYR:CG	2.56	0.41
2:1:623:VAL:HG22	2:1:684:PHE:CZ	2.55	0.41
8:7:8:ARG:CZ	44:W:178:ALA:HA	2.50	0.41
8:7:38:LEU:HD21	8:7:47:PRO:HD3	2.02	0.41
11:A:754:SER:HA	11:A:757:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1095:LEU:HD13	11:A:1401:LEU:HD22	2.01	0.41
11:A:1181:PRO:HB2	11:A:1197:TYR:CE1	2.55	0.41
12:B:598:VAL:HG22	12:B:601:VAL:HG23	2.01	0.41
12:B:633:LEU:HA	12:B:633:LEU:HD23	1.85	0.41
13:C:38:PHE:CE1	13:C:245:VAL:HA	2.56	0.41
22:Di:110:TYR:HB3	22:Di:111:SER:H	1.65	0.41
34:K:4:PRO:HA	34:K:5:PRO:HD3	1.94	0.41
38:O:184:ALA:HA	38:O:190:ALA:CB	2.51	0.41
47:b:35:ILE:HD13	47:b:52:TYR:HA	2.02	0.41
3:2:475:PHE:CE1	3:2:498:GLU:HB3	2.55	0.41
4:3:48:LEU:HD13	4:3:90:LEU:HD21	2.02	0.41
5:4:88:LEU:HD21	5:4:170:ILE:HD11	2.03	0.41
6:5:101:TYR:CE2	6:5:103:LEU:HB3	2.55	0.41
9:8:184:LEU:HD13	9:8:222:LEU:HG	2.03	0.41
11:A:689:ILE:CD1	12:B:981:LEU:HB3	2.51	0.41
11:A:790:GLN:HA	11:A:821:GLY:O	2.21	0.41
11:A:935:GLN:O	11:A:939:VAL:HG23	2.20	0.41
11:A:1153:ARG:O	11:A:1157:ILE:HG12	2.20	0.41
11:A:1196:TYR:CG	11:A:1246:ILE:HG23	2.56	0.41
11:A:1207:ILE:HD12	11:A:1207:ILE:HA	1.97	0.41
11:A:1211:LEU:HD11	11:A:1258:ARG:HB3	2.02	0.41
11:A:1309:MET:HG2	11:A:1334:TRP:CE3	2.56	0.41
12:B:25:ALA:O	12:B:29:VAL:HG23	2.21	0.41
12:B:132:VAL:HG13	12:B:140:LEU:HB3	2.01	0.41
12:B:206:TYR:HB3	12:B:208:PHE:CZ	2.55	0.41
12:B:854:ILE:HG22	12:B:921:ILE:HD13	2.02	0.41
13:C:11:ILE:HG13	34:K:108:ALA:HB1	2.03	0.41
13:C:69:GLY:CA	35:L:57:ALA:HB1	2.51	0.41
13:C:100:GLU:O	13:C:122:SER:HA	2.20	0.41
15:DA:1085:THR:HG23	20:DG:134:HIS:NE2	2.36	0.41
26:Dk:165:VAL:HG22	26:Dk:194:LEU:HD12	2.03	0.41
27:Dm:31:LEU:H	27:Dm:31:LEU:HD23	1.86	0.41
28:E:28:VAL:HG22	28:E:62:VAL:HG11	2.03	0.41
31:H:14:ASP:HB3	31:H:29:HIS:HB2	2.03	0.41
33:J:6:ARG:HD2	33:J:13:ILE:HD13	2.02	0.41
37:N:66:DC:H2'	37:N:67:DC:C5	2.56	0.41
37:N:217:DA:H1'	41:T:-217:DT:O2	2.21	0.41
38:O:262:CYS:SG	38:O:325:PHE:CD1	3.12	0.41
38:O:305:PHE:CZ	41:T:-2:DT:H1'	2.54	0.41
40:R:145:LEU:HD12	40:R:145:LEU:HA	1.96	0.41
41:T:7:DT:H2'	41:T:8:DT:C5	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:e:38:LYS:HA	46:e:39:PRO:HD3	1.97	0.41
1:0:431:LYS:HG2	1:0:457:ILE:HG23	2.03	0.41
1:0:527:THR:O	1:0:530:ARG:HG2	2.21	0.41
4:3:418:PHE:CZ	4:3:436:SER:HA	2.56	0.41
11:A:42:LYS:HE2	11:A:42:LYS:HB2	1.94	0.41
11:A:787:VAL:HG22	11:A:824:GLU:O	2.20	0.41
11:A:1154:ALA:HB3	11:A:1309:MET:SD	2.61	0.41
12:B:677:MET:HB3	12:B:682:LEU:HG	2.01	0.41
12:B:978:ILE:O	12:B:982:ILE:HG13	2.21	0.41
15:DA:414:ILE:HG22	15:DA:416:TRP:H	1.86	0.41
15:DA:899:LYS:O	15:DA:1196:ARG:HD3	2.21	0.41
18:DE:786:THR:HG23	18:DE:790:LEU:O	2.21	0.41
31:H:58:LEU:CG	31:H:143:LEU:HD11	2.51	0.41
38:O:190:ALA:HB1	38:O:200:VAL:HG11	2.03	0.41
11:A:1054:MET:SD	11:A:1060:LEU:HD12	2.61	0.40
11:A:1312:PRO:HB3	11:A:1335:ILE:HD13	2.01	0.40
12:B:724:TYR:N	12:B:724:TYR:CD1	2.84	0.40
15:DA:802:HIS:HD2	15:DA:884:GLN:HB3	1.86	0.40
15:DA:823:ARG:HD2	15:DA:864:LEU:HD23	2.03	0.40
15:DA:838:SER:O	15:DA:842:ILE:HG13	2.22	0.40
18:DE:464:TYR:CZ	18:DE:794:ALA:HB2	2.56	0.40
25:Dc:92:PHE:CG	25:Dc:93:PRO:HD2	2.55	0.40
37:N:-2:DG:N2	41:T:3:DC:C2	2.89	0.40
37:N:66:DC:H2"	37:N:67:DC:C6	2.56	0.40
38:O:202:MET:HE3	38:O:213:ILE:CD1	2.51	0.40
41:T:-80:DA:H1'	41:T:-79:DT:O4'	2.21	0.40
1:0:568:LEU:HD11	1:0:606:PHE:HB3	2.02	0.40
2:1:74:SER:O	2:1:208:SER:HA	2.22	0.40
2:1:335:ARG:HE	2:1:365:VAL:HG23	1.86	0.40
3:2:435:SER:HB2	3:2:436:PRO:HD2	2.03	0.40
10:9:246:SER:HA	10:9:249:LEU:HD12	2.02	0.40
11:A:516:GLN:HA	11:A:520:MET:HG2	2.03	0.40
11:A:871:VAL:HB	11:A:1088:GLY:HA3	2.03	0.40
11:A:872:MET:HE2	11:A:1086:MET:SD	2.61	0.40
11:A:1473:LEU:CD1	29:F:64:ARG:HG2	2.52	0.40
12:B:550:MET:HE1	12:B:574:VAL:HG12	2.02	0.40
12:B:635:LEU:HD13	12:B:661:VAL:HG11	2.03	0.40
23:DJ:119:PHE:O	23:DJ:123:LEU:HD13	2.21	0.40
17:Dd:863:LEU:HD23	17:Dd:863:LEU:H	1.85	0.40
31:H:9:ILE:O	31:H:32:SER:HA	2.22	0.40
31:H:13:LYS:HA	31:H:13:LYS:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:110:LEU:HD23	32:I:110:LEU:HA	1.84	0.40
36:M:127:ARG:HD2	36:M:183:VAL:HB	2.04	0.40
37:N:144:DG:C5	37:N:145:DC:C4	3.09	0.40
38:O:163:PRO:HB2	38:O:321:ILE:HG22	2.04	0.40
38:O:276:THR:HB	38:O:335:PHE:HZ	1.86	0.40
40:R:191:PHE:HE2	40:R:236:LYS:HD3	1.84	0.40
41:T:-117:DA:C6	41:T:-116:DG:C6	3.09	0.40
4:3:282:TYR:HA	4:3:283:PRO:HD3	1.91	0.40
11:A:1020:LEU:HD22	11:A:1076:PHE:CG	2.57	0.40
12:B:513:GLU:HA	12:B:726:SER:OG	2.21	0.40
12:B:908:MET:HG3	12:B:920:LYS:HB2	2.03	0.40
14:D:37:VAL:HG21	30:G:2:PHE:CG	2.56	0.40
16:DB:73:TYR:HB2	16:DB:149:ASN:OD1	2.21	0.40
29:F:108:ARG:O	29:F:115:TYR:HA	2.20	0.40
31:H:58:LEU:HD12	31:H:145:MET:HG2	2.02	0.40
37:N:17:DG:N2	41:T:-16:DC:C2	2.89	0.40
38:O:204:ILE:CD1	38:O:207:PRO:HG2	2.50	0.40
38:O:231:ARG:HA	38:O:253:PHE:CZ	2.57	0.40
41:T:-6:DT:C4	41:T:-5:DT:O4	2.75	0.40
44:W:187:ILE:O	44:W:191:LEU:HG	2.21	0.40
45:X:155:LEU:HD21	45:X:201:LEU:HB2	2.03	0.40
1:0:194:ILE:HD13	1:0:280:LEU:HD11	2.03	0.40
2:1:370:LYS:HB2	2:1:371:PRO:HD3	2.04	0.40
2:1:644:PHE:HB2	2:1:646:ILE:HD12	2.03	0.40
3:2:525:ILE:HD12	3:2:528:MET:HE1	2.03	0.40
8:7:9:CYS:SG	8:7:31:CYS:SG	3.19	0.40
11:A:276:LEU:HD13	11:A:342:ARG:NH2	2.37	0.40
11:A:353:ASN:O	11:A:357:LYS:HE3	2.21	0.40
11:A:365:THR:HG22	11:A:482:PHE:CE2	2.56	0.40
11:A:725:LEU:O	11:A:733:LEU:HD13	2.22	0.40
11:A:1156:ASP:O	11:A:1160:ARG:HG3	2.22	0.40
11:A:1486:ILE:HA	11:A:1487:PRO:HD3	1.99	0.40
12:B:453:TRP:CD1	12:B:453:TRP:N	2.89	0.40
14:D:57:LEU:HD13	14:D:61:PHE:CE1	2.56	0.40
17:Dd:881:ARG:HG2	17:Dd:885:ILE:HD11	2.03	0.40
30:G:107:PHE:O	30:G:160:ILE:HA	2.21	0.40
32:I:15:ARG:HD3	32:I:37:TYR:CD2	2.56	0.40
37:N:53:DC:H2'	37:N:54:DC:C6	2.56	0.40
37:N:156:DG:C2	41:T:-155:DG:C2	3.09	0.40
38:O:328:ILE:O	38:O:332:LEU:HG	2.22	0.40
40:R:62:LEU:HD12	40:R:62:LEU:HA	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:T:-110:DT:H1'	41:T:-109:DA:C4	2.57	0.40
42:U:50:LEU:HD21	43:V:10:THR:O	2.22	0.40
45:X:151:LEU:HD13	45:X:171:ILE:HG13	2.03	0.40
46:a:66:LEU:HB3	46:a:67:PRO:HD3	2.03	0.40
4:3:45:PHE:CZ	4:3:57:MET:HE2	2.57	0.40
5:4:375:VAL:O	5:4:380:HIS:N	2.51	0.40
11:A:785:ILE:HD13	11:A:785:ILE:HG21	1.86	0.40
11:A:870:SER:HB2	11:A:882:SER:HB3	2.03	0.40
12:B:637:LYS:HB3	12:B:637:LYS:HE3	1.81	0.40
12:B:647:GLU:C	12:B:649:ASN:N	2.80	0.40
14:D:74:PHE:CE1	14:D:83:VAL:HG21	2.56	0.40
15:DA:1165:LEU:HG	15:DA:1195:VAL:HG21	2.03	0.40
16:DB:603:LYS:H	16:DB:603:LYS:HG2	1.71	0.40
17:Dd:878:LEU:O	17:Dd:882:ILE:HG13	2.22	0.40
19:Df:223:TYR:CD2	19:Df:255:MET:HE1	2.56	0.40
28:E:61:LEU:HB2	28:E:73:PHE:CE1	2.57	0.40
28:E:110:MET:SD	28:E:118:LEU:HD11	2.61	0.40
28:E:173:ILE:HG23	28:E:209:VAL:HA	2.04	0.40
29:F:105:ILE:HG21	29:F:117:ASP:HB3	2.04	0.40
30:G:144:ARG:HH21	30:G:167:TYR:HB3	1.86	0.40
31:H:6:PHE:CZ	31:H:125:LEU:HD21	2.57	0.40
33:J:21:TYR:O	33:J:25:LEU:HG	2.22	0.40
36:M:242:LEU:HB2	36:M:244:LEU:HG	2.04	0.40
38:O:168:ILE:HD12	38:O:258:MET:HG2	2.01	0.40
41:T:-48:DA:C6	41:T:-47:DG:C6	3.09	0.40
43:V:3:TYR:CE2	43:V:98:CYS:HB3	2.57	0.40
44:W:17:LEU:O	44:W:21:VAL:HG22	2.20	0.40
45:X:216:PHE:CD1	45:X:216:PHE:N	2.87	0.40
49:h:39:ALA:HA	49:h:60:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	601/782 (77%)	583 (97%)	18 (3%)	0	100	100
2	1	710/760 (93%)	679 (96%)	31 (4%)	0	100	100
3	2	253/548 (46%)	245 (97%)	8 (3%)	0	100	100
4	3	413/462 (89%)	400 (97%)	13 (3%)	0	100	100
5	4	341/395 (86%)	334 (98%)	7 (2%)	0	100	100
6	5	259/308 (84%)	246 (95%)	13 (5%)	0	100	100
7	6	67/71 (94%)	65 (97%)	2 (3%)	0	100	100
8	7	208/309 (67%)	196 (94%)	12 (6%)	0	100	100
9	8	297/346 (86%)	287 (97%)	10 (3%)	0	100	100
10	9	285/323 (88%)	279 (98%)	6 (2%)	0	100	100
11	A	1413/1984 (71%)	1379 (98%)	34 (2%)	0	100	100
12	B	1130/1300 (87%)	1096 (97%)	34 (3%)	0	100	100
13	C	253/275 (92%)	247 (98%)	6 (2%)	0	100	100
14	D	126/184 (68%)	122 (97%)	4 (3%)	0	100	100
15	DA	542/1893 (29%)	526 (97%)	16 (3%)	0	100	100
16	DB	959/1199 (80%)	928 (97%)	31 (3%)	0	100	100
17	DD	153/1085 (14%)	152 (99%)	1 (1%)	0	100	100
17	Dd	154/1085 (14%)	151 (98%)	3 (2%)	0	100	100
18	DE	540/800 (68%)	526 (97%)	14 (3%)	0	100	100
18	De	531/800 (66%)	507 (96%)	24 (4%)	0	100	100
19	DF	404/677 (60%)	393 (97%)	11 (3%)	0	100	100
19	Df	399/677 (59%)	388 (97%)	11 (3%)	0	100	100
20	DG	139/349 (40%)	132 (95%)	7 (5%)	0	100	100
21	DH	207/310 (67%)	196 (95%)	11 (5%)	0	100	100
22	DI	118/264 (45%)	114 (97%)	4 (3%)	0	100	100
22	Di	119/264 (45%)	114 (96%)	5 (4%)	0	100	100
23	DJ	86/218 (39%)	80 (93%)	6 (7%)	0	100	100
23	Dj	91/218 (42%)	84 (92%)	7 (8%)	0	100	100
24	DL	72/161 (45%)	70 (97%)	2 (3%)	0	100	100
24	DI	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
25	Dc	125/929 (14%)	124 (99%)	1 (1%)	0	100	100
26	Dk	96/211 (46%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Dm	85/124 (68%)	80 (94%)	5 (6%)	0	100	100
28	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
29	F	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
30	G	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
31	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
32	I	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
33	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
34	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
35	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
36	M	248/316 (78%)	241 (97%)	7 (3%)	0	100	100
38	O	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
39	Q	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
40	R	218/249 (88%)	215 (99%)	3 (1%)	0	100	100
42	U	109/376 (29%)	104 (95%)	5 (5%)	0	100	100
43	V	97/109 (89%)	93 (96%)	4 (4%)	0	100	100
44	W	198/439 (45%)	197 (100%)	1 (0%)	0	100	100
45	X	169/291 (58%)	163 (96%)	6 (4%)	0	100	100
46	a	95/136 (70%)	95 (100%)	0	0	100	100
46	e	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
47	b	80/103 (78%)	78 (98%)	2 (2%)	0	100	100
47	f	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
48	c	107/130 (82%)	106 (99%)	1 (1%)	0	100	100
48	g	104/130 (80%)	101 (97%)	3 (3%)	0	100	100
49	d	95/126 (75%)	94 (99%)	1 (1%)	0	100	100
49	h	93/126 (74%)	93 (100%)	0	0	100	100
All	All	14307/24124 (59%)	13872 (97%)	435 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	536/688 (78%)	535 (100%)	1 (0%)	87	87
2	1	624/664 (94%)	621 (100%)	3 (0%)	81	83
3	2	241/484 (50%)	241 (100%)	0	100	100
4	3	351/399 (88%)	351 (100%)	0	100	100
5	4	311/352 (88%)	309 (99%)	2 (1%)	78	83
6	5	234/272 (86%)	234 (100%)	0	100	100
7	6	62/64 (97%)	62 (100%)	0	100	100
8	7	194/283 (69%)	194 (100%)	0	100	100
9	8	259/299 (87%)	258 (100%)	1 (0%)	84	84
10	9	259/296 (88%)	259 (100%)	0	100	100
11	A	1254/1763 (71%)	1252 (100%)	2 (0%)	87	87
12	B	994/1127 (88%)	994 (100%)	0	100	100
13	C	234/252 (93%)	234 (100%)	0	100	100
14	D	118/160 (74%)	117 (99%)	1 (1%)	73	80
15	DA	495/1682 (29%)	492 (99%)	3 (1%)	78	83
16	DB	876/1083 (81%)	875 (100%)	1 (0%)	88	89
17	DD	144/815 (18%)	143 (99%)	1 (1%)	76	81
17	Dd	146/815 (18%)	145 (99%)	1 (1%)	76	81
18	DE	478/657 (73%)	478 (100%)	0	100	100
18	De	475/657 (72%)	473 (100%)	2 (0%)	84	84
19	DF	324/574 (56%)	321 (99%)	3 (1%)	70	79
19	Df	322/574 (56%)	320 (99%)	2 (1%)	78	83
20	DG	133/322 (41%)	130 (98%)	3 (2%)	44	64
21	DH	181/270 (67%)	180 (99%)	1 (1%)	78	83
22	DI	106/235 (45%)	105 (99%)	1 (1%)	70	79
22	Di	107/235 (46%)	107 (100%)	0	100	100
23	DJ	79/154 (51%)	79 (100%)	0	100	100
23	Dj	83/154 (54%)	83 (100%)	0	100	100
24	DL	69/141 (49%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Dl	98/141 (70%)	97 (99%)	1 (1%)	68	78
25	Dc	113/833 (14%)	113 (100%)	0	100	100
26	Dk	87/182 (48%)	87 (100%)	0	100	100
27	Dm	80/106 (76%)	79 (99%)	1 (1%)	61	74
28	E	191/192 (100%)	191 (100%)	0	100	100
29	F	69/111 (62%)	69 (100%)	0	100	100
30	G	152/153 (99%)	149 (98%)	3 (2%)	48	66
31	H	129/131 (98%)	129 (100%)	0	100	100
32	I	103/112 (92%)	103 (100%)	0	100	100
33	J	53/56 (95%)	53 (100%)	0	100	100
34	K	104/106 (98%)	104 (100%)	0	100	100
35	L	41/55 (74%)	41 (100%)	0	100	100
36	M	215/268 (80%)	215 (100%)	0	100	100
38	O	154/293 (53%)	154 (100%)	0	100	100
39	Q	121/448 (27%)	121 (100%)	0	100	100
40	R	196/218 (90%)	196 (100%)	0	100	100
42	U	105/324 (32%)	105 (100%)	0	100	100
43	V	90/98 (92%)	90 (100%)	0	100	100
44	W	182/373 (49%)	182 (100%)	0	100	100
45	X	154/261 (59%)	154 (100%)	0	100	100
46	a	85/111 (77%)	85 (100%)	0	100	100
46	e	86/111 (78%)	86 (100%)	0	100	100
47	b	67/79 (85%)	67 (100%)	0	100	100
47	f	65/79 (82%)	65 (100%)	0	100	100
48	c	86/101 (85%)	86 (100%)	0	100	100
48	g	84/101 (83%)	84 (100%)	0	100	100
49	d	83/106 (78%)	83 (100%)	0	100	100
49	h	81/106 (76%)	81 (100%)	0	100	100
All	All	12763/20726 (62%)	12730 (100%)	33 (0%)	84	86

