Full wwPDB EM Validation Report

Aug 5, 2026 – 02:25 AM EDT

PDB ID	:	8SG9 / pdb_00008sg9
EMDB ID	:	EMD-40453
Title	:	CCT G beta 5 complex closed state 3
Authors	:	Wang, S.; Sass, M.; Willardson, B.M.; Shen, P.S.
Deposited on	:	2023-04-12
Resolution	:	2.90 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:

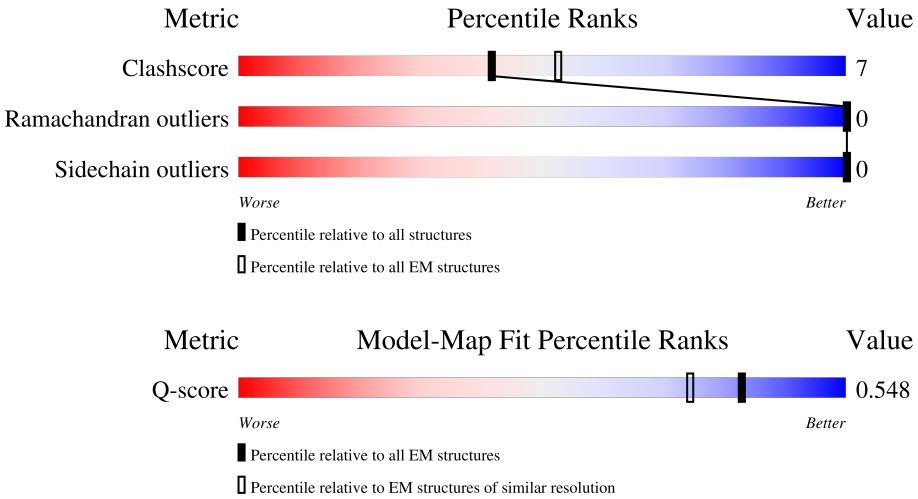
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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 <=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	N	395	14% 84%
2	A	536	84% 16%
2	a	536	81% 18%
3	B	526	82% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	b	526	83% 17%
4	D	520	86% 14%
4	d	520	84% 16%
5	E	540	81% 18%
5	e	540	82% 18%
6	G	528	80% 20%
6	g	528	80% 19%
7	H	528	82% 18%
7	h	528	85% 15%
8	Q	538	83% 17%
8	q	538	85% 14%
9	Z	527	80% 20%
9	z	527	83% 17%

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
12	AF3	D	603	-	-	X	-
12	AF3	G	603	-	-	X	-
12	AF3	H	603	-	-	X	-
12	AF3	Z	603	-	-	X	-
12	AF3	d	603	-	-	X	-
12	AF3	q	603	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 65583 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 Guanine nucleotide-binding protein subunit beta-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	63	Total	C	N	O	S	0	0
			474	298	76	93	7		

- Molecule 2 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	536	Total	C	N	O	S	0	0
			4069	2548	711	787	23		
2	a	532	Total	C	N	O	S	0	0
			4041	2533	707	778	23		

- Molecule 3 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	526	Total	C	N	O	S	0	0
			3952	2473	696	764	19		
3	b	525	Total	C	N	O	S	0	0
			3943	2467	694	763	19		

- Molecule 4 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	520	Total	C	N	O	S	0	0
			3923	2453	683	764	23		
4	d	520	Total	C	N	O	S	0	0
			3917	2450	680	764	23		

- Molecule 5 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	535	Total	C	N	O	S	1	0
			4132	2590	719	792	31		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	540	Total	C	N	O	S	1	0
			4169	2610	724	804	31		

- Molecule 6 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	526	Total	C	N	O	S	0	0
			4089	2548	726	785	30		
6	g	523	Total	C	N	O	S	0	0
			4063	2532	719	782	30		

- Molecule 7 is a protein called T-complex protein 1 subunit eta, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	528	Total	C	N	O	S	0	0
			4054	2561	699	769	25		
7	h	525	Total	C	N	O	S	0	0
			4032	2548	696	763	25		

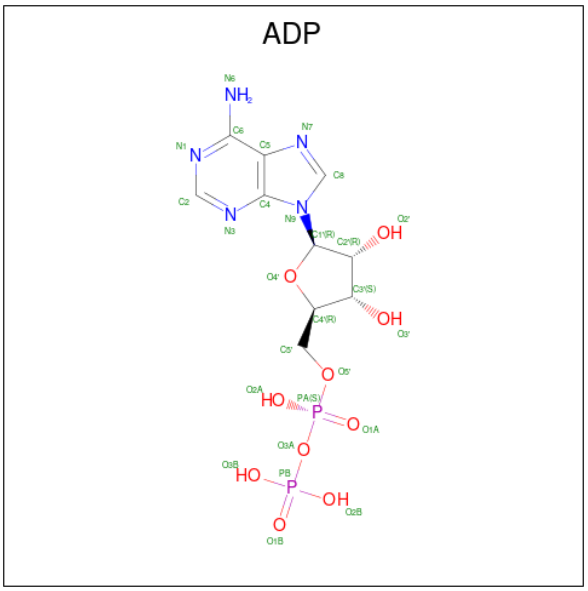
- Molecule 8 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	538	Total	C	N	O	S	0	0
			4086	2579	696	784	27		
8	q	533	Total	C	N	O	S	0	0
			4053	2558	690	778	27		

- Molecule 9 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	525	Total	C	N	O	S	0	0
			4022	2528	704	769	21		
9	z	527	Total	C	N	O	S	0	0
			4033	2534	706	772	21		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	a	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	b	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	e	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	g	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	h	1	Total	C	N	O	P	0
			27	10	5	10	2	

Continued on next page...

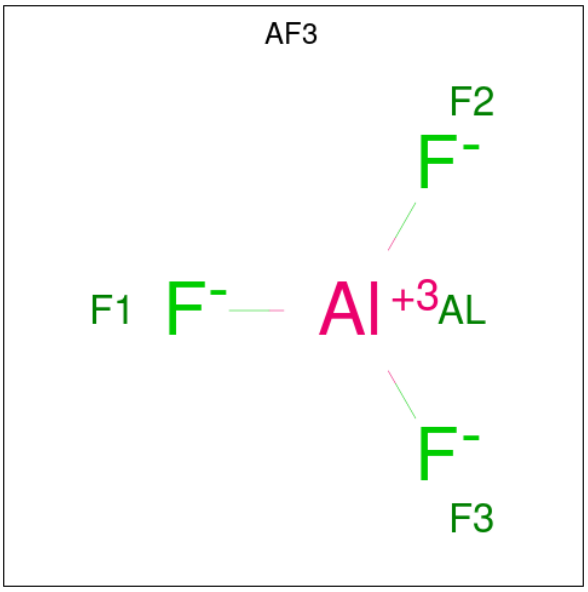
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
10	q	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	z	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	
11	B	1	Total	Mg	0
			1	1	
11	D	1	Total	Mg	0
			1	1	
11	E	1	Total	Mg	0
			1	1	
11	G	1	Total	Mg	0
			1	1	
11	H	1	Total	Mg	0
			1	1	
11	Q	1	Total	Mg	0
			1	1	
11	Z	1	Total	Mg	0
			1	1	
11	a	1	Total	Mg	0
			1	1	
11	b	1	Total	Mg	0
			1	1	
11	d	1	Total	Mg	0
			1	1	
11	e	1	Total	Mg	0
			1	1	
11	g	1	Total	Mg	0
			1	1	
11	h	1	Total	Mg	0
			1	1	
11	q	1	Total	Mg	0
			1	1	
11	z	1	Total	Mg	0
			1	1	

- Molecule 12 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total Al F 4 1 3	0
12	B	1	Total Al F 4 1 3	0
12	D	1	Total Al F 4 1 3	0
12	E	1	Total Al F 4 1 3	0
12	G	1	Total Al F 4 1 3	0
12	H	1	Total Al F 4 1 3	0
12	Q	1	Total Al F 4 1 3	0
12	Z	1	Total Al F 4 1 3	0
12	a	1	Total Al F 4 1 3	0
12	b	1	Total Al F 4 1 3	0
12	d	1	Total Al F 4 1 3	0
12	e	1	Total Al F 4 1 3	0
12	g	1	Total Al F 4 1 3	0
12	h	1	Total Al F 4 1 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
12	q	1	Total Al F 4 1 3	0
12	z	1	Total Al F 4 1 3	0

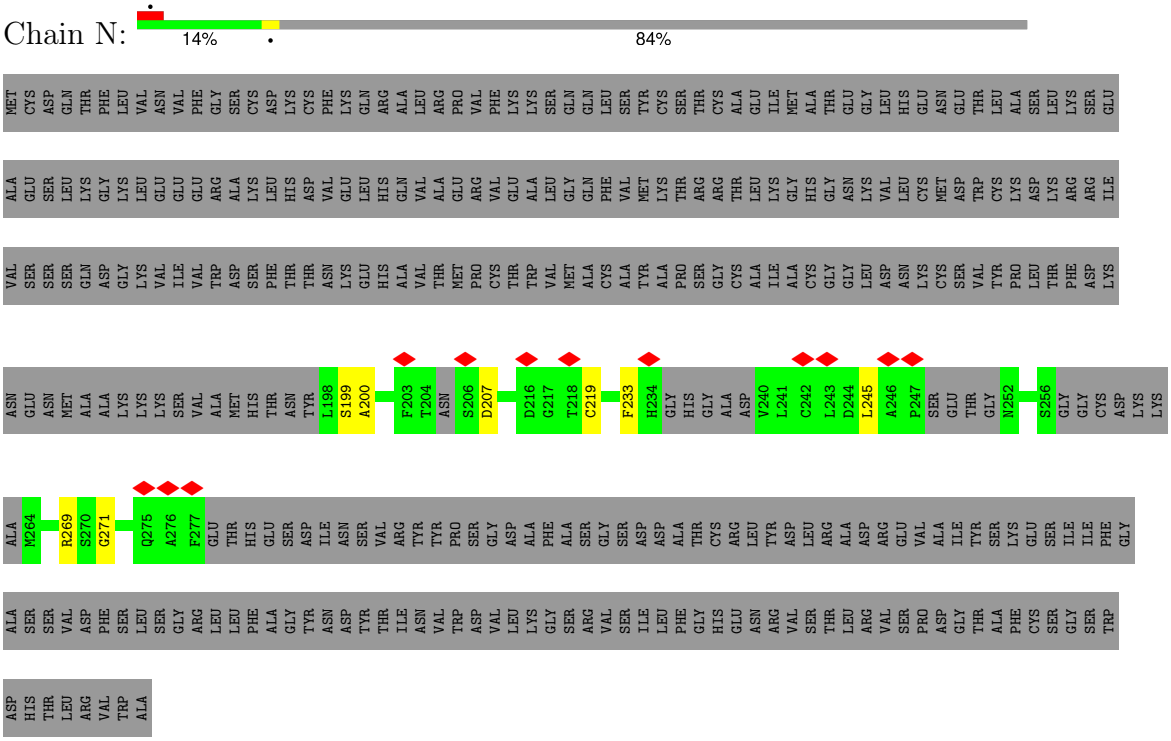
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	AltConf
13	A	2	Total O 2 2	0
13	B	2	Total O 2 2	0
13	D	1	Total O 1 1	0
13	E	1	Total O 1 1	0
13	G	1	Total O 1 1	0
13	H	1	Total O 1 1	0
13	Q	1	Total O 1 1	0
13	Z	1	Total O 1 1	0
13	a	2	Total O 2 2	0
13	b	1	Total O 1 1	0
13	d	1	Total O 1 1	0
13	e	1	Total O 1 1	0
13	g	1	Total O 1 1	0
13	h	1	Total O 1 1	0
13	q	1	Total O 1 1	0
13	z	1	Total O 1 1	0

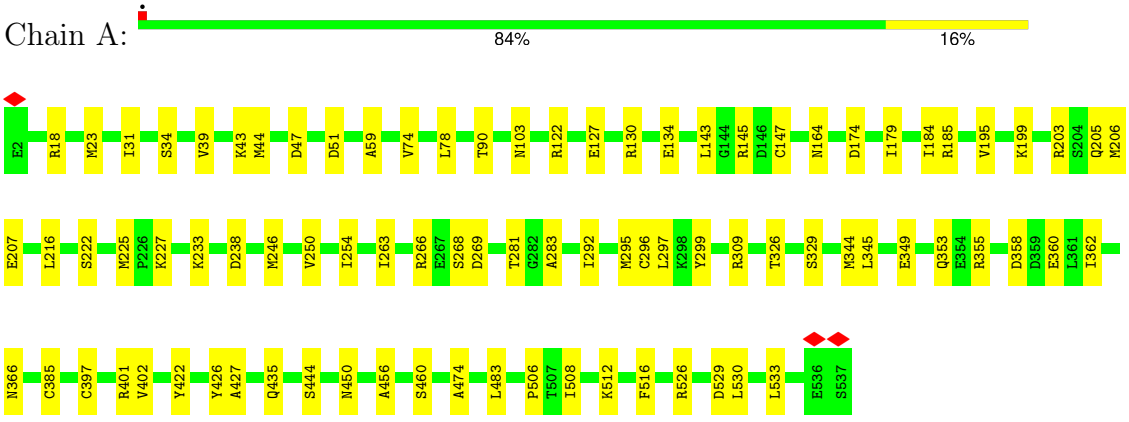
3 Residue-property plots (i)

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: Guanine nucleotide-binding protein subunit beta-5

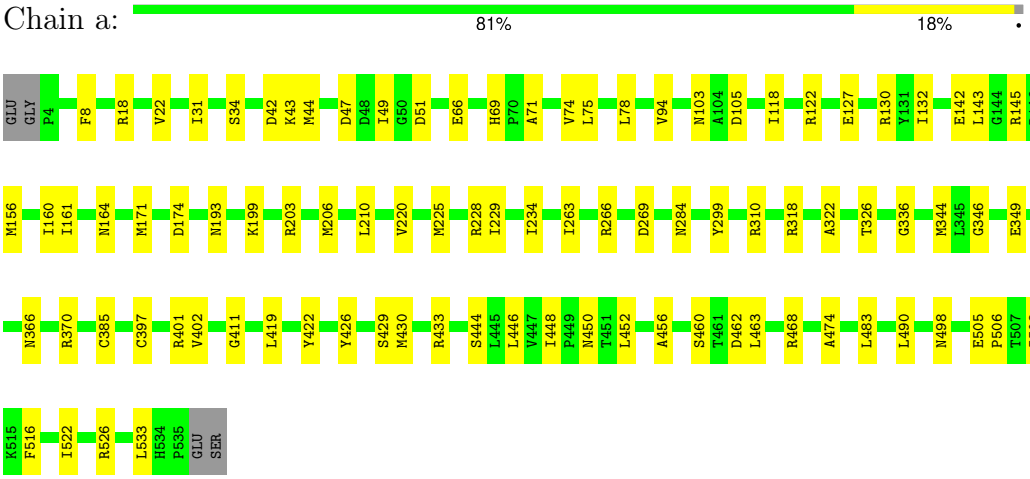


• Molecule 2: T-complex protein 1 subunit alpha



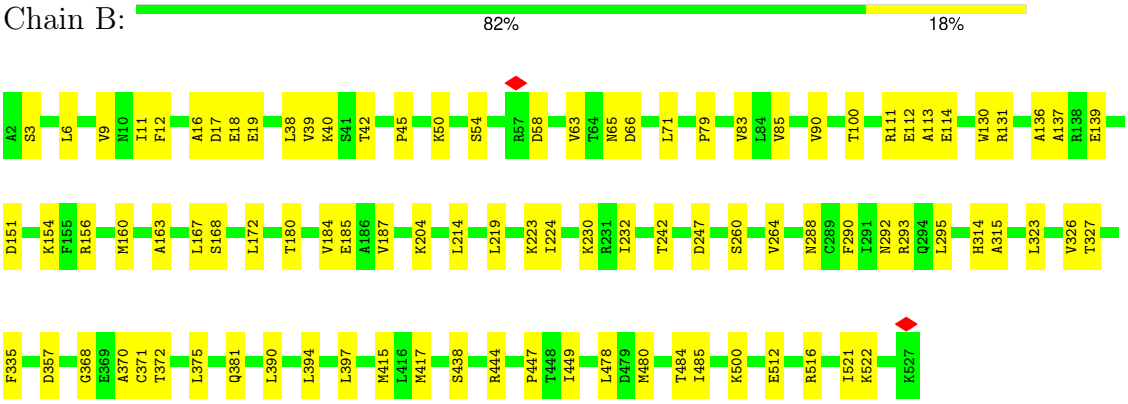
• Molecule 2: T-complex protein 1 subunit alpha

Chain a:



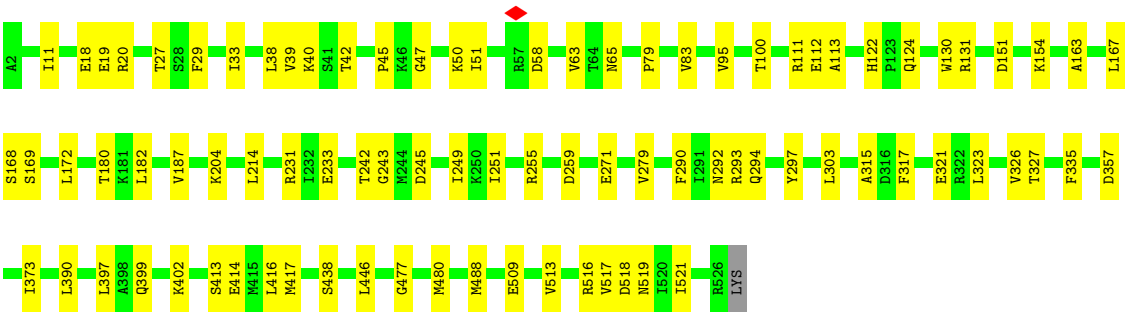
• Molecule 3: T-complex protein 1 subunit beta

Chain B:



• Molecule 3: T-complex protein 1 subunit beta

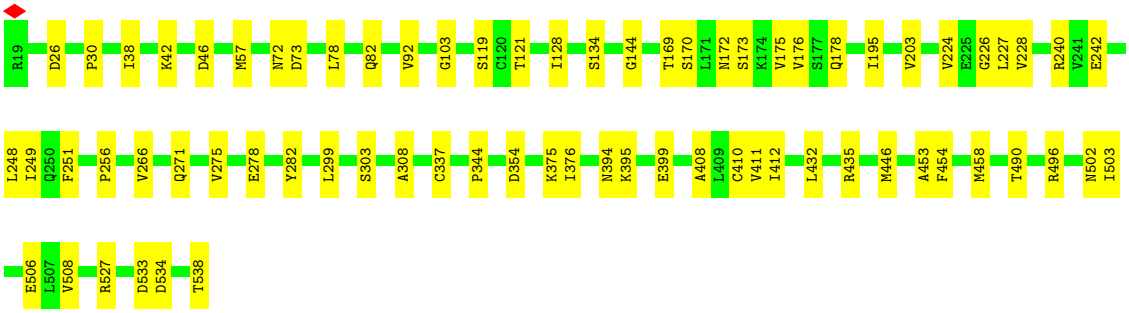
Chain b:



• Molecule 4: T-complex protein 1 subunit delta

Chain D:

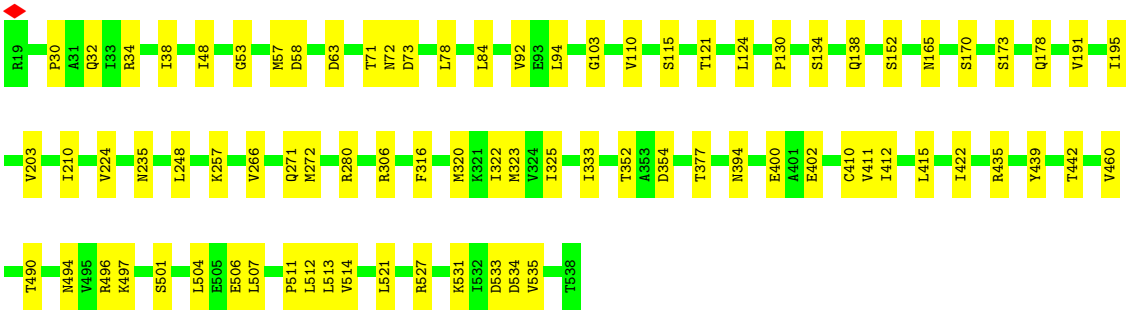




• Molecule 4: T-complex protein 1 subunit delta

Chain d:

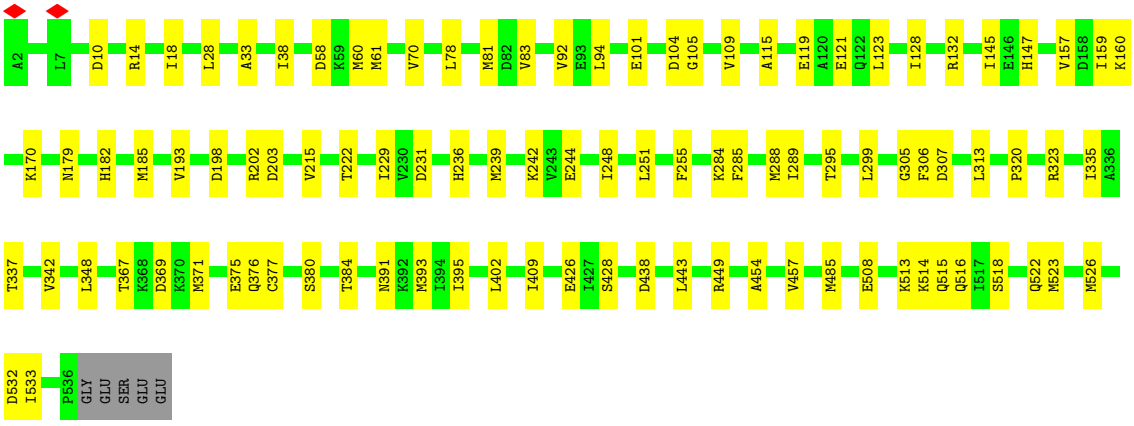




• Molecule 5: T-complex protein 1 subunit epsilon

Chain E:

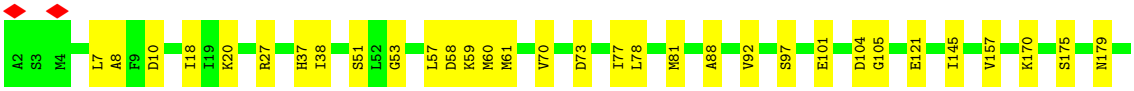


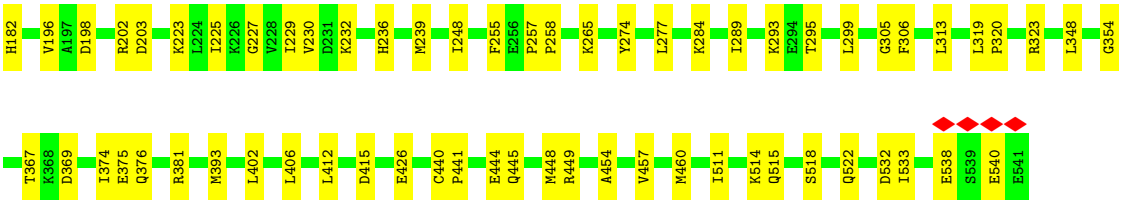


• Molecule 5: T-complex protein 1 subunit epsilon

Chain e:



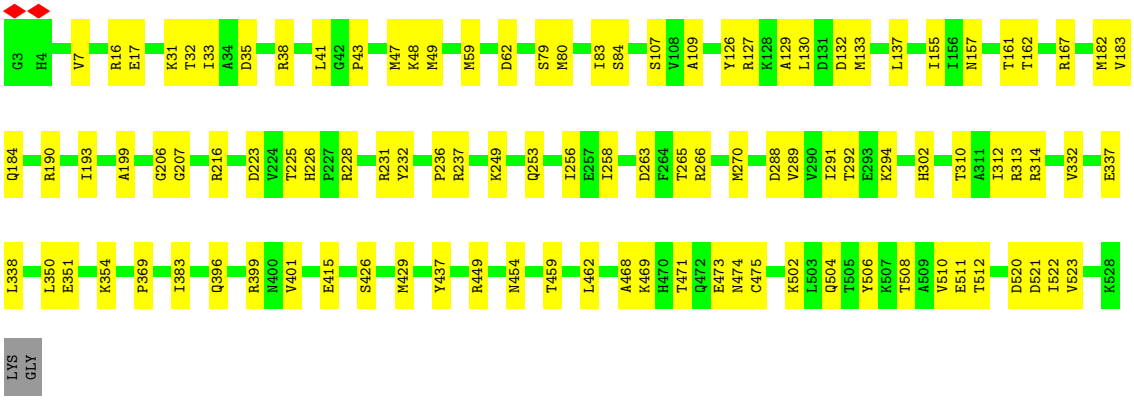




• Molecule 6: T-complex protein 1 subunit gamma

Chain G:

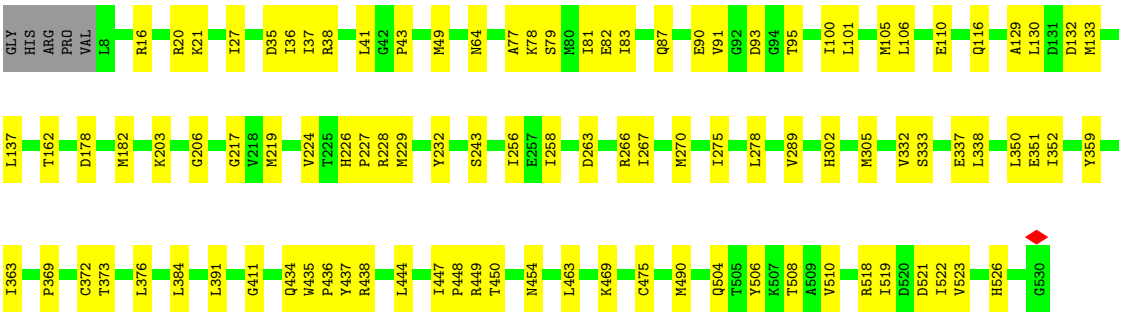




• Molecule 6: T-complex protein 1 subunit gamma

Chain g:

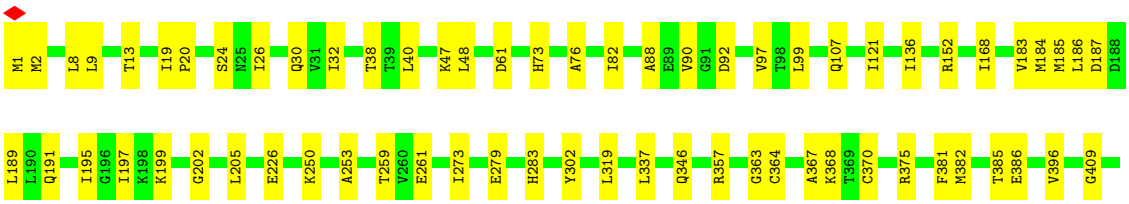


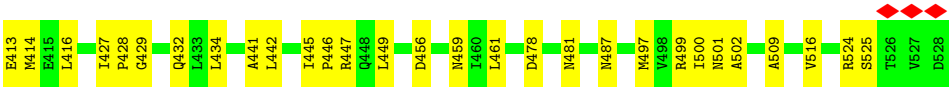


• Molecule 7: T-complex protein 1 subunit eta, N-terminally processed

Chain H:



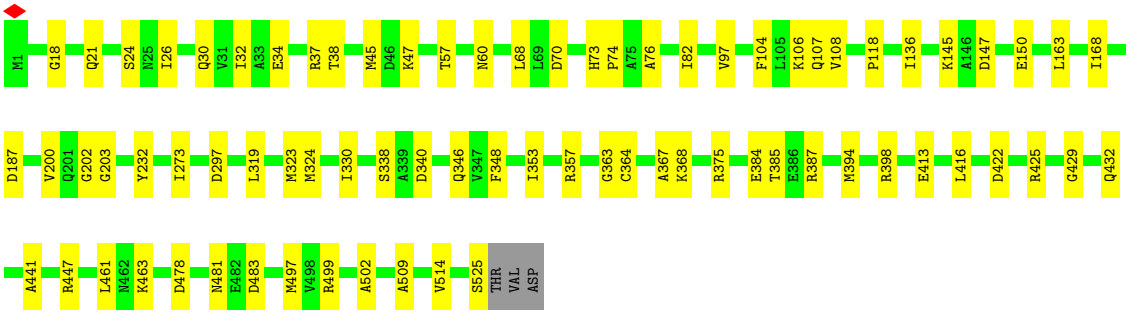




• Molecule 7: T-complex protein 1 subunit eta, N-terminally processed

Chain h:

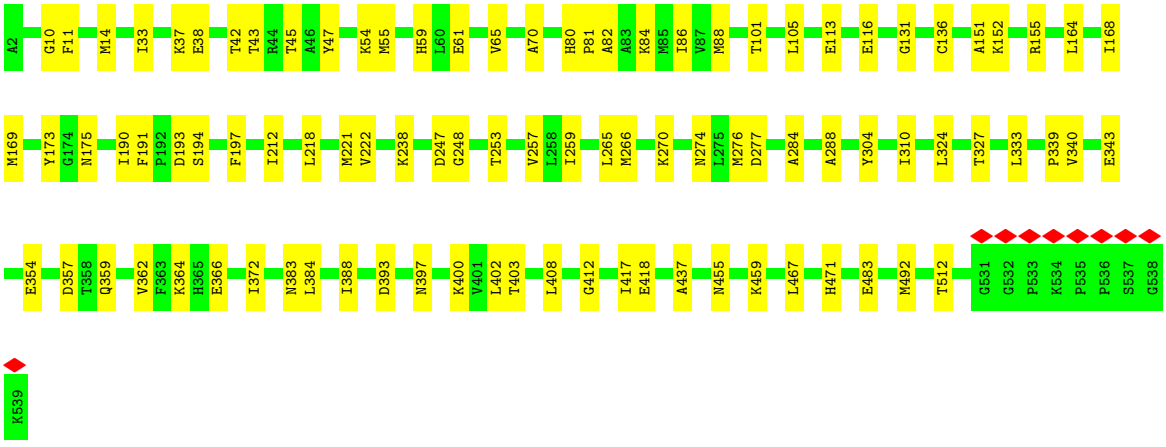




• Molecule 8: T-complex protein 1 subunit theta

Chain Q:

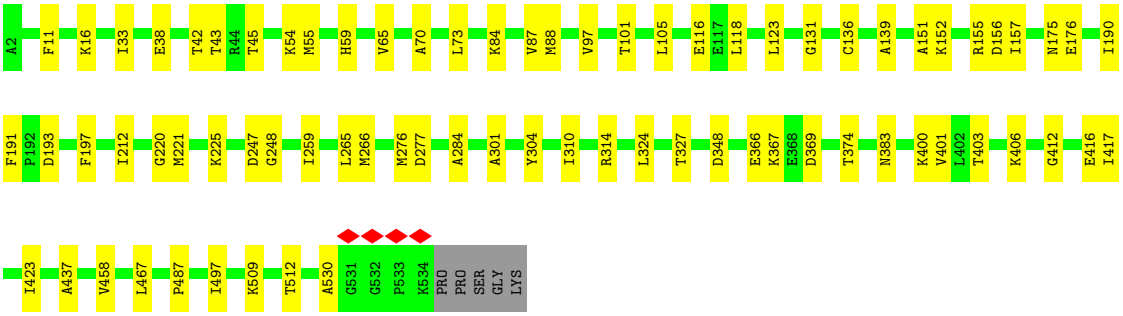




• Molecule 8: T-complex protein 1 subunit theta

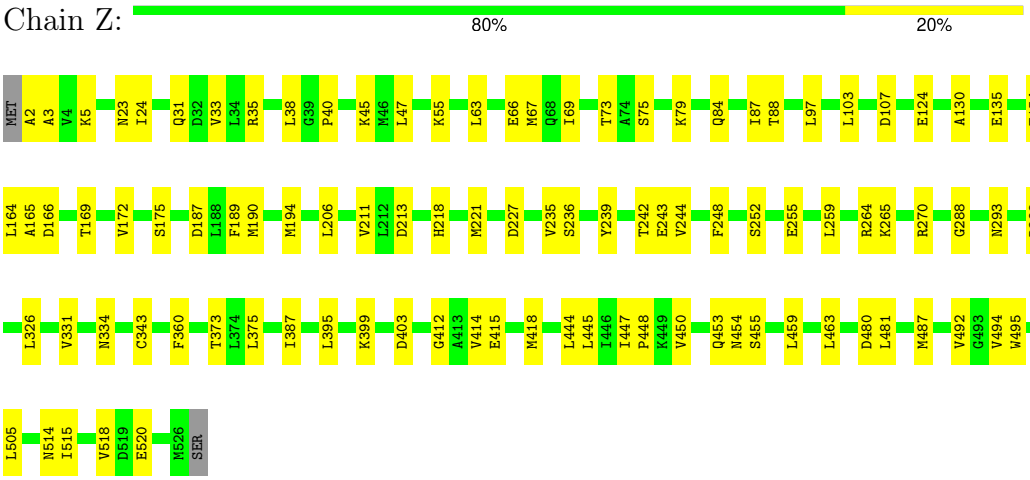
Chain q:





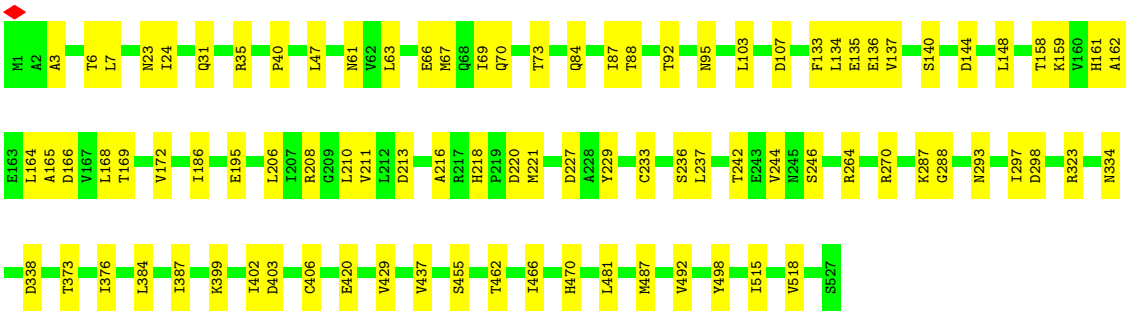
• Molecule 9: T-complex protein 1 subunit zeta

Chain Z:



• Molecule 9: T-complex protein 1 subunit zeta

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96135	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 ($e^-/Å^2$)	40.42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.932	Depositor
Minimum map value	-0.305	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.109	Depositor
Map size (Å)	317.4, 317.4, 317.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AF3, MG, ADP

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	N	0.08	0/479	0.24	0/644
2	A	0.12	0/4109	0.26	0/5548
2	a	0.13	0/4081	0.28	1/5510 (0.0%)
3	B	0.13	0/3995	0.25	0/5386
3	b	0.13	0/3986	0.26	0/5375
4	D	0.12	0/3955	0.24	0/5338
4	d	0.12	0/3949	0.25	0/5331
5	E	0.13	0/4183	0.28	0/5635
5	e	0.13	0/4220	0.27	0/5684
6	G	0.13	0/4136	0.26	0/5579
6	g	0.13	0/4108	0.26	0/5539
7	H	0.13	0/4111	0.26	0/5550
7	h	0.13	0/4089	0.26	0/5519
8	Q	0.12	0/4147	0.25	0/5606
8	q	0.12	0/4112	0.27	1/5558 (0.0%)
9	Z	0.13	0/4069	0.25	0/5486
9	z	0.12	0/4080	0.25	0/5501
All	All	0.13	0/65809	0.26	2/88789 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	49	ILE	N-CA-C	-6.18	107.26	113.20
8	q	530	ALA	CB-CA-C	-5.10	110.29	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	N	474	0	446	6	0
2	A	4069	0	4224	52	0
2	a	4041	0	4205	62	0
3	B	3952	0	4070	66	0
3	b	3943	0	4057	59	0
4	D	3923	0	4131	45	0
4	d	3917	0	4120	53	0
5	E	4132	0	4246	64	0
5	e	4169	0	4272	75	0
6	G	4089	0	4224	67	0
6	g	4063	0	4201	74	0
7	H	4054	0	4160	70	0
7	h	4032	0	4140	55	0
8	Q	4086	0	4160	59	0
8	q	4053	0	4125	52	0
9	Z	4022	0	4161	76	0
9	z	4033	0	4171	55	0
10	A	27	0	12	1	0
10	B	27	0	12	2	0
10	D	27	0	12	1	0
10	E	27	0	12	0	0
10	G	27	0	12	2	0
10	H	27	0	12	2	0
10	Q	27	0	12	2	0
10	Z	27	0	12	2	0
10	a	27	0	12	1	0
10	b	27	0	12	2	0
10	d	27	0	12	2	0
10	e	27	0	12	2	0
10	g	27	0	12	2	0
10	h	27	0	12	1	0
10	q	27	0	12	3	0
10	z	27	0	12	1	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	G	1	0	0	0	0
11	H	1	0	0	0	0
11	Q	1	0	0	0	0
11	Z	1	0	0	0	0
11	a	1	0	0	0	0
11	b	1	0	0	0	0
11	d	1	0	0	0	0
11	e	1	0	0	0	0
11	g	1	0	0	0	0
11	h	1	0	0	0	0
11	q	1	0	0	0	0
11	z	1	0	0	0	0
12	A	4	0	0	1	0
12	B	4	0	0	1	0
12	D	4	0	0	2	0
12	E	4	0	0	0	0
12	G	4	0	0	3	0
12	H	4	0	0	2	0
12	Q	4	0	0	1	0
12	Z	4	0	0	2	0
12	a	4	0	0	1	0
12	b	4	0	0	0	0
12	d	4	0	0	2	0
12	e	4	0	0	1	0
12	g	4	0	0	1	0
12	h	4	0	0	0	0
12	q	4	0	0	2	0
12	z	4	0	0	1	0
13	A	2	0	0	0	0
13	B	2	0	0	0	0
13	D	1	0	0	0	0
13	E	1	0	0	0	0
13	G	1	0	0	0	0
13	H	1	0	0	0	0
13	Q	1	0	0	0	0
13	Z	1	0	0	0	0
13	a	2	0	0	0	0
13	b	1	0	0	0	0
13	d	1	0	0	0	0
13	e	1	0	0	0	0
13	g	1	0	0	0	0
13	h	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	q	1	0	0	0	0
13	z	1	0	0	0	0
All	All	65583	0	67305	899	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 7.