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	521	GLU
2	1	87	LEU
2	1	203	ASN
2	1	673	ASP
5	4	93	GLU
5	4	379	LEU
9	8	86	ASN
11	A	79	THR
11	A	546	ARG
14	D	129	GLN
15	DA	404	MET
15	DA	475	LEU
15	DA	1165	LEU
16	DB	21	GLU
17	DD	888	LYS
19	DF	297	LEU
19	DF	301	VAL
19	DF	339	GLN
20	DG	143	VAL
20	DG	161	ASP
20	DG	181	TRP
21	DH	161	LYS
22	DI	69	ASP
17	Dd	948	GLU
18	De	250	GLU
18	De	512	ASP
19	Df	72	ASP
19	Df	323	VAL
24	DI	106	ARG
27	Dm	31	LEU
30	G	39	THR
30	G	138	GLN
30	G	166	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	366	ASN
2	1	201	HIS
2	1	203	ASN
2	1	612	HIS
2	1	613	HIS
3	2	119	GLN

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Mol	Chain	Res	Type
3	2	402	ASN
4	3	83	GLN
4	3	211	GLN
4	3	390	GLN
5	4	220	HIS
6	5	155	GLN
6	5	205	GLN
8	7	57	ASN
8	7	129	ASN
9	8	221	GLN
10	9	43	ASN
11	A	267	GLN
11	A	330	GLN
11	A	606	HIS
11	A	671	ASN
11	A	721	HIS
11	A	742	ASN
11	A	765	ASN
11	A	861	GLN
11	A	905	ASN
11	A	1005	HIS
11	A	1397	HIS
12	B	23	GLN
12	B	197	GLN
12	B	227	ASN
12	B	312	GLN
12	B	420	GLN
12	B	486	ASN
12	B	941	GLN
13	C	5	ASN
13	C	260	GLN
15	DA	409	HIS
15	DA	569	ASN
15	DA	600	GLN
15	DA	802	HIS
15	DA	837	HIS
15	DA	860	ASN
15	DA	896	GLN
15	DA	1058	HIS
16	DB	183	GLN
16	DB	235	HIS
16	DB	285	HIS

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Mol	Chain	Res	Type
16	DB	348	GLN
16	DB	352	GLN
16	DB	415	HIS
16	DB	432	HIS
16	DB	450	GLN
16	DB	454	HIS
16	DB	471	GLN
16	DB	486	GLN
16	DB	495	GLN
16	DB	509	ASN
16	DB	593	HIS
16	DB	644	GLN
16	DB	652	GLN
16	DB	663	GLN
16	DB	745	GLN
16	DB	750	GLN
16	DB	882	HIS
16	DB	908	GLN
16	DB	916	ASN
17	DD	925	ASN
17	DD	936	GLN
17	DD	1059	ASN
18	DE	223	HIS
18	DE	256	HIS
18	DE	420	ASN
18	DE	424	GLN
18	DE	471	GLN
18	DE	636	HIS
18	DE	782	HIS
19	DF	87	HIS
19	DF	119	ASN
19	DF	270	ASN
19	DF	275	ASN
19	DF	385	HIS
19	DF	422	HIS
20	DG	53	HIS
22	DI	98	GLN
23	DJ	160	GLN
23	DJ	210	ASN
23	DJ	215	HIS
24	DL	117	GLN
25	Dc	78	HIS

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Mol	Chain	Res	Type
25	Dc	94	HIS
17	Dd	889	HIS
17	Dd	912	ASN
18	De	223	HIS
18	De	232	HIS
18	De	420	ASN
19	Df	134	HIS
19	Df	214	HIS
19	Df	325	ASN
19	Df	422	HIS
23	Dj	122	GLN
24	Di	86	GLN
24	Di	105	HIS
27	Dm	48	ASN
30	G	28	GLN
30	G	91	GLN
31	H	29	HIS
31	H	131	ASN
32	I	60	HIS
32	I	100	HIS
34	K	49	GLN
34	K	89	ASN
35	L	23	HIS
36	M	140	ASN
38	O	277	HIS
39	Q	10	ASN
39	Q	53	ASN
40	R	14	GLN
40	R	81	HIS
43	V	35	GLN
43	V	39	GLN
43	V	70	ASN
44	W	143	GLN
46	a	109	ASN
48	c	32	HIS
49	d	48	GLN
49	d	68	ASN
49	h	83	HIS
49	h	85	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 46 ligands modelled in this entry, 18 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	2A1	N	302	50	4,4,4	1.73	1 (25%)	3,4,4	3.88	2 (66%)
50	2A1	N	301	50	4,4,4	2.46	1 (25%)	3,4,4	2.50	1 (33%)
51	ALA	2	602	50	3,4,5	0.41	0	2,4,6	17.08	1 (50%)
50	2A1	0	806	50	4,4,4	2.23	1 (25%)	3,4,4	4.00	1 (33%)
50	2A1	0	811	50	4,4,4	2.34	1 (25%)	3,4,4	3.32	1 (33%)
50	2A1	2	603	50,51	4,4,4	2.58	2 (50%)	3,4,4	1.98	1 (33%)
50	2A1	0	801	50	4,4,4	2.12	3 (75%)	3,4,4	0.38	0
50	2A1	0	803	50	4,4,4	2.20	1 (25%)	3,4,4	3.86	2 (66%)
50	2A1	N	303	50	4,4,4	2.00	1 (25%)	3,4,4	3.83	1 (33%)
50	2A1	0	804	50	4,4,4	2.00	1 (25%)	3,4,4	3.66	2 (66%)
50	2A1	0	814	50	4,4,4	2.53	2 (50%)	3,4,4	4.84	1 (33%)
51	ALA	2	606	50	5,5,5	1.47	0	6,6,6	1.15	0
50	2A1	2	605	50,51	4,4,4	2.42	1 (25%)	3,4,4	2.59	1 (33%)
50	2A1	0	802	50	4,4,4	2.75	1 (25%)	3,4,4	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	2A1	0	815	50	4,4,4	2.12	1 (25%)	3,4,4	4.72	2 (66%)
52	SF4	1	1000	2	0,12,12	-	-	-	-	-
50	2A1	0	812	50	4,4,4	2.82	2 (50%)	3,4,4	1.76	1 (33%)
50	2A1	N	306	-	4,4,4	2.31	1 (25%)	3,4,4	2.76	1 (33%)
50	2A1	0	813	50	4,4,4	3.19	2 (50%)	3,4,4	3.19	1 (33%)
50	2A1	N	305	50	4,4,4	3.05	2 (50%)	3,4,4	3.49	1 (33%)
50	2A1	0	807	50,51	4,4,4	3.67	2 (50%)	3,4,4	0.88	0
50	2A1	0	810	50	4,4,4	1.90	1 (25%)	3,4,4	0.90	0
50	2A1	0	809	-	4,4,4	2.30	1 (25%)	3,4,4	2.71	1 (33%)
50	2A1	2	604	50	4,4,4	3.04	3 (75%)	3,4,4	4.06	2 (66%)
50	2A1	N	304	50	4,4,4	3.11	2 (50%)	3,4,4	5.59	2 (66%)
50	2A1	2	601	51	4,4,4	2.29	1 (25%)	3,4,4	3.38	1 (33%)
50	2A1	0	805	50	4,4,4	2.42	1 (25%)	3,4,4	3.74	2 (66%)
51	ALA	0	808	50	5,5,5	1.61	2 (40%)	6,6,6	2.72	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	2A1	N	302	50	-	0/2/2/2	-
50	2A1	N	301	50	-	2/2/2/2	-
51	ALA	2	602	50	-	0/0/2/4	-
50	2A1	0	806	50	-	1/2/2/2	-
50	2A1	0	811	50	-	0/2/2/2	-
50	2A1	2	603	50,51	-	1/2/2/2	-
50	2A1	0	801	50	-	2/2/2/2	-
50	2A1	0	803	50	-	0/2/2/2	-
50	2A1	N	303	50	-	2/2/2/2	-
50	2A1	0	804	50	-	2/2/2/2	-
50	2A1	0	814	50	-	0/2/2/2	-
51	ALA	2	606	50	-	0/4/4/4	-
50	2A1	2	605	50,51	-	1/2/2/2	-
50	2A1	0	802	50	-	2/2/2/2	-
50	2A1	0	815	50	-	2/2/2/2	-
52	SF4	1	1000	2	-	-	0/6/5/5
50	2A1	0	812	50	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	2A1	N	306	-	-	1/2/2/2	-
50	2A1	0	813	50	-	0/2/2/2	-
50	2A1	N	305	50	-	0/2/2/2	-
50	2A1	0	807	50,51	-	2/2/2/2	-
50	2A1	0	810	50	-	0/2/2/2	-
50	2A1	0	809	-	-	0/2/2/2	-
50	2A1	2	604	50	-	0/2/2/2	-
50	2A1	N	304	50	-	2/2/2/2	-
50	2A1	2	601	51	-	0/2/2/2	-
50	2A1	0	805	50	-	0/2/2/2	-
51	ALA	0	808	50	-	0/4/4/4	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	0	807	2A1	O-C	-5.70	1.18	1.42
50	N	304	2A1	O-C	-5.51	1.19	1.42
50	0	802	2A1	O-C	-4.89	1.21	1.42
50	0	813	2A1	O-C	-4.67	1.22	1.42
50	N	301	2A1	O-C	-4.65	1.22	1.42
50	0	807	2A1	C-CA	4.63	1.59	1.52
50	N	305	2A1	O-C	-4.59	1.23	1.42
50	2	604	2A1	O-C	-4.56	1.23	1.42
50	0	805	2A1	O-C	-4.55	1.23	1.42
50	2	605	2A1	O-C	-4.54	1.23	1.42
50	0	811	2A1	O-C	-4.50	1.23	1.42
50	N	306	2A1	O-C	-4.46	1.23	1.42
50	0	809	2A1	O-C	-4.45	1.23	1.42
50	0	814	2A1	O-C	-4.36	1.24	1.42
50	0	803	2A1	O-C	-4.17	1.24	1.42
50	0	815	2A1	O-C	-4.14	1.24	1.42
50	2	601	2A1	O-C	-4.11	1.25	1.42
50	2	603	2A1	O-C	-4.05	1.25	1.42
50	0	813	2A1	C-CA	-4.05	1.46	1.52
50	0	806	2A1	O-C	-4.04	1.25	1.42
50	0	812	2A1	C-CA	-4.00	1.46	1.52
50	N	303	2A1	O-C	-3.80	1.26	1.42
50	0	804	2A1	O-C	-3.78	1.26	1.42
50	0	812	2A1	O-C	-3.77	1.26	1.42
50	N	305	2A1	C-CA	3.54	1.58	1.52
50	0	810	2A1	O-C	-3.49	1.27	1.42
50	2	604	2A1	CA-N	-3.39	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	N	302	2A1	O-C	-3.12	1.29	1.42
50	2	603	2A1	CA-N	-3.01	1.40	1.49
50	0	801	2A1	O-C	-2.73	1.30	1.42
50	N	304	2A1	C-CA	2.48	1.56	1.52
50	0	814	2A1	CA-N	-2.47	1.42	1.49
51	0	808	ALA	CA-C	-2.42	1.51	1.54
50	0	801	2A1	C-CA	-2.38	1.48	1.52
51	0	808	ALA	CA-N	-2.25	1.40	1.48
50	0	801	2A1	CA-N	-2.14	1.43	1.49
50	2	604	2A1	C-CA	-2.12	1.49	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	2	602	ALA	O-C-CA	-24.15	47.80	124.28
50	N	304	2A1	O-C-CA	9.19	129.31	112.42
50	0	814	2A1	O-C-CA	8.12	127.34	112.42
50	0	815	2A1	O-C-CA	7.33	125.90	112.42
50	0	806	2A1	O-C-CA	6.69	124.72	112.42
50	N	303	2A1	O-C-CA	6.37	124.14	112.42
50	0	803	2A1	O-C-CA	6.15	123.73	112.42
50	2	604	2A1	O-C-CA	6.05	123.54	112.42
50	0	804	2A1	O-C-CA	5.91	123.29	112.42
50	N	305	2A1	O-C-CA	5.88	123.23	112.42
51	0	808	ALA	OXT-C-O	-5.80	110.92	124.09
50	2	601	2A1	O-C-CA	5.79	123.07	112.42
50	0	811	2A1	O-C-CA	5.73	122.96	112.42
50	0	813	2A1	O-C-CA	5.15	121.89	112.42
50	0	805	2A1	O-C-CA	5.06	121.71	112.42
50	N	302	2A1	O-C-CA	5.05	121.71	112.42
50	N	306	2A1	O-C-CA	4.70	121.06	112.42
50	0	809	2A1	O-C-CA	4.61	120.90	112.42
50	N	302	2A1	C3-CA-C	-4.43	104.71	111.33
50	2	605	2A1	O-C-CA	4.35	120.41	112.42
50	N	301	2A1	O-C-CA	4.09	119.94	112.42
50	0	805	2A1	C3-CA-C	-3.85	105.58	111.33
50	0	815	2A1	C3-CA-C	-3.58	105.98	111.33
50	2	603	2A1	O-C-CA	3.35	118.59	112.42
50	2	604	2A1	C3-CA-C	-3.01	106.83	111.33
50	0	812	2A1	O-C-CA	2.93	117.81	112.42
50	N	304	2A1	C3-CA-C	-2.66	107.36	111.33
51	0	808	ALA	O-C-CA	2.55	130.12	121.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	0	803	2A1	C3-CA-C	-2.47	107.63	111.33
50	0	804	2A1	C3-CA-C	-2.23	108.00	111.33

There are no chirality outliers.

All (22) torsion outliers are listed below:

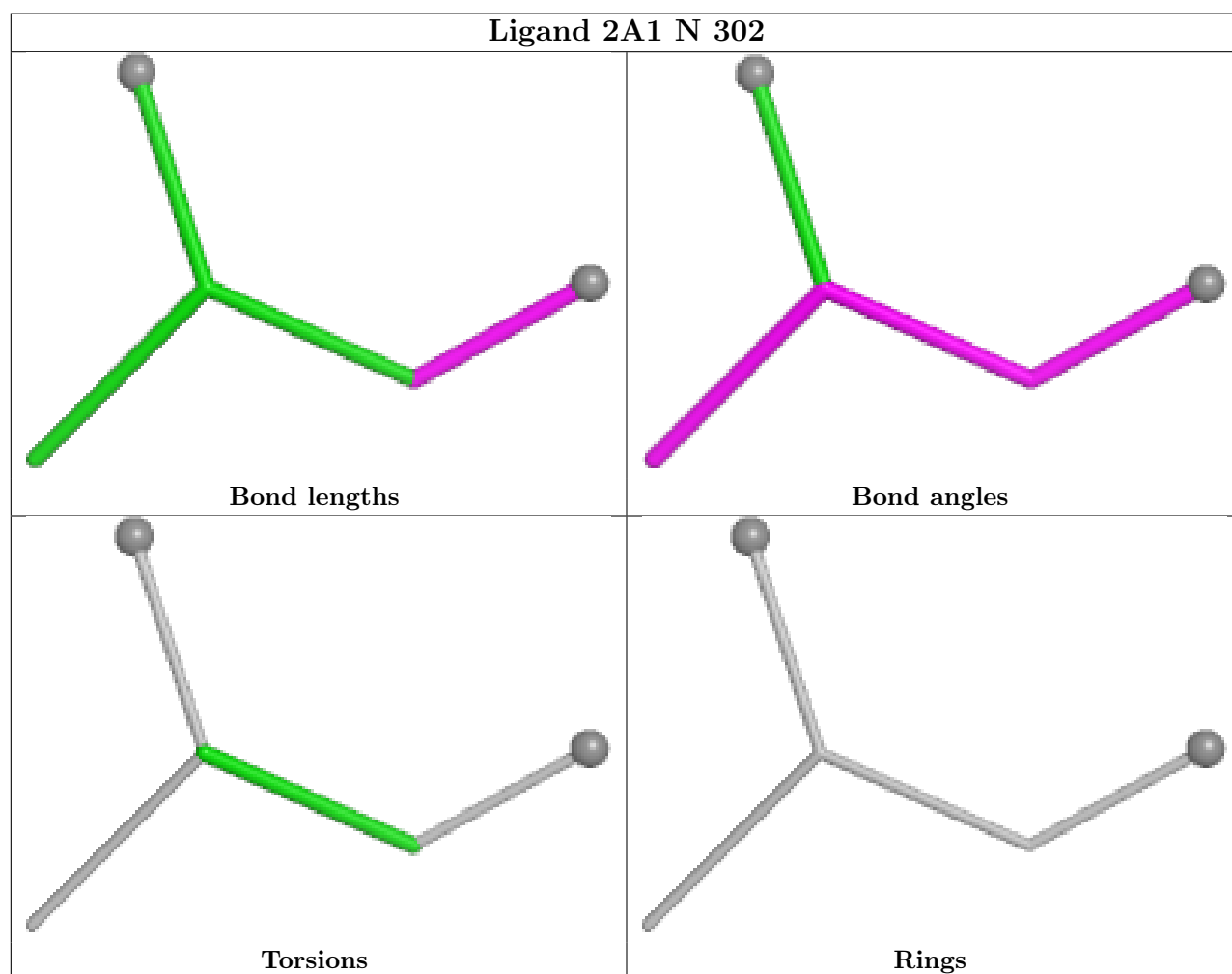
Mol	Chain	Res	Type	Atoms
50	0	801	2A1	O-C-CA-N
50	0	801	2A1	O-C-CA-C3
50	0	802	2A1	O-C-CA-N
50	0	802	2A1	O-C-CA-C3
50	0	804	2A1	O-C-CA-N
50	0	804	2A1	O-C-CA-C3
50	0	807	2A1	O-C-CA-N
50	0	807	2A1	O-C-CA-C3
50	0	812	2A1	O-C-CA-N
50	0	812	2A1	O-C-CA-C3
50	0	815	2A1	O-C-CA-N
50	0	815	2A1	O-C-CA-C3
50	2	603	2A1	O-C-CA-C3
50	2	605	2A1	O-C-CA-C3
50	N	301	2A1	O-C-CA-C3
50	N	303	2A1	O-C-CA-C3
50	N	304	2A1	O-C-CA-C3
50	N	301	2A1	O-C-CA-N
50	N	303	2A1	O-C-CA-N
50	N	304	2A1	O-C-CA-N
50	0	806	2A1	O-C-CA-C3
50	N	306	2A1	O-C-CA-C3

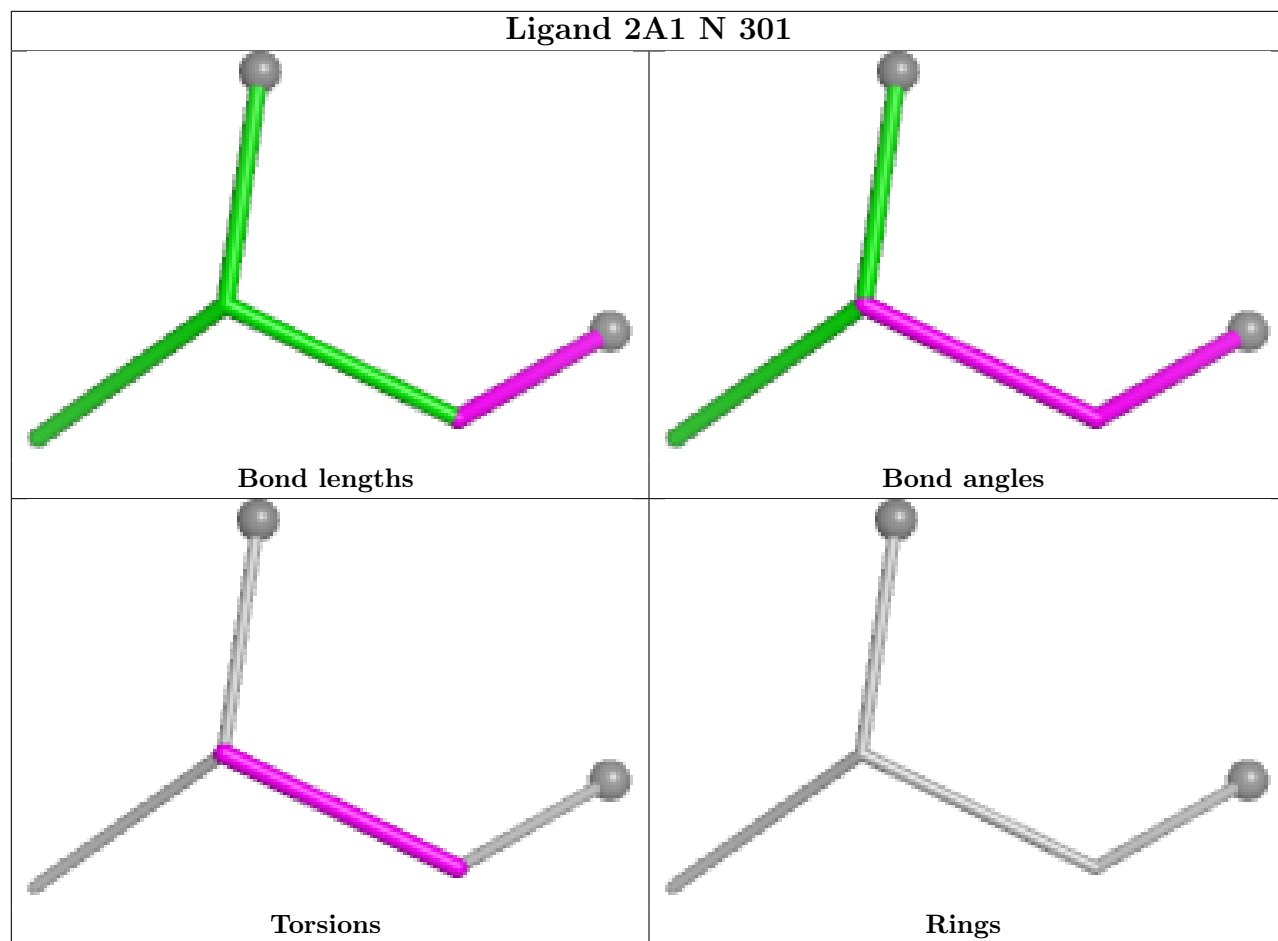
There are no ring outliers.

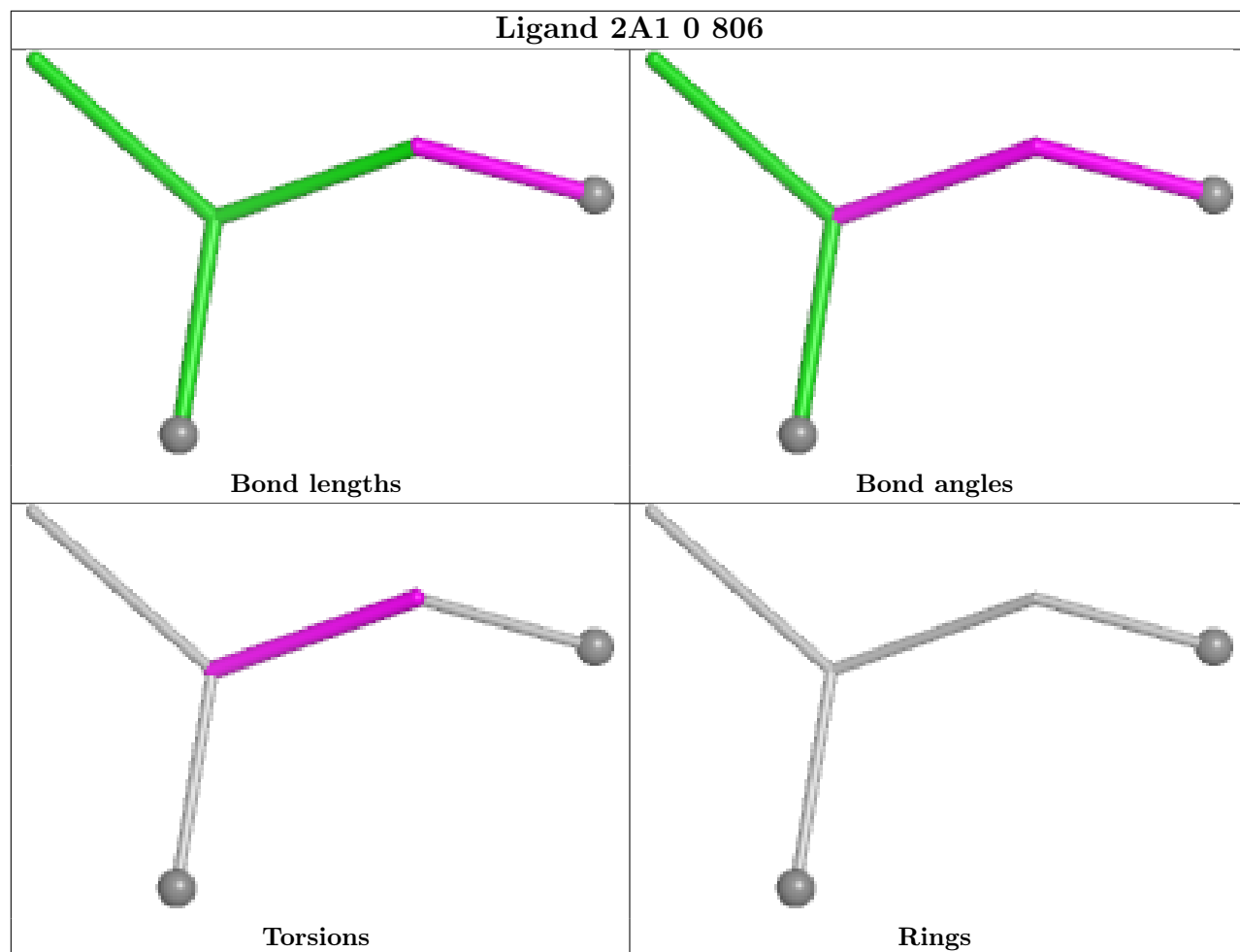
6 monomers are involved in 3 short contacts:

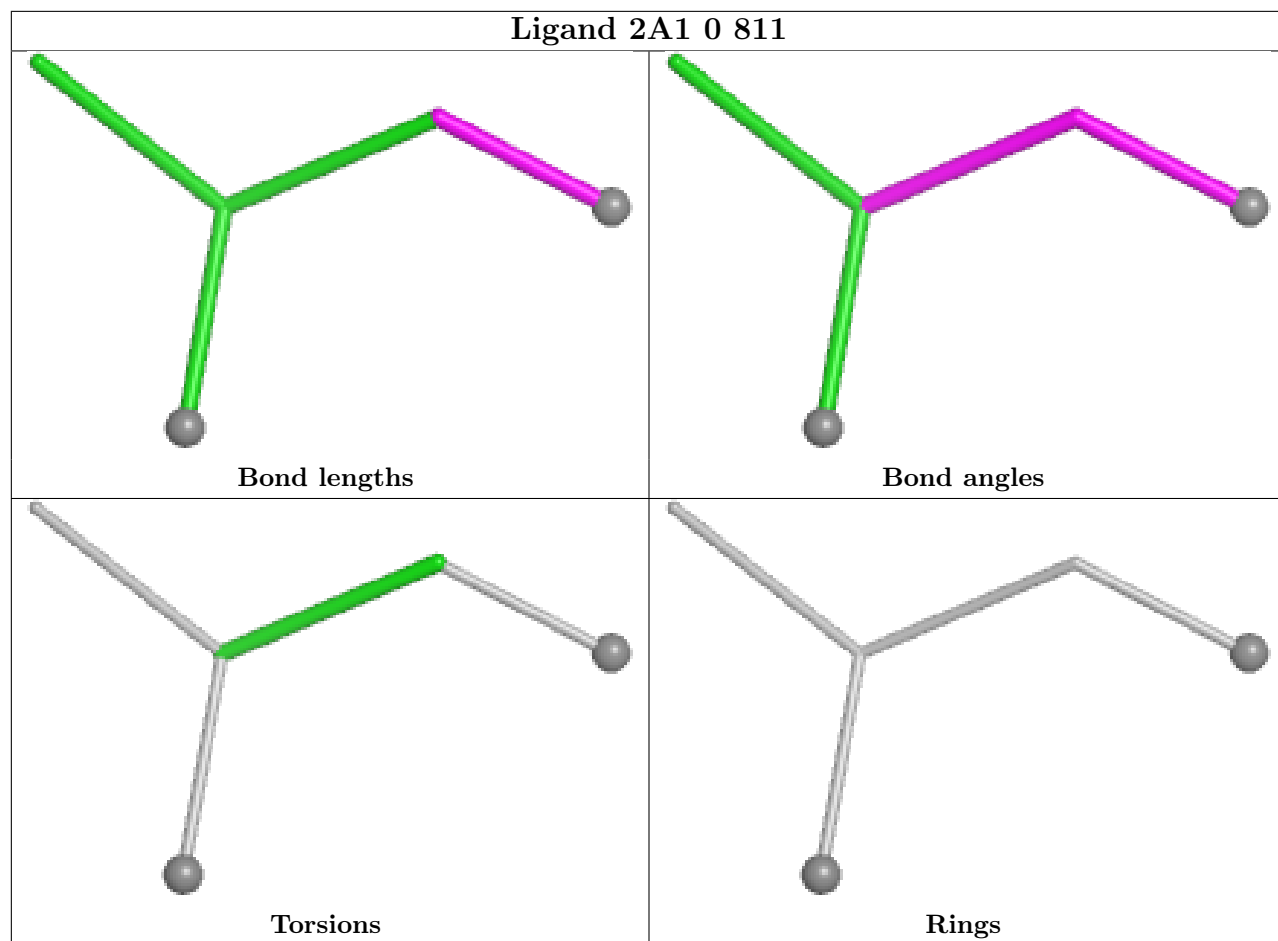
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	0	801	2A1	1	0
50	0	802	2A1	1	0
50	0	812	2A1	1	0
50	0	813	2A1	1	0
50	0	807	2A1	1	0
51	0	808	ALA	1	0

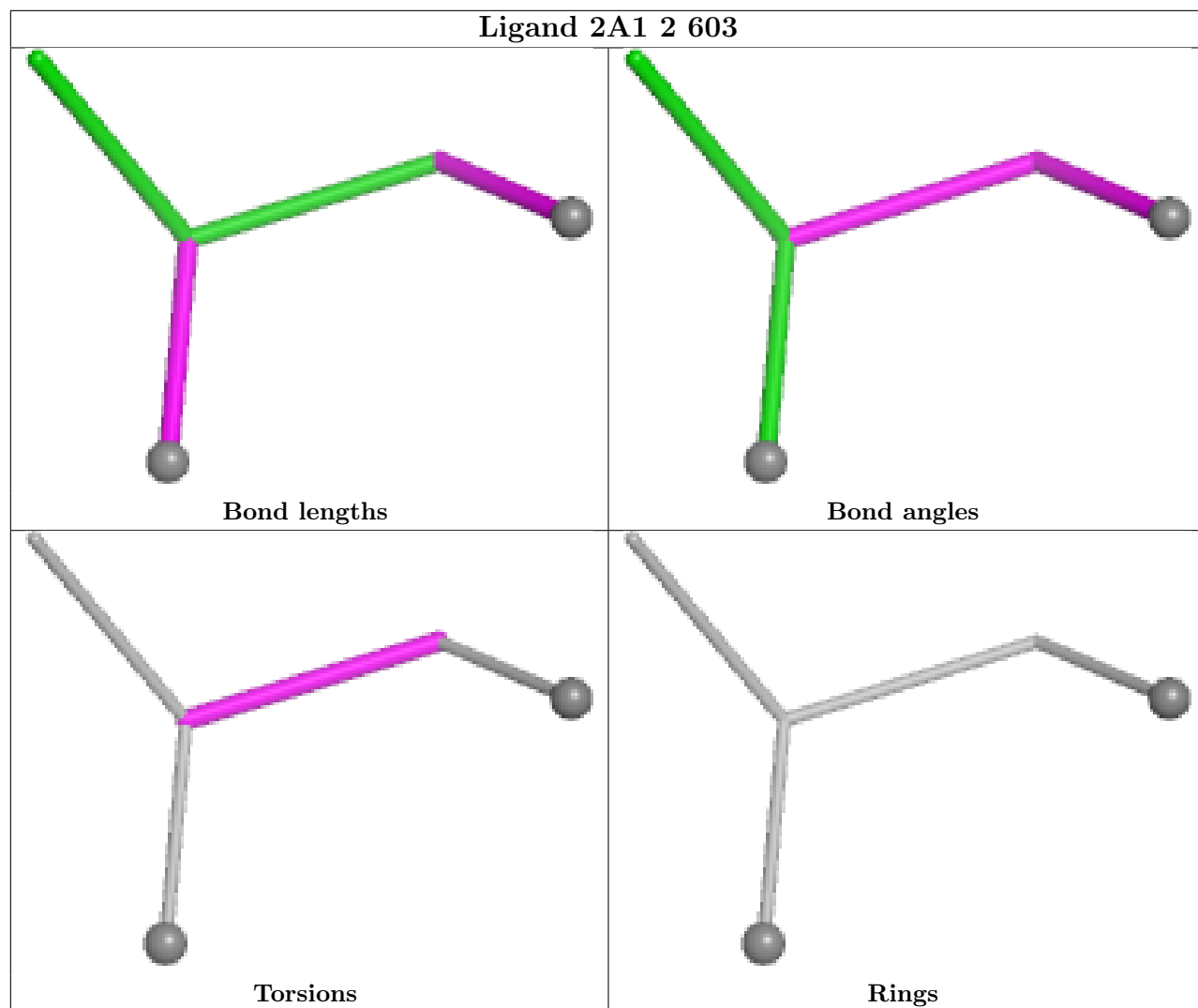
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