All (899) 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)
3:B:79:PRO:HB2	5:E:60:MET:HE2	1.52	0.92
6:G:292:THR:HG22	6:G:294:LYS:H	1.45	0.80
3:b:11:ILE:HD11	5:e:88:ALA:HB2	1.65	0.78
5:E:426:GLU:OE2	5:E:513:LYS:NZ	2.17	0.77
6:g:289:VAL:HG21	6:g:350:LEU:HD13	1.68	0.76
3:B:219:LEU:HB2	3:B:372:THR:HG21	1.70	0.74
9:Z:190:MET:HE2	9:Z:326:LEU:HD12	1.71	0.73
6:g:133:MET:HE3	6:g:444:LEU:HD11	1.69	0.73
3:b:39:VAL:HG22	3:b:100:THR:HG23	1.71	0.72
6:g:206:GLY:HA3	9:z:87:ILE:HG13	1.70	0.72
5:E:305:GLY:HA2	5:E:323:ARG:HB2	1.72	0.72
6:g:35:ASP:OD1	6:g:38:ARG:NH1	2.23	0.72
9:z:242:THR:HG22	9:z:244:VAL:H	1.54	0.71
6:g:266:ARG:HG3	6:g:270:MET:HE3	1.72	0.71
6:g:27:ILE:HD13	6:g:110:GLU:HB2	1.72	0.71
3:B:50:LYS:HD3	4:D:534:ASP:HB3	1.71	0.71
7:H:82:ILE:HG21	7:H:509:ALA:HB2	1.73	0.71
4:D:78:LEU:HB3	4:D:92:VAL:HG22	1.73	0.70
7:h:82:ILE:HG21	7:h:509:ALA:HB2	1.71	0.70
7:H:346:GLN:HB2	7:H:363:GLY:HA3	1.73	0.70
5:e:305:GLY:HA2	5:e:323:ARG:HB2	1.72	0.70
7:h:145:LYS:HD2	7:h:147:ASP:H	1.55	0.70
6:G:132:ASP:OD2	6:G:437:TYR:OH	2.08	0.70
4:d:30:PRO:HB3	4:d:533:ASP:HB2	1.73	0.69
2:a:164:ASN:ND2	2:a:206:MET:SD	2.65	0.69
2:A:474:ALA:HB2	2:A:483:LEU:HB2	1.74	0.69
4:D:30:PRO:HB3	4:D:533:ASP:HB2	1.75	0.69
9:z:264:ARG:NH2	9:z:298:ASP:OD2	2.26	0.69
5:E:185:MET:HE3	5:E:402:LEU:HD21	1.74	0.69
5:E:60:MET:HG3	5:E:70:VAL:HG22	1.76	0.68
6:G:313:ARG:HG2	6:G:314:ARG:HG3	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:35:ASP:OD1	6:G:38:ARG:NH1	2.27	0.68
3:B:38:LEU:O	3:B:50:LYS:NZ	2.27	0.67
5:e:515:GLN:HE22	7:h:203:GLY:HA2	1.58	0.67
4:D:128:ILE:HG23	4:D:446:MET:HE2	1.77	0.67
6:G:237:ARG:H	6:G:288:ASP:HB2	1.60	0.67
6:g:469:LYS:NZ	6:g:475:CYS:SG	2.68	0.67
2:A:222:SER:H	2:A:225:MET:HE3	1.57	0.67
3:B:39:VAL:HG22	3:B:100:THR:HG23	1.77	0.66
3:B:112:GLU:HB3	3:B:438:SER:HB3	1.78	0.66
9:Z:31:GLN:O	9:Z:35:ARG:HG3	1.95	0.66
8:Q:354:GLU:OE1	8:Q:359:GLN:NE2	2.29	0.66
2:a:474:ALA:HB2	2:a:483:LEU:HB2	1.78	0.66
8:Q:253:THR:HG1	9:Z:239:TYR:HH	1.42	0.65
2:A:18:ARG:HH22	4:D:57:MET:HE2	1.61	0.65
7:H:456:ASP:OD2	7:H:459:ASN:ND2	2.30	0.65
3:b:112:GLU:HB3	3:b:438:SER:HB3	1.77	0.65
9:z:84:GLN:OE1	9:z:88:THR:OG1	2.14	0.65
7:h:32:ILE:HG13	7:h:76:ALA:HB1	1.77	0.65
2:A:205:GLN:OE1	6:G:127:ARG:NH2	2.30	0.65
4:d:78:LEU:HB3	4:d:92:VAL:HG22	1.77	0.65
7:h:346:GLN:HB2	7:h:363:GLY:HA3	1.79	0.65
5:E:242:LYS:NZ	5:E:244:GLU:OE2	2.30	0.64
9:z:229:TYR:HE2	9:z:287:LYS:HD3	1.62	0.64
3:B:17:ASP:OD2	3:B:18:GLU:N	2.30	0.64
9:Z:242:THR:HG22	9:Z:244:VAL:H	1.62	0.64
8:Q:169:MET:SD	10:Q:601:ADP:N6	2.69	0.64
2:a:103:ASN:ND2	2:a:444:SER:OG	2.27	0.64
9:Z:252:SER:OG	9:Z:255:GLU:OE1	2.15	0.64
3:b:50:LYS:HD3	4:d:534:ASP:HB3	1.80	0.64
3:B:478:LEU:HB3	3:B:480:MET:HE3	1.79	0.64
2:a:18:ARG:HH22	4:d:57:MET:HE2	1.63	0.63
3:B:45:PRO:HG2	3:B:480:MET:HG3	1.80	0.63
4:D:119:SER:HB2	4:D:453:ALA:HB1	1.79	0.63
9:Z:453:GLN:HG3	9:Z:459:LEU:HD21	1.80	0.63
9:z:148:LEU:HD11	9:z:402:ILE:HD11	1.80	0.63
5:e:51:SER:OG	5:e:59:LYS:NZ	2.29	0.63
6:G:469:LYS:NZ	6:G:475:CYS:SG	2.71	0.63
2:a:44:MET:HE3	6:g:519:ILE:HD13	1.81	0.63
6:G:206:GLY:HA3	9:Z:87:ILE:HG13	1.80	0.63
4:d:235:ASN:ND2	4:d:322:ILE:O	2.31	0.62
5:e:198:ASP:HB3	5:e:202:ARG:HB2	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:z:166:ASP:O	9:z:169:THR:OG1	2.17	0.62
9:z:218:HIS:HB3	9:z:221:MET:HG2	1.80	0.62
2:A:199:LYS:HB3	2:A:385:CYS:HB3	1.82	0.62
2:a:132:ILE:HD11	2:a:419:LEU:HD11	1.80	0.62
6:G:383:ILE:HD12	9:Z:514:ASN:HD22	1.65	0.62
2:a:229:ILE:HD13	2:a:284:ASN:HB3	1.81	0.62
5:e:10:ASP:OD2	7:h:24:SER:OG	2.16	0.62
7:H:524:ARG:NH1	8:Q:61:GLU:OE2	2.33	0.62
3:b:131:ARG:NH2	5:e:179:ASN:OD1	2.32	0.62
7:H:32:ILE:HG13	7:H:76:ALA:HB1	1.82	0.62
2:A:59:ALA:HB2	2:A:90:THR:HG21	1.81	0.62
7:h:319:LEU:HB3	7:h:330:ILE:HD11	1.81	0.61
6:g:504:GLN:NE2	6:g:508:THR:OG1	2.33	0.61
5:e:230:VAL:HG12	5:e:232:LYS:H	1.63	0.61
6:g:203:LYS:HB2	6:g:384:LEU:HD13	1.83	0.61
6:G:302:HIS:HB2	9:Z:334:ASN:HB2	1.82	0.61
6:g:64:ASN:HB2	6:g:95:THR:HG21	1.82	0.61
3:b:38:LEU:O	3:b:50:LYS:NZ	2.25	0.61
9:Z:218:HIS:HB3	9:Z:221:MET:HG3	1.83	0.61
6:g:449:ARG:HB2	6:g:463:LEU:HD11	1.82	0.61
8:q:139:ALA:HB2	8:q:423:ILE:HD11	1.83	0.61
5:e:518:SER:O	5:e:522:GLN:HG2	2.01	0.60
4:D:432:LEU:HD23	4:D:458:MET:HE2	1.82	0.60
9:Z:84:GLN:OE1	9:Z:88:THR:OG1	2.18	0.60
9:Z:38:LEU:O	9:Z:454:ASN:ND2	2.34	0.60
6:G:155:ILE:HG21	6:G:401:VAL:HG21	1.83	0.60
9:Z:487:MET:HE1	9:Z:492:VAL:HG21	1.82	0.60
5:e:225:ILE:HD13	5:e:229:ILE:HD11	1.83	0.60
8:q:175:ASN:HD21	8:q:212:ILE:HD11	1.66	0.60
2:A:353:GLN:O	6:G:190:ARG:NH1	2.34	0.60
6:g:101:LEU:O	6:g:105:MET:HG3	2.01	0.60
7:h:97:VAL:HG12	7:h:502:ALA:HA	1.84	0.60
4:d:352:THR:OG1	4:d:354:ASP:OD1	2.19	0.60
9:Z:24:ILE:HD13	9:Z:107:ASP:HB2	1.84	0.60
5:E:438:ASP:OD1	5:E:449:ARG:NH2	2.34	0.60
6:G:226:HIS:HD2	6:G:228:ARG:H	1.49	0.60
8:Q:247:ASP:OD1	8:Q:248:GLY:N	2.34	0.60
2:A:103:ASN:OD1	2:A:444:SER:OG	2.19	0.59
6:G:16:ARG:HG3	6:G:523:VAL:HG22	1.82	0.59
8:Q:221:MET:HG3	8:Q:327:THR:HG21	1.83	0.59
3:b:231:ARG:NH1	3:b:233:GLU:OE2	2.34	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:233:PHE:HE1	1:N:271:GLY:HA2	1.67	0.59
8:Q:364:LYS:NZ	8:Q:366:GLU:OE2	2.35	0.59
7:h:74:PRO:HB2	8:q:55:MET:HE2	1.85	0.59
7:H:250:LYS:HB2	7:H:253:ALA:HB2	1.85	0.59
5:e:367:THR:HG23	5:e:369:ASP:H	1.67	0.59
6:g:87:GLN:NE2	6:g:93:ASP:O	2.36	0.59
1:N:269:ARG:HG2	5:E:307:ASP:HA	1.84	0.59
2:a:34:SER:OG	2:a:43:LYS:NZ	2.36	0.59
7:h:478:ASP:OD2	7:h:481:ASN:ND2	2.34	0.59
2:A:44:MET:HB2	6:G:522:ILE:HG12	1.84	0.58
6:G:396:GLN:OE1	6:G:399:ARG:NH2	2.36	0.58
7:h:384:GLU:OE1	7:h:387:ARG:NH1	2.35	0.58
10:q:601:ADP:O1B	12:q:603:AF3:F2	2.11	0.58
3:B:71:LEU:HB3	3:B:85:VAL:HG22	1.85	0.58
2:a:47:ASP:HB3	2:a:51:ASP:HB2	1.85	0.58
5:e:60:MET:HG3	5:e:70:VAL:HG22	1.83	0.58
4:d:103:GLY:HA3	4:d:410:CYS:HB3	1.84	0.58
9:z:61:ASN:HB2	9:z:92:THR:HG21	1.84	0.58
2:A:34:SER:OG	2:A:43:LYS:NZ	2.36	0.58
2:a:42:ASP:OD1	6:g:518:ARG:NH2	2.36	0.58
6:g:79:SER:O	6:g:83:ILE:HG12	2.04	0.58
8:q:38:GLU:O	8:q:42:THR:HG23	2.04	0.58
9:Z:189:PHE:O	9:Z:323:ARG:NH1	2.37	0.58
2:a:353:GLN:NE2	2:a:360:GLU:OE1	2.36	0.58
3:B:131:ARG:NH2	5:E:179:ASN:OD1	2.36	0.58
9:Z:135:GLU:OE1	9:Z:498:TYR:OH	2.19	0.58
3:b:251:ILE:HG13	5:e:277:LEU:HD11	1.86	0.58
6:G:41:LEU:O	6:G:454:ASN:ND2	2.36	0.58
8:q:155:ARG:HH21	8:q:193:ASP:HA	1.69	0.58
7:h:499:ARG:NH2	10:h:601:ADP:O3'	2.37	0.57
9:z:210:LEU:HD21	9:z:323:ARG:HB3	1.85	0.57
8:Q:45:THR:HG1	8:Q:54:LYS:HZ1	1.50	0.57
5:E:518:SER:O	5:E:522:GLN:HG2	2.03	0.57
7:h:34:GLU:HA	7:h:37:ARG:HG3	1.86	0.57
7:H:152:ARG:NH2	7:H:184:MET:SD	2.77	0.57
5:e:415:ASP:HB3	5:e:511:ILE:HD11	1.86	0.57
4:D:248:LEU:HD23	4:D:299:LEU:HB2	1.87	0.57
7:h:447:ARG:HB2	7:h:461:LEU:HD11	1.85	0.57
5:e:78:LEU:HB3	5:e:92:VAL:HG22	1.87	0.57
5:e:248:ILE:N	5:e:354:GLY:O	2.34	0.57
4:d:195:ILE:HG21	4:d:203:VAL:HG22	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:289:VAL:HG11	6:G:350:LEU:HD13	1.86	0.56
7:H:499:ARG:NH2	10:H:601:ADP:O3'	2.38	0.56
3:B:163:ALA:HB3	3:B:180:THR:HG23	1.86	0.56
3:b:163:ALA:HB3	3:b:180:THR:HG23	1.88	0.56
5:E:248:ILE:HD12	5:E:337:THR:HG21	1.88	0.56
6:G:289:VAL:HG12	6:G:310:THR:HB	1.87	0.56
3:b:326:VAL:HG13	3:b:327:THR:HG23	1.86	0.56
4:D:228:VAL:HG22	4:D:375:LYS:HG2	1.87	0.56
5:E:236:HIS:HB3	5:E:239:MET:HG3	1.87	0.56
6:G:332:VAL:HG21	6:G:338:LEU:HD13	1.87	0.56
8:q:220:GLY:O	8:q:374:THR:OG1	2.18	0.56
3:B:415:MET:HE1	3:B:444:ARG:HG3	1.87	0.56
9:Z:47:LEU:HB2	9:Z:55:LYS:HB3	1.86	0.56
2:a:505:GLU:OE2	2:a:510:LYS:NZ	2.27	0.56
3:B:151:ASP:HB3	3:B:154:LYS:HB2	1.88	0.56
5:e:203:ASP:OD2	7:h:357:ARG:NH2	2.35	0.56
7:h:422:ASP:OD1	7:h:425:ARG:NH2	2.38	0.56
2:A:130:ARG:NH1	2:A:134:GLU:OE1	2.39	0.56
6:G:130:LEU:HB2	6:G:510:VAL:HG11	1.88	0.56
9:z:420:GLU:HG3	9:z:470:HIS:HD2	1.70	0.56
2:A:450:ASN:ND2	2:A:460:SER:OG	2.34	0.56
3:b:122:HIS:HD2	3:b:124:GLN:HB2	1.70	0.56
6:g:332:VAL:HG21	6:g:338:LEU:HD13	1.88	0.56
5:E:78:LEU:HB3	5:E:92:VAL:HG22	1.86	0.56
6:g:41:LEU:O	6:g:454:ASN:ND2	2.36	0.56
8:Q:84:LYS:O	8:Q:88:MET:HG3	2.05	0.55
9:Z:455:SER:OG	9:Z:481:LEU:O	2.23	0.55
7:h:107:GLN:HG3	7:h:441:ALA:HB2	1.88	0.55
9:Z:264:ARG:NH2	9:Z:298:ASP:OD2	2.38	0.55
8:Q:284:ALA:HB2	8:Q:310:ILE:HD11	1.88	0.55
8:Q:412:GLY:HA3	8:Q:492:MET:HE2	1.89	0.55
2:a:75:LEU:HD23	2:a:94:VAL:HG13	1.88	0.55
2:a:456:ALA:HB2	2:a:490:LEU:HD12	1.88	0.55
5:E:377:CYS:HB2	5:E:380:SER:HB3	1.88	0.55
5:e:239:MET:SD	5:e:320:PRO:HA	2.47	0.55
6:G:48:LYS:HG2	9:Z:520:GLU:HB3	1.89	0.55
8:Q:47:TYR:O	8:Q:455:ASN:ND2	2.38	0.55
2:a:143:LEU:HB3	2:a:147:CYS:HB2	1.88	0.55
3:b:413:SER:O	3:b:417:MET:HG3	2.06	0.55
2:a:145:ARG:NH2	2:a:174:ASP:OD1	2.40	0.55
8:q:73:LEU:HD13	8:q:87:VAL:HG22	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:183:VAL:HG21	6:G:199:ALA:HB2	1.89	0.55
6:G:468:ALA:O	6:G:471:THR:OG1	2.25	0.55
7:H:279:GLU:HG3	7:H:283:HIS:HD2	1.72	0.55
9:z:164:LEU:HD21	9:z:387:ILE:HG12	1.88	0.55
8:Q:175:ASN:HD21	8:Q:212:ILE:HD11	1.70	0.55
9:Z:38:LEU:HD21	9:Z:447:ILE:HG23	1.89	0.55
4:d:138:GLN:OE1	4:d:527:ARG:NH1	2.38	0.55
5:e:20:LYS:HB3	7:h:70:ASP:HB3	1.87	0.55
5:e:293:LYS:HD2	5:e:319:LEU:HD11	1.89	0.55
9:z:31:GLN:O	9:z:35:ARG:HG3	2.07	0.55
2:A:508:ILE:HD11	2:A:512:LYS:HE3	1.88	0.54
8:Q:190:ILE:HG22	8:Q:191:PHE:H	1.72	0.54
5:e:37:HIS:CE1	5:e:533:ILE:HD11	2.42	0.54
7:h:463:LYS:NZ	7:h:483:ASP:OD1	2.31	0.54
7:H:38:THR:OG1	7:H:47:LYS:NZ	2.37	0.54
7:H:456:ASP:OD2	2:a:433:ARG:NH2	2.40	0.54
6:g:129:ALA:O	6:g:133:MET:HG3	2.07	0.54
10:g:601:ADP:O1B	12:g:603:AF3:F3	2.16	0.54
9:z:462:THR:O	9:z:466:ILE:HG12	2.07	0.54
2:A:281:THR:HG23	2:A:345:LEU:HD11	1.89	0.54
6:G:62:ASP:OD1	12:G:603:AF3:F3	2.16	0.54
6:g:302:HIS:HB2	9:z:334:ASN:HB2	1.89	0.54
9:z:24:ILE:HD13	9:z:107:ASP:HB2	1.89	0.54
7:H:187:ASP:HB3	7:H:368:LYS:HD2	1.90	0.54
8:q:97:VAL:HG13	8:q:401:VAL:HG21	1.89	0.54
2:A:122:ARG:HG3	4:D:178:GLN:HG3	1.89	0.54
2:A:203:ARG:HD3	2:A:207:GLU:HG2	1.89	0.54
4:D:72:ASN:ND2	4:D:173:SER:O	2.38	0.54
5:E:170:LYS:O	5:E:182:HIS:NE2	2.41	0.54
7:h:145:LYS:NZ	7:h:150:GLU:HB2	2.23	0.54
2:A:227:LYS:HD3	2:A:353:GLN:HG2	1.90	0.54
4:d:210:ILE:HG21	4:d:402:GLU:HG3	1.89	0.54
9:z:227:ASP:O	9:z:288:GLY:N	2.40	0.54
2:a:326:THR:OG1	2:a:344:MET:SD	2.63	0.53
6:g:132:ASP:OD2	6:g:437:TYR:OH	2.21	0.53
4:D:26:ASP:OD1	4:D:26:ASP:N	2.41	0.53
8:Q:155:ARG:HH21	8:Q:193:ASP:HA	1.73	0.53
4:D:38:ILE:HG21	4:D:121:THR:OG1	2.07	0.53
5:E:255:PHE:HB2	5:E:306:PHE:HB3	1.90	0.53
8:q:277:ASP:HB2	8:q:304:TYR:CZ	2.43	0.53
8:q:70:ALA:HB2	8:q:101:THR:HG21	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:z:40:PRO:HD3	9:z:158:THR:HG22	1.90	0.53
8:Q:248:GLY:H	8:Q:276:MET:HE1	1.74	0.53
10:Z:601:ADP:O2B	12:Z:603:AF3:F1	2.17	0.53
4:d:72:ASN:ND2	4:d:173:SER:O	2.41	0.53
5:e:375:GLU:HG2	5:e:376:GLN:HG3	1.91	0.53
4:d:497:LYS:HE2	4:d:501:SER:HB3	1.91	0.53
2:A:164:ASN:ND2	2:A:206:MET:SD	2.82	0.53
9:Z:97:LEU:HD13	9:Z:450:VAL:HG21	1.91	0.53
6:g:229:MET:HG3	6:g:305:MET:HE2	1.91	0.53
9:z:216:ALA:HB1	9:z:221:MET:HG3	1.91	0.53
5:E:198:ASP:HB3	5:E:202:ARG:HB2	1.91	0.53
6:G:265:THR:HG21	9:Z:265:LYS:HB3	1.90	0.53
8:Q:238:LYS:HB2	8:Q:288:ALA:HA	1.91	0.53
2:a:429:SER:O	2:a:430:MET:HE2	2.09	0.53
7:h:429:GLY:HA2	7:h:432:GLN:HB3	1.90	0.53
2:a:152:ALA:O	2:a:156:MET:HG3	2.09	0.53
4:D:195:ILE:HG21	4:D:203:VAL:HG22	1.91	0.52
5:E:285:PHE:HA	5:E:288:MET:HE3	1.91	0.52
10:Q:601:ADP:O2B	12:Q:603:AF3:F2	2.18	0.52
5:e:295:THR:HG21	5:e:348:LEU:HG	1.91	0.52
10:z:601:ADP:O1B	12:z:603:AF3:F3	2.17	0.52
7:h:364:CYS:HB2	7:h:367:ALA:HB2	1.91	0.52
9:Z:399:LYS:NZ	9:Z:403:ASP:OD2	2.40	0.52
3:B:63:VAL:HG12	3:B:381:GLN:HB3	1.91	0.52
7:h:45:MET:O	7:h:60:ASN:ND2	2.43	0.52
8:q:84:LYS:O	8:q:88:MET:HG3	2.10	0.52
7:H:447:ARG:HB2	7:H:461:LEU:HD11	1.92	0.52
3:b:95:VAL:HG12	3:b:399:GLN:HG3	1.90	0.52
4:d:496:ARG:NH1	4:d:506:GLU:OE1	2.42	0.52
8:q:400:LYS:O	8:q:403:THR:OG1	2.22	0.52
5:E:289:ILE:HG13	5:E:313:LEU:HB3	1.92	0.52
5:E:335:ILE:HD11	7:H:226:GLU:HB2	1.91	0.52
3:B:375:LEU:HD21	3:B:390:LEU:HD11	1.92	0.52
10:G:601:ADP:O2B	12:G:603:AF3:F1	2.17	0.52
2:a:299:TYR:OH	6:g:337:GLU:OE2	2.14	0.52
3:b:249:ILE:HG21	5:e:277:LEU:HG	1.90	0.52
4:D:354:ASP:OD1	4:D:354:ASP:N	2.42	0.52
8:Q:417:ILE:HG13	8:Q:467:LEU:HD13	1.91	0.52
3:b:414:GLU:HG2	3:b:446:LEU:HD23	1.91	0.52
6:g:376:LEU:HB3	6:g:384:LEU:HD22	1.91	0.52
7:h:38:THR:HG1	7:h:47:LYS:HZ3	1.51	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:9:LEU:HD13	7:H:13:THR:HG21	1.92	0.52
7:h:57:THR:HG21	7:h:68:LEU:HG	1.92	0.52
6:G:182:MET:HE3	6:G:369:PRO:HG2	1.91	0.51
7:H:497:MET:HA	7:H:500:ILE:HB	1.92	0.51
9:Z:40:PRO:HD3	9:Z:158:THR:HG22	1.92	0.51
9:Z:47:LEU:HD13	9:Z:66:GLU:HB2	1.93	0.51
2:a:127:GLU:HG3	2:a:426:TYR:CZ	2.45	0.51
4:d:38:ILE:HG21	4:d:121:THR:OG1	2.10	0.51
5:e:538:GLU:HG3	5:e:540:GLU:HB3	1.92	0.51
6:g:256:ILE:HB	9:z:246:SER:HA	1.92	0.51
5:E:38:ILE:HG21	5:E:121:GLU:HB2	1.92	0.51
6:g:411:GLY:HA3	6:g:490:MET:HE3	1.92	0.51
8:q:73:LEU:HD11	8:q:105:LEU:HD21	1.92	0.51
8:Q:136:CYS:HB2	8:Q:512:THR:HG21	1.92	0.51
6:g:130:LEU:HB2	6:g:510:VAL:HG11	1.91	0.51
8:q:221:MET:HG2	8:q:327:THR:HG21	1.91	0.51
5:E:532:ASP:OD2	7:H:47:LYS:NZ	2.33	0.51
7:H:88:ALA:HB1	8:Q:357:ASP:HB2	1.92	0.51
3:b:83:VAL:HG22	5:e:393:MET:HE3	1.92	0.51
3:B:160:MET:HE2	3:B:184:VAL:HG11	1.93	0.51
6:G:223:ASP:OD1	6:G:231:ARG:NH1	2.43	0.51
8:Q:277:ASP:HB2	8:Q:304:TYR:CZ	2.45	0.51
5:e:104:ASP:OD1	5:e:105:GLY:N	2.43	0.51
3:B:326:VAL:HG13	3:B:327:THR:HG23	1.93	0.51
5:E:508:GLU:OE1	5:E:513:LYS:HE3	2.11	0.51
8:q:151:ALA:HB3	8:q:406:LYS:HE2	1.93	0.51
2:a:263:ILE:HG23	4:d:272:MET:HE1	1.93	0.51
7:H:414:MET:HE2	7:H:446:PRO:HG3	1.93	0.51
3:b:204:LYS:NZ	3:b:357:ASP:OD2	2.37	0.51
5:e:38:ILE:HG21	5:e:121:GLU:HB2	1.93	0.51
8:q:458:VAL:HB	8:q:487:PRO:HG3	1.93	0.51
7:H:478:ASP:OD2	7:H:481:ASN:ND2	2.43	0.51
9:Z:103:LEU:HD21	9:Z:515:ILE:HG21	1.93	0.51
3:b:517:VAL:HG11	5:e:60:MET:HE3	1.93	0.51
3:B:58:ASP:OD2	3:B:58:ASP:N	2.44	0.50
3:B:83:VAL:HG22	5:E:393:MET:SD	2.51	0.50
7:H:168:ILE:HG21	7:H:385:THR:HG23	1.92	0.50
2:a:122:ARG:HG3	4:d:178:GLN:HG3	1.93	0.50
8:q:191:PHE:HB2	8:q:197:PHE:HD1	1.75	0.50
2:a:142:GLU:HG2	2:a:143:LEU:HD22	1.92	0.50
7:H:186:LEU:HD11	7:H:195:ILE:HD11	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:164:LEU:HD21	9:Z:387:ILE:HG12	1.92	0.50
5:e:18:ILE:HA	7:h:73:HIS:HB2	1.94	0.50
6:g:226:HIS:ND1	6:g:305:MET:HE1	2.26	0.50
2:A:78:LEU:HD11	2:A:516:PHE:HB3	1.92	0.50
5:E:14:ARG:NH1	7:H:20:PRO:HB2	2.26	0.50
7:H:90:VAL:HG12	7:H:92:ASP:H	1.77	0.50
2:a:118:ILE:HG23	2:a:522:ILE:HG12	1.93	0.50
6:g:258:ILE:HG23	6:g:263:ASP:HB2	1.93	0.50
8:Q:81:PRO:HA	8:Q:84:LYS:HB2	1.92	0.50
3:b:47:GLY:O	4:d:531:LYS:NZ	2.44	0.50
9:z:47:LEU:HD13	9:z:66:GLU:HB2	1.94	0.50
9:Z:227:ASP:O	9:Z:288:GLY:N	2.37	0.50
7:h:145:LYS:HZ1	7:h:150:GLU:HB2	1.76	0.50
3:B:415:MET:HE3	3:B:447:PRO:HG3	1.94	0.50
2:A:145:ARG:NH2	2:A:174:ASP:OD1	2.45	0.50
4:D:454:PHE:O	4:D:458:MET:HG2	2.12	0.50
7:h:26:ILE:O	7:h:30:GLN:HG2	2.12	0.50
5:E:231:ASP:HA	5:E:371:MET:HG2	1.93	0.50
7:H:273:ILE:HD11	8:Q:266:MET:HA	1.94	0.50
3:b:45:PRO:HD2	3:b:480:MET:HE2	1.94	0.50
3:b:51:ILE:HG12	3:b:63:VAL:HG22	1.94	0.50
2:a:8:PHE:HB2	4:d:84:LEU:HD11	1.93	0.49
2:a:228:ARG:HG3	2:a:352:VAL:HG22	1.93	0.49
3:b:242:THR:HG21	3:b:335:PHE:CE2	2.47	0.49
4:d:48:ILE:HD11	4:d:110:VAL:HG11	1.93	0.49
7:h:145:LYS:HZ3	7:h:147:ASP:HB3	1.76	0.49
2:A:353:GLN:HE21	2:A:360:GLU:HB3	1.77	0.49
10:A:601:ADP:O2B	12:A:603:AF3:F3	2.19	0.49
9:Z:414:VAL:O	9:Z:418:MET:HG3	2.12	0.49
2:a:462:ASP:OD1	2:a:463:LEU:N	2.45	0.49
2:a:533:LEU:HD12	4:d:63:ASP:HA	1.95	0.49
4:d:513:LEU:HD23	4:d:513:LEU:O	2.12	0.49
8:q:225:LYS:HE2	8:q:314:ARG:O	2.12	0.49
9:z:213:ASP:OD1	9:z:213:ASP:N	2.41	0.49
3:B:136:ALA:O	3:B:139:GLU:HG3	2.12	0.49
10:a:601:ADP:O2B	12:a:603:AF3:F3	2.20	0.49
5:e:306:PHE:CE1	5:e:323:ARG:HB3	2.47	0.49
8:q:247:ASP:OD1	8:q:248:GLY:N	2.44	0.49
5:E:94:LEU:HB2	5:E:523:MET:HG3	1.95	0.49
7:H:427:ILE:HB	7:H:428:PRO:HD2	1.94	0.49
10:H:601:ADP:O3B	12:H:603:AF3:F1	2.21	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:q:73:LEU:HD11	8:q:105:LEU:HD11	1.94	0.49
8:q:417:ILE:HG13	8:q:467:LEU:HD13	1.93	0.49
7:H:136:ILE:HD11	7:H:416:LEU:HD11	1.93	0.49
9:Z:154:THR:HG21	9:Z:495:TRP:H	1.75	0.49
4:d:494:ASN:ND2	4:d:501:SER:OG	2.39	0.49
5:e:27:ARG:NH2	5:e:532:ASP:OD2	2.38	0.49
8:q:118:LEU:HD22	8:q:123:LEU:HD12	1.94	0.49
6:G:504:GLN:NE2	6:G:508:THR:OG1	2.45	0.49
2:a:402:VAL:HG23	2:a:506:PRO:HG3	1.95	0.49
3:b:271:GLU:HG2	5:e:274:TYR:CZ	2.48	0.49
8:q:190:ILE:HG22	8:q:191:PHE:H	1.78	0.49
8:q:284:ALA:HB2	8:q:310:ILE:HD11	1.95	0.49
9:z:338:ASP:N	9:z:338:ASP:OD1	2.45	0.49
6:G:415:GLU:OE2	6:G:502:LYS:NZ	2.32	0.49
7:H:121:ILE:HG12	7:H:434:LEU:HD11	1.94	0.49
8:Q:459:LYS:NZ	6:g:116:GLN:O	2.45	0.49
6:g:16:ARG:HB2	6:g:523:VAL:HG12	1.93	0.49
7:H:279:GLU:OE1	7:H:302:TYR:OH	2.30	0.49
7:H:525:SER:HB3	8:Q:59:HIS:HB2	1.94	0.49
9:Z:63:LEU:O	9:Z:67:MET:HG3	2.12	0.49
4:d:439:TYR:O	4:d:442:THR:OG1	2.31	0.49
5:E:18:ILE:HA	7:H:73:HIS:HB2	1.94	0.49
5:E:375:GLU:HG3	5:E:376:GLN:HG3	1.94	0.49
6:g:77:ALA:O	6:g:81:ILE:HG12	2.13	0.49
9:z:211:VAL:HG23	9:z:373:THR:HG21	1.93	0.49
4:D:503:ILE:HG13	4:D:508:VAL:HB	1.94	0.49
7:H:202:GLY:O	7:H:375:ARG:NH2	2.46	0.49
4:d:323:MET:HE3	4:d:325:ILE:HD11	1.94	0.49
3:b:65:ASN:ND2	3:b:169:SER:O	2.46	0.48
8:q:276:MET:HE2	8:q:301:ALA:HB2	1.94	0.48
1:N:245:LEU:HD23	1:N:245:LEU:H	1.78	0.48
8:Q:37:LYS:HB2	8:Q:113:GLU:OE2	2.13	0.48
2:a:31:ILE:O	2:a:43:LYS:HE3	2.13	0.48
8:Q:173:TYR:OH	8:Q:483:GLU:OE2	2.30	0.48
9:Z:172:VAL:HG13	9:Z:395:LEU:HD23	1.94	0.48
9:Z:412:GLY:HA2	9:Z:415:GLU:OE2	2.14	0.48
9:Z:480:ASP:HB2	9:Z:487:MET:HG2	1.95	0.48
5:e:236:HIS:HB2	5:e:239:MET:HE3	1.94	0.48
2:A:47:ASP:HB3	2:A:51:ASP:HB2	1.94	0.48
3:B:521:ILE:HB	5:E:61:MET:SD	2.54	0.48
6:G:184:GLN:HG3	6:G:193:ILE:HG12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:526:ARG:HE	4:d:58:ASP:CG	2.22	0.48
3:b:477:GLY:C	3:b:488:MET:HE3	2.38	0.48
7:h:187:ASP:HB3	7:h:368:LYS:HD3	1.96	0.48
3:B:326:VAL:HG23	3:B:368:GLY:HA2	1.95	0.48
5:E:147:HIS:NE2	5:E:428:SER:OG	2.39	0.48
6:G:520:ASP:OD1	6:G:521:ASP:N	2.46	0.48
7:H:185:MET:HE3	7:H:370:CYS:SG	2.53	0.48
7:H:429:GLY:HA2	7:H:432:GLN:HB3	1.96	0.48
8:Q:193:ASP:OD1	8:Q:194:SER:N	2.46	0.48
8:Q:400:LYS:O	8:Q:403:THR:OG1	2.24	0.48
3:b:79:PRO:HB2	5:e:60:MET:SD	2.52	0.48
2:A:130:ARG:NH2	2:A:422:TYR:OH	2.46	0.48
10:G:601:ADP:O2B	12:G:603:AF3:F2	2.21	0.48
7:H:107:GLN:HG3	7:H:441:ALA:HB2	1.94	0.48
8:Q:11:PHE:CE1	9:Z:69:ILE:HD11	2.48	0.48
4:d:48:ILE:HG13	4:d:48:ILE:O	2.13	0.48
5:e:101:GLU:HG2	5:e:515:GLN:NE2	2.28	0.48
8:q:45:THR:HG1	8:q:54:LYS:HZ1	1.52	0.48
9:z:455:SER:OG	9:z:481:LEU:O	2.32	0.48
6:G:225:THR:HG22	6:G:313:ARG:HB2	1.95	0.48
7:H:197:ILE:HG21	7:H:386:GLU:HG3	1.95	0.48
9:Z:418:MET:HE1	9:Z:505:LEU:HD11	1.96	0.48
2:a:78:LEU:HD11	2:a:516:PHE:HB3	1.95	0.48
2:a:349:GLU:HB2	2:a:366:ASN:HB3	1.96	0.48
3:b:279:VAL:HG11	3:b:303:LEU:HB3	1.96	0.48
5:e:73:ASP:OD1	12:e:603:AF3:F2	2.22	0.48
9:z:195:GLU:HB3	9:z:384:LEU:HD13	1.95	0.48
7:H:516:VAL:HG21	8:Q:55:MET:HE3	1.94	0.48
8:Q:327:THR:HB	8:Q:372:ILE:HB	1.96	0.48
9:Z:166:ASP:O	9:Z:169:THR:OG1	2.31	0.48
2:a:336:GLY:O	4:d:280:ARG:NH1	2.44	0.48
5:e:170:LYS:O	5:e:182:HIS:NE2	2.42	0.48
7:h:145:LYS:NZ	7:h:147:ASP:O	2.44	0.48
6:G:226:HIS:CD2	6:G:228:ARG:H	2.29	0.48
2:a:132:ILE:HG13	2:a:419:LEU:HD21	1.95	0.48
8:q:324:LEU:HA	8:q:327:THR:HG22	1.96	0.48
9:z:103:LEU:HD21	9:z:515:ILE:HG21	1.95	0.48
7:H:253:ALA:HA	8:Q:257:VAL:HB	1.96	0.48
7:H:413:GLU:OE1	7:H:445:ILE:HB	2.14	0.48
9:Z:213:ASP:N	9:Z:213:ASP:OD1	2.44	0.47
3:b:113:ALA:HB2	3:b:130:TRP:CH2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:g:434:GLN:OE1	6:g:438:ARG:NH2	2.47	0.47
3:B:295:LEU:HD23	3:B:314:HIS:HB2	1.97	0.47
4:D:496:ARG:NH2	4:D:506:GLU:OE2	2.38	0.47
3:B:3:SER:N	4:d:32:GLN:OE1	2.46	0.47
4:D:303:SER:HB3	4:D:308:ALA:HB2	1.97	0.47
8:Q:324:LEU:HA	8:Q:327:THR:HG22	1.97	0.47
6:g:20:ARG:HG2	6:g:20:ARG:HH11	1.79	0.47
7:h:394:MET:O	7:h:398:ARG:HG2	2.14	0.47
3:B:131:ARG:NH2	3:B:512:GLU:OE2	2.40	0.47
6:G:157:ASN:O	6:G:161:THR:HG23	2.15	0.47
2:a:411:GLY:O	2:a:498:ASN:ND2	2.42	0.47
5:E:485:MET:SD	5:E:485:MET:N	2.87	0.47
4:d:415:LEU:HD13	4:d:511:PRO:HB3	1.95	0.47
10:d:601:ADP:O2B	12:d:603:AF3:F3	2.22	0.47
5:e:175:SER:OG	10:e:601:ADP:O1A	2.23	0.47
3:B:214:LEU:HD11	3:B:371:CYS:HB3	1.95	0.47
3:B:247:ASP:OD1	3:B:247:ASP:N	2.47	0.47
4:D:170:SER:HB2	4:D:411:VAL:HG21	1.97	0.47
5:e:445:GLN:HB3	5:e:449:ARG:NH1	2.29	0.47
8:q:259:ILE:HG21	8:q:265:LEU:HB2	1.97	0.47
9:z:399:LYS:NZ	9:z:403:ASP:OD2	2.46	0.47
2:A:326:THR:HB	2:A:344:MET:HG3	1.96	0.47
3:B:168:SER:OG	10:B:601:ADP:N7	2.45	0.47
4:D:227:LEU:HD23	4:D:376:ILE:HD12	1.97	0.47
4:D:266:VAL:HG13	4:D:271:GLN:HB2	1.96	0.47
6:G:31:LYS:HD3	6:G:107:SER:HB2	1.97	0.47
7:H:61:ASP:OD1	12:H:603:AF3:F3	2.22	0.47
7:H:73:HIS:HB3	7:H:76:ALA:HB3	1.97	0.47
5:e:454:ALA:O	5:e:457:VAL:HG12	2.15	0.47
9:z:23:ASN:OD1	9:z:73:THR:OG1	2.28	0.47
9:z:63:LEU:O	9:z:67:MET:HG3	2.14	0.47
3:B:113:ALA:HB2	3:B:130:TRP:CH2	2.50	0.47
5:E:295:THR:HG21	5:E:348:LEU:HG	1.97	0.47
7:H:446:PRO:HA	7:H:449:LEU:HD12	1.97	0.47
9:Z:159:LYS:NZ	12:Z:603:AF3:F1	2.37	0.47
9:z:135:GLU:OE2	9:z:498:TYR:OH	2.30	0.47
3:B:111:ARG:O	3:B:114:GLU:HG2	2.13	0.47
5:E:159:ILE:HG23	5:E:160:LYS:HD3	1.96	0.47
6:G:79:SER:O	6:G:83:ILE:HG23	2.15	0.47
9:Z:235:VAL:O	9:Z:293:ASN:ND2	2.38	0.47
5:e:532:ASP:HB3	7:h:47:LYS:HD2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:q:11:PHE:CE1	9:z:69:ILE:HD11	2.50	0.47
2:A:227:LYS:HB3	2:A:353:GLN:HB3	1.96	0.47
2:A:268:SER:HB2	2:A:295:MET:HE1	1.97	0.47
2:A:299:TYR:OH	6:G:337:GLU:OE2	2.31	0.47
3:B:9:VAL:HG13	3:B:11:ILE:HD11	1.97	0.47
5:E:229:ILE:HG22	5:E:384:THR:HG21	1.97	0.46
6:G:354:LYS:NZ	9:Z:187:ASP:OD1	2.34	0.46
7:h:200:VAL:HG11	7:h:353:ILE:HG22	1.97	0.46
9:z:84:GLN:HG2	9:z:95:ASN:OD1	2.15	0.46
5:E:115:ALA:O	5:E:119:GLU:HG2	2.15	0.46
9:Z:211:VAL:HG23	9:Z:373:THR:HG21	1.96	0.46
5:e:97:SER:HB3	7:h:202:GLY:HA2	1.97	0.46
7:h:145:LYS:HD2	7:h:147:ASP:N	2.28	0.46
9:z:140:SER:HA	9:z:406:CYS:HA	1.97	0.46
2:A:39:VAL:HG21	2:A:456:ALA:HB2	1.97	0.46
5:E:255:PHE:HB2	5:E:306:PHE:CB	2.45	0.46
6:G:17:GLU:N	6:G:17:GLU:OE1	2.48	0.46
4:d:134:SER:HG	4:d:527:ARG:HE	1.55	0.46
6:g:133:MET:HE2	6:g:506:TYR:CD1	2.50	0.46
5:E:109:VAL:HG13	5:E:516:GLN:HG2	1.97	0.46
4:d:266:VAL:HG13	4:d:271:GLN:HB2	1.98	0.46
6:g:90:GLU:HG3	6:g:91:VAL:HG13	1.98	0.46
6:g:137:LEU:HD11	6:g:506:TYR:CD1	2.49	0.46
7:h:168:ILE:HG21	7:h:385:THR:HG23	1.97	0.46
8:q:156:ASP:OD1	8:q:157:ILE:N	2.48	0.46
9:z:233:CYS:SG	9:z:293:ASN:ND2	2.89	0.46
2:a:450:ASN:OD1	2:a:460:SER:OG	2.33	0.46
5:E:526:MET:HE3	7:H:381:PHE:HD2	1.81	0.46
9:z:186:ILE:HD11	9:z:402:ILE:HG21	1.98	0.46
10:D:601:ADP:O2B	12:D:603:AF3:F1	2.24	0.46
7:H:187:ASP:OD1	7:H:187:ASP:N	2.45	0.46
5:e:289:ILE:HG13	5:e:313:LEU:HB3	1.97	0.46
1:N:207:ASP:OD1	1:N:207:ASP:N	2.49	0.46
7:H:2:MET:HE1	9:z:7:LEU:HD23	1.98	0.46
8:Q:418:GLU:OE1	8:Q:471:HIS:ND1	2.43	0.46
8:q:33:ILE:HD13	8:q:116:GLU:HB2	1.97	0.46
8:q:190:ILE:HG22	8:q:191:PHE:N	2.30	0.46
8:Q:402:LEU:HD21	8:Q:408:LEU:HD21	1.98	0.46
9:Z:415:GLU:OE2	9:Z:447:ILE:HB	2.16	0.46
2:A:397:CYS:O	2:A:401:ARG:HG2	2.16	0.46
3:B:3:SER:HB3	3:B:6:LEU:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:220:VAL:HB	2:a:225:MET:HE3	1.96	0.46
3:b:45:PRO:HG3	10:b:601:ADP:C5	2.51	0.46
2:A:292:ILE:HG23	2:A:296:CYS:HB2	1.96	0.45
7:H:1:MET:HE3	6:g:21:LYS:HB3	1.97	0.45
5:e:255:PHE:HB2	5:e:306:PHE:HB2	1.97	0.45
3:B:40:LYS:HD2	3:B:449:ILE:HD13	1.98	0.45
3:B:516:ARG:NH2	5:E:58:ASP:OD1	2.44	0.45
5:E:81:MET:HG2	5:E:83:VAL:HG13	1.98	0.45
5:E:157:VAL:HG12	5:E:157:VAL:O	2.17	0.45
8:Q:38:GLU:O	8:Q:42:THR:HG23	2.15	0.45
8:Q:218:LEU:HD21	8:Q:362:VAL:HG13	1.98	0.45
3:b:122:HIS:CD2	3:b:124:GLN:HB2	2.50	0.45
9:z:159:LYS:HD3	9:z:159:LYS:HA	1.64	0.45
2:A:127:GLU:HG3	2:A:426:TYR:CZ	2.51	0.45
2:A:533:LEU:HD13	4:D:82:GLN:HG2	1.99	0.45
4:D:490:THR:OG1	4:D:502:ASN:OD1	2.33	0.45
5:E:306:PHE:CE2	5:E:323:ARG:HB3	2.52	0.45
6:G:83:ILE:HD13	6:G:512:THR:HG21	1.98	0.45
7:H:205:LEU:HD21	7:H:381:PHE:CE1	2.52	0.45
3:b:167:LEU:HD22	3:b:172:LEU:HD12	1.98	0.45
4:d:316:PHE:O	4:d:320:MET:HG3	2.16	0.45
3:B:66:ASP:OD1	12:B:603:AF3:F2	2.25	0.45
3:B:293:ARG:HA	3:B:315:ALA:O	2.15	0.45
5:E:185:MET:HE1	5:E:222:THR:HG21	1.98	0.45
4:d:490:THR:HB	4:d:504:LEU:HD23	1.97	0.45
8:q:136:CYS:SG	8:q:512:THR:HG21	2.56	0.45
4:D:169:THR:HA	4:D:172:ASN:OD1	2.16	0.45
3:b:293:ARG:HA	3:b:315:ALA:O	2.17	0.45
3:b:293:ARG:HH21	3:b:294:GLN:HE21	1.64	0.45
4:d:134:SER:OG	4:d:527:ARG:NE	2.31	0.45
6:g:228:ARG:NH2	6:g:305:MET:SD	2.80	0.45
4:D:103:GLY:HA3	4:D:410:CYS:HB3	1.99	0.45
6:G:43:PRO:HA	6:G:162:THR:HA	1.97	0.45
8:Q:33:ILE:HG21	8:Q:116:GLU:HB2	1.99	0.45
8:Q:191:PHE:HB2	8:Q:197:PHE:HD1	1.82	0.45
4:d:165:ASN:CG	4:d:507:LEU:HD12	2.41	0.45
6:G:49:MET:HE3	9:Z:518:VAL:HG11	1.99	0.45
2:a:234:ILE:N	2:a:346:GLY:O	2.49	0.45
2:a:266:ARG:HA	2:a:269:ASP:HB2	1.99	0.45
5:e:196:VAL:O	5:e:196:VAL:HG23	2.17	0.45
5:E:28:LEU:HB3	5:E:33:ALA:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:32:THR:HG23	9:Z:3:ALA:HB1	1.97	0.45
6:G:232:TYR:HD2	6:G:351:GLU:HG3	1.82	0.45
7:H:8:LEU:HA	8:Q:80:HIS:HB2	1.99	0.45
3:b:33:ILE:HD11	3:b:111:ARG:HB2	1.99	0.45
7:h:323:MET:HE2	7:h:330:ILE:H	1.82	0.45
3:b:255:ARG:HD3	5:e:265:LYS:HD2	1.98	0.45
5:e:255:PHE:HB2	5:e:306:PHE:CB	2.47	0.45
5:e:284:LYS:HD2	5:e:284:LYS:HA	1.76	0.45
5:e:444:GLU:O	5:e:448:MET:HG2	2.17	0.45
6:g:447:ILE:HB	6:g:448:PRO:HD3	1.99	0.45
9:z:161:HIS:ND1	9:z:162:ALA:N	2.65	0.45
4:D:144:GLY:HA2	4:D:432:LEU:HD11	1.99	0.45
6:g:182:MET:HE3	6:g:369:PRO:HG2	1.98	0.45
2:A:205:GLN:HG3	6:G:511:GLU:OE2	2.17	0.44
5:E:367:THR:HG23	5:E:369:ASP:H	1.82	0.44
8:Q:222:VAL:HG22	8:Q:362:VAL:HG22	1.99	0.44
9:Z:244:VAL:HG12	9:Z:244:VAL:O	2.17	0.44
2:a:74:VAL:HG13	4:d:394:ASN:HD22	1.82	0.44
3:b:323:LEU:O	3:b:327:THR:OG1	2.29	0.44
4:d:73:ASP:OD1	12:d:603:AF3:F2	2.25	0.44
5:e:157:VAL:HG12	5:e:157:VAL:O	2.17	0.44
8:q:497:ILE:HD13	10:q:601:ADP:C6	2.52	0.44
5:E:132:ARG:NH2	5:E:443:LEU:HD22	2.33	0.44
7:H:97:VAL:HG12	7:H:502:ALA:HA	1.99	0.44
9:Z:194:MET:HE1	9:Z:213:ASP:HB3	1.98	0.44
3:b:516:ARG:NH2	5:e:58:ASP:OD1	2.49	0.44
6:g:41:LEU:HD22	6:g:450:THR:HG23	2.00	0.44
2:A:238:ASP:HB3	2:A:329:SER:HA	1.99	0.44
6:G:182:MET:HE1	6:G:216:ARG:HA	1.99	0.44
7:H:205:LEU:HD21	7:H:381:PHE:HE1	1.83	0.44
9:Z:159:LYS:NZ	10:Z:601:ADP:O2B	2.36	0.44
6:g:78:LYS:O	6:g:82:GLU:HG2	2.18	0.44
6:G:253:GLN:O	6:G:253:GLN:HG3	2.17	0.44
3:b:521:ILE:HB	5:e:61:MET:SD	2.58	0.44
4:d:257:LYS:HD2	4:d:306:ARG:HD3	1.99	0.44
5:e:78:LEU:HD23	5:e:81:MET:SD	2.57	0.44
6:g:182:MET:HE2	6:g:372:CYS:HB3	1.99	0.44
6:G:291:ILE:HG12	6:G:312:ILE:HD13	1.98	0.44
9:Z:492:VAL:HG23	9:Z:494:VAL:HG23	1.99	0.44
2:a:69:HIS:HD1	2:a:71:ALA:H	1.65	0.44
5:e:53:GLY:H	10:e:601:ADP:H5'1	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:415:GLU:OE2	9:Z:448:PRO:HD3	2.17	0.44
3:b:245:ASP:HB2	3:b:297:TYR:CZ	2.53	0.44
5:e:223:LYS:HE3	5:e:225:ILE:HD11	1.99	0.44
7:h:338:SER:OG	7:h:340:ASP:OD1	2.26	0.44
7:h:525:SER:HB2	8:q:59:HIS:HB2	2.00	0.44
9:z:134:LEU:HA	9:z:137:VAL:HG12	1.99	0.44
3:B:187:VAL:HG21	3:B:397:LEU:HB2	1.99	0.44
7:H:442:LEU:HD23	7:H:442:LEU:HA	1.87	0.44
7:h:104:PHE:O	7:h:108:VAL:HG22	2.18	0.44
8:q:176:GLU:OE1	8:q:176:GLU:N	2.43	0.44
2:A:233:LYS:HB2	2:A:283:ALA:HA	1.99	0.44
3:B:260:SER:HB2	4:D:278:GLU:OE1	2.17	0.44
9:Z:23:ASN:OD1	9:Z:73:THR:OG1	2.36	0.44
2:a:160:ILE:HD12	6:g:518:ARG:HG3	2.00	0.44
6:g:226:HIS:HB3	6:g:305:MET:HE1	1.99	0.44
7:h:163:LEU:HD22	7:h:168:ILE:HD11	1.99	0.44
8:q:225:LYS:HB3	8:q:225:LYS:HE3	1.66	0.44
6:G:33:ILE:HG21	6:G:80:MET:HB3	1.99	0.44
6:G:236:PRO:HG3	6:G:350:LEU:HB2	2.00	0.44
6:G:258:ILE:HG23	6:G:263:ASP:HB2	2.00	0.44
7:H:259:THR:HG22	7:H:261:GLU:H	1.83	0.44
2:a:199:LYS:HB3	2:a:385:CYS:HB3	1.99	0.44
3:b:187:VAL:HG21	3:b:397:LEU:HB2	2.00	0.44
4:d:170:SER:HB3	4:d:411:VAL:HG21	1.99	0.44
5:e:101:GLU:OE1	7:h:375:ARG:NH2	2.51	0.44
6:g:83:ILE:HG23	6:g:508:THR:HG22	2.00	0.44
7:h:297:ASP:OD1	7:h:297:ASP:N	2.51	0.44
8:q:16:LYS:HE3	9:z:70:GLN:HG3	1.99	0.44
3:B:224:ILE:HD12	3:B:230:LYS:HD3	2.00	0.43
5:E:454:ALA:O	5:E:457:VAL:HG12	2.18	0.43
6:G:462:LEU:HD23	6:G:462:LEU:HA	1.91	0.43
2:a:193:ASN:O	2:a:318:ARG:NH2	2.51	0.43
5:e:402:LEU:HD23	5:e:402:LEU:HA	1.85	0.43
4:D:73:ASP:OD1	12:D:603:AF3:F3	2.26	0.43
4:D:240:ARG:NH1	4:D:242:GLU:OE2	2.30	0.43
6:G:137:LEU:HD11	6:G:506:TYR:CD1	2.53	0.43
8:Q:131:GLY:HA3	8:Q:437:ALA:HB3	2.00	0.43
9:Z:165:ALA:O	9:Z:169:THR:HG23	2.18	0.43
7:h:324:MET:HE3	7:h:368:LYS:HB2	2.01	0.43
9:Z:2:ALA:HB3	9:Z:5:LYS:HG3	1.99	0.43
9:Z:331:VAL:HB	9:Z:343:CYS:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:g:226:HIS:CG	6:g:227:PRO:HD2	2.53	0.43
7:h:73:HIS:HB3	7:h:76:ALA:HB3	2.00	0.43
8:q:348:ASP:OD2	8:q:366:GLU:N	2.44	0.43
9:z:133:PHE:O	9:z:136:GLU:HG3	2.19	0.43
2:A:143:LEU:HB2	2:A:147:CYS:HB2	1.99	0.43
2:A:355:ARG:NH2	2:A:358:ASP:OD1	2.46	0.43
9:Z:236:SER:O	9:Z:270:ARG:NH2	2.51	0.43
3:b:413:SER:O	3:b:416:LEU:HG	2.19	0.43
3:B:242:THR:HG21	3:B:335:PHE:CE2	2.54	0.43
5:E:101:GLU:HG2	5:E:515:GLN:NE2	2.34	0.43
6:G:7:VAL:H	5:e:7:LEU:HD21	1.84	0.43
3:b:58:ASP:OD1	3:b:58:ASP:N	2.48	0.43
5:e:457:VAL:HA	5:e:460:MET:HE3	1.99	0.43
7:h:398:ARG:HB3	7:h:497:MET:SD	2.59	0.43
7:h:413:GLU:OE2	7:h:499:ARG:NE	2.51	0.43
9:z:168:LEU:O	9:z:172:VAL:HG12	2.18	0.43
9:z:487:MET:HE2	9:z:492:VAL:HG21	2.01	0.43
2:A:246:MET:HE2	2:A:250:VAL:HG11	2.00	0.43
2:A:402:VAL:HG23	2:A:506:PRO:HG3	2.01	0.43
3:B:19:GLU:OE2	3:B:522:LYS:NZ	2.40	0.43
3:B:326:VAL:HB	3:B:370:ALA:HB3	2.00	0.43
3:b:168:SER:OG	10:b:601:ADP:N7	2.40	0.43
5:e:37:HIS:NE2	5:e:533:ILE:HD11	2.34	0.43
5:e:426:GLU:OE2	5:e:426:GLU:N	2.52	0.43
2:A:179:ILE:HD13	2:A:195:VAL:HG23	2.00	0.43
4:D:271:GLN:O	4:D:275:VAL:HG23	2.19	0.43
8:Q:270:LYS:O	8:Q:274:ASN:ND2	2.34	0.43
9:Z:375:LEU:HD12	9:Z:375:LEU:HA	1.85	0.43
5:e:77:ILE:O	5:e:81:MET:HG3	2.19	0.43
8:q:131:GLY:HA3	8:q:437:ALA:HB3	1.99	0.43
2:A:297:LEU:HD11	2:A:309:ARG:HH12	1.84	0.43
4:D:395:LYS:O	4:D:399:GLU:HG2	2.19	0.43
9:Z:35:ARG:HH21	9:Z:453:GLN:CD	2.27	0.43
2:a:171:MET:HG3	2:a:210:LEU:HB2	2.01	0.43
2:a:397:CYS:O	2:a:401:ARG:HG2	2.19	0.43
3:b:182:LEU:HD11	3:b:214:LEU:N	2.33	0.43
4:d:224:VAL:HG23	4:d:377:THR:HG22	2.00	0.43
5:e:145:ILE:HG23	5:e:514:LYS:HD2	1.99	0.43
7:h:18:GLY:O	7:h:21:GLN:HG3	2.19	0.43
8:q:151:ALA:O	8:q:152:LYS:HG2	2.18	0.43
2:A:266:ARG:HA	2:A:269:ASP:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:167:LEU:HD22	3:B:172:LEU:HD12	2.01	0.43
4:D:224:VAL:HG12	4:D:226:GLY:H	1.84	0.43
5:E:145:ILE:HG23	5:E:514:LYS:HD2	2.00	0.43
6:G:109:ALA:HB2	6:G:126:TYR:OH	2.19	0.43
2:a:310:ARG:HA	2:a:310:ARG:HD3	1.80	0.43
6:g:243:SER:OG	6:g:333:SER:O	2.24	0.43
9:z:3:ALA:O	9:z:6:THR:OG1	2.32	0.43
9:z:236:SER:O	9:z:270:ARG:NH2	2.52	0.43
9:z:376:ILE:HG22	9:z:384:LEU:HD22	2.00	0.43
4:D:42:LYS:HZ3	4:D:46:ASP:CG	2.26	0.42
3:b:317:PHE:O	3:b:321:GLU:HG3	2.19	0.42
4:d:512:LEU:C	4:d:514:VAL:H	2.27	0.42
6:g:217:GLY:HA3	6:g:363:ILE:O	2.20	0.42
3:B:12:PHE:HB3	3:B:16:ALA:HB3	2.00	0.42
3:B:232:ILE:HD13	3:B:288:ASN:HB3	2.01	0.42
3:B:323:LEU:HA	3:B:326:VAL:HG12	2.00	0.42
6:G:83:ILE:HG13	6:G:84:SER:N	2.35	0.42
6:G:167:ARG:NH1	9:Z:124:GLU:OE1	2.49	0.42
7:H:189:LEU:HD22	7:H:191:GLN:HE21	1.84	0.42
9:Z:33:VAL:HG11	9:Z:67:MET:SD	2.60	0.42
9:Z:75:SER:O	9:Z:79:LYS:HG2	2.19	0.42
9:Z:175:SER:HB2	9:Z:206:LEU:HD13	2.00	0.42
9:z:206:LEU:HD23	9:z:208:ARG:HH12	1.84	0.42
2:A:216:LEU:HB2	2:A:362:ILE:HB	2.01	0.42
3:B:54:SER:HA	4:D:538:THR:HB	2.00	0.42
7:H:279:GLU:HG3	7:H:283:HIS:CD2	2.52	0.42
8:Q:259:ILE:HG21	8:Q:265:LEU:HB2	2.00	0.42
9:Z:154:THR:HG21	9:Z:494:VAL:HA	2.00	0.42
9:Z:221:MET:HE1	9:Z:312:ALA:HB3	2.00	0.42
3:b:20:ARG:HD2	3:b:20:ARG:HA	1.82	0.42
8:q:43:THR:HG21	8:q:105:LEU:HD22	2.00	0.42
8:q:101:THR:N	12:q:603:AF3:F1	2.33	0.42
8:q:509:LYS:HB2	8:q:509:LYS:HE2	1.83	0.42
2:A:184:ILE:O	2:A:185:ARG:HG2	2.20	0.42
8:Q:10:GLY:O	8:Q:14:MET:HG3	2.19	0.42
3:b:509:GLU:O	3:b:513:VAL:HG13	2.20	0.42
7:h:118:PRO:HB3	7:h:514:VAL:HG12	2.01	0.42
2:A:23:MET:HE2	5:e:8:ALA:HA	2.00	0.42
3:B:156:ARG:NH2	3:B:185:GLU:OE2	2.46	0.42
5:E:193:VAL:HG21	5:E:409:ILE:HB	2.00	0.42
5:E:533:ILE:HD13	7:H:48:LEU:HD22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:340:VAL:HG22	8:Q:343:GLU:CD	2.45	0.42
3:b:18:GLU:OE2	3:b:519:ASN:ND2	2.48	0.42
5:e:402:LEU:O	5:e:406:LEU:HG	2.18	0.42
7:h:30:GLN:OE1	7:h:106:LYS:HB2	2.19	0.42
8:q:65:VAL:HG12	8:q:383:ASN:HB3	2.01	0.42
3:B:480:MET:HE2	3:B:480:MET:HA	2.02	0.42
7:H:19:ILE:HD12	7:H:19:ILE:H	1.83	0.42
8:Q:393:ASP:O	8:Q:397:ASN:ND2	2.53	0.42
3:b:259:ASP:OD1	3:b:259:ASP:N	2.53	0.42
5:e:299:LEU:HD12	5:e:320:PRO:O	2.18	0.42
6:g:27:ILE:HG21	6:g:110:GLU:HB2	2.02	0.42
8:q:45:THR:OG1	8:q:54:LYS:NZ	2.29	0.42
3:B:223:LYS:HB2	3:B:223:LYS:HE3	1.89	0.42
5:E:198:ASP:OD2	5:E:202:ARG:HD3	2.19	0.42
6:G:207:GLY:O	9:Z:503:GLN:NE2	2.42	0.42
9:Z:130:ALA:HB1	9:Z:418:MET:HE2	2.01	0.42
2:a:160:ILE:HG23	2:a:161:ILE:HG23	2.02	0.42
7:h:273:ILE:HD11	8:q:266:MET:HA	2.01	0.42
2:A:74:VAL:HG13	4:D:394:ASN:HD22	1.85	0.42
5:E:104:ASP:OD1	5:E:105:GLY:N	2.51	0.42
6:G:473:GLU:HG2	6:G:474:ASN:N	2.35	0.42
8:Q:248:GLY:N	8:Q:276:MET:HE1	2.34	0.42
2:a:66:GLU:HG3	6:g:526:HIS:HB2	2.02	0.42
3:b:40:LYS:C	3:b:42:THR:H	2.27	0.42
6:g:435:TRP:HB2	6:g:436:PRO:HD3	2.01	0.42
3:B:40:LYS:C	3:B:42:THR:H	2.28	0.42
3:B:45:PRO:HG3	10:B:601:ADP:C5	2.55	0.42
3:B:204:LYS:NZ	3:B:357:ASP:OD2	2.44	0.42
3:B:290:PHE:CE2	3:B:292:ASN:HB2	2.55	0.42
8:Q:191:PHE:HB2	8:Q:197:PHE:CD1	2.55	0.42
3:b:151:ASP:HB3	3:b:154:LYS:HB2	2.01	0.42
4:d:34:ARG:NE	4:d:130:PRO:HG3	2.35	0.42
5:e:412:LEU:HD23	5:e:412:LEU:HA	1.90	0.42
6:g:266:ARG:HD2	6:g:266:ARG:HA	1.67	0.42
3:B:90:VAL:HG21	5:E:391:ASN:HA	2.02	0.42
3:B:484:THR:OG1	3:B:485:ILE:N	2.53	0.42
4:D:408:ALA:O	4:D:412:ILE:HG12	2.19	0.42
5:E:229:ILE:HG12	5:E:371:MET:HE2	2.01	0.42
7:H:26:ILE:O	7:H:30:GLN:HG2	2.20	0.42
7:H:183:VAL:HG11	7:H:396:VAL:HG12	2.02	0.42
7:H:427:ILE:HD11	7:H:432:GLN:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:444:LEU:HD23	9:Z:444:LEU:HA	1.89	0.42
6:g:41:LEU:HD13	6:g:100:ILE:HD12	2.02	0.42
8:q:412:GLY:N	10:q:601:ADP:O2'	2.38	0.42
3:B:137:ALA:HB1	3:B:417:MET:HB3	2.01	0.41
5:E:203:ASP:OD2	7:H:357:ARG:NH2	2.38	0.41
8:Q:11:PHE:HE1	9:Z:69:ILE:HD11	1.85	0.41
6:g:178:ASP:O	6:g:182:MET:HG2	2.20	0.41
2:A:427:ALA:O	2:A:435:GLN:HG2	2.20	0.41
3:b:323:LEU:HA	3:b:326:VAL:HG12	2.01	0.41
6:g:224:VAL:HB	6:g:229:MET:HE3	2.01	0.41
6:g:352:ILE:HG22	6:g:359:TYR:HD1	1.85	0.41
7:h:136:ILE:HD11	7:h:416:LEU:HD11	2.02	0.41
4:d:534:ASP:OD1	4:d:535:VAL:N	2.53	0.41
5:e:196:VAL:HG12	5:e:381:ARG:O	2.20	0.41
6:g:20:ARG:HG2	6:g:20:ARG:NH1	2.34	0.41
6:g:411:GLY:N	10:g:601:ADP:O2'	2.34	0.41
9:z:218:HIS:CD2	9:z:220:ASP:HB2	2.55	0.41
9:z:237:LEU:HB2	9:z:297:ILE:HG12	2.02	0.41
1:N:199:SER:OG	1:N:200:ALA:N	2.53	0.41
1:N:219:CYS:SG	1:N:233:PHE:HB2	2.60	0.41
2:A:349:GLU:HB3	2:A:366:ASN:HB2	2.01	0.41
2:A:529:ASP:OD2	2:A:530:LEU:N	2.52	0.41
3:B:42:THR:HB	3:B:65:ASN:OD1	2.20	0.41
3:B:264:VAL:HG12	4:D:256:PRO:HB2	2.02	0.41
4:D:435:ARG:HA	4:D:435:ARG:HD3	1.84	0.41
7:H:499:ARG:HA	7:H:499:ARG:HD3	1.87	0.41
3:b:29:PHE:O	3:b:33:ILE:HG12	2.20	0.41
5:e:257:PRO:HA	5:e:258:PRO:HD3	1.95	0.41
6:g:36:ILE:HG22	6:g:37:ILE:HG23	2.01	0.41
8:q:55:MET:HG2	8:q:65:VAL:HB	2.03	0.41
8:q:151:ALA:HB3	8:q:406:LYS:HB3	2.02	0.41
2:A:254:ILE:HD11	2:A:263:ILE:HD12	2.03	0.41
5:E:10:ASP:OD2	7:H:24:SER:OG	2.31	0.41
6:G:47:MET:HE2	6:G:59:MET:HG2	2.03	0.41
8:Q:70:ALA:HB2	8:Q:101:THR:HG21	2.02	0.41
2:a:322:ALA:HA	2:a:370:ARG:HB3	2.03	0.41
2:a:448:ILE:O	2:a:452:LEU:HG	2.19	0.41
4:d:191:VAL:HG21	4:d:412:ILE:HB	2.03	0.41
3:B:500:LYS:HA	3:B:500:LYS:HD3	1.95	0.41
4:D:176:VAL:O	4:D:176:VAL:HG23	2.21	0.41
4:D:337:CYS:SG	4:D:344:PRO:HD3	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:203:ARG:H	2:a:203:ARG:HG3	1.67	0.41
4:d:53:GLY:H	10:d:601:ADP:H5'1	1.86	0.41
4:D:134:SER:HB2	4:D:527:ARG:HE	1.85	0.41
5:E:101:GLU:OE1	7:H:375:ARG:NH2	2.53	0.41
5:E:123:LEU:HD22	5:E:128:ILE:HD12	2.01	0.41
9:Z:194:MET:HE2	9:Z:360:PHE:HE2	1.86	0.41
9:Z:504:LEU:HD23	9:Z:504:LEU:HA	1.92	0.41
6:g:43:PRO:HA	6:g:162:THR:HA	2.01	0.41
5:E:251:LEU:HD23	5:E:342:VAL:HB	2.01	0.41
6:G:129:ALA:O	6:G:133:MET:HG3	2.20	0.41
6:G:266:ARG:HG3	6:G:270:MET:HE2	2.02	0.41
8:Q:82:ALA:O	8:Q:86:ILE:HG12	2.20	0.41
8:Q:384:LEU:O	8:Q:388:ILE:HG12	2.21	0.41
4:d:115:SER:OG	4:d:460:VAL:HG11	2.21	0.41
5:E:284:LYS:HD2	5:E:284:LYS:HA	1.70	0.41
7:H:40:LEU:HD13	7:H:99:LEU:HD12	2.03	0.41
7:H:364:CYS:HB2	7:H:367:ALA:HB2	2.03	0.41
8:Q:164:LEU:O	8:Q:168:ILE:HG12	2.20	0.41
9:Z:45:LYS:HG3	9:Z:63:LEU:HD22	2.02	0.41
9:Z:130:ALA:HB1	9:Z:418:MET:CE	2.50	0.41
9:Z:248:PHE:CD1	9:Z:259:LEU:HD13	2.56	0.41
2:a:130:ARG:NH2	2:a:422:TYR:OH	2.54	0.41
2:a:446:LEU:HD11	2:a:468:ARG:HD2	2.03	0.41
3:b:402:LYS:HB2	3:b:402:LYS:HE3	1.90	0.41
4:d:78:LEU:HD23	4:d:78:LEU:HA	1.86	0.41
5:e:227:GLY:HA3	5:e:374:ILE:O	2.21	0.41
5:e:440:CYS:SG	5:e:444:GLU:HB2	2.61	0.41
6:g:232:TYR:HD2	6:g:351:GLU:HG3	1.86	0.41
6:g:521:ASP:OD1	6:g:522:ILE:N	2.54	0.41
9:z:429:VAL:HG21	9:z:437:VAL:HG21	2.03	0.41
3:B:79:PRO:O	3:B:83:VAL:HG23	2.21	0.41
7:H:199:LYS:HB3	7:H:382:MET:SD	2.61	0.41
7:H:319:LEU:HD23	7:H:319:LEU:HA	1.96	0.41
8:Q:151:ALA:O	8:Q:152:LYS:HG2	2.21	0.41
2:a:266:ARG:HA	2:a:266:ARG:HD2	1.92	0.41
2:a:508:ILE:HD12	2:a:508:ILE:HA	1.90	0.41
3:b:243:GLY:HA2	3:b:294:GLN:OE1	2.21	0.41
3:b:518:ASP:HB3	5:e:57:LEU:HD13	2.03	0.41
6:g:463:LEU:HD23	6:g:463:LEU:HA	1.91	0.41
9:z:165:ALA:O	9:z:169:THR:HG23	2.21	0.41
3:B:187:VAL:HG23	3:B:394:LEU:HD23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:249:LYS:NZ	9:Z:243:GLU:O	2.42	0.40
6:G:449:ARG:HG3	6:G:459:THR:HG21	2.02	0.40
8:Q:65:VAL:HG12	8:Q:383:ASN:HB3	2.03	0.40
2:a:514:LEU:HD23	2:a:514:LEU:HA	1.92	0.40
4:d:435:ARG:HA	4:d:435:ARG:HD3	1.80	0.40
6:g:226:HIS:HB3	6:g:305:MET:CE	2.51	0.40
6:g:267:ILE:HD13	6:g:267:ILE:HA	1.94	0.40
6:g:391:LEU:HD23	6:g:391:LEU:HA	1.89	0.40
9:z:144:ASP:OD1	9:z:144:ASP:N	2.52	0.40
3:B:50:LYS:O	3:B:63:VAL:HA	2.21	0.40
3:B:113:ALA:HB2	3:B:130:TRP:HH2	1.84	0.40
5:E:299:LEU:HD12	5:E:320:PRO:O	2.21	0.40
6:G:256:ILE:HD11	9:Z:244:VAL:HB	2.04	0.40
6:G:426:SER:HA	6:G:429:MET:HE2	2.03	0.40
8:Q:333:LEU:HD11	8:Q:339:PRO:HB3	2.02	0.40
4:d:152:SER:HA	4:d:422:ILE:HG22	2.03	0.40
7:h:187:ASP:OD1	7:h:187:ASP:N	2.48	0.40
8:q:416:GLU:OE2	8:q:416:GLU:N	2.52	0.40
5:E:215:VAL:HA	5:E:395:ILE:HD11	2.03	0.40
9:Z:445:LEU:HD22	9:Z:463:LEU:HD11	2.02	0.40
2:a:22:VAL:HG21	2:a:105:ASP:CB	2.51	0.40
4:d:248:LEU:HD21	4:d:333:ILE:HD12	2.02	0.40
5:e:236:HIS:HB3	5:e:239:MET:HG3	2.04	0.40
6:g:106:LEU:HD23	6:g:106:LEU:HA	1.95	0.40
6:g:278:LEU:HD23	6:g:278:LEU:HA	1.94	0.40
7:h:232:TYR:HD1	7:h:348:PHE:HD2	1.70	0.40
8:q:367:LYS:HG3	8:q:369:ASP:HB2	2.03	0.40
9:z:67:MET:HB3	9:z:69:ILE:HG12	2.04	0.40
4:D:256:PRO:HD3	4:D:282:TYR:CD2	2.57	0.40
7:H:337:LEU:HD23	7:H:337:LEU:HA	1.86	0.40
3:b:19:GLU:OE2	3:b:27:THR:HG21	2.22	0.40
4:d:71:THR:HA	4:d:400:GLU:OE1	2.21	0.40
6:g:219:MET:H	6:g:373:THR:HG21	1.86	0.40
6:g:226:HIS:CG	6:g:305:MET:HE1	2.57	0.40
6:g:275:ILE:HD13	6:g:275:ILE:HA	1.91	0.40
2:A:31:ILE:O	2:A:43:LYS:HE3	2.21	0.40
2:A:526:ARG:NH1	4:D:175:VAL:HA	2.36	0.40
4:D:249:ILE:HD12	4:D:251:PHE:CE2	2.56	0.40
7:H:409:GLY:HA3	7:H:487:ASN:ND2	2.37	0.40
7:H:501:ASN:C	7:H:501:ASN:HD22	2.29	0.40
8:Q:43:THR:HB	8:Q:105:LEU:HD23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:22:VAL:HG21	2:a:105:ASP:HB2	2.02	0.40
3:b:290:PHE:CE2	3:b:292:ASN:HB2	2.57	0.40
3:b:373:ILE:HD13	3:b:390:LEU:HD21	2.04	0.40
4:d:94:LEU:HD11	4:d:521:LEU:HB3	2.03	0.40
4:d:124:LEU:HD21	4:d:130:PRO:HB3	2.03	0.40
5:e:441:PRO:O	5:e:445:GLN:HG3	2.21	0.40
6:g:49:MET:HG3	9:z:518:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	N	53/395 (13%)	48 (91%)	5 (9%)	0	100	100
2	A	534/536 (100%)	512 (96%)	22 (4%)	0	100	100
2	a	530/536 (99%)	511 (96%)	19 (4%)	0	100	100
3	B	524/526 (100%)	508 (97%)	16 (3%)	0	100	100
3	b	523/526 (99%)	507 (97%)	16 (3%)	0	100	100
4	D	518/520 (100%)	506 (98%)	12 (2%)	0	100	100
4	d	518/520 (100%)	494 (95%)	24 (5%)	0	100	100
5	E	534/540 (99%)	519 (97%)	15 (3%)	0	100	100
5	e	539/540 (100%)	522 (97%)	17 (3%)	0	100	100
6	G	524/528 (99%)	508 (97%)	16 (3%)	0	100	100
6	g	521/528 (99%)	507 (97%)	14 (3%)	0	100	100
7	H	526/528 (100%)	508 (97%)	18 (3%)	0	100	100
7	h	523/528 (99%)	504 (96%)	19 (4%)	0	100	100
8	Q	536/538 (100%)	522 (97%)	14 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	q	531/538 (99%)	518 (98%)	13 (2%)	0	100	100
9	Z	523/527 (99%)	509 (97%)	14 (3%)	0	100	100
9	z	525/527 (100%)	513 (98%)	12 (2%)	0	100	100
All	All	8482/8881 (96%)	8216 (97%)	266 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	N	54/334 (16%)	54 (100%)	0	100	100
2	A	447/447 (100%)	447 (100%)	0	100	100
2	a	444/447 (99%)	444 (100%)	0	100	100
3	B	418/418 (100%)	418 (100%)	0	100	100
3	b	417/418 (100%)	417 (100%)	0	100	100
4	D	442/442 (100%)	442 (100%)	0	100	100
4	d	441/442 (100%)	441 (100%)	0	100	100
5	E	452/455 (99%)	452 (100%)	0	100	100
5	e	456/455 (100%)	456 (100%)	0	100	100
6	G	456/457 (100%)	456 (100%)	0	100	100
6	g	453/457 (99%)	453 (100%)	0	100	100
7	H	435/435 (100%)	435 (100%)	0	100	100
7	h	432/435 (99%)	432 (100%)	0	100	100
8	Q	442/442 (100%)	442 (100%)	0	100	100
8	q	438/442 (99%)	438 (100%)	0	100	100
9	Z	437/439 (100%)	437 (100%)	0	100	100
9	z	438/439 (100%)	438 (100%)	0	100	100
All	All	7102/7404 (96%)	7102 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	193	ASN
2	A	262	GLN
2	A	284	ASN
2	A	353	GLN
2	A	393	HIS
3	B	78	ASN
3	B	337	HIS
3	B	380	GLN
4	D	25	GLN
4	D	165	ASN
4	D	262	ASN
4	D	263	GLN
4	D	350	GLN
5	E	55	ASN
5	E	291	GLN
5	E	379	ASN
5	E	504	GLN
5	E	515	GLN
6	G	28	ASN
6	G	302	HIS
6	G	390	ASN
6	G	472	GLN
7	H	60	ASN
7	H	107	GLN
7	H	117	HIS
7	H	130	GLN
7	H	282	HIS
7	H	331	GLN
7	H	335	ASN
7	H	352	GLN
7	H	359	ASN
7	H	448	GLN
7	H	459	ASN
8	Q	53	ASN
8	Q	91	HIS
8	Q	140	HIS
8	Q	309	ASN
8	Q	397	ASN
9	Z	70	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	Z	467	GLN
9	Z	482	ASN
9	Z	514	ASN
2	a	193	ASN
2	a	284	ASN
3	b	73	ASN
3	b	285	HIS
3	b	294	GLN
3	b	298	ASN
3	b	337	HIS
4	d	262	ASN
5	e	316	GLN
5	e	504	GLN
5	e	515	GLN
6	g	390	ASN
6	g	400	ASN
6	g	420	HIS
7	h	86	GLN
7	h	359	ASN
8	q	53	ASN
8	q	79	GLN
8	q	91	HIS
8	q	93	GLN
8	q	303	HIS
9	z	61	ASN
9	z	182	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 16 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
10	ADP	a	601	11,12	28,29,29	1.38	4 (14%)	43,45,45	1.81	9 (20%)
10	ADP	z	601	11,12	28,29,29	1.39	4 (14%)	43,45,45	1.84	10 (23%)
10	ADP	B	601	11,12	28,29,29	1.41	4 (14%)	43,45,45	1.82	10 (23%)
10	ADP	g	601	11,12	28,29,29	1.39	5 (17%)	43,45,45	1.82	9 (20%)
12	AF3	d	603	10	0,3,3	-	-	-		
10	ADP	G	601	11,12	28,29,29	1.38	5 (17%)	43,45,45	1.82	10 (23%)
10	ADP	h	601	11,12	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
10	ADP	b	601	11,12	28,29,29	1.40	4 (14%)	43,45,45	1.87	11 (25%)
10	ADP	A	601	11,12	28,29,29	1.38	4 (14%)	43,45,45	1.82	10 (23%)
10	ADP	d	601	11,12	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
10	ADP	e	601	11,12	28,29,29	1.40	4 (14%)	43,45,45	1.83	10 (23%)
12	AF3	Q	603	10	0,3,3	-	-	-		
12	AF3	Z	603	10	0,3,3	-	-	-		
12	AF3	A	603	10	0,3,3	-	-	-		
12	AF3	z	603	10	0,3,3	-	-	-		
12	AF3	h	603	10	0,3,3	-	-	-		
10	ADP	q	601	11,12	28,29,29	1.39	4 (14%)	43,45,45	1.83	10 (23%)
12	AF3	G	603	6,10	0,3,3	-	-	-		
12	AF3	b	603	10	0,3,3	-	-	-		
12	AF3	e	603	10	0,3,3	-	-	-		
12	AF3	H	603	10	0,3,3	-	-	-		
10	ADP	Z	601	11,12	28,29,29	1.38	4 (14%)	43,45,45	1.84	9 (20%)
10	ADP	D	601	11,12	28,29,29	1.39	4 (14%)	43,45,45	1.82	8 (18%)
10	ADP	Q	601	11,12	28,29,29	1.38	4 (14%)	43,45,45	1.83	10 (23%)
12	AF3	q	603	10	0,3,3	-	-	-		
12	AF3	B	603	10	0,3,3	-	-	-		
10	ADP	H	601	11,12	28,29,29	1.41	4 (14%)	43,45,45	1.85	10 (23%)
12	AF3	g	603	10	0,3,3	-	-	-		
12	AF3	E	603	10	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	AF3	D	603	10	0,3,3	-	-	-		
12	AF3	a	603	10,2	0,3,3	-	-	-		
10	ADP	E	601	11,12	28,29,29	1.40	4 (14%)	43,45,45	1.85	10 (23%)