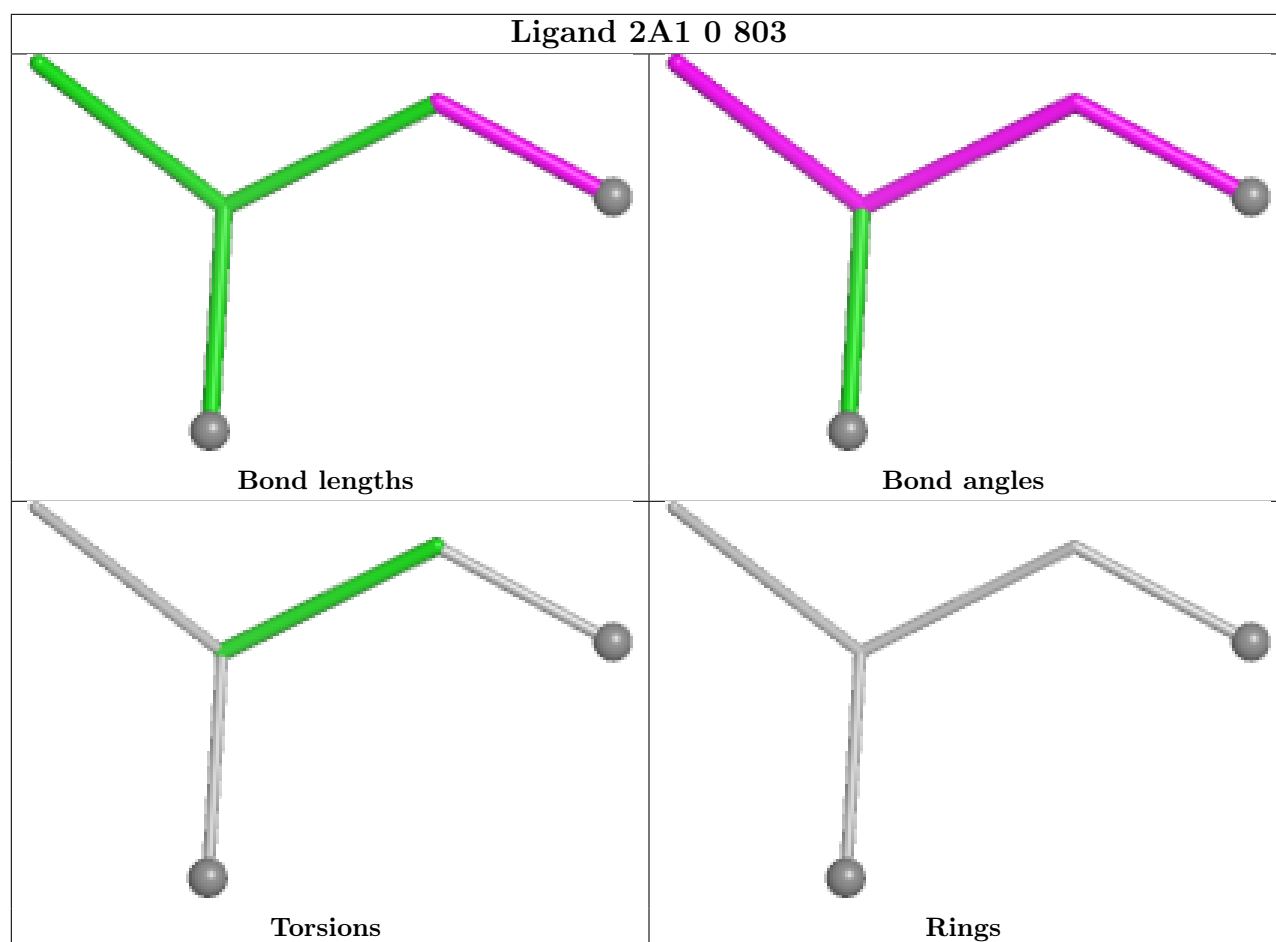


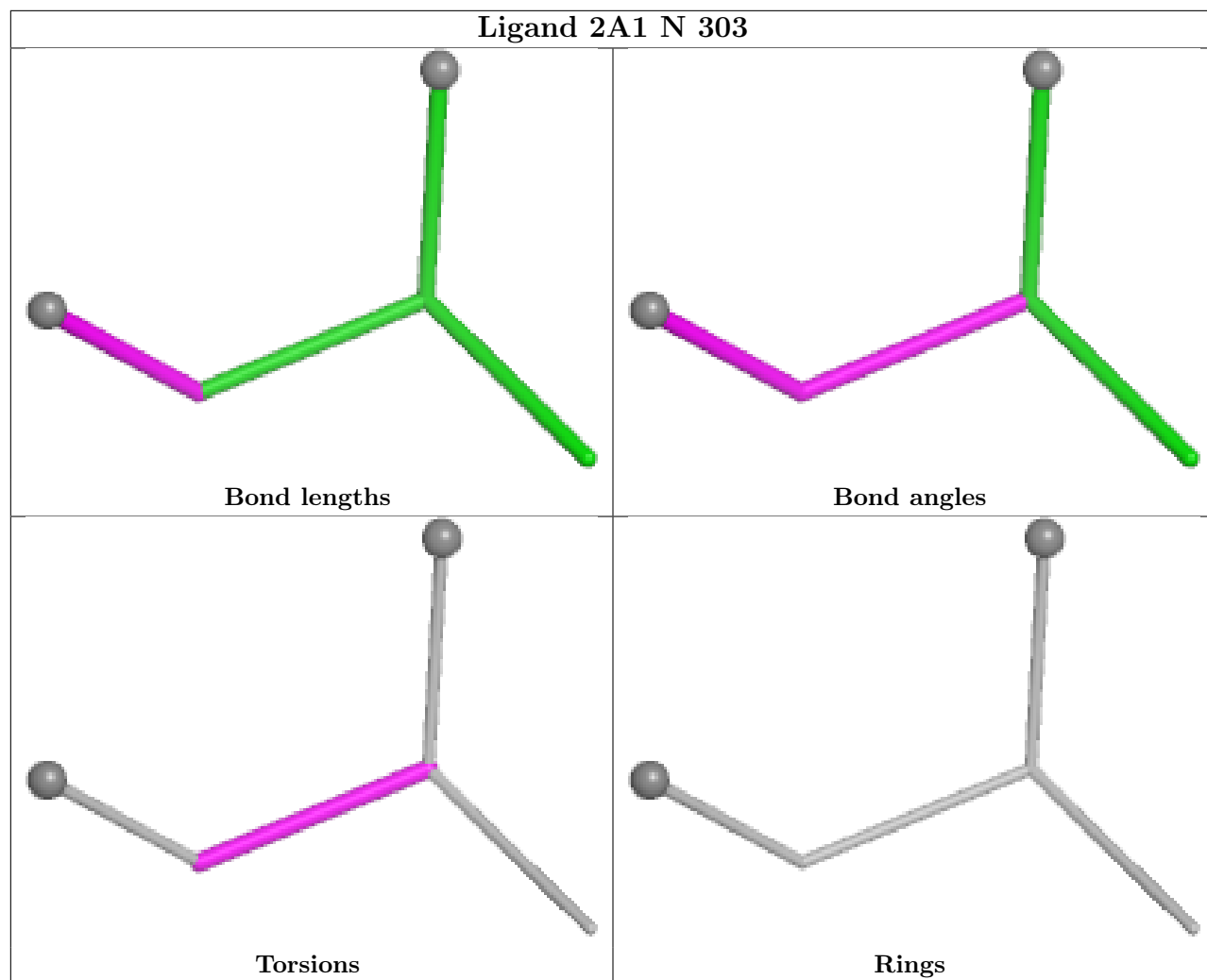


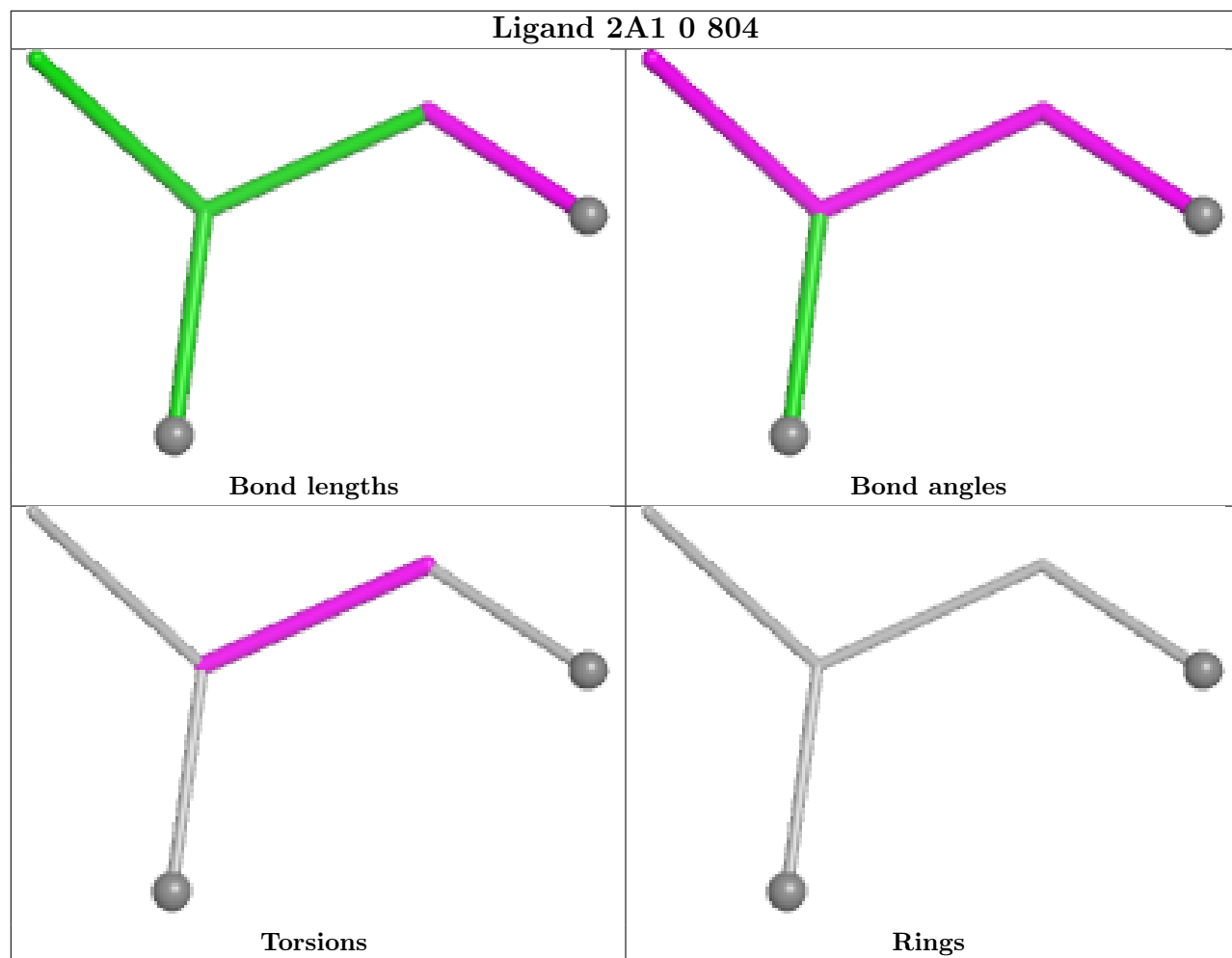


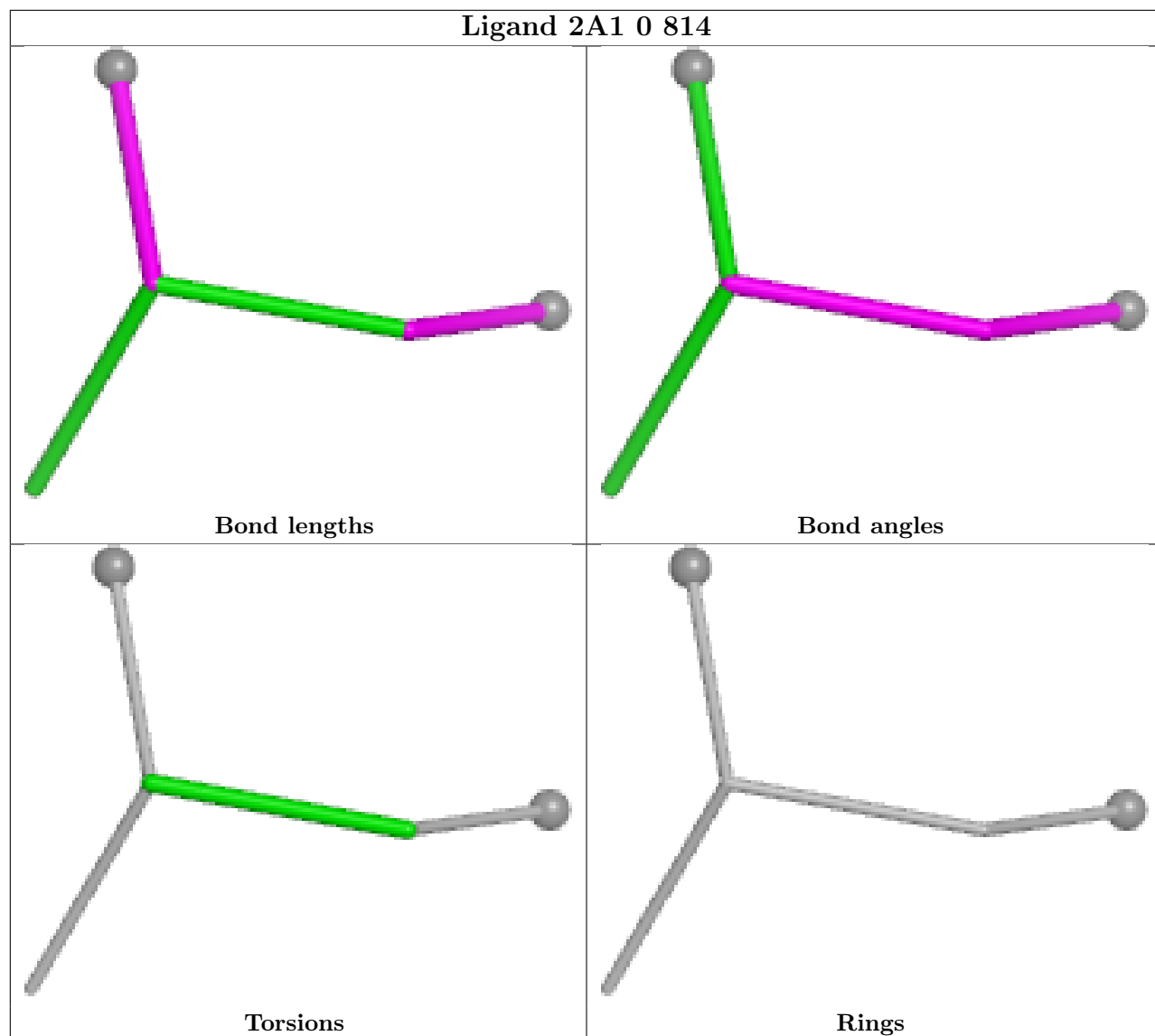


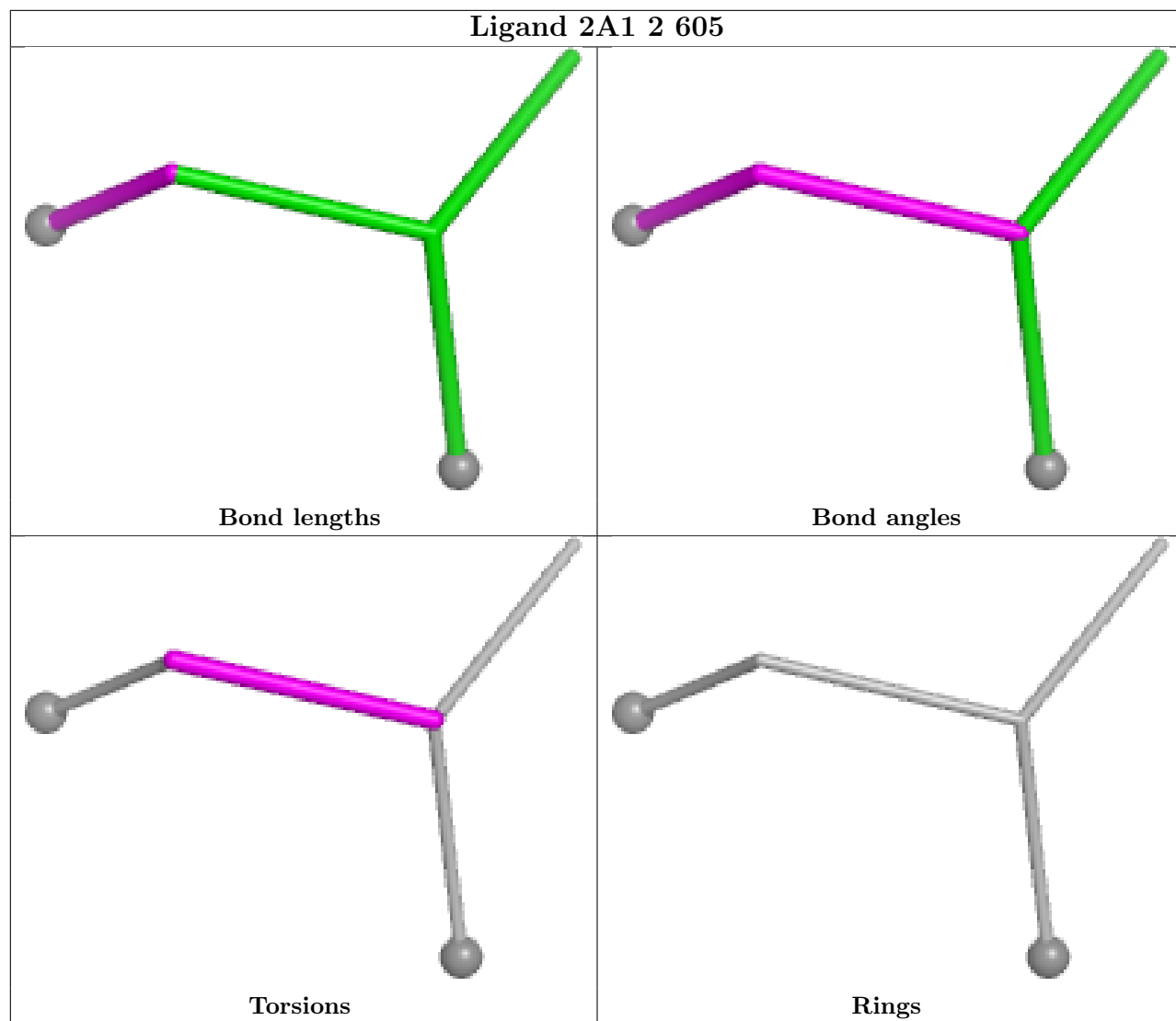


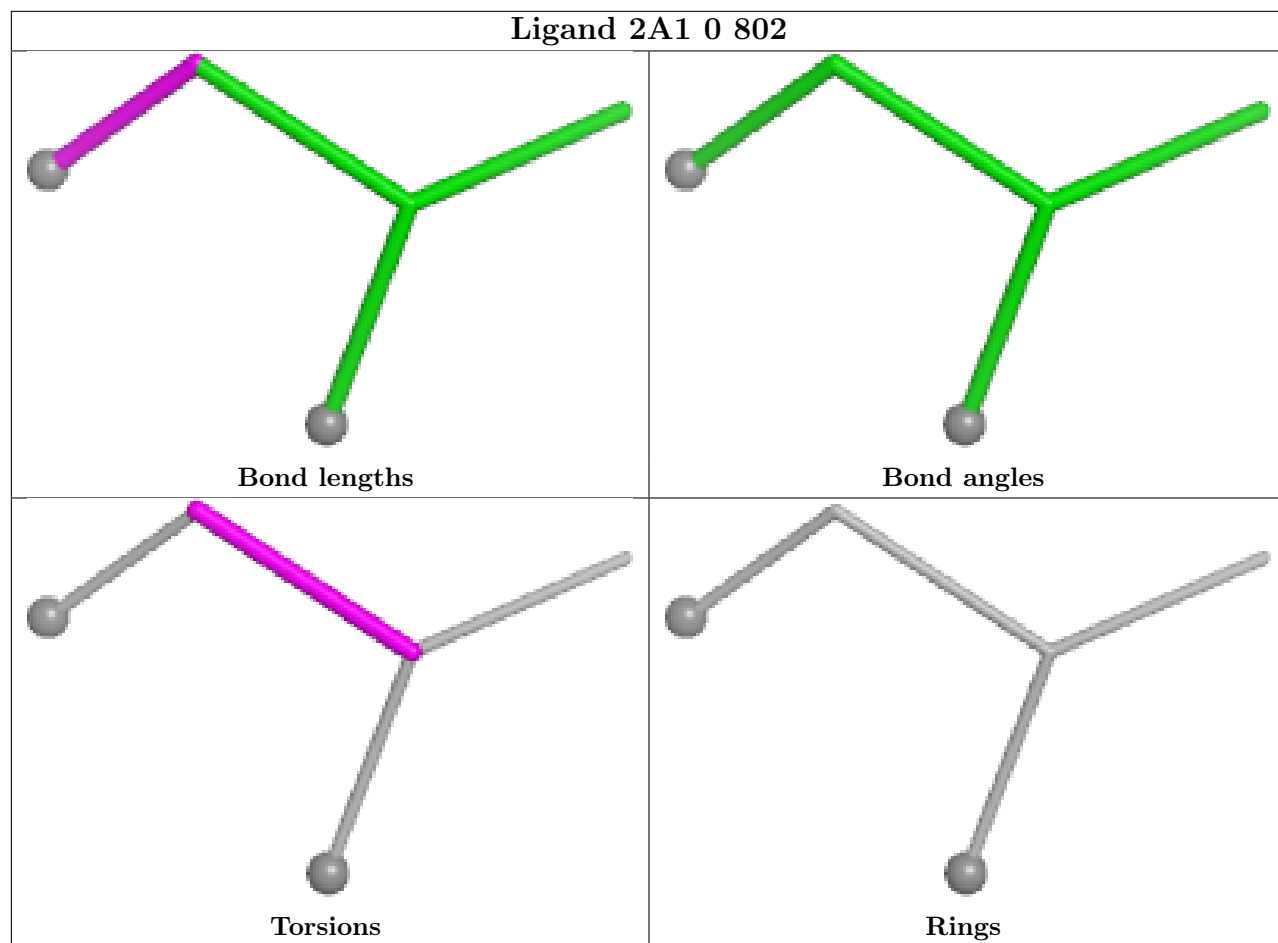


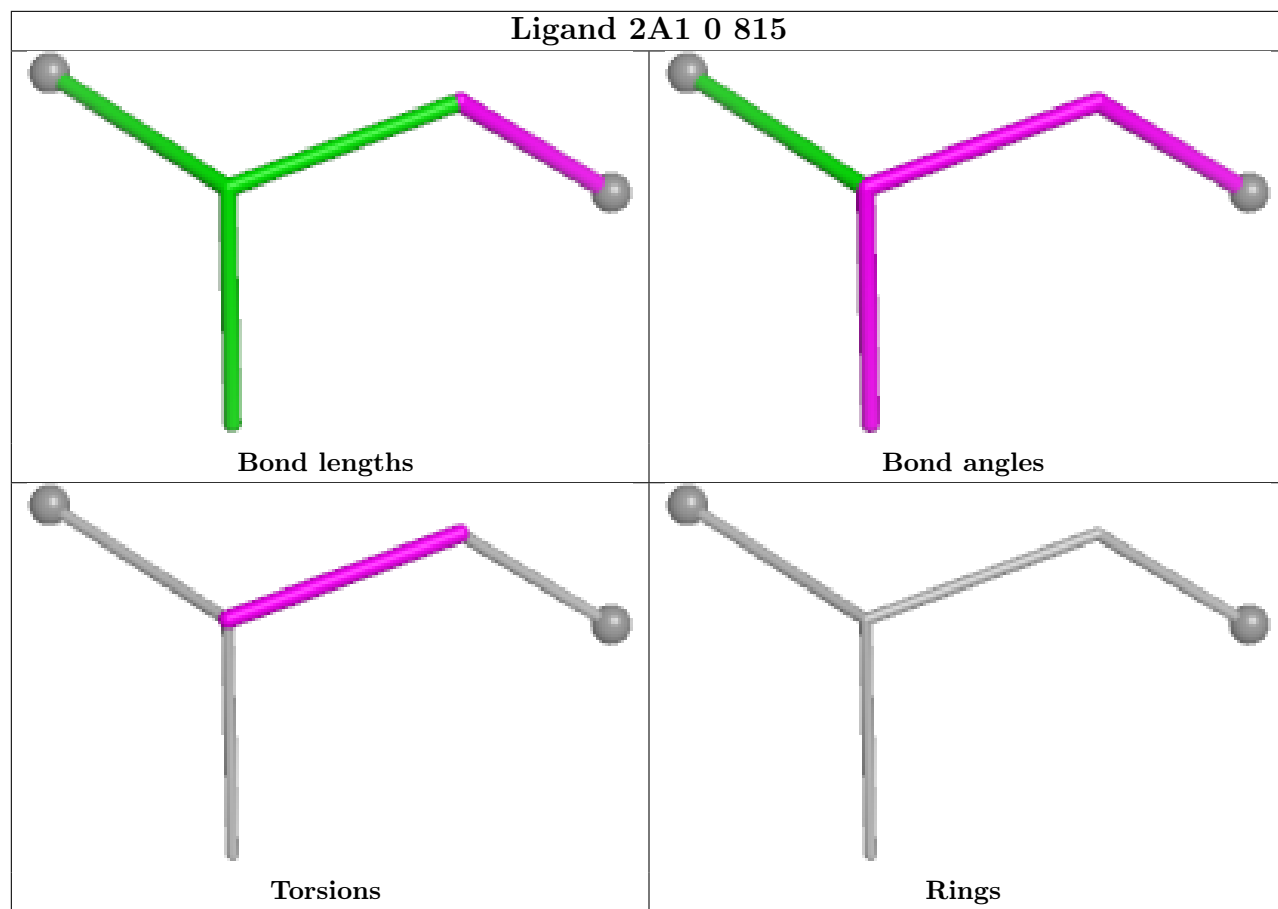


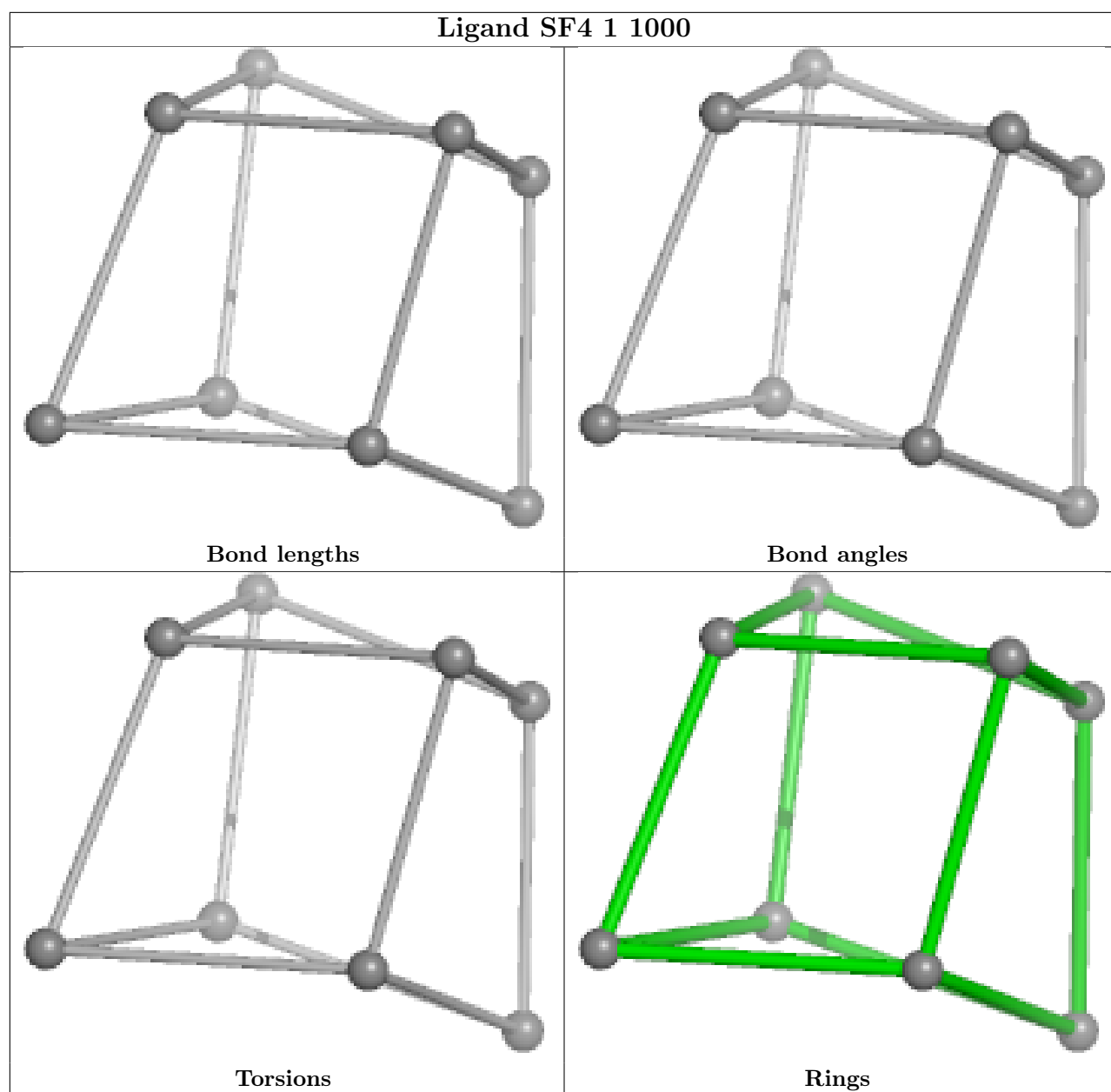