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
10	ADP	a	601	11,12	-	4/16/32/32	0/3/3/3
10	ADP	z	601	11,12	-	2/16/32/32	0/3/3/3
10	ADP	B	601	11,12	-	1/16/32/32	0/3/3/3
10	ADP	g	601	11,12	-	4/16/32/32	0/3/3/3
10	ADP	e	601	11,12	-	1/16/32/32	0/3/3/3
10	ADP	G	601	11,12	-	2/16/32/32	0/3/3/3
10	ADP	Z	601	11,12	-	4/16/32/32	0/3/3/3
10	ADP	h	601	11,12	-	1/16/32/32	0/3/3/3
10	ADP	b	601	11,12	-	1/16/32/32	0/3/3/3
10	ADP	A	601	11,12	-	3/16/32/32	0/3/3/3
10	ADP	D	601	11,12	-	1/16/32/32	0/3/3/3
10	ADP	Q	601	11,12	-	7/16/32/32	0/3/3/3
10	ADP	E	601	11,12	-	2/16/32/32	0/3/3/3
10	ADP	d	601	11,12	-	1/16/32/32	0/3/3/3
10	ADP	H	601	11,12	-	4/16/32/32	0/3/3/3
10	ADP	q	601	11,12	-	5/16/32/32	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	e	601	ADP	C5-C4	4.58	1.47	1.39
10	B	601	ADP	C5-C4	4.57	1.47	1.39
10	E	601	ADP	C5-C4	4.57	1.47	1.39
10	a	601	ADP	C5-C4	4.56	1.47	1.39
10	b	601	ADP	C5-C4	4.56	1.47	1.39
10	z	601	ADP	C5-C4	4.56	1.47	1.39
10	d	601	ADP	C5-C4	4.55	1.47	1.39
10	h	601	ADP	C5-C4	4.55	1.47	1.39
10	Q	601	ADP	C5-C4	4.54	1.47	1.39
10	q	601	ADP	C5-C4	4.53	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	601	ADP	C5-C4	4.53	1.47	1.39
10	D	601	ADP	C5-C4	4.52	1.47	1.39
10	Z	601	ADP	C5-C4	4.52	1.47	1.39
10	H	601	ADP	C5-C4	4.52	1.47	1.39
10	g	601	ADP	C5-C4	4.51	1.47	1.39
10	A	601	ADP	C5-C4	4.50	1.47	1.39
10	B	601	ADP	C5-C6	2.68	1.48	1.41
10	G	601	ADP	C5-C6	2.67	1.48	1.41
10	A	601	ADP	C5-C6	2.67	1.48	1.41
10	D	601	ADP	C5-C6	2.66	1.48	1.41
10	e	601	ADP	C5-C6	2.66	1.48	1.41
10	b	601	ADP	C5-C6	2.66	1.48	1.41
10	h	601	ADP	C5-C6	2.66	1.48	1.41
10	E	601	ADP	C5-C6	2.66	1.48	1.41
10	Q	601	ADP	C5-C6	2.65	1.48	1.41
10	z	601	ADP	C5-C6	2.65	1.48	1.41
10	a	601	ADP	C5-C6	2.64	1.48	1.41
10	Z	601	ADP	C5-C6	2.64	1.48	1.41
10	d	601	ADP	C5-C6	2.64	1.48	1.41
10	H	601	ADP	C5-C6	2.64	1.48	1.41
10	g	601	ADP	C5-C6	2.63	1.48	1.41
10	q	601	ADP	C5-C6	2.62	1.48	1.41
10	q	601	ADP	C5-N7	-2.39	1.34	1.39
10	b	601	ADP	C5-N7	-2.37	1.34	1.39
10	D	601	ADP	C5-N7	-2.36	1.34	1.39
10	Q	601	ADP	C5-N7	-2.35	1.34	1.39
10	a	601	ADP	C5-N7	-2.34	1.34	1.39
10	h	601	ADP	C5-N7	-2.34	1.34	1.39
10	g	601	ADP	C5-N7	-2.34	1.34	1.39
10	q	601	ADP	C8-N7	2.34	1.36	1.31
10	z	601	ADP	C5-N7	-2.34	1.34	1.39
10	h	601	ADP	C8-N7	2.33	1.36	1.31
10	G	601	ADP	C5-N7	-2.33	1.34	1.39
10	A	601	ADP	C5-N7	-2.33	1.34	1.39
10	d	601	ADP	C8-N7	2.32	1.36	1.31
10	H	601	ADP	C5-N7	-2.32	1.34	1.39
10	Q	601	ADP	C8-N7	2.31	1.36	1.31
10	B	601	ADP	C5-N7	-2.31	1.34	1.39
10	B	601	ADP	C8-N7	2.31	1.36	1.31
10	d	601	ADP	C5-N7	-2.31	1.34	1.39
10	e	601	ADP	C5-N7	-2.31	1.34	1.39
10	E	601	ADP	C8-N7	2.31	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	e	601	ADP	C8-N7	2.31	1.36	1.31
10	Z	601	ADP	C5-N7	-2.31	1.34	1.39
10	H	601	ADP	C8-N7	2.31	1.36	1.31
10	a	601	ADP	C8-N7	2.30	1.36	1.31
10	A	601	ADP	C8-N7	2.30	1.36	1.31
10	D	601	ADP	C8-N7	2.30	1.36	1.31
10	E	601	ADP	C5-N7	-2.29	1.34	1.39
10	b	601	ADP	C8-N7	2.28	1.36	1.31
10	z	601	ADP	C8-N7	2.28	1.36	1.31
10	Z	601	ADP	C8-N7	2.27	1.36	1.31
10	g	601	ADP	C8-N7	2.25	1.36	1.31
10	G	601	ADP	C8-N7	2.25	1.36	1.31
10	g	601	ADP	C4-N9	-2.07	1.33	1.37
10	G	601	ADP	C4-N9	-2.01	1.33	1.37