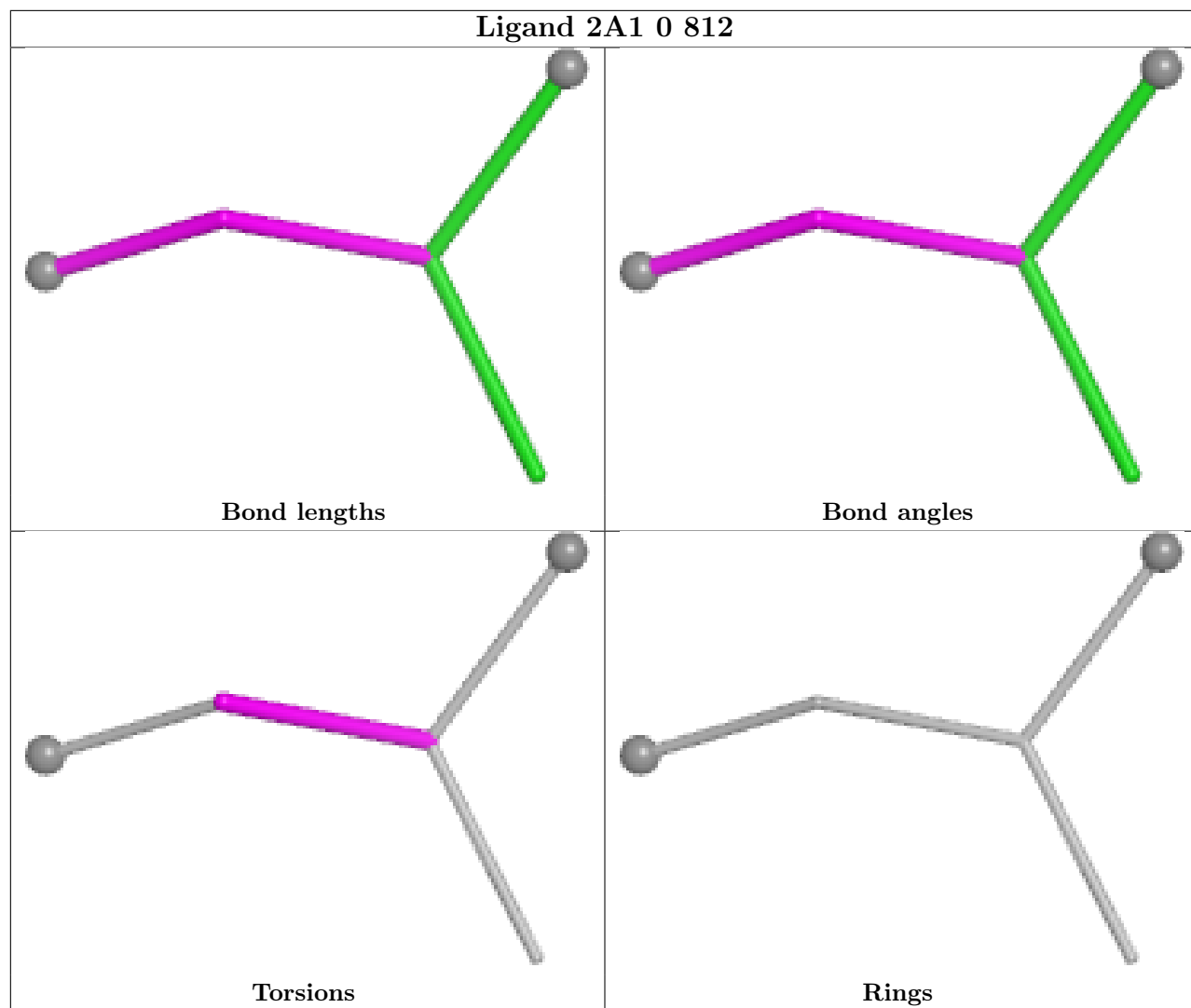


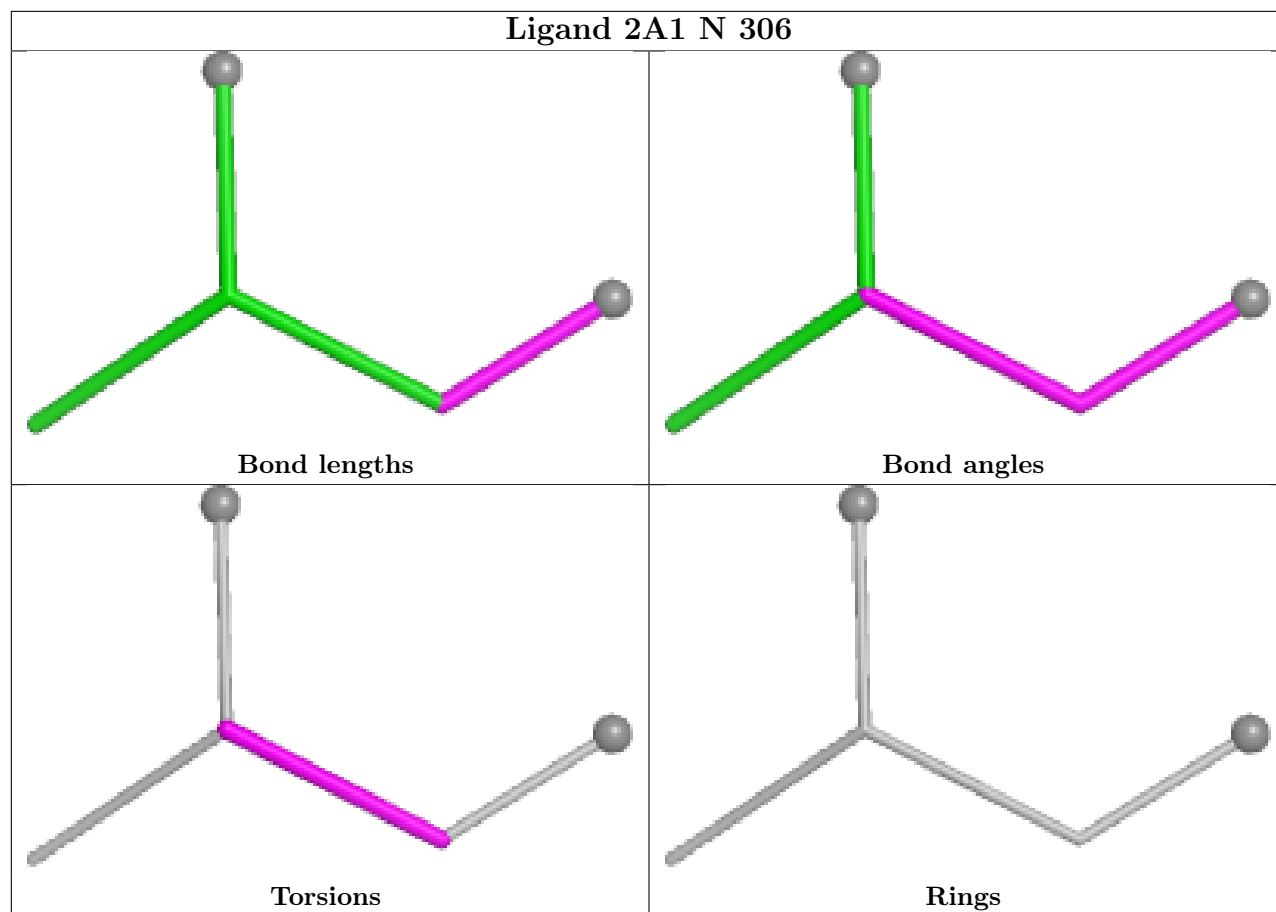


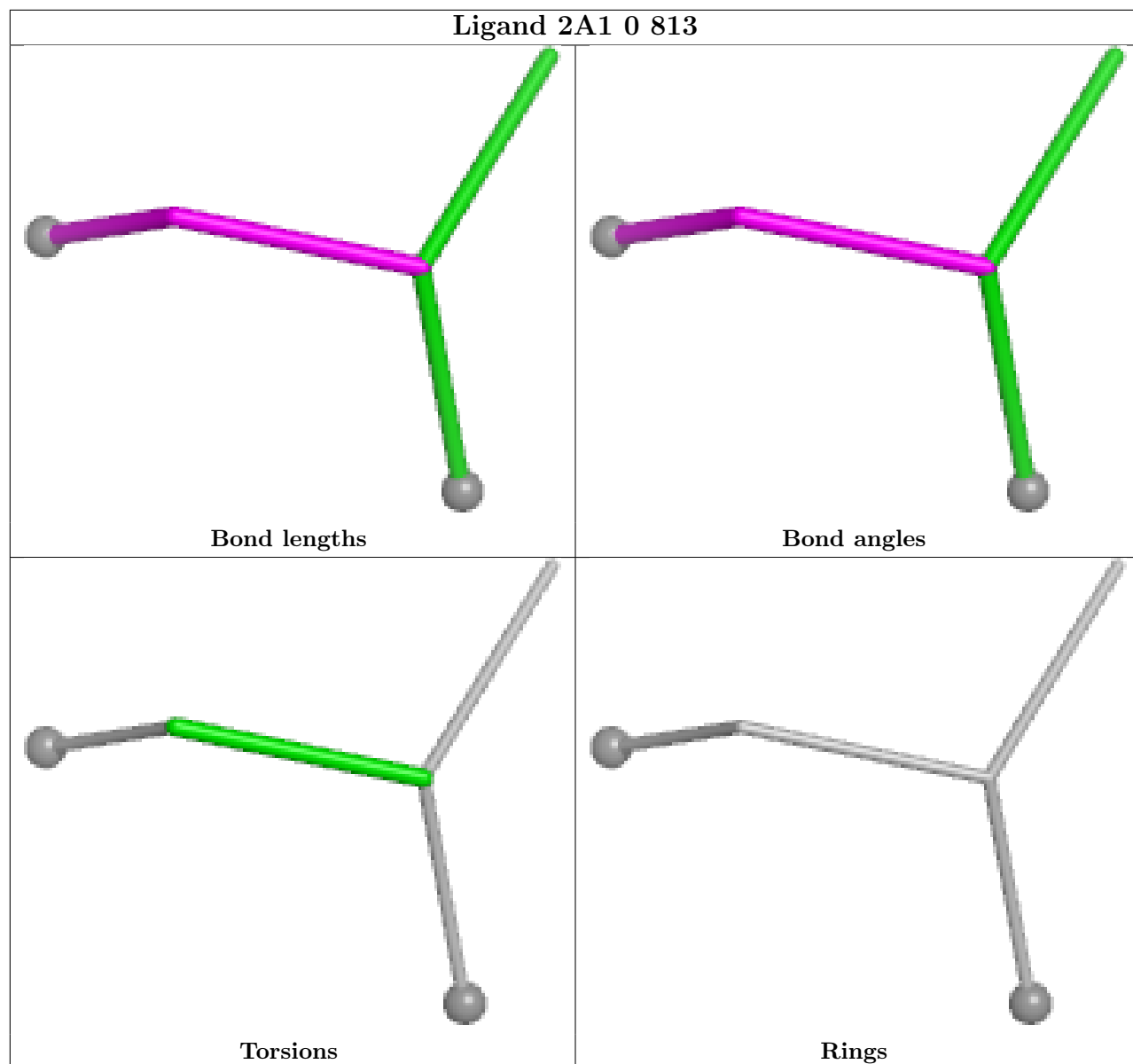


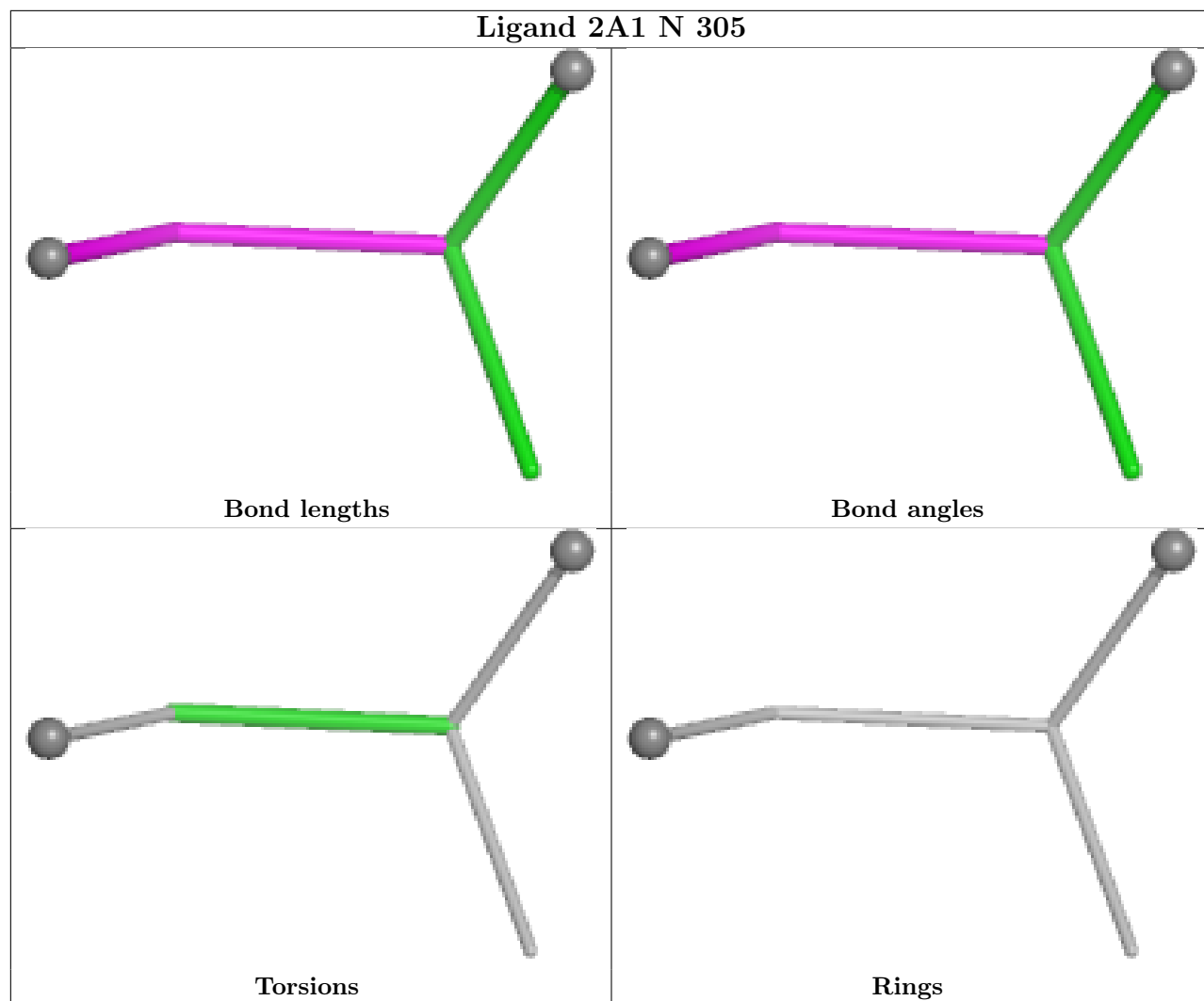


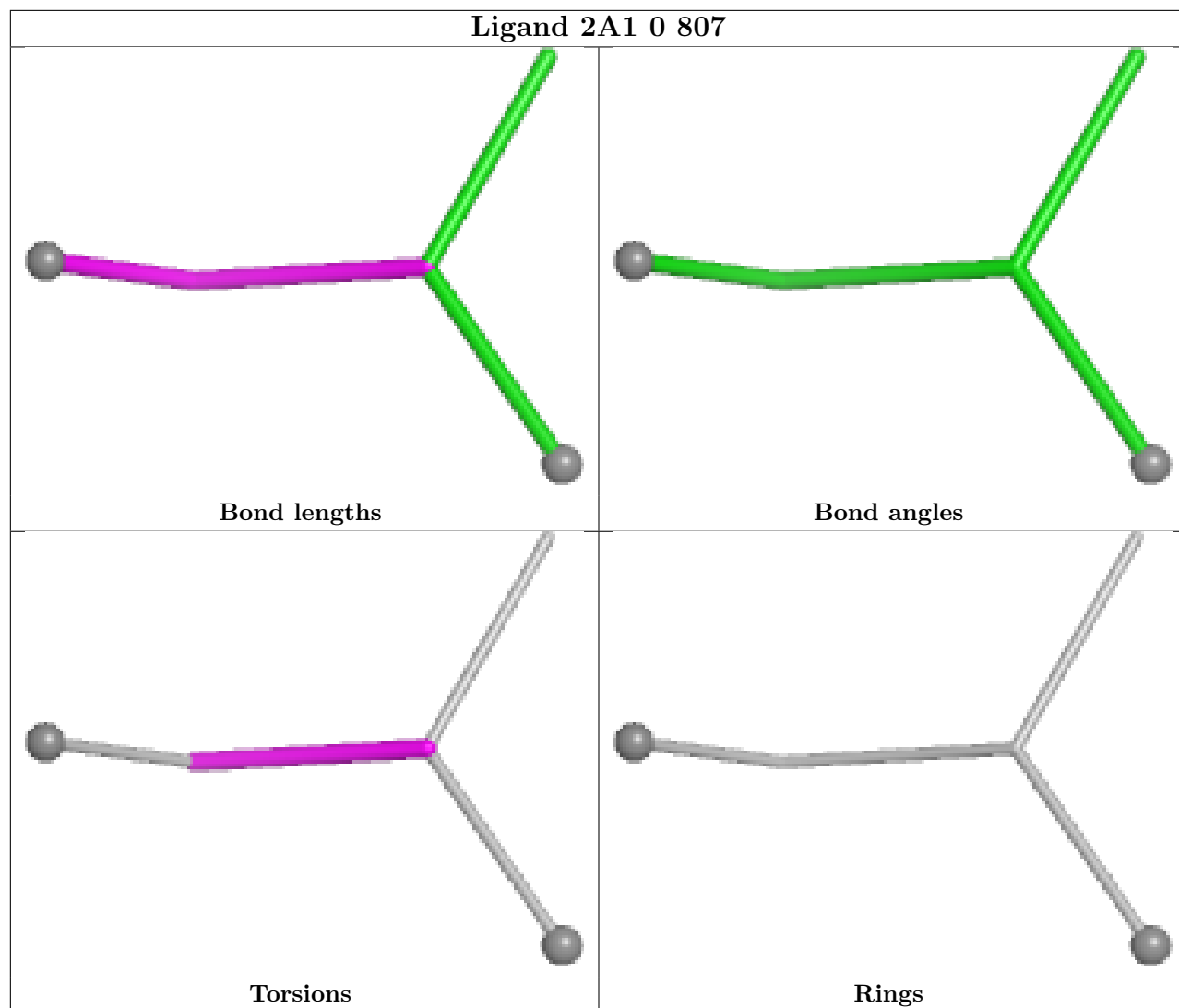


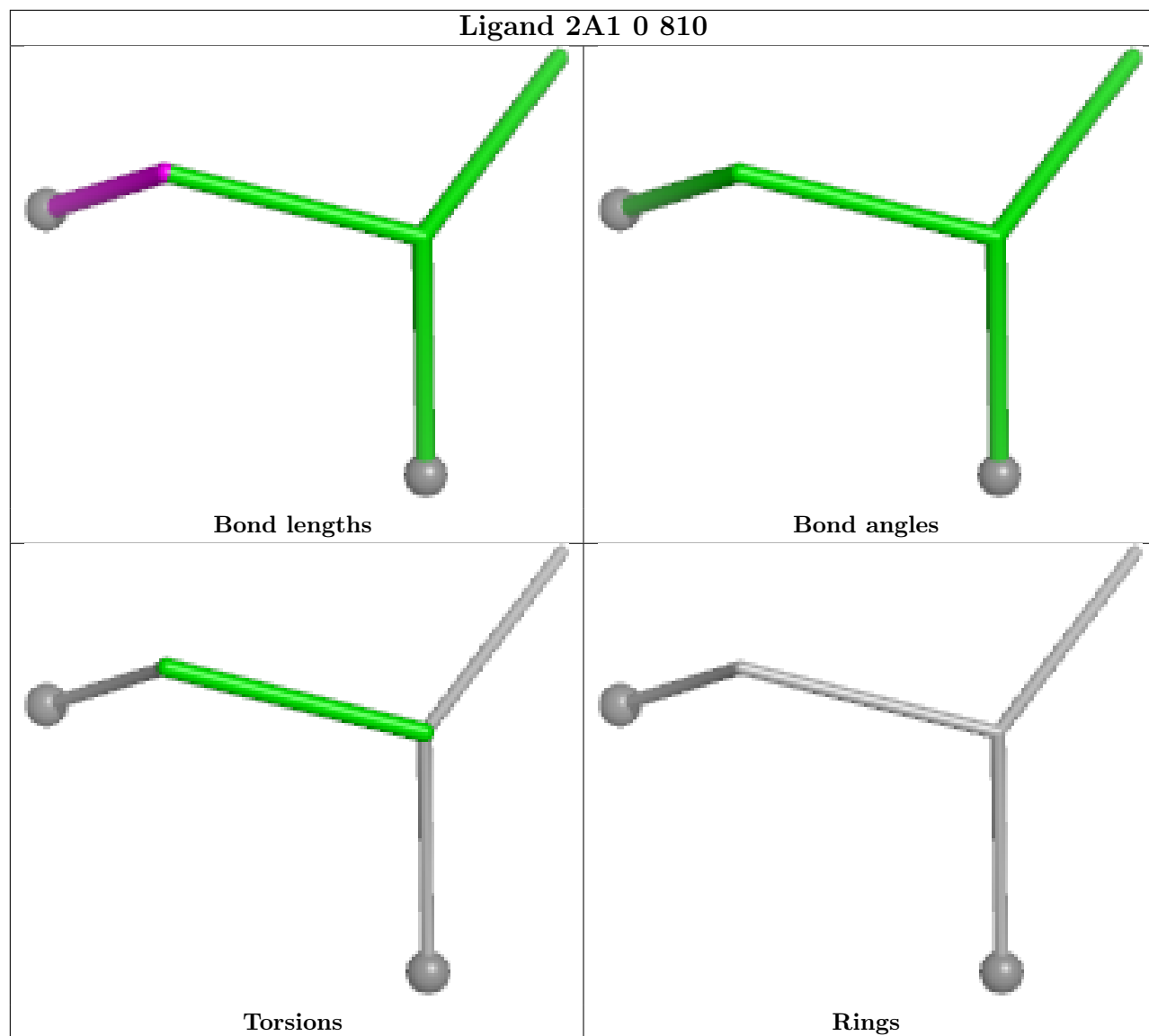


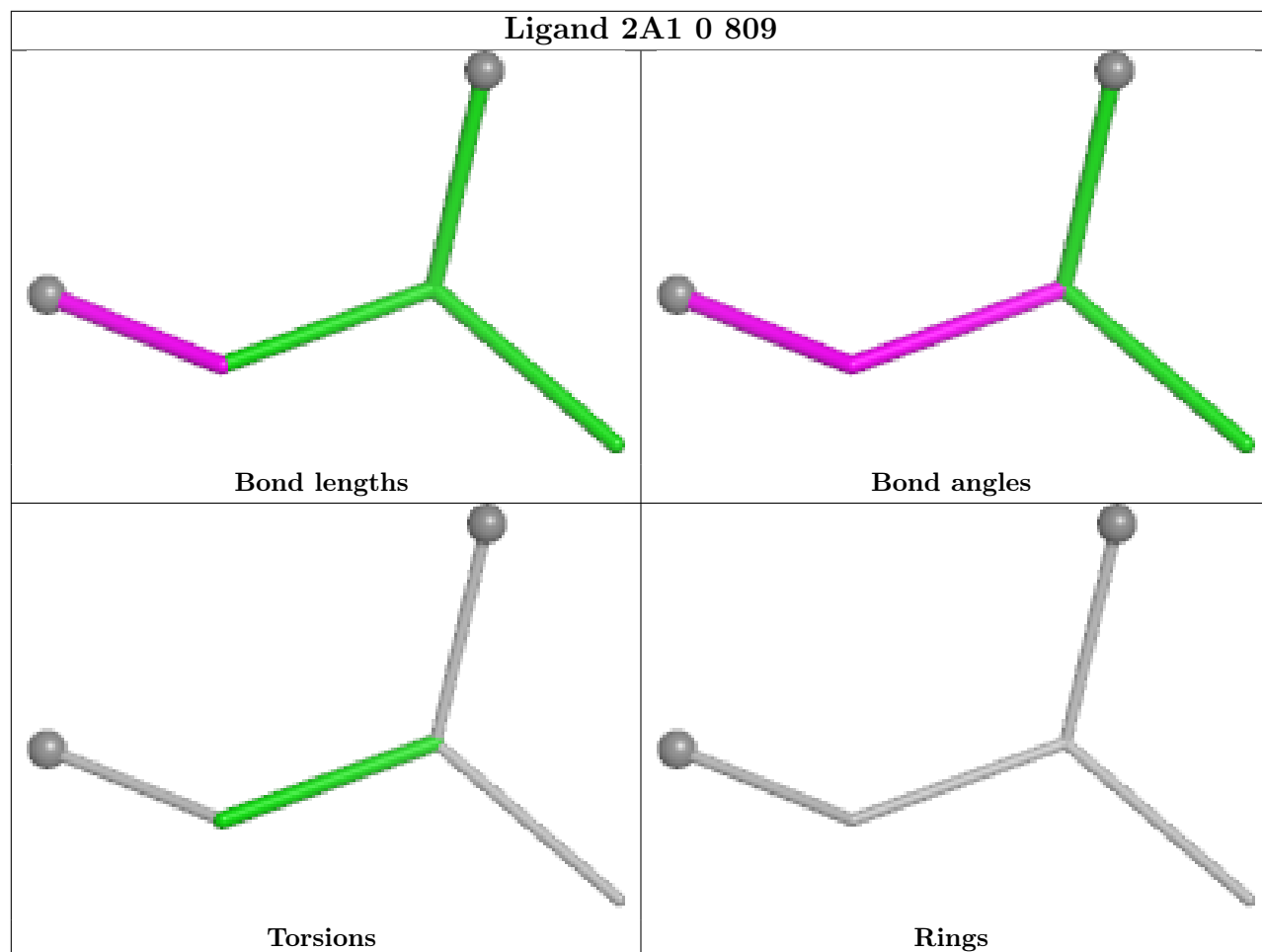


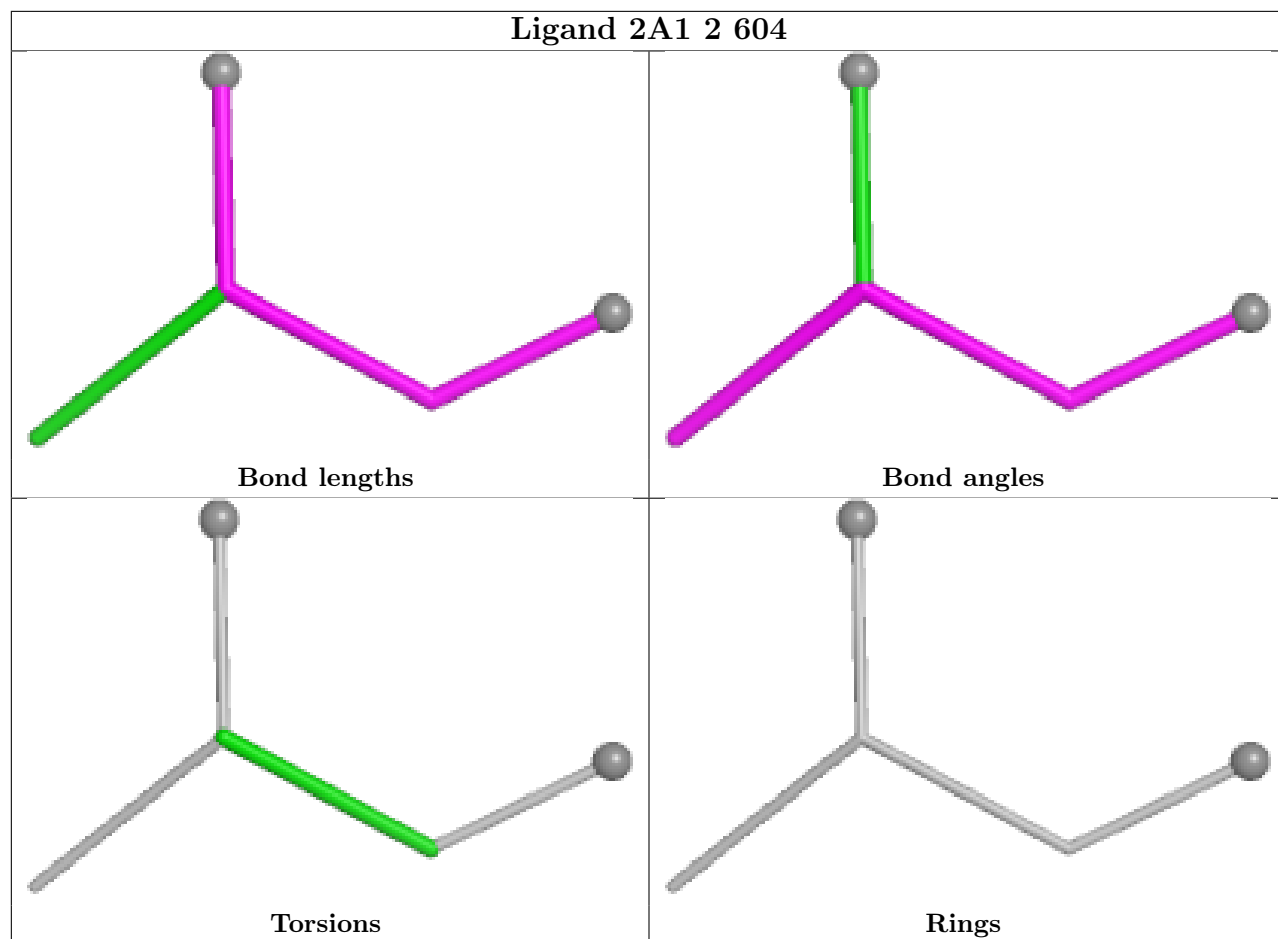


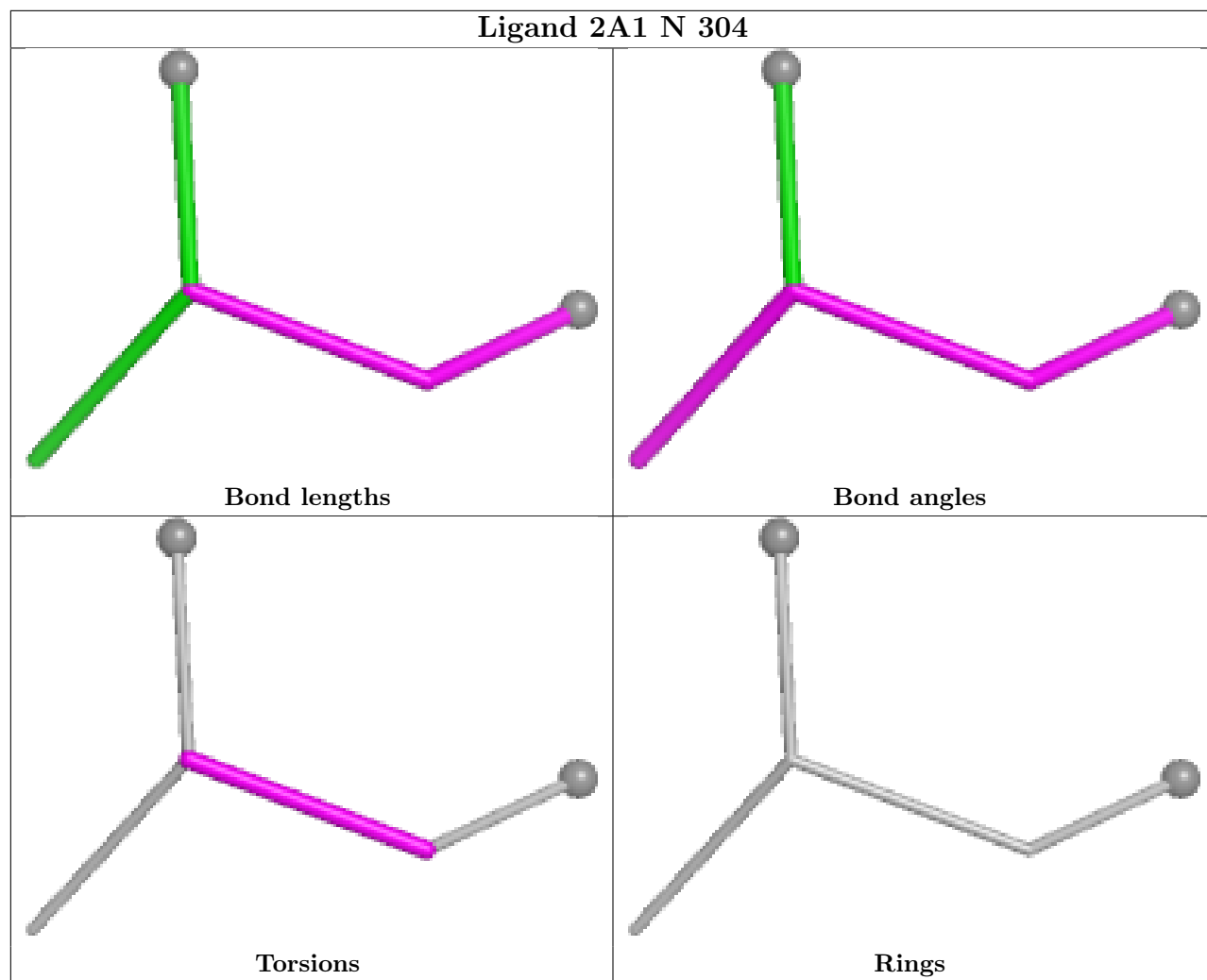


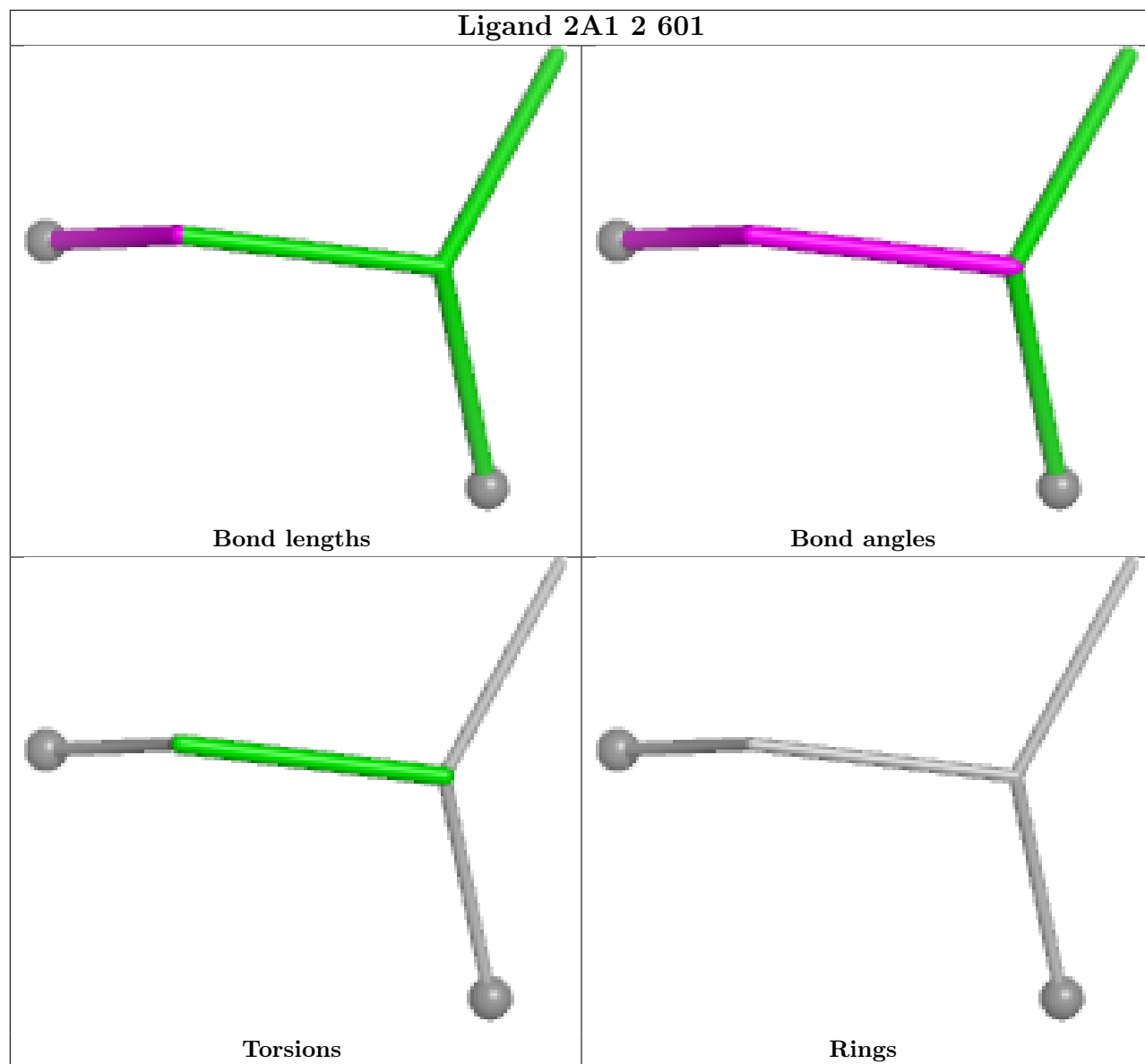


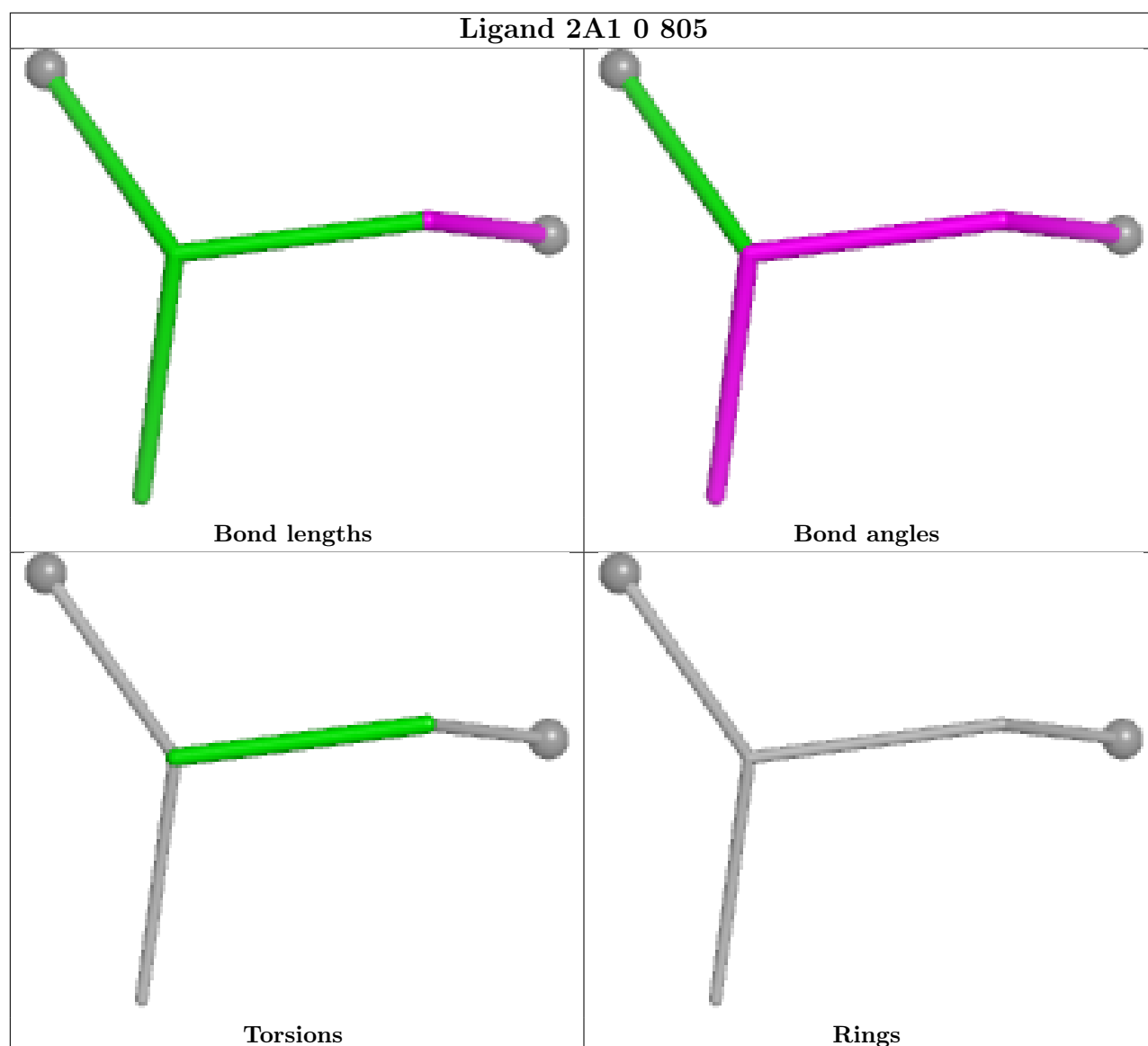












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

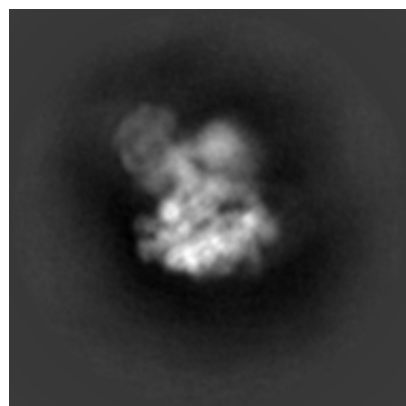
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57691. These allow visual inspection of the internal detail of the map and identification of artifacts.