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	601	ADP	C5-C4-N3	-5.92	118.57	126.72
10	d	601	ADP	C5-C4-N3	-5.88	118.61	126.72
10	e	601	ADP	C5-C4-N3	-5.85	118.66	126.72
10	D	601	ADP	C5-C4-N3	-5.84	118.68	126.72
10	b	601	ADP	C5-C4-N3	-5.83	118.69	126.72
10	h	601	ADP	C5-C4-N3	-5.81	118.72	126.72
10	Z	601	ADP	C5-C4-N3	-5.78	118.76	126.72
10	H	601	ADP	C5-C4-N3	-5.78	118.76	126.72
10	Q	601	ADP	C5-C4-N3	-5.78	118.76	126.72
10	z	601	ADP	C5-C4-N3	-5.77	118.77	126.72
10	B	601	ADP	C5-C4-N3	-5.75	118.81	126.72
10	a	601	ADP	C5-C4-N3	-5.74	118.82	126.72
10	q	601	ADP	C5-C4-N3	-5.72	118.83	126.72
10	A	601	ADP	C5-C4-N3	-5.69	118.89	126.72
10	G	601	ADP	C5-C4-N3	-5.69	118.89	126.72
10	g	601	ADP	C5-C4-N3	-5.64	118.94	126.72
10	z	601	ADP	N3-C4-N9	4.62	135.02	127.17
10	E	601	ADP	N3-C4-N9	4.62	135.02	127.17
10	Z	601	ADP	N3-C4-N9	4.59	134.98	127.17
10	e	601	ADP	N3-C4-N9	4.59	134.97	127.17
10	d	601	ADP	N3-C4-N9	4.57	134.94	127.17
10	b	601	ADP	N3-C4-N9	4.56	134.92	127.17
10	D	601	ADP	N3-C4-N9	4.56	134.92	127.17
10	a	601	ADP	N3-C4-N9	4.55	134.91	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	601	ADP	N3-C4-N9	4.53	134.87	127.17
10	H	601	ADP	N3-C4-N9	4.52	134.86	127.17
10	A	601	ADP	N3-C4-N9	4.52	134.85	127.17
10	h	601	ADP	N3-C4-N9	4.51	134.84	127.17
10	Q	601	ADP	N3-C4-N9	4.50	134.82	127.17
10	G	601	ADP	N3-C4-N9	4.47	134.78	127.17
10	q	601	ADP	N3-C4-N9	4.47	134.77	127.17
10	g	601	ADP	N3-C4-N9	4.39	134.62	127.17
10	d	601	ADP	C2-N3-C4	3.74	120.95	111.83
10	E	601	ADP	C2-N3-C4	3.73	120.94	111.83
10	D	601	ADP	C2-N3-C4	3.73	120.93	111.83
10	Q	601	ADP	C2-N3-C4	3.72	120.91	111.83
10	b	601	ADP	C2-N3-C4	3.71	120.90	111.83
10	B	601	ADP	C2-N3-C4	3.70	120.87	111.83
10	h	601	ADP	C2-N3-C4	3.70	120.87	111.83
10	Z	601	ADP	C2-N3-C4	3.68	120.81	111.83
10	e	601	ADP	C2-N3-C4	3.67	120.81	111.83
10	H	601	ADP	C2-N3-C4	3.67	120.80	111.83
10	q	601	ADP	C2-N3-C4	3.67	120.79	111.83
10	z	601	ADP	C2-N3-C4	3.67	120.79	111.83
10	A	601	ADP	C2-N3-C4	3.66	120.76	111.83
10	a	601	ADP	C2-N3-C4	3.66	120.76	111.83
10	g	601	ADP	C4-C5-N7	-3.60	106.47	110.58
10	G	601	ADP	C2-N3-C4	3.59	120.61	111.83
10	g	601	ADP	C2-N3-C4	3.58	120.58	111.83
10	h	601	ADP	C4-C5-N7	-3.58	106.49	110.58
10	E	601	ADP	C4-C5-N7	-3.57	106.50	110.58
10	b	601	ADP	C4-C5-N7	-3.56	106.52	110.58
10	d	601	ADP	C4-C5-N7	-3.54	106.54	110.58
10	Q	601	ADP	C4-C5-N7	-3.53	106.55	110.58
10	H	601	ADP	C4-C5-N7	-3.52	106.55	110.58
10	D	601	ADP	C4-C5-N7	-3.51	106.57	110.58
10	e	601	ADP	C4-C5-N7	-3.51	106.57	110.58
10	a	601	ADP	C4-C5-N7	-3.51	106.57	110.58
10	B	601	ADP	C4-C5-N7	-3.50	106.58	110.58
10	q	601	ADP	C4-C5-N7	-3.50	106.58	110.58
10	G	601	ADP	C4-C5-N7	-3.50	106.58	110.58
10	A	601	ADP	C4-C5-N7	-3.47	106.61	110.58
10	Z	601	ADP	C4-C5-N7	-3.41	106.68	110.58
10	z	601	ADP	C4-C5-N7	-3.41	106.69	110.58
10	B	601	ADP	N3-C2-N1	-3.29	123.60	128.58
10	q	601	ADP	N3-C2-N1	-3.28	123.62	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	d	601	ADP	N3-C2-N1	-3.24	123.67	128.58
10	h	601	ADP	N3-C2-N1	-3.24	123.67	128.58
10	D	601	ADP	N3-C2-N1	-3.24	123.68	128.58
10	A	601	ADP	N3-C2-N1	-3.24	123.68	128.58
10	Q	601	ADP	N3-C2-N1	-3.24	123.68	128.58
10	b	601	ADP	N3-C2-N1	-3.23	123.69	128.58
10	H	601	ADP	N3-C2-N1	-3.23	123.69	128.58
10	a	601	ADP	N3-C2-N1	-3.22	123.70	128.58
10	Z	601	ADP	N3-C2-N1	-3.22	123.71	128.58
10	E	601	ADP	N3-C2-N1	-3.21	123.72	128.58
10	z	601	ADP	N3-C2-N1	-3.21	123.72	128.58
10	e	601	ADP	N3-C2-N1	-3.13	123.85	128.58
10	g	601	ADP	N3-C2-N1	-3.09	123.90	128.58
10	G	601	ADP	N3-C2-N1	-3.07	123.93	128.58
10	A	601	ADP	C4-N9-C8	2.83	108.71	105.74
10	z	601	ADP	C4-N9-C8	2.80	108.68	105.74
10	a	601	ADP	C4-N9-C8	2.80	108.67	105.74
10	g	601	ADP	C4-N9-C8	2.74	108.61	105.74
10	Z	601	ADP	C4-N9-C8	2.73	108.60	105.74
10	G	601	ADP	C4-N9-C8	2.73	108.60	105.74
10	B	601	ADP	C4-N9-C8	2.71	108.58	105.74
10	H	601	ADP	C4-N9-C8	2.70	108.58	105.74
10	q	601	ADP	C4-N9-C8	2.67	108.54	105.74
10	E	601	ADP	C4-N9-C8	2.65	108.52	105.74
10	Q	601	ADP	C4-N9-C8	2.65	108.52	105.74
10	e	601	ADP	C4-N9-C8	2.65	108.52	105.74
10	h	601	ADP	C4-N9-C8	2.64	108.51	105.74
10	b	601	ADP	C4-N9-C8	2.64	108.50	105.74
10	h	601	ADP	C5-N7-C8	2.59	107.53	103.45
10	g	601	ADP	C5-N7-C8	2.59	107.53	103.45
10	b	601	ADP	C5-N7-C8	2.59	107.52	103.45
10	a	601	ADP	C5-N7-C8	2.58	107.51	103.45
10	E	601	ADP	C5-N7-C8	2.58	107.50	103.45
10	D	601	ADP	C5-N7-C8	2.57	107.49	103.45
10	A	601	ADP	C5-N7-C8	2.57	107.49	103.45
10	H	601	ADP	C5-N7-C8	2.57	107.48	103.45
10	D	601	ADP	C4-N9-C8	2.57	108.43	105.74
10	Q	601	ADP	C5-N7-C8	2.55	107.47	103.45
10	d	601	ADP	C5-N7-C8	2.55	107.46	103.45
10	q	601	ADP	C5-N7-C8	2.55	107.46	103.45
10	B	601	ADP	C5-N7-C8	2.55	107.45	103.45
10	e	601	ADP	C5-N7-C8	2.55	107.45	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	d	601	ADP	C4-N9-C8	2.54	108.41	105.74
10	G	601	ADP	C5-N7-C8	2.54	107.44	103.45
10	z	601	ADP	C5-N7-C8	2.50	107.38	103.45
10	Z	601	ADP	C5-N7-C8	2.46	107.32	103.45
10	Z	601	ADP	C3'-C2'-C1'	2.35	105.92	101.46
10	b	601	ADP	C3'-C2'-C1'	2.33	105.87	101.46
10	E	601	ADP	C3'-C2'-C1'	2.30	105.82	101.46
10	z	601	ADP	C3'-C2'-C1'	2.30	105.82	101.46
10	b	601	ADP	O4'-C1'-N9	2.25	112.40	108.09
10	e	601	ADP	C3'-C2'-C1'	2.20	105.62	101.46
10	h	601	ADP	C6-C5-N7	2.18	136.29	132.09
10	Q	601	ADP	C6-C5-N7	2.18	136.28	132.09
10	B	601	ADP	C6-C5-N7	2.17	136.26	132.09
10	g	601	ADP	C6-C5-N7	2.16	136.26	132.09
10	b	601	ADP	C6-C5-N7	2.16	136.25	132.09
10	q	601	ADP	C6-C5-N7	2.16	136.25	132.09
10	A	601	ADP	C3'-C2'-C1'	2.14	105.52	101.46
10	D	601	ADP	C6-C5-N7	2.13	136.20	132.09
10	a	601	ADP	C6-C5-N7	2.13	136.20	132.09
10	A	601	ADP	C6-C5-N7	2.13	136.19	132.09
10	G	601	ADP	C3'-C2'-C1'	2.13	105.48	101.46
10	H	601	ADP	C6-C5-N7	2.12	136.18	132.09
10	A	601	ADP	N9-C8-N7	-2.12	110.93	113.94
10	Q	601	ADP	C3'-C2'-C1'	2.11	105.46	101.46
10	d	601	ADP	C6-C5-N7	2.11	136.16	132.09
10	q	601	ADP	C3'-C2'-C1'	2.11	105.46	101.46
10	E	601	ADP	C6-C5-N7	2.11	136.16	132.09
10	G	601	ADP	C6-C5-N7	2.10	136.15	132.09
10	g	601	ADP	N9-C8-N7	-2.10	110.96	113.94
10	a	601	ADP	N9-C8-N7	-2.09	110.97	113.94
10	e	601	ADP	C6-C5-N7	2.08	136.10	132.09
10	H	601	ADP	O3B-PB-O2B	2.07	115.57	107.80
10	d	601	ADP	C3'-C2'-C1'	2.07	105.38	101.46
10	H	601	ADP	N9-C8-N7	-2.06	111.01	113.94
10	q	601	ADP	N9-C8-N7	-2.05	111.02	113.94
10	Z	601	ADP	C6-C5-N7	2.05	136.03	132.09
10	h	601	ADP	N9-C8-N7	-2.05	111.03	113.94
10	z	601	ADP	C6-C5-N7	2.04	136.03	132.09
10	G	601	ADP	N9-C8-N7	-2.04	111.04	113.94
10	Q	601	ADP	N9-C8-N7	-2.04	111.05	113.94
10	z	601	ADP	N9-C8-N7	-2.03	111.05	113.94
10	B	601	ADP	N9-C8-N7	-2.03	111.06	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	601	ADP	C3'-C2'-C1'	2.02	105.29	101.46
10	b	601	ADP	N9-C8-N7	-2.02	111.07	113.94
10	E	601	ADP	N9-C8-N7	-2.02	111.07	113.94
10	e	601	ADP	N9-C8-N7	-2.00	111.09	113.94

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	601	ADP	C5'-O5'-PA-O1A
10	A	601	ADP	C5'-O5'-PA-O2A
10	A	601	ADP	C5'-O5'-PA-O3A
10	E	601	ADP	C5'-O5'-PA-O1A
10	H	601	ADP	C5'-O5'-PA-O3A
10	Q	601	ADP	C5'-O5'-PA-O1A
10	Q	601	ADP	C5'-O5'-PA-O2A
10	Q	601	ADP	C5'-O5'-PA-O3A
10	a	601	ADP	C5'-O5'-PA-O1A
10	a	601	ADP	C5'-O5'-PA-O2A
10	a	601	ADP	C5'-O5'-PA-O3A
10	g	601	ADP	C5'-O5'-PA-O1A
10	q	601	ADP	C5'-O5'-PA-O1A
10	q	601	ADP	C5'-O5'-PA-O3A
10	Q	601	ADP	C3'-C4'-C5'-O5'
10	z	601	ADP	O4'-C4'-C5'-O5'
10	z	601	ADP	C3'-C4'-C5'-O5'
10	Z	601	ADP	O4'-C4'-C5'-O5'
10	Z	601	ADP	C3'-C4'-C5'-O5'
10	B	601	ADP	PB-O3A-PA-O5'
10	D	601	ADP	PB-O3A-PA-O5'
10	b	601	ADP	PB-O3A-PA-O5'
10	d	601	ADP	PB-O3A-PA-O5'
10	e	601	ADP	PB-O3A-PA-O5'
10	h	601	ADP	PB-O3A-PA-O5'
10	Q	601	ADP	O4'-C4'-C5'-O5'
10	H	601	ADP	PA-O3A-PB-O1B
10	Q	601	ADP	PB-O3A-PA-O2A
10	Z	601	ADP	C5'-O5'-PA-O1A
10	g	601	ADP	C5'-O5'-PA-O2A
10	g	601	ADP	C5'-O5'-PA-O3A
10	q	601	ADP	C5'-O5'-PA-O2A
10	Z	601	ADP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	q	601	ADP	PB-O3A-PA-O1A
10	E	601	ADP	PB-O3A-PA-O5'
10	q	601	ADP	C3'-C4'-C5'-O5'
10	H	601	ADP	PA-O3A-PB-O2B
10	H	601	ADP	PA-O3A-PB-O3B
10	Q	601	ADP	PB-O3A-PA-O1A
10	a	601	ADP	PB-O3A-PA-O2A
10	G	601	ADP	PB-O3A-PA-O1A
10	G	601	ADP	PB-O3A-PA-O2A
10	g	601	ADP	PB-O3A-PA-O2A

There are no ring outliers.