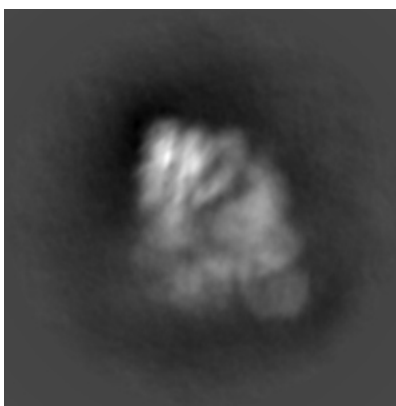
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

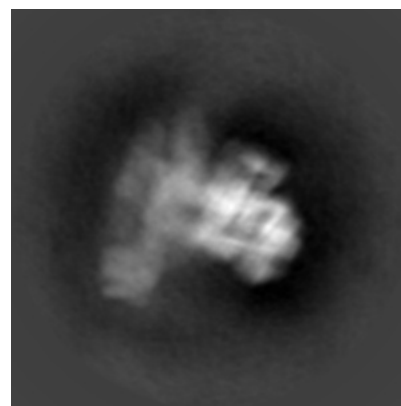
6.1.1 Primary map



X

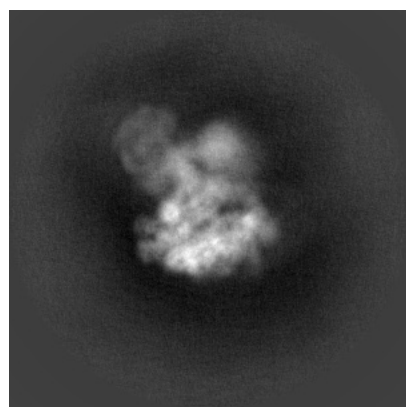


Y

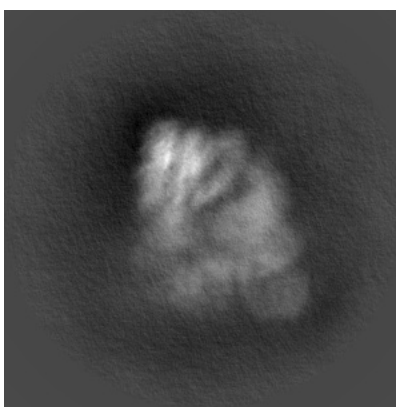


Z

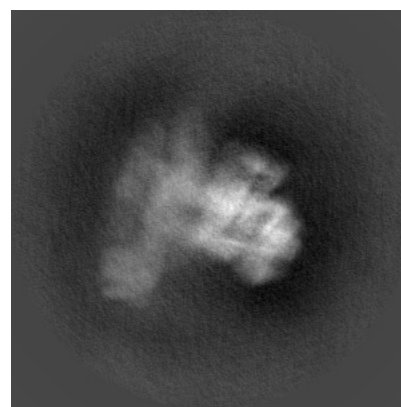
6.1.2 Raw map



X



Y

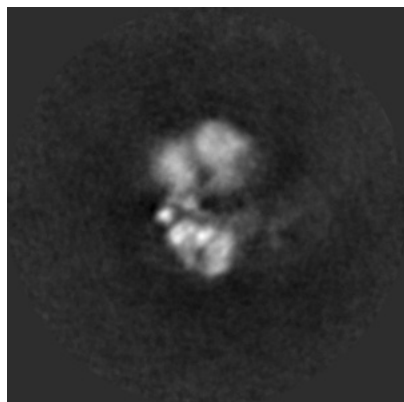


Z

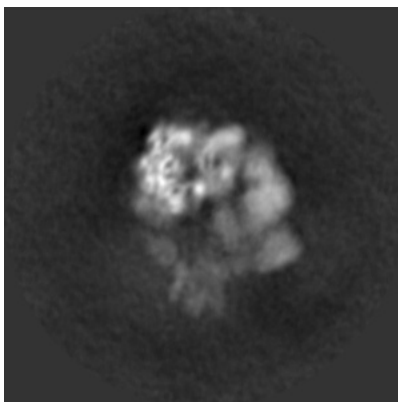
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

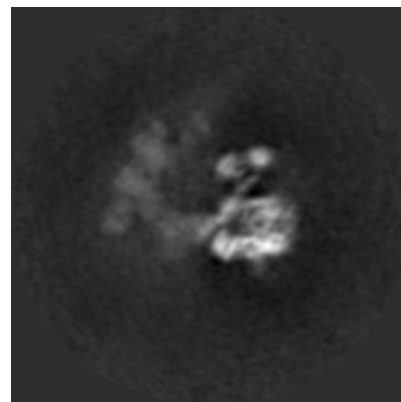
6.2.1 Primary map



X Index: 256

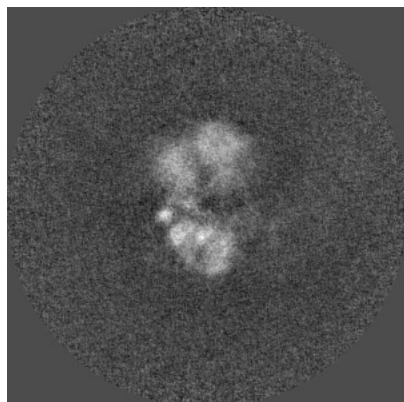


Y Index: 256

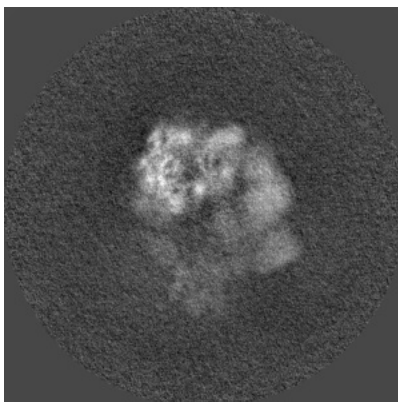


Z Index: 256

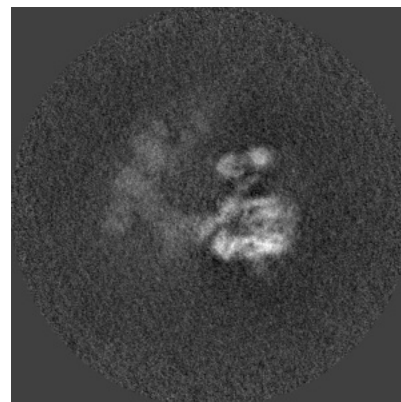
6.2.2 Raw map



X Index: 256



Y Index: 256

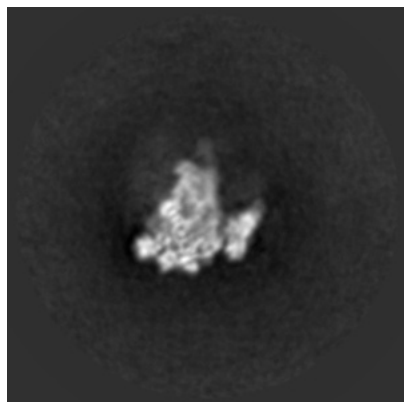


Z Index: 256

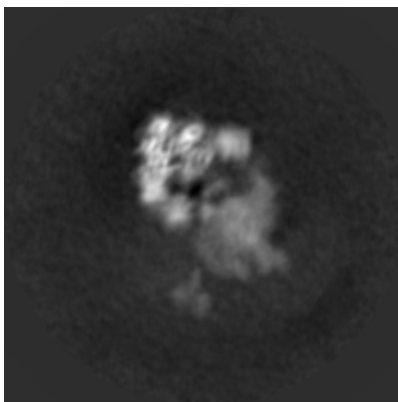
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

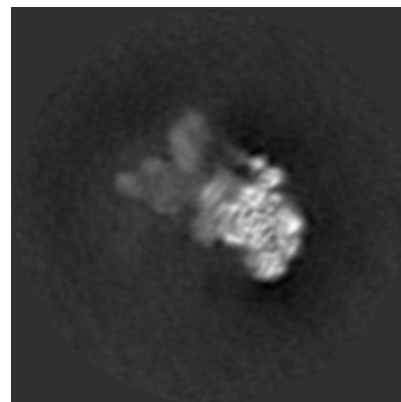
6.3.1 Primary map



X Index: 334

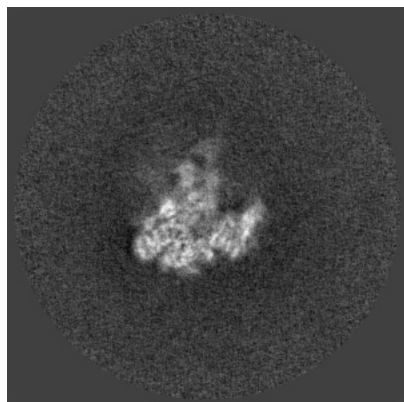


Y Index: 228

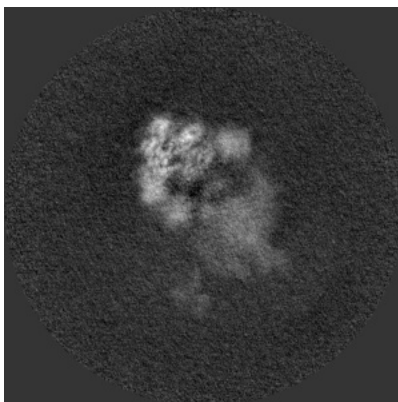


Z Index: 204

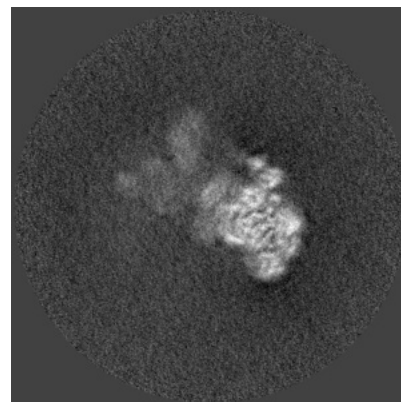
6.3.2 Raw map



X Index: 327



Y Index: 228



Z Index: 203

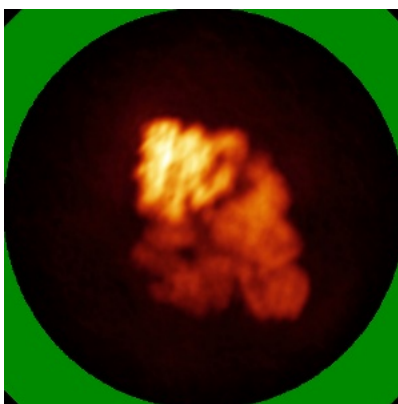
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

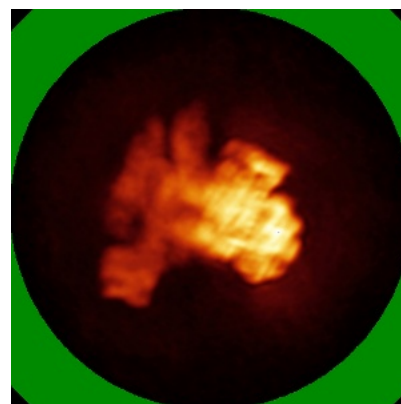
6.4.1 Primary map



X

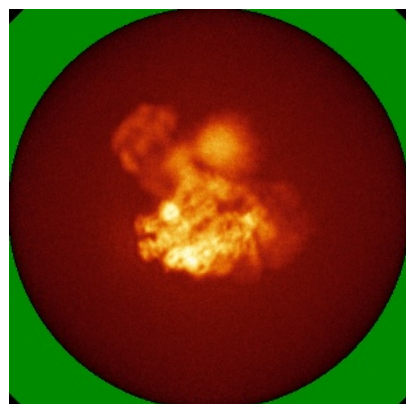


Y

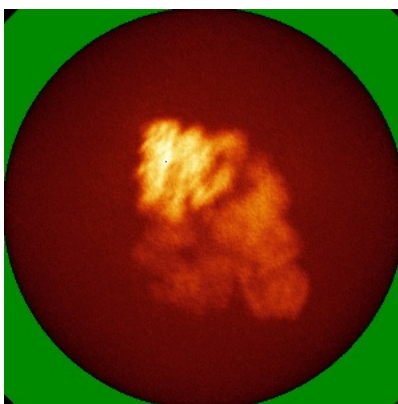


Z

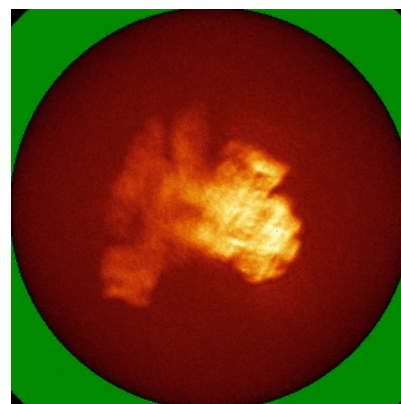
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



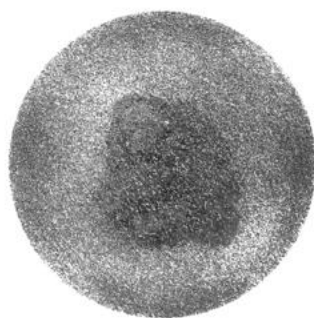
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

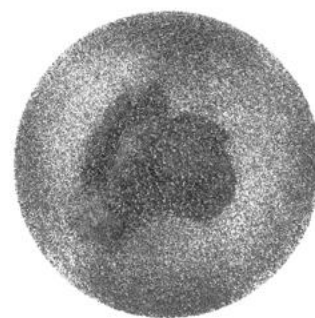
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

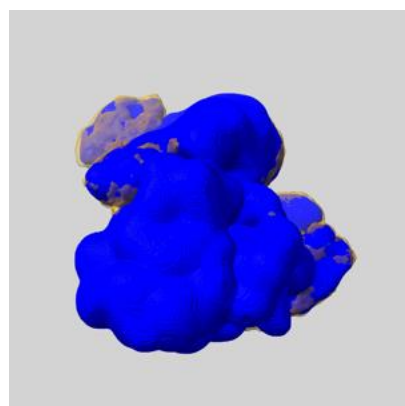
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

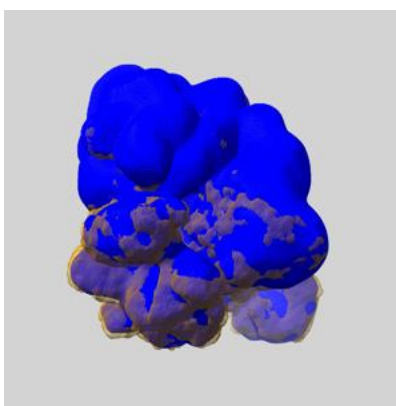
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

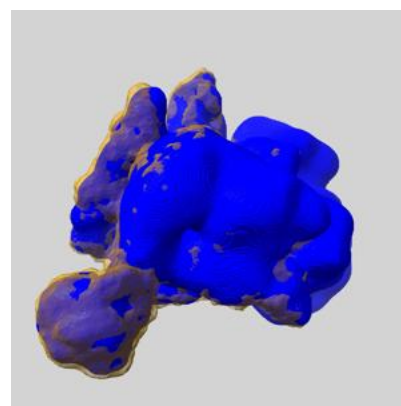
6.6.1 emd_57691_msk_1.map [i](#)



X



Y

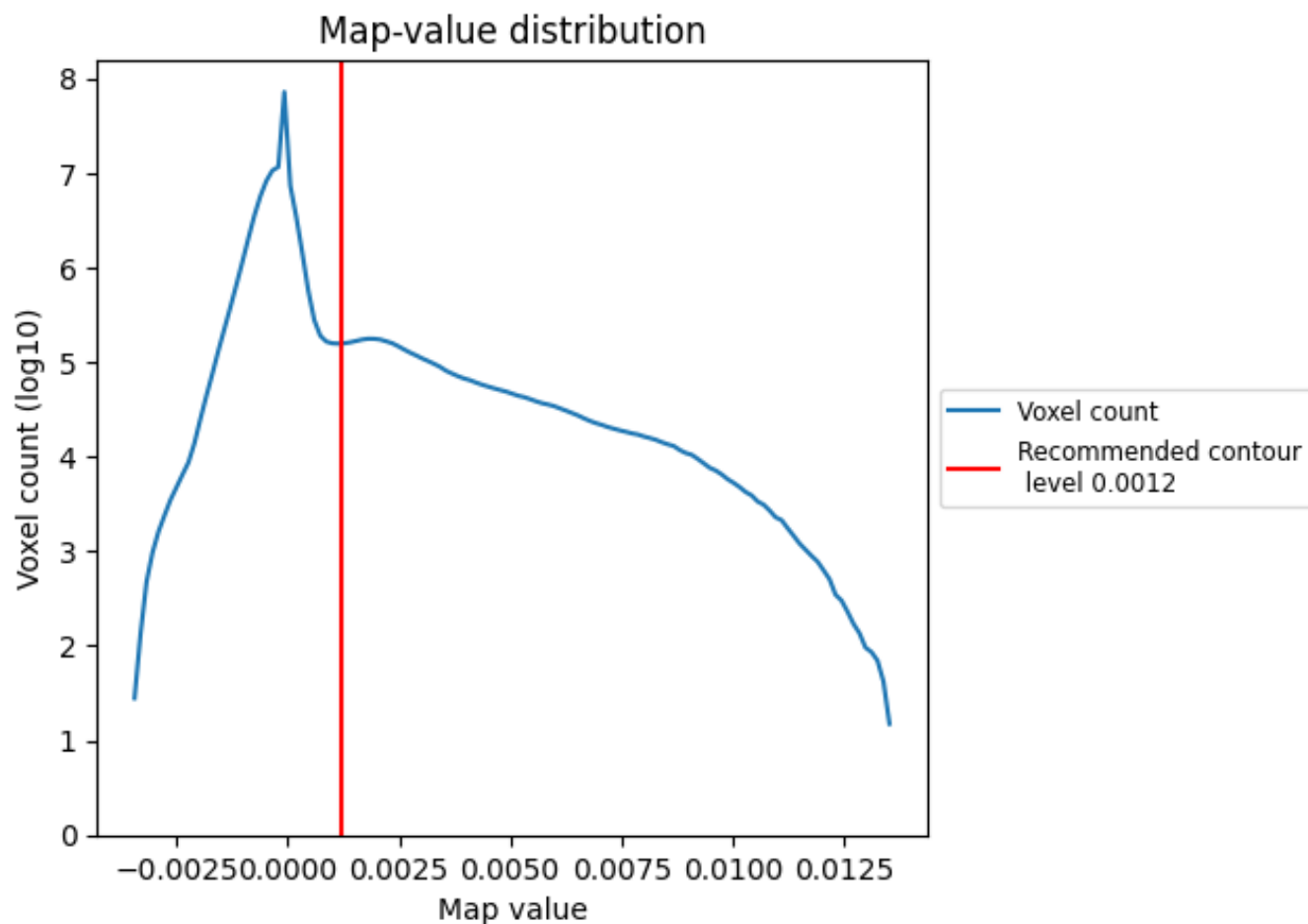


Z

7 Map analysis [i](#)

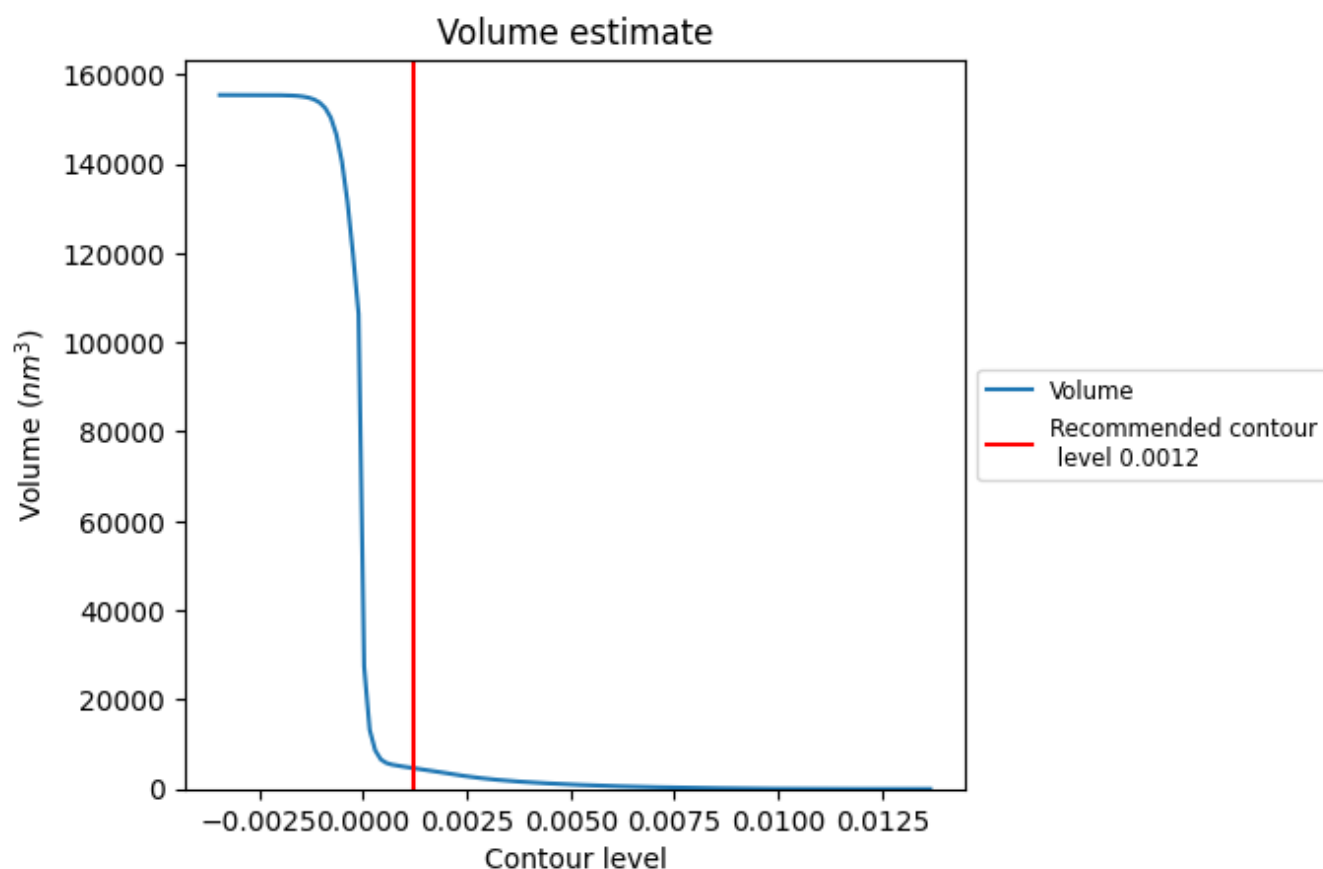
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

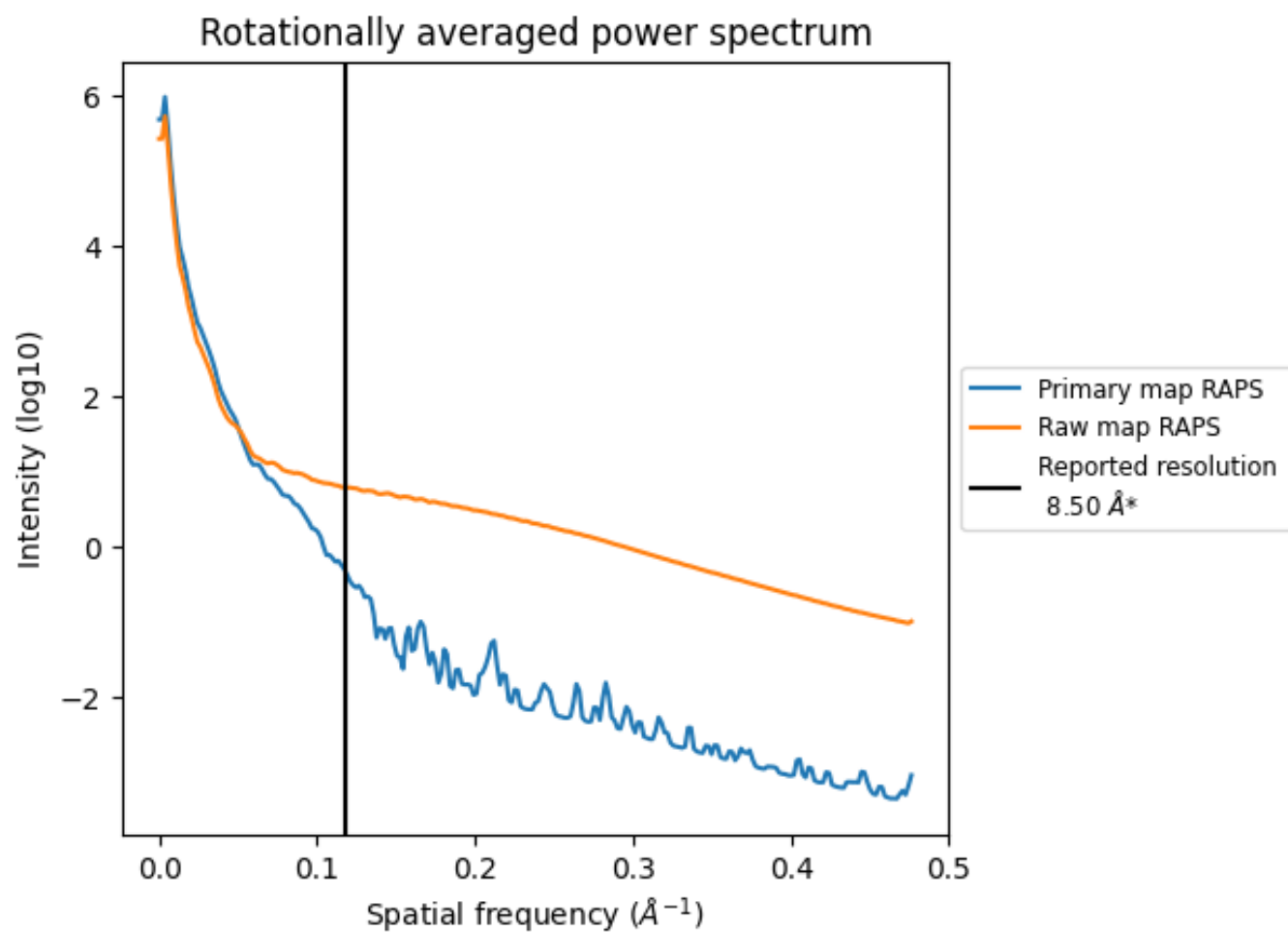
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4699 nm^3 ; this corresponds to an approximate mass of 4245 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

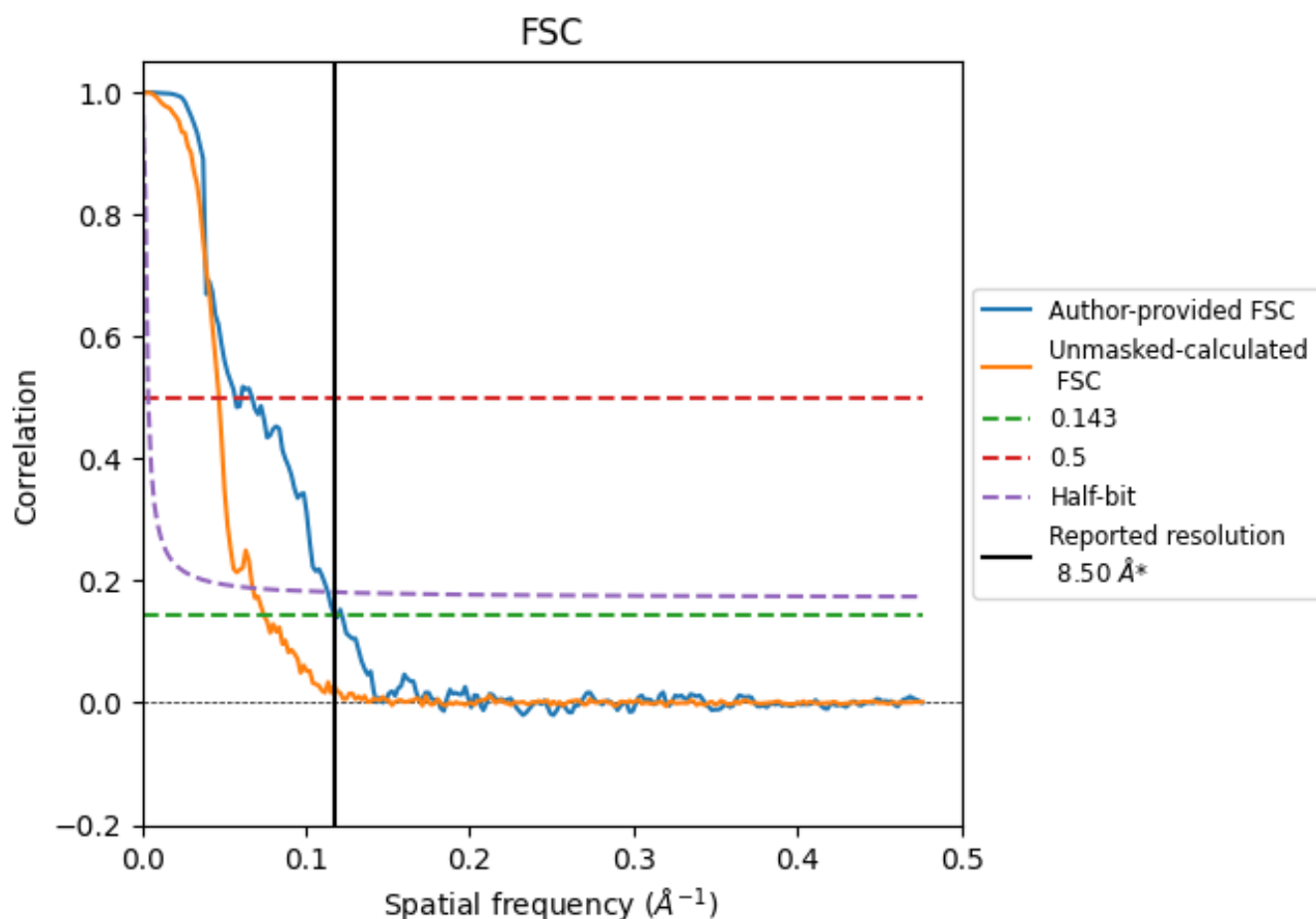


*Reported resolution corresponds to spatial frequency of 0.118 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.118 Å⁻¹

8.2 Resolution estimates [i](#)

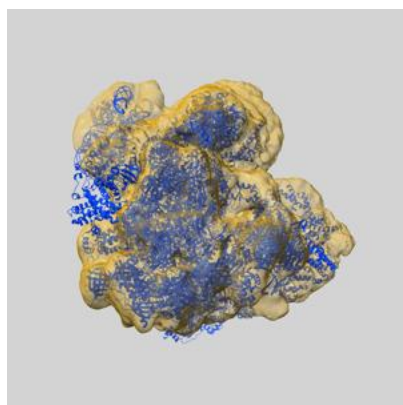
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.50	-	-
Author-provided FSC curve	8.47	17.67	8.83
Unmasked-calculated*	13.44	21.37	14.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 13.44 differs from the reported value 8.5 by more than 10 %

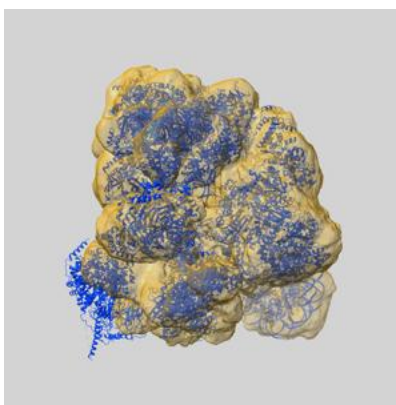
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57691 and PDB model 30FF. Per-residue inclusion information can be found in section [3](#) on page [20](#).

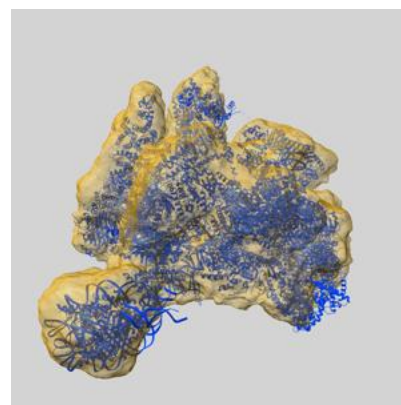
9.1 Map-model overlay [i](#)



X



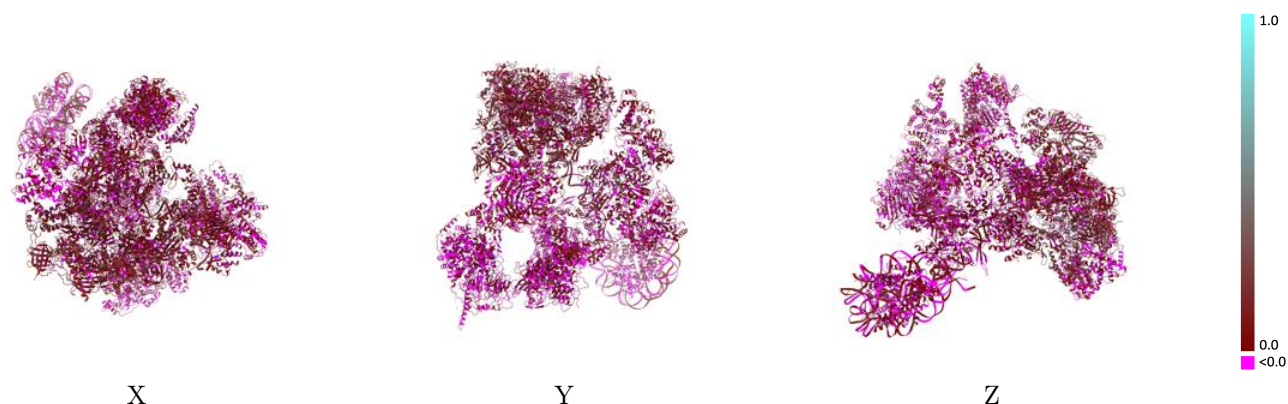
Y



Z

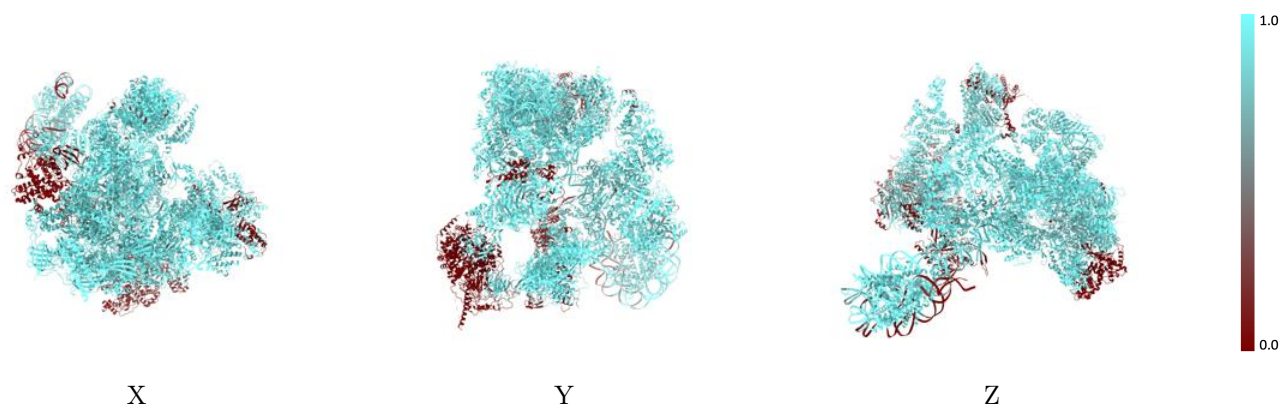
The images above show the 3D surface view of the map at the recommended contour level 0.0012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



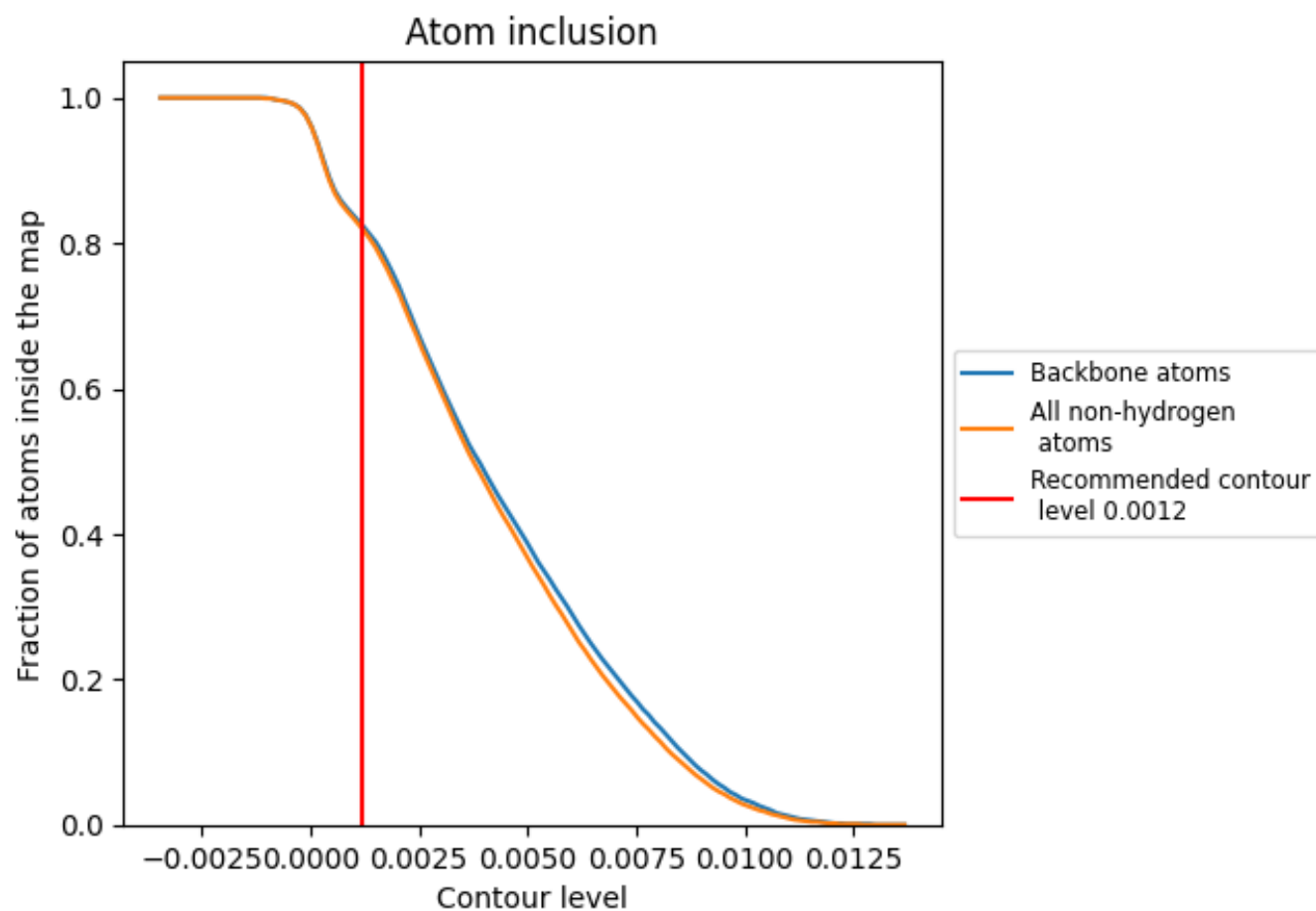
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8190	 0.0530
0	 0.9960	 0.0420
1	 0.9920	 0.0500
2	 1.0000	 0.0480
3	 0.9860	 0.0470
4	 0.9780	 0.0490
5	 1.0000	 0.0320
6	 1.0000	 0.0330
7	 0.6810	 0.0350
8	 0.5810	 0.0290
9	 0.1680	 -0.0070
A	 0.9970	 0.1070
B	 1.0000	 0.1120
C	 0.9990	 0.1280
D	 0.9990	 0.0920
DA	 0.5590	 0.0160
DB	 0.8010	 0.0130
DD	 0.5470	 0.0170
DE	 0.9520	 0.0380
DF	 0.9020	 0.0280
DG	 0.1030	 -0.0060
DH	 0.8400	 0.0440
DI	 0.8400	 0.0250
DJ	 0.7150	 0.0360
DL	 0.4590	 0.0110
Dc	 0.0000	 0.0020
Dd	 0.0000	 0.0020
De	 0.3160	 0.0020
Df	 0.7590	 0.0260
Di	 0.1280	 -0.0260
Dj	 0.0430	 0.0220
Dk	 0.0000	 -0.0200
Dl	 0.1430	 0.0070
Dm	 0.0000	 -0.0230
E	 0.9980	 0.1150



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Chain	Atom inclusion	Q-score
F	 1.0000	 0.1280
G	 0.9990	 0.0930
H	 0.9990	 0.1120
I	 1.0000	 0.0770
J	 1.0000	 0.1090
K	 1.0000	 0.1170
L	 1.0000	 0.1050
M	 0.9980	 0.1110
N	 0.7700	 0.0550
O	 1.0000	 0.0970
Q	 1.0000	 0.0650
R	 0.9990	 0.0990
T	 0.7490	 0.0470
U	 0.9850	 0.0880
V	 0.9820	 0.0840
W	 0.9850	 0.0930
X	 1.0000	 0.1010
a	 0.9640	 0.0110
b	 0.9790	 -0.0030
c	 0.9240	 -0.0050
d	 0.9990	 0.0130
e	 0.9340	 0.0360
f	 0.9440	 -0.0080
g	 0.9960	 0.0280
h	 0.9960	 0.0210