28 monomers are involved in 34 short contacts:

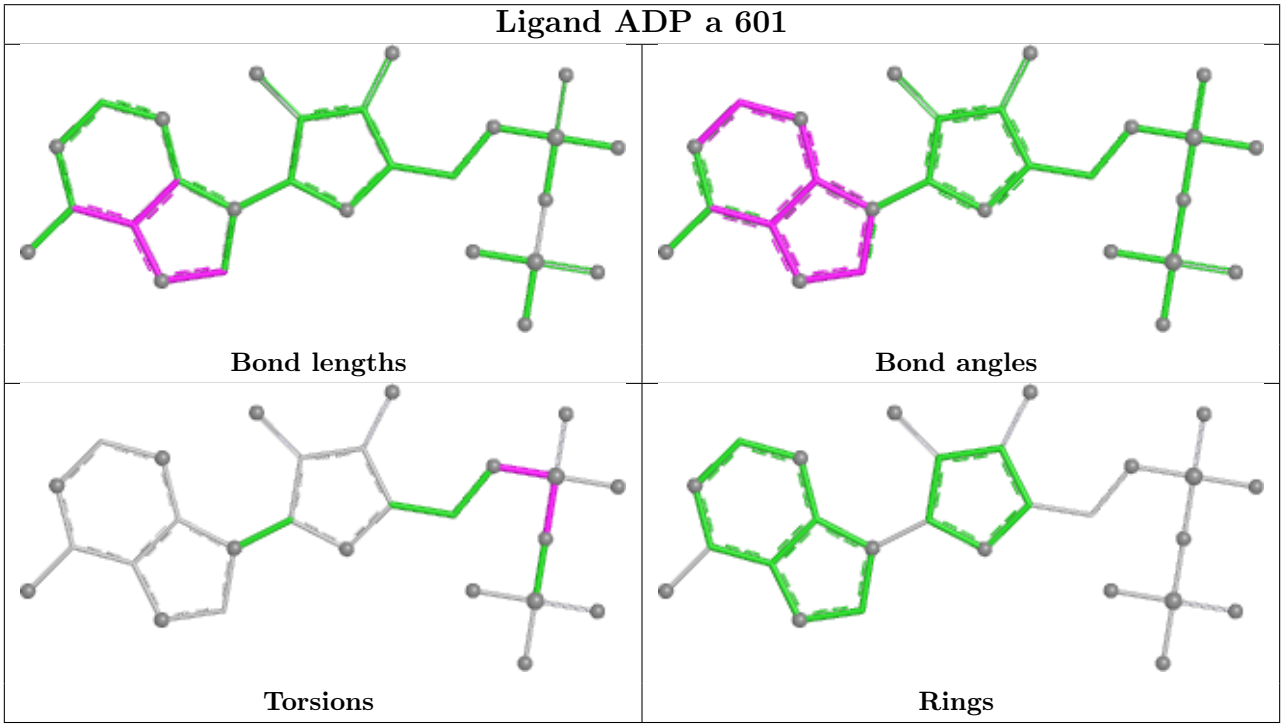
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	a	601	ADP	1	0
10	z	601	ADP	1	0
10	B	601	ADP	2	0
10	g	601	ADP	2	0
12	d	603	AF3	2	0
10	G	601	ADP	2	0
10	h	601	ADP	1	0
10	b	601	ADP	2	0
10	A	601	ADP	1	0
10	d	601	ADP	2	0
10	e	601	ADP	2	0
12	Q	603	AF3	1	0
12	Z	603	AF3	2	0
12	A	603	AF3	1	0
12	z	603	AF3	1	0
10	q	601	ADP	3	0
12	G	603	AF3	3	0
12	e	603	AF3	1	0
12	H	603	AF3	2	0
10	Z	601	ADP	2	0
10	D	601	ADP	1	0
10	Q	601	ADP	2	0
12	q	603	AF3	2	0
12	B	603	AF3	1	0
10	H	601	ADP	2	0
12	g	603	AF3	1	0
12	D	603	AF3	2	0

Continued on next page...

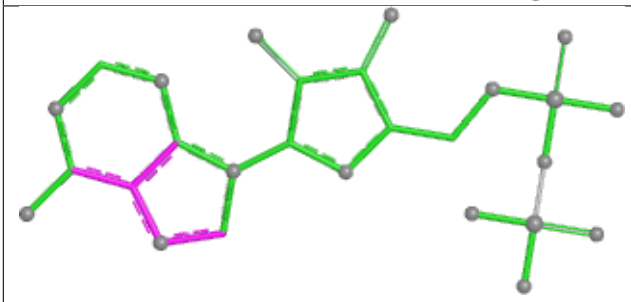
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	a	603	AF3	1	0

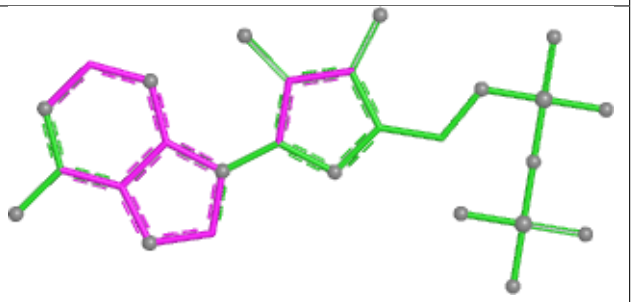
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



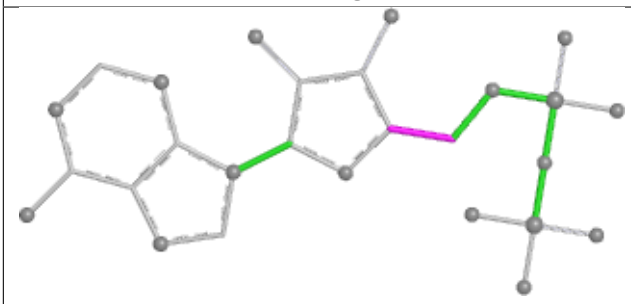
Ligand ADP z 601



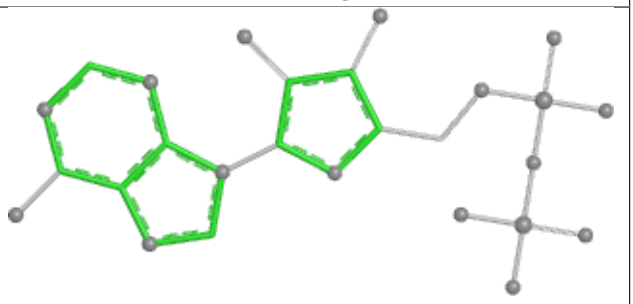
Bond lengths



Bond angles

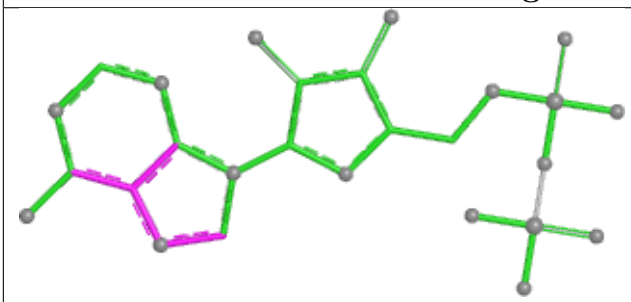


Torsions

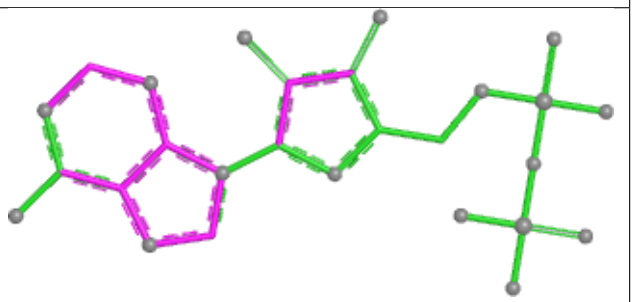


Rings

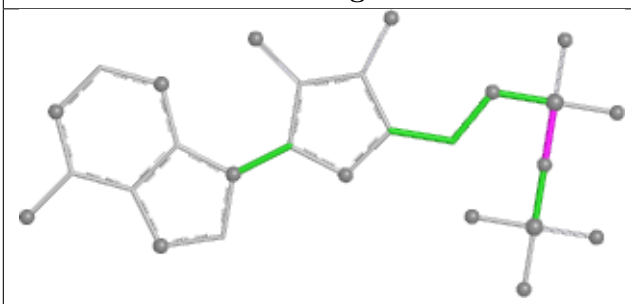
Ligand ADP B 601



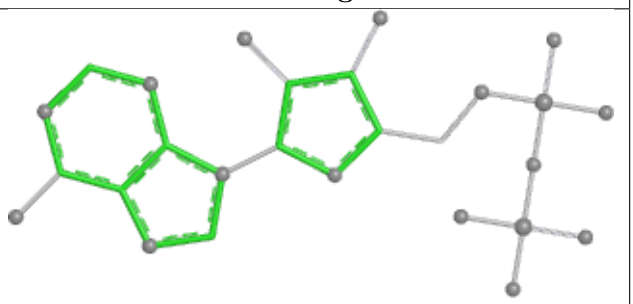
Bond lengths



Bond angles

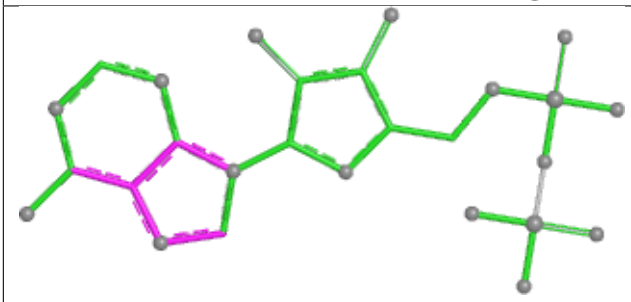


Torsions

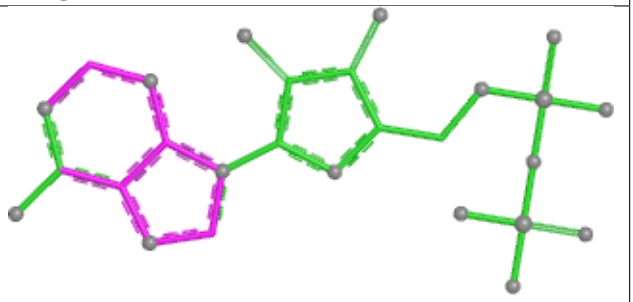


Rings

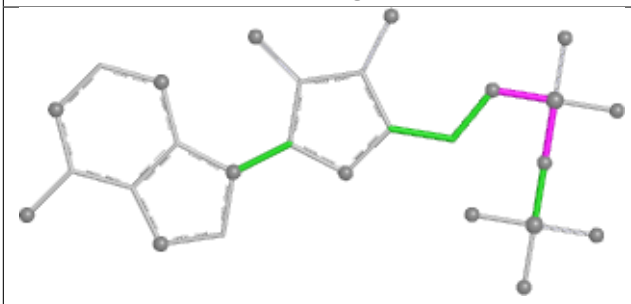
Ligand ADP g 601



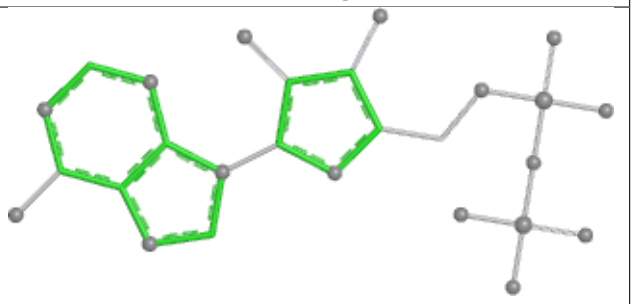
Bond lengths



Bond angles

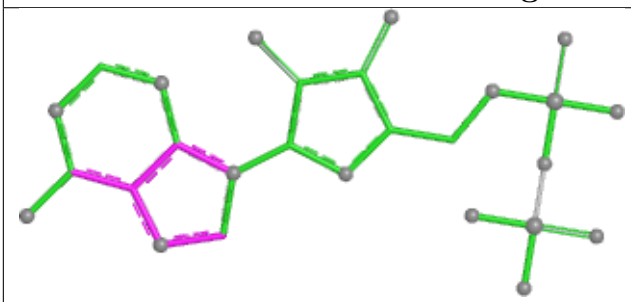


Torsions

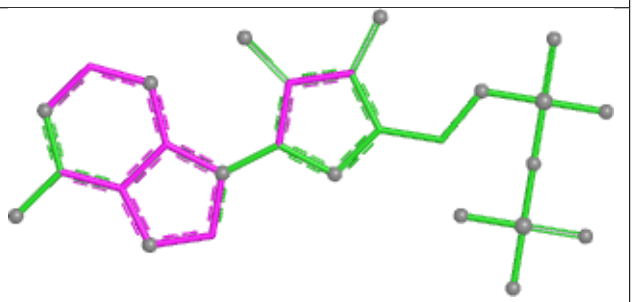


Rings

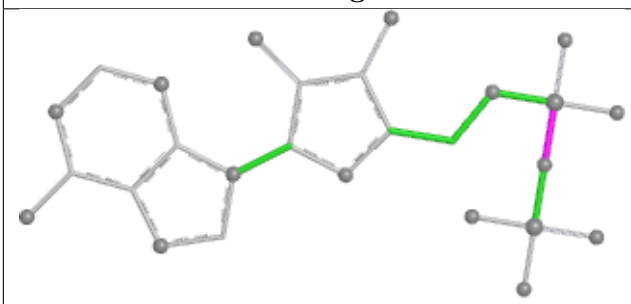
Ligand ADP G 601



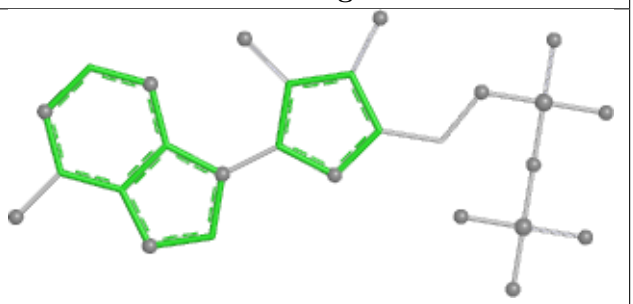
Bond lengths



Bond angles

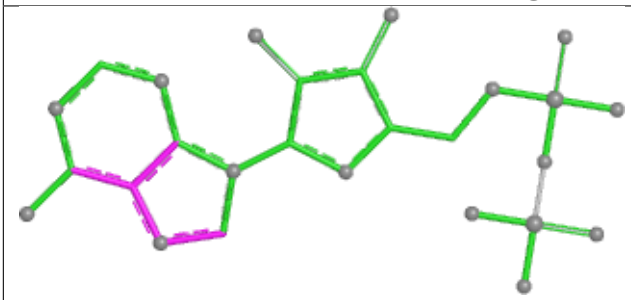


Torsions

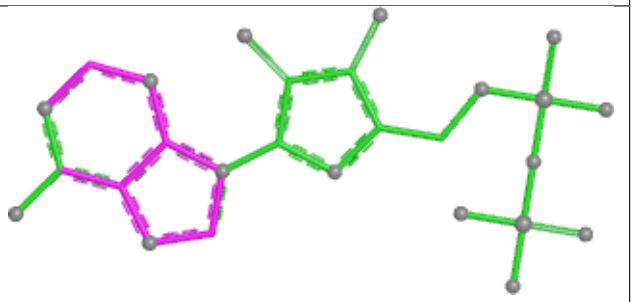


Rings

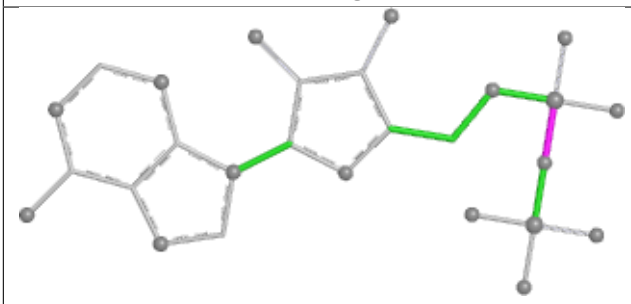
Ligand ADP h 601



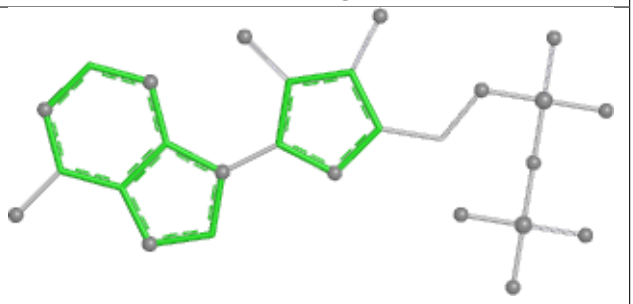
Bond lengths



Bond angles

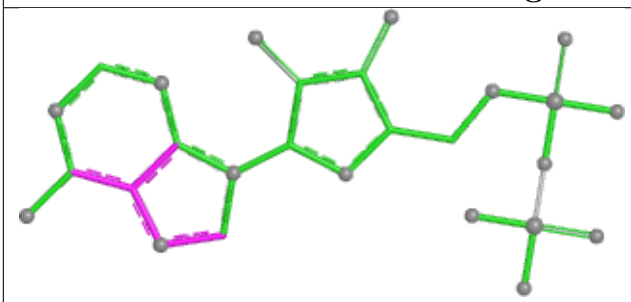


Torsions

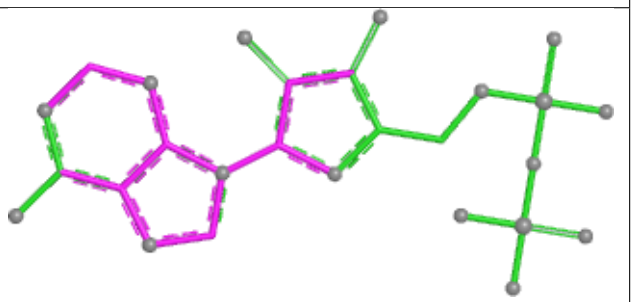


Rings

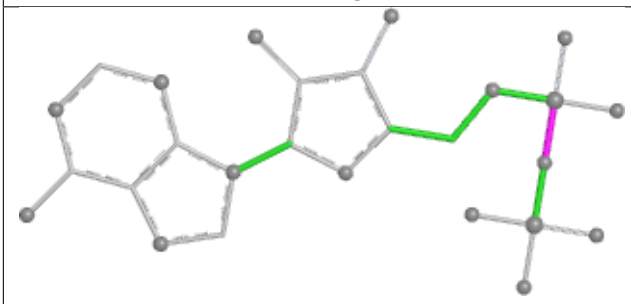
Ligand ADP b 601



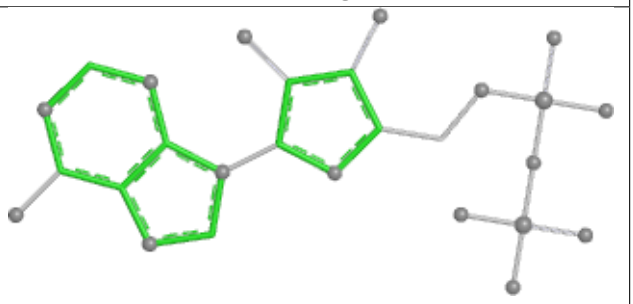
Bond lengths



Bond angles

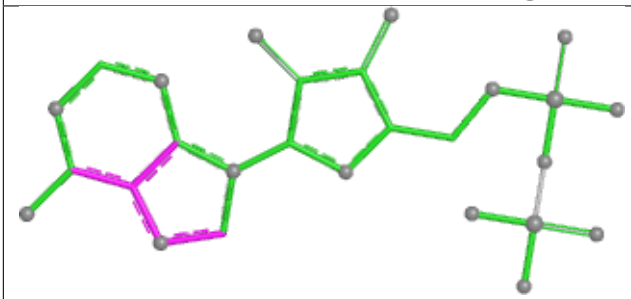


Torsions

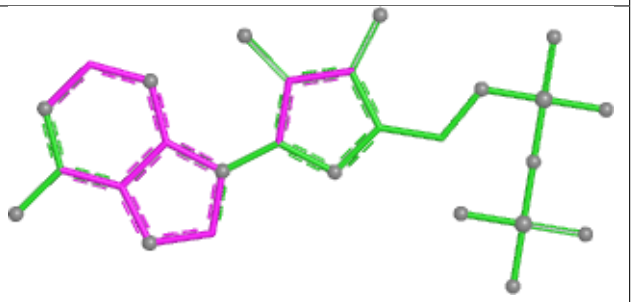


Rings

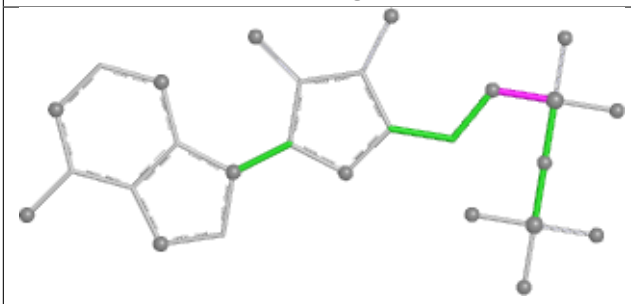
Ligand ADP A 601



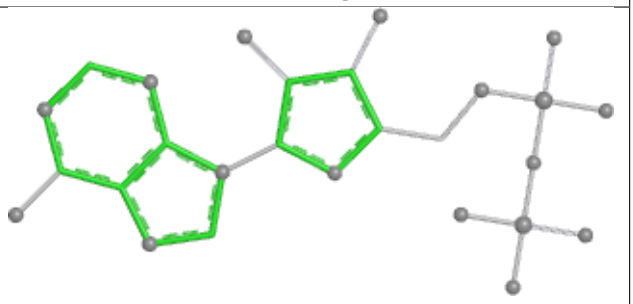
Bond lengths



Bond angles

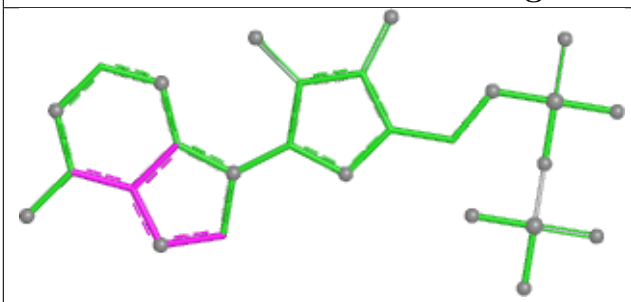


Torsions

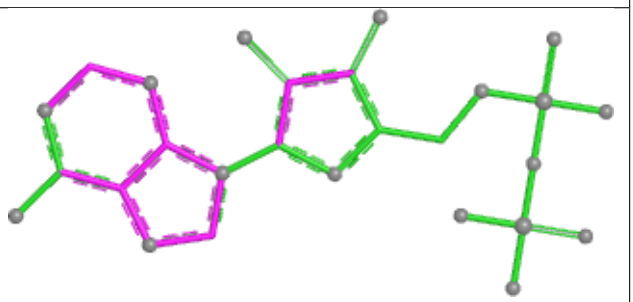


Rings

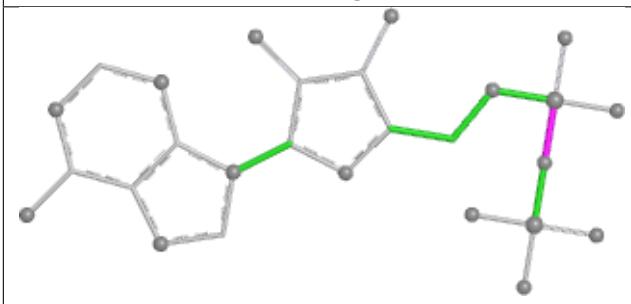
Ligand ADP d 601



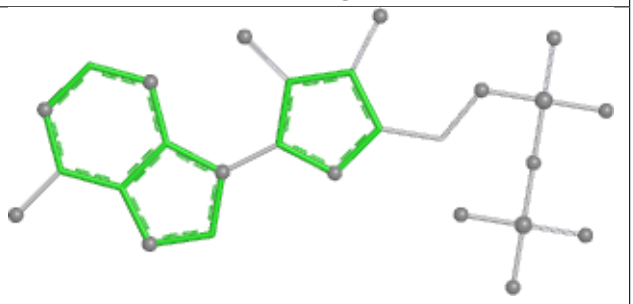
Bond lengths



Bond angles

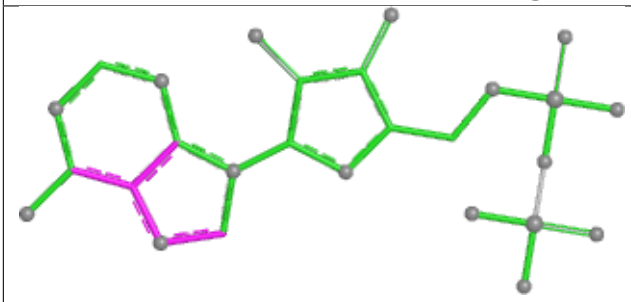


Torsions

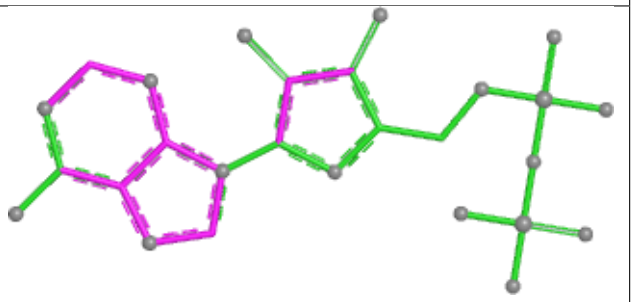


Rings

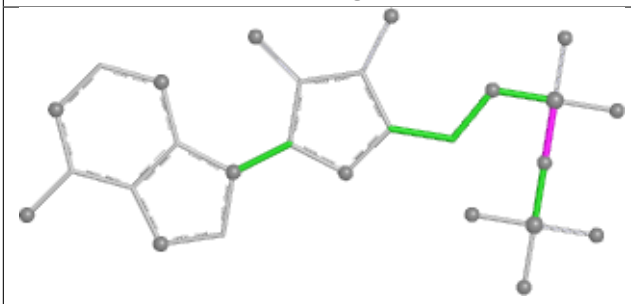
Ligand ADP e 601



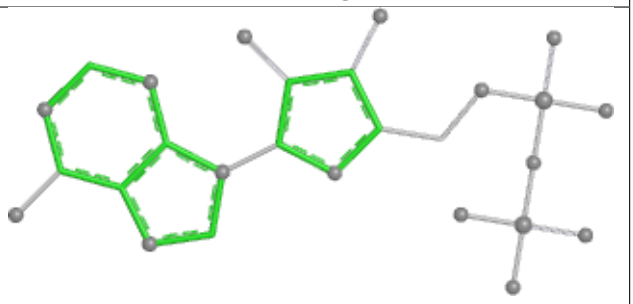
Bond lengths



Bond angles

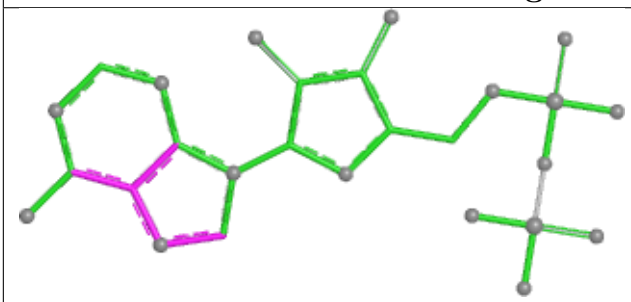


Torsions

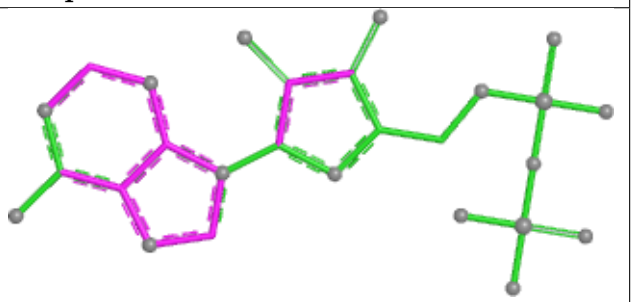


Rings

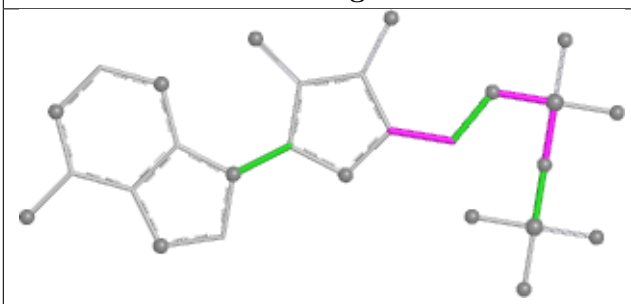
Ligand ADP q 601



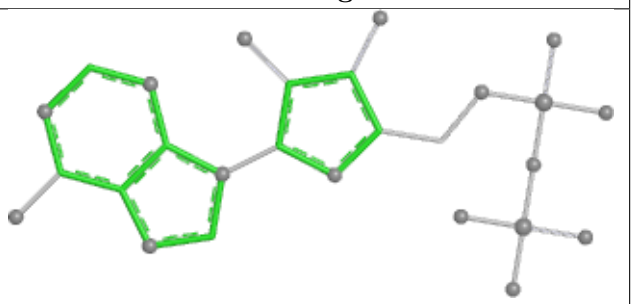
Bond lengths



Bond angles

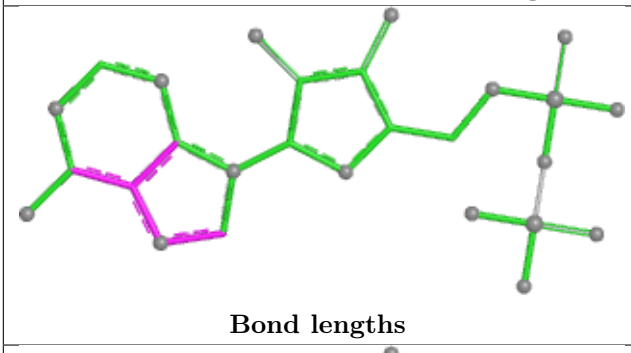


Torsions

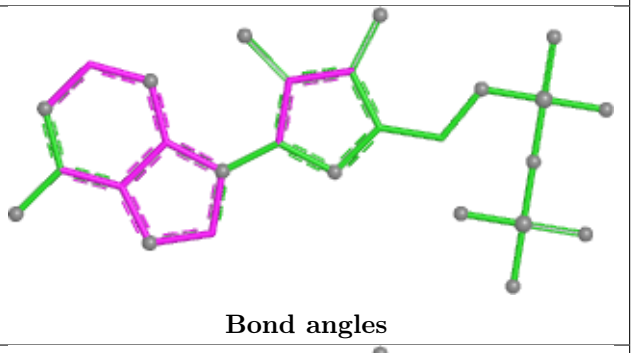


Rings

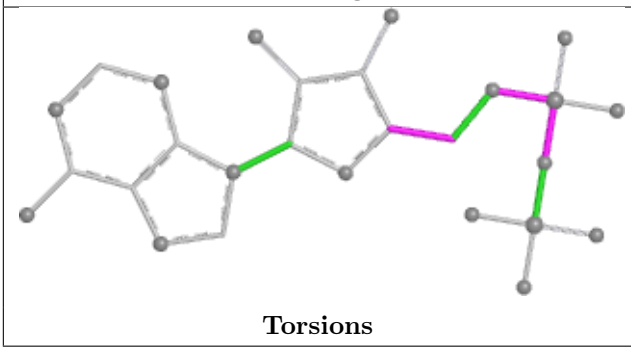
Ligand ADP Z 601



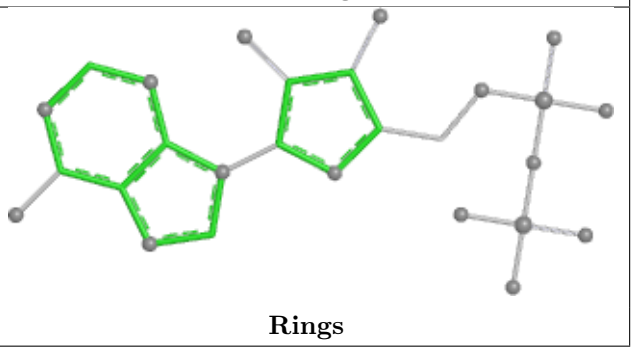
Bond lengths



Bond angles

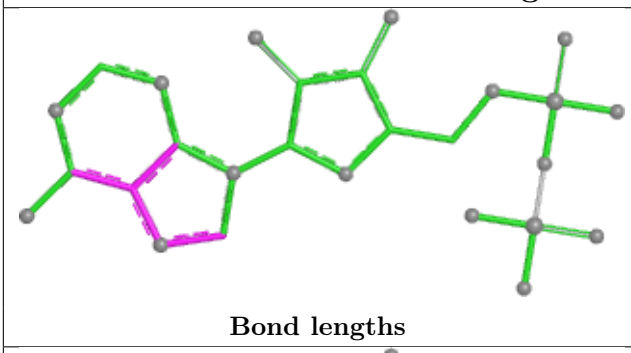


Torsions

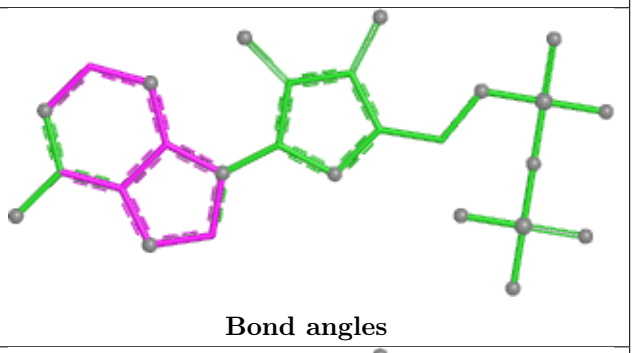


Rings

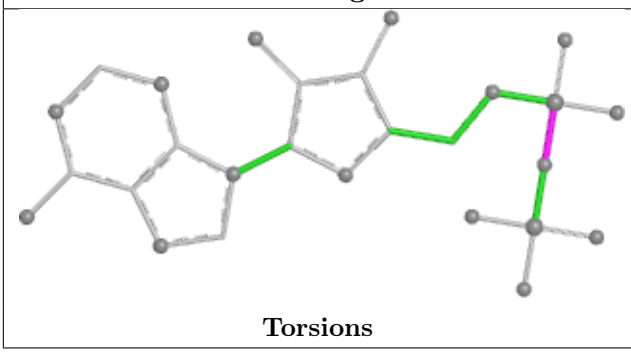
Ligand ADP D 601



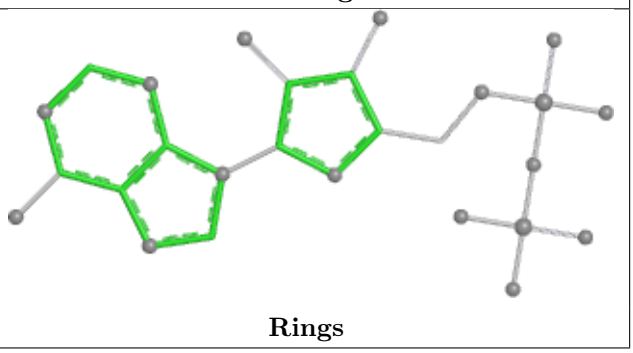
Bond lengths



Bond angles

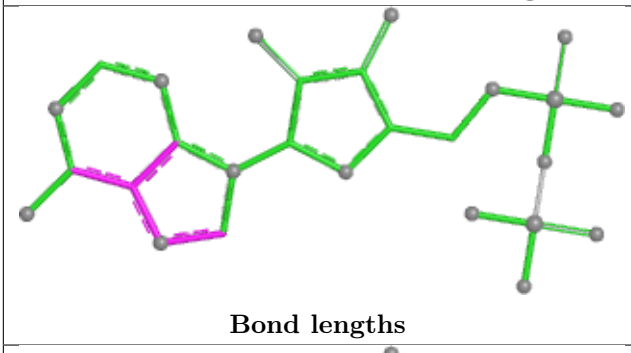


Torsions

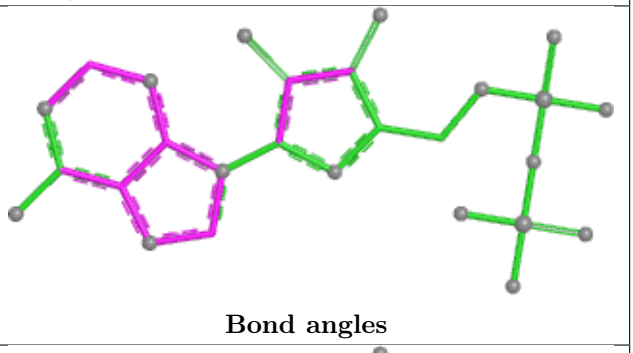


Rings

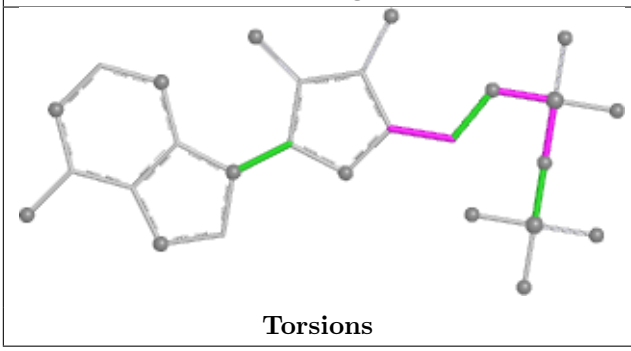
Ligand ADP Q 601



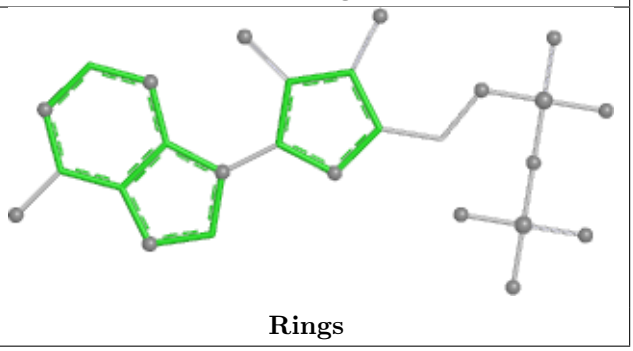
Bond lengths



Bond angles

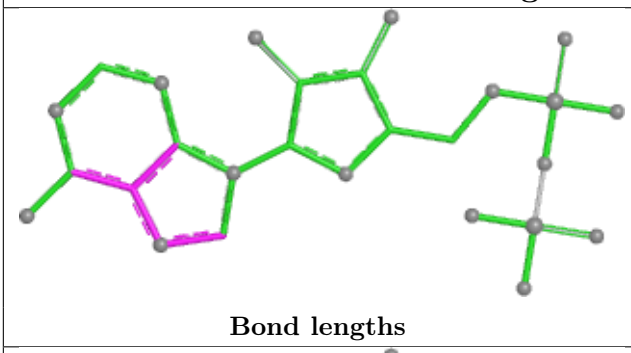


Torsions

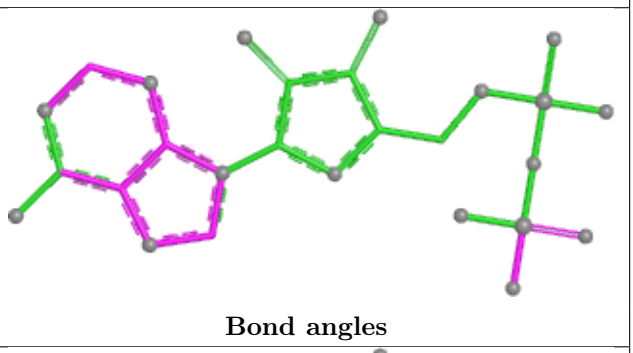


Rings

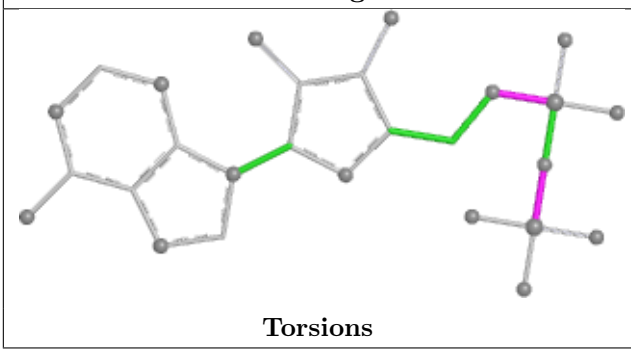
Ligand ADP H 601



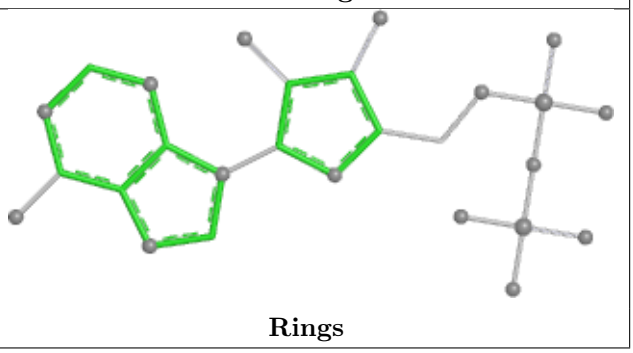
Bond lengths



Bond angles

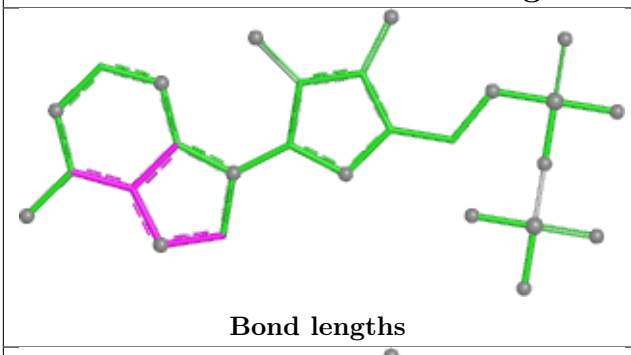


Torsions

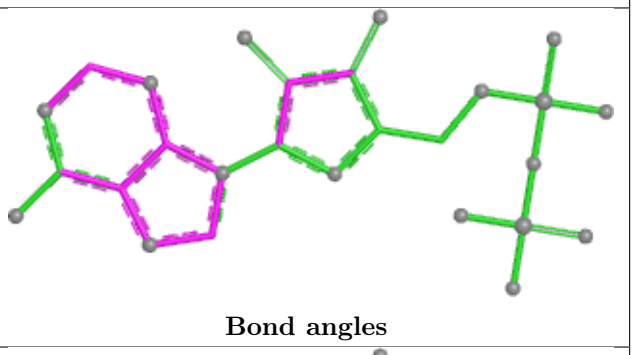


Rings

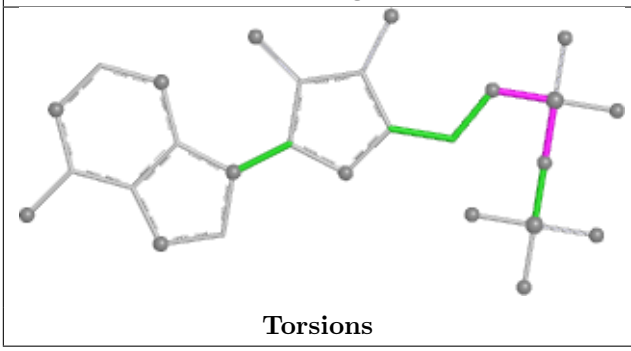
Ligand ADP E 601



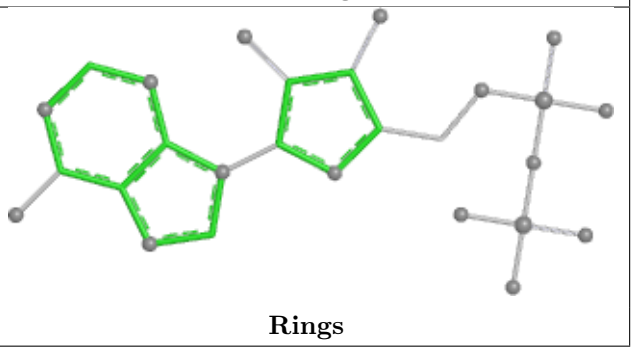
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

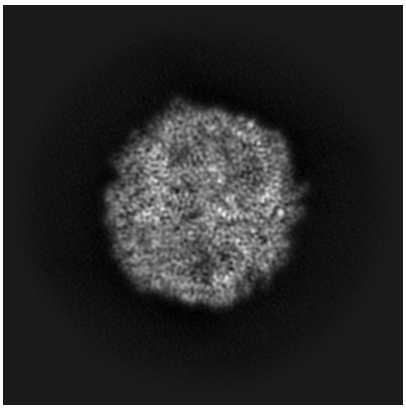
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40453. These allow visual inspection of the internal detail of the map and identification of artifacts.

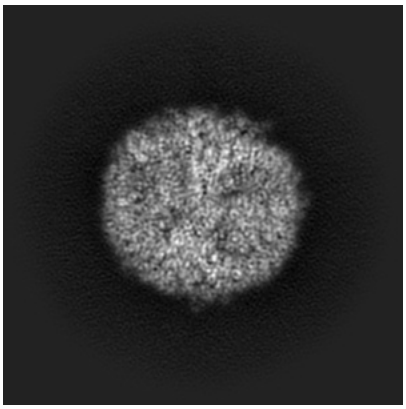
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

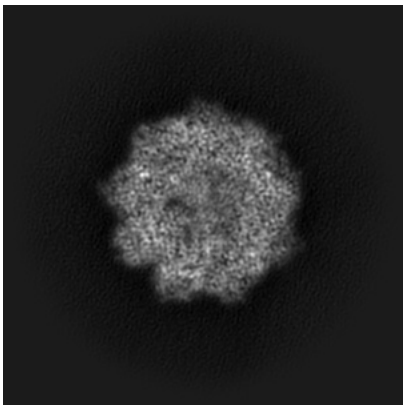
6.1.1 Primary map



X

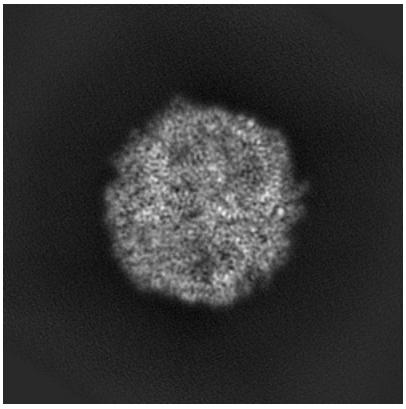


Y

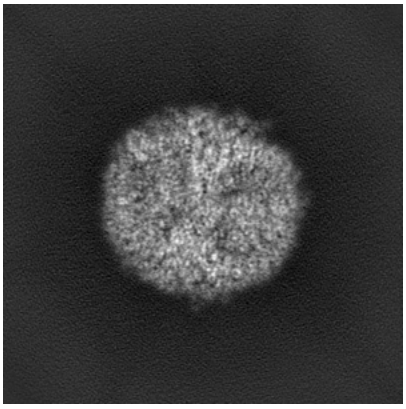


Z

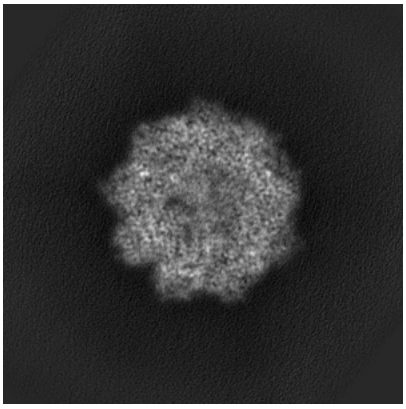
6.1.2 Raw map



X



Y

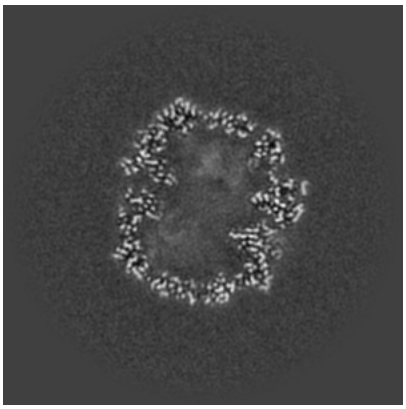


Z

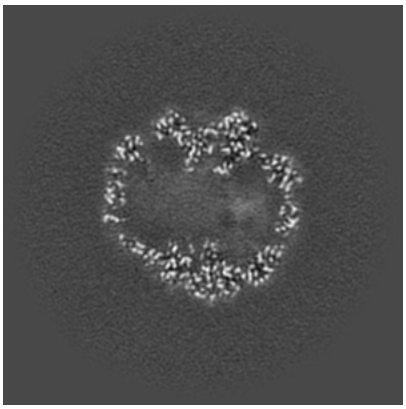
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

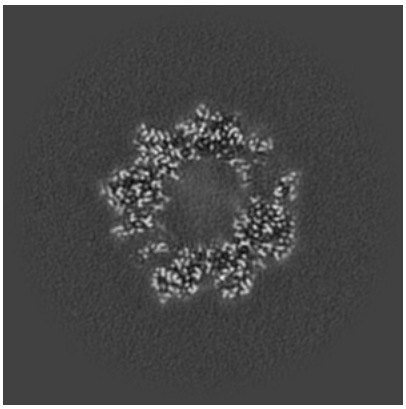
6.2.1 Primary map



X Index: 150

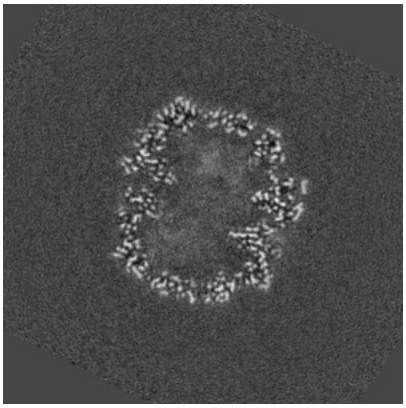


Y Index: 150

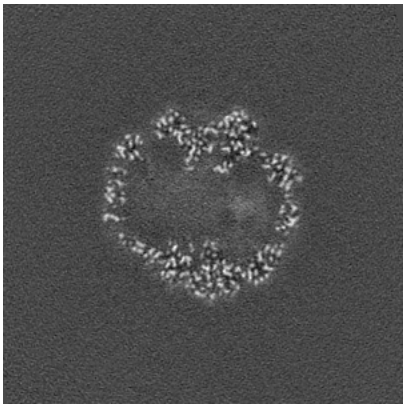


Z Index: 150

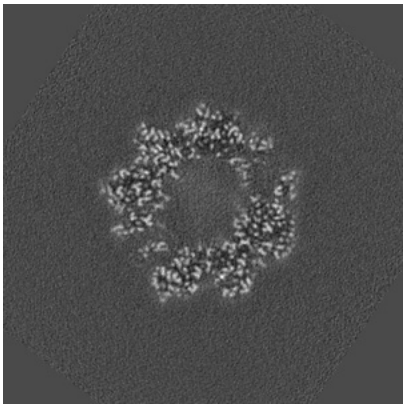
6.2.2 Raw map



X Index: 150



Y Index: 150

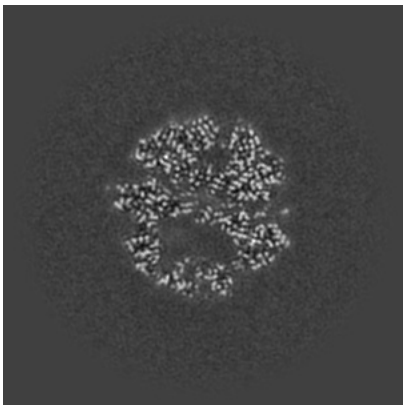


Z Index: 150

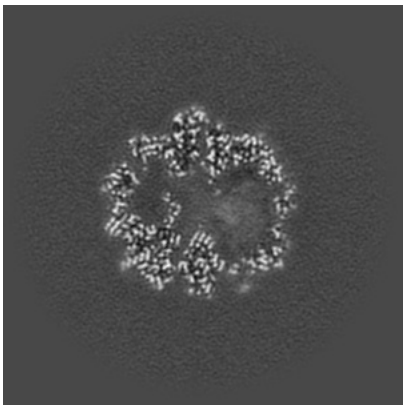
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

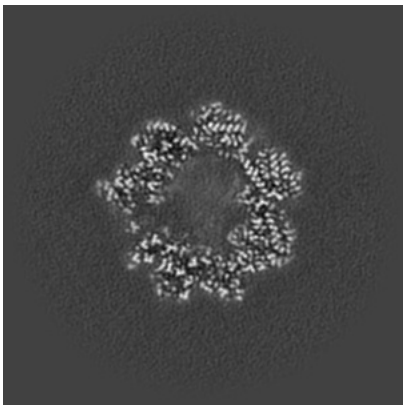
6.3.1 Primary map



X Index: 182

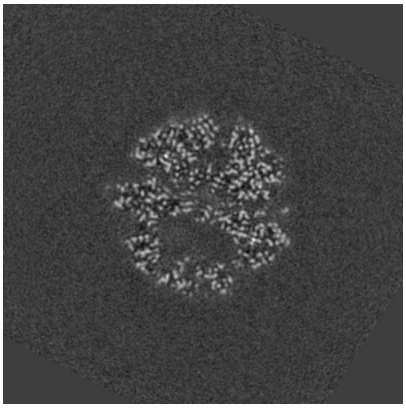


Y Index: 172

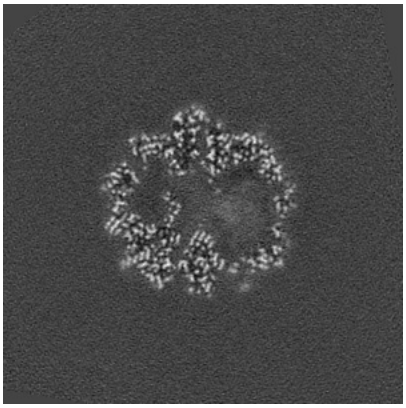


Z Index: 143

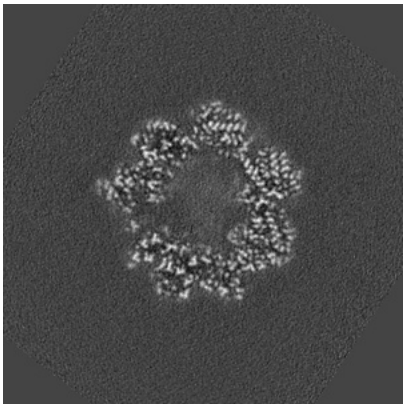
6.3.2 Raw map



X Index: 182



Y Index: 172

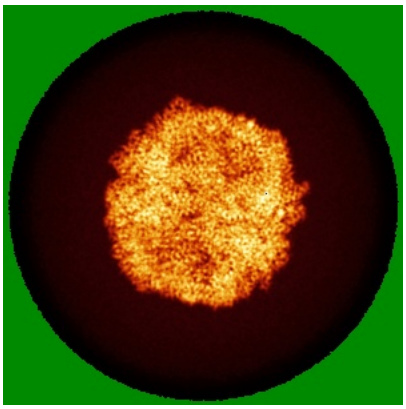


Z Index: 143

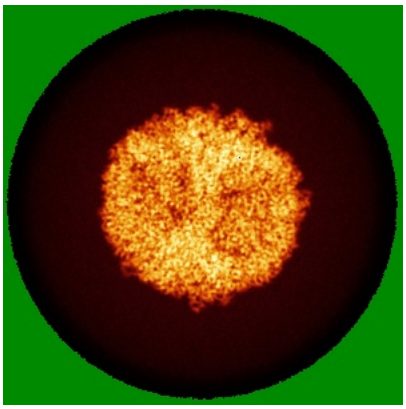
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

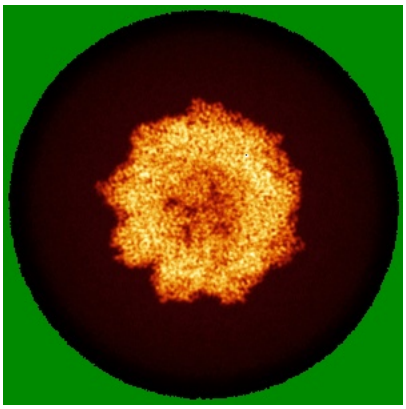
6.4.1 Primary map



X

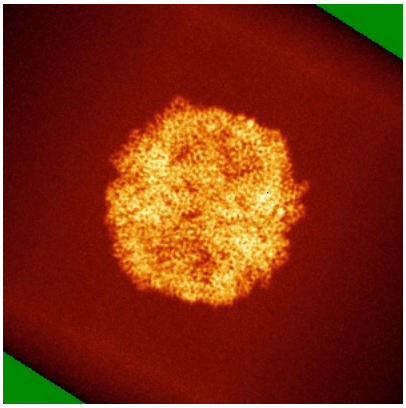


Y

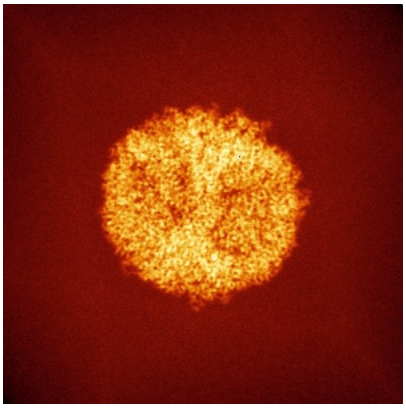


Z

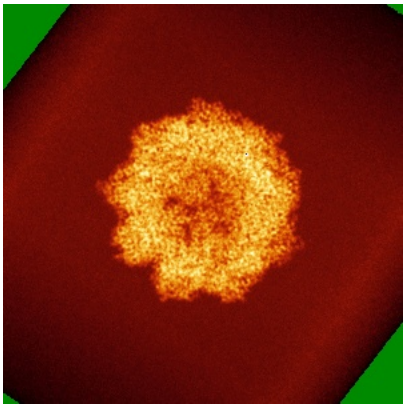
6.4.2 Raw map



X



Y

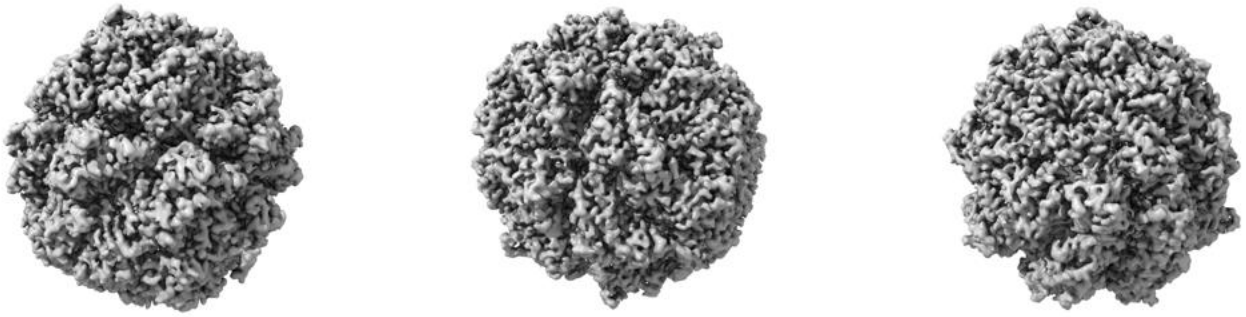


Z

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)

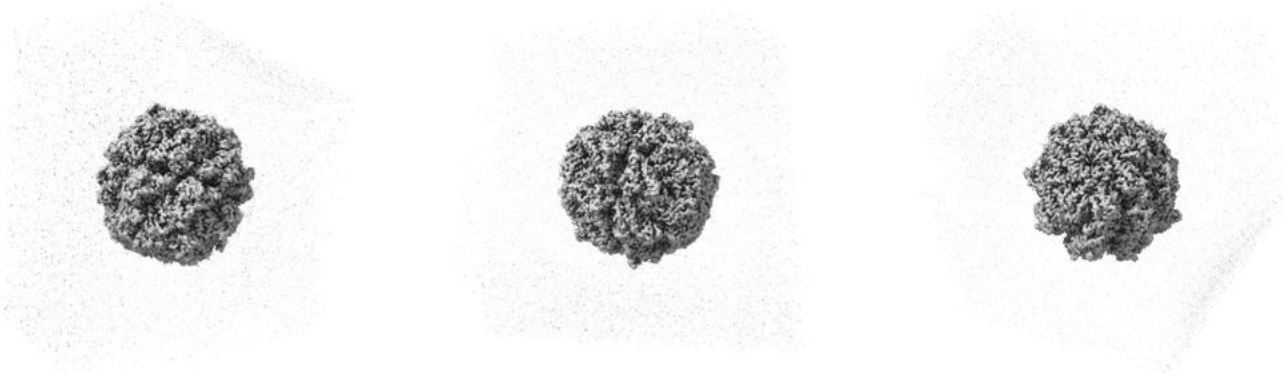
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.109. 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.

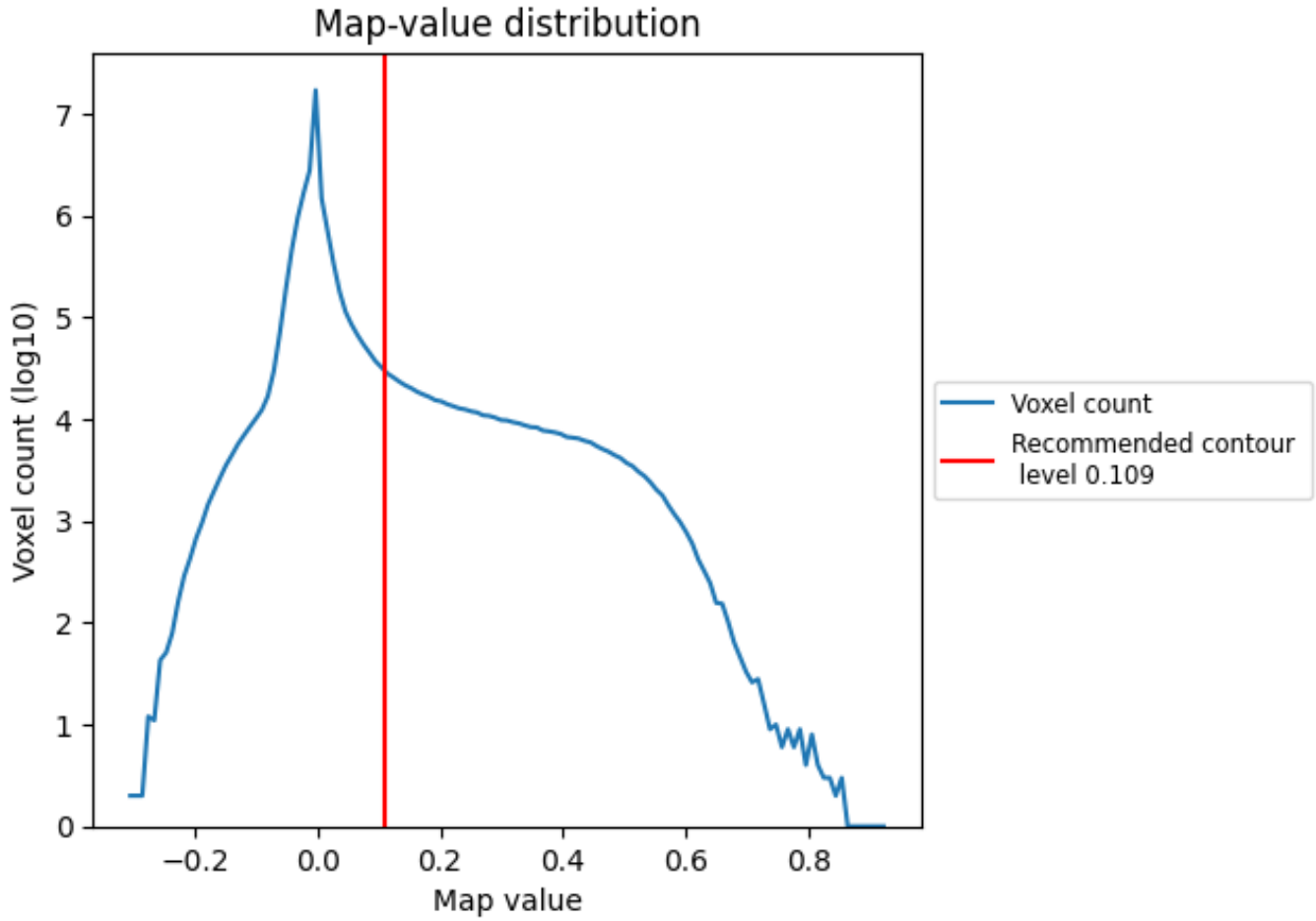
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

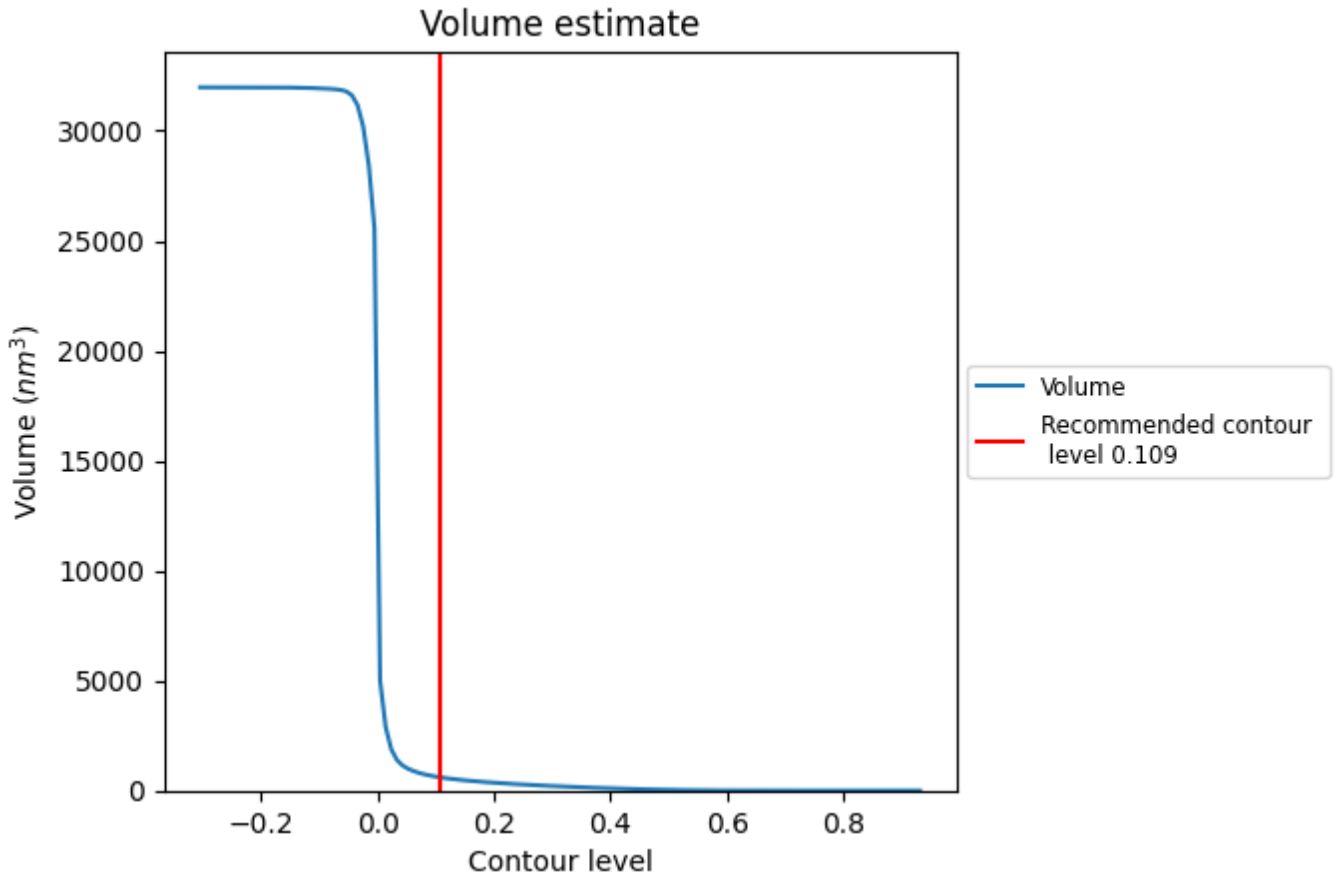
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

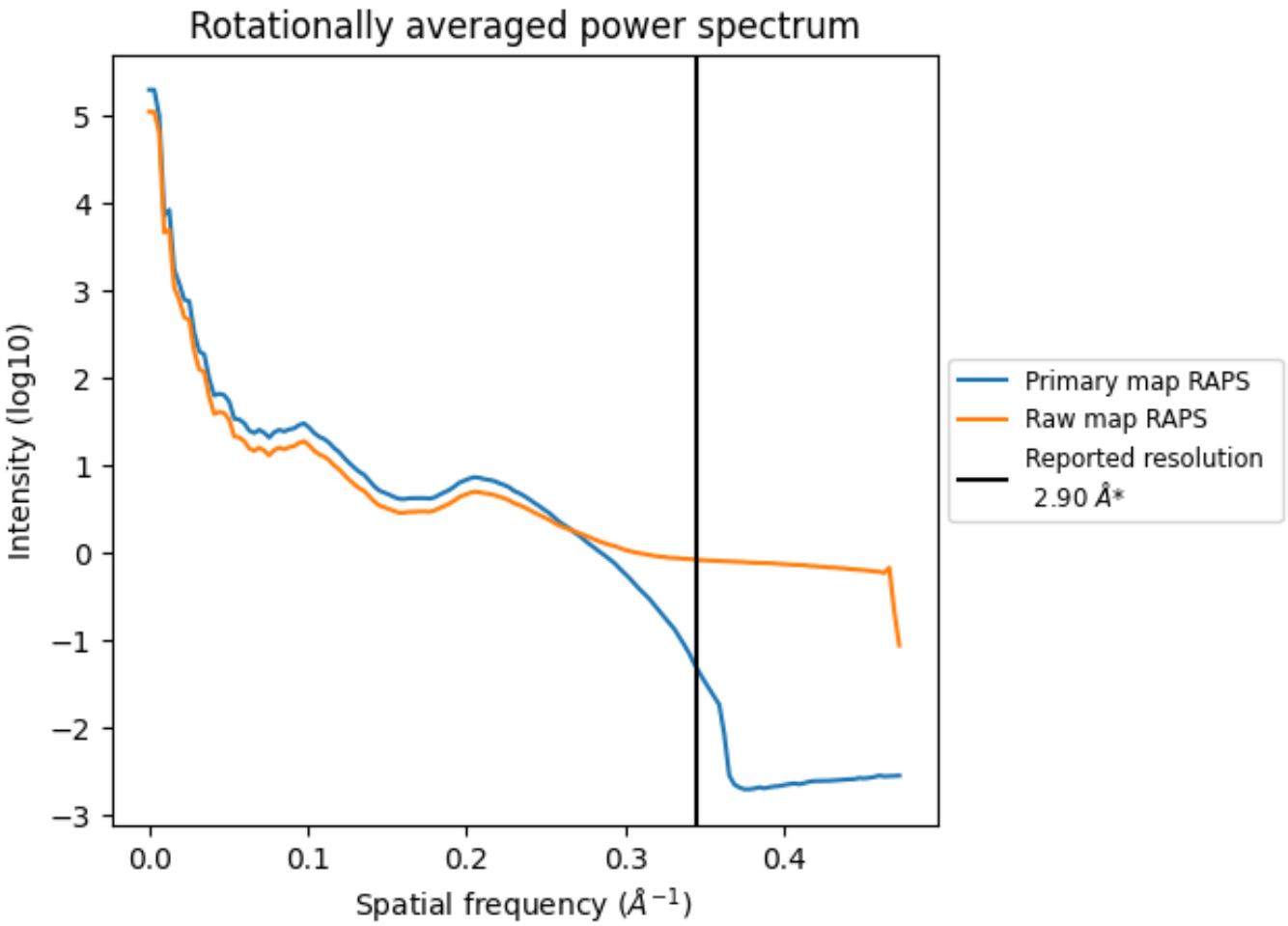
7.2 Volume estimate



The volume at the recommended contour level is 595 nm^3; this corresponds to an approximate mass of 538 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 (i)

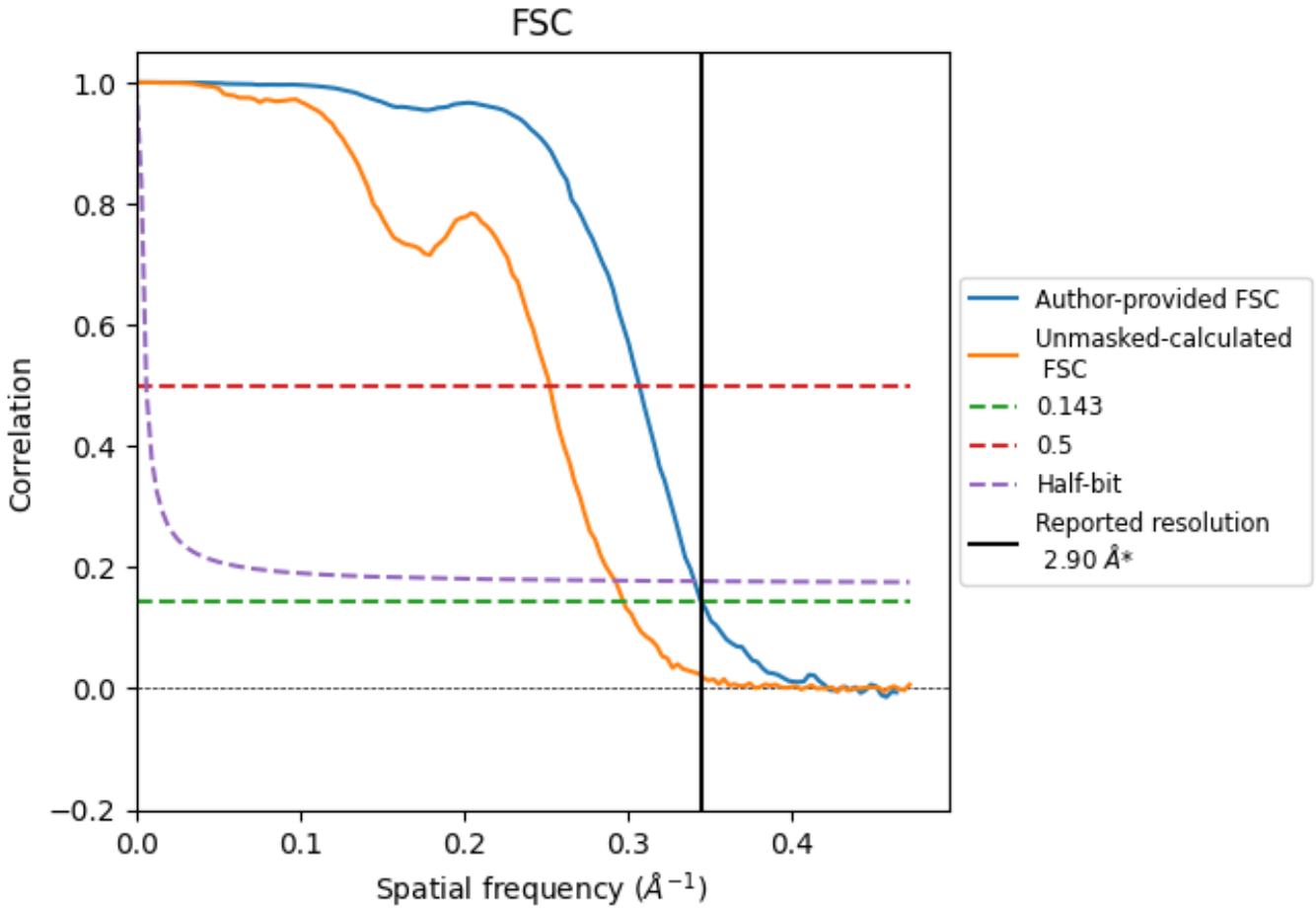


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

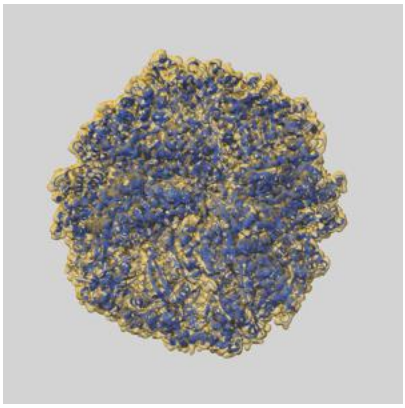
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.25	2.93
Unmasked-calculated*	3.36	3.96	3.42

*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 3.36 differs from the reported value 2.9 by more than 10 %

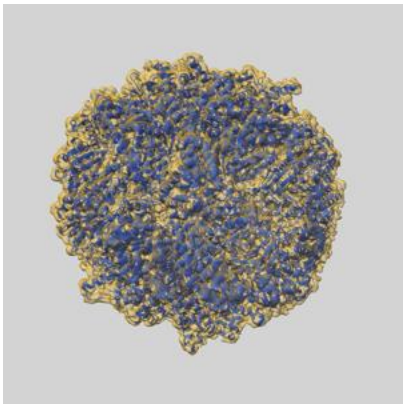
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40453 and PDB model 8SG9. Per-residue inclusion information can be found in section 3 on page 10.

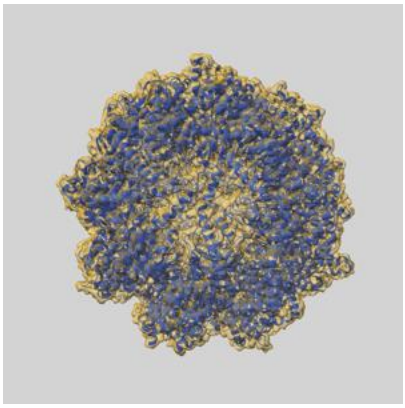
9.1 Map-model overlay



X



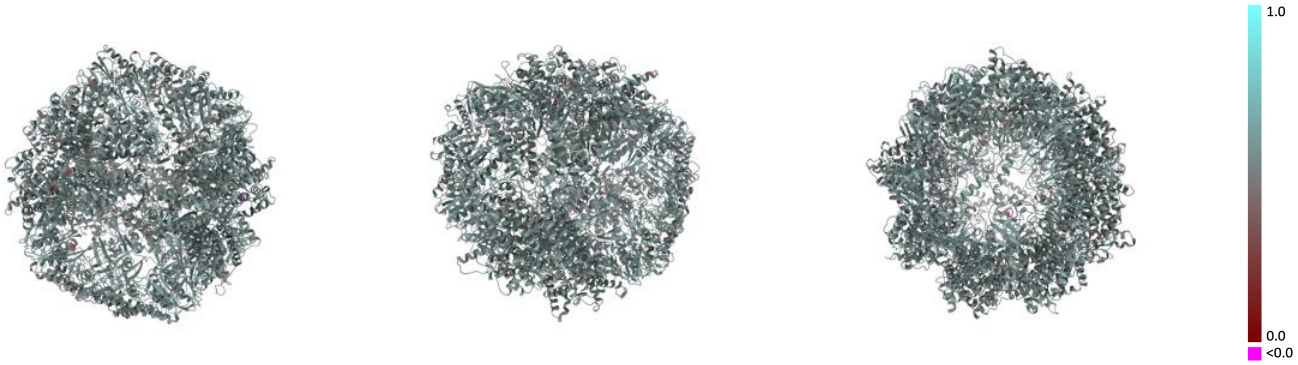
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.109 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.

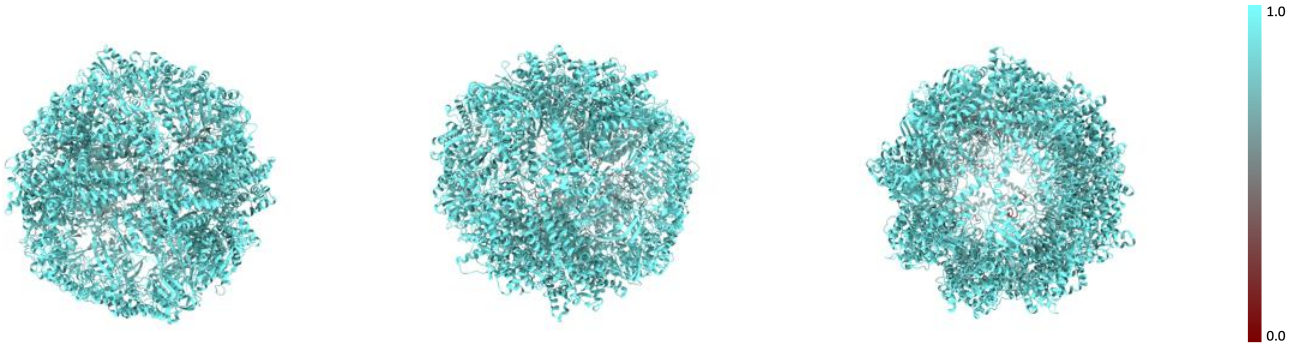
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

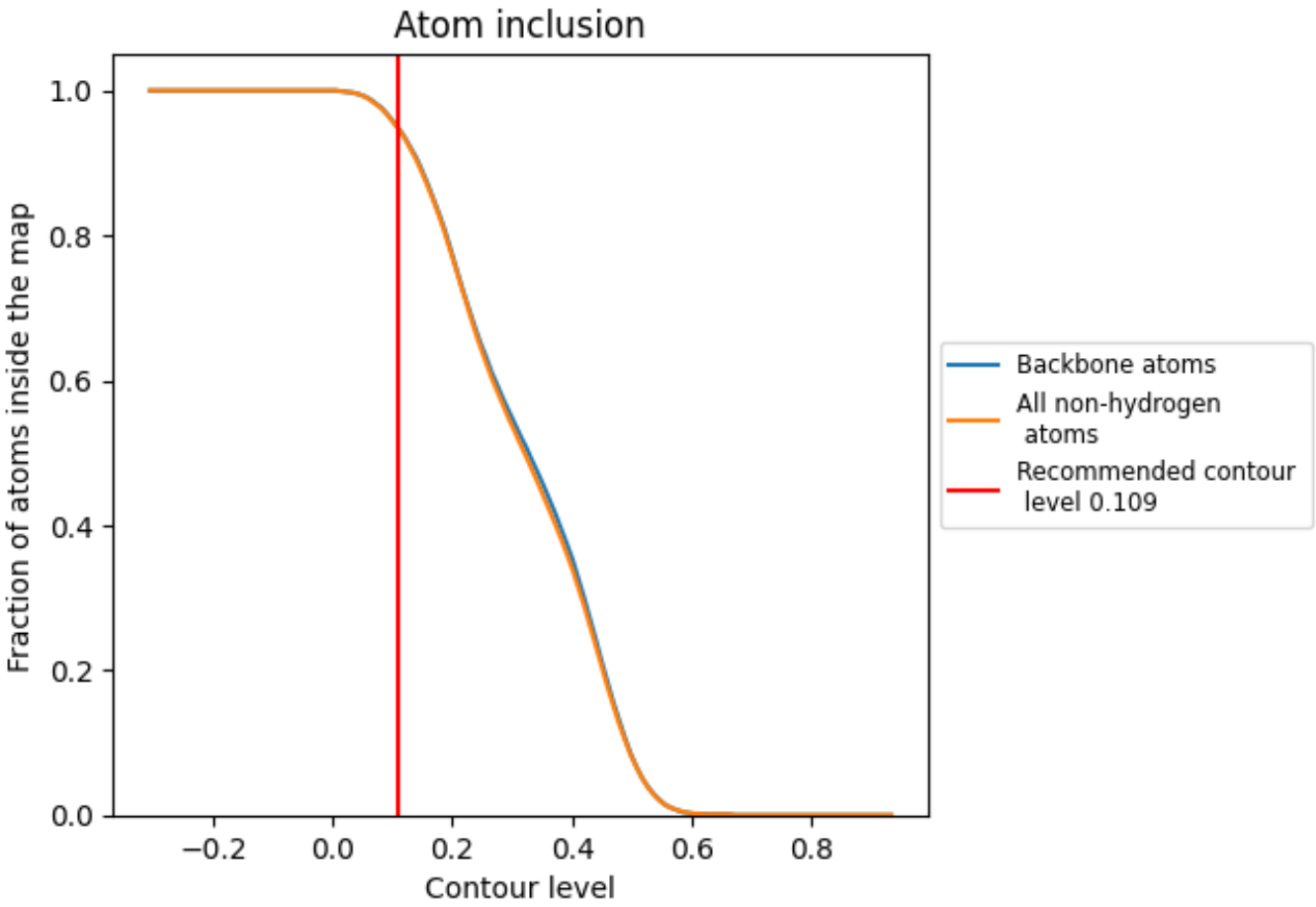
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.109).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9480	0.5480
A	0.9480	0.5460
B	0.9600	0.5540
D	0.9580	0.5500
E	0.9510	0.5500
G	0.9540	0.5500
H	0.9500	0.5480
N	0.5750	0.4620
Q	0.9410	0.5400
Z	0.9540	0.5450
a	0.9550	0.5450
b	0.9610	0.5570
d	0.9560	0.5480
e	0.9410	0.5470
g	0.9540	0.5520
h	0.9560	0.5530
q	0.9470	0.5470
z	0.9480	0.5460

