



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:57 AM UTC

PDB ID : 4A3F / pdb_00004a3f
Title : RNA Polymerase II initial transcribing complex with a 6nt DNA-RNA hybrid and soaked with AMPCPP
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on : 2011-09-30
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

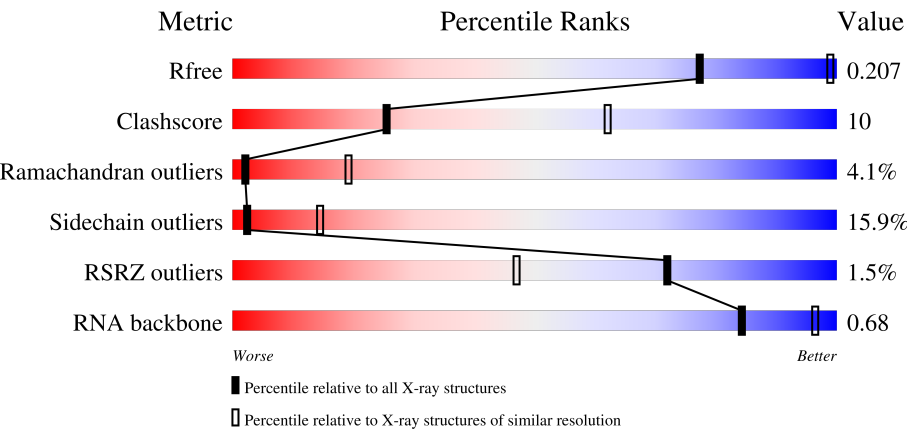
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



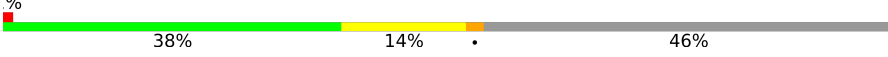
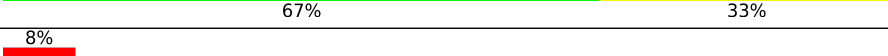
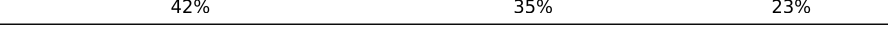
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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

Mol	Chain	Length	Quality of chain
1	A	1732	2% 51%24%6%18%
2	B	1224	2% 54%28%7%9%
3	C	318	47%31%5%16%
4	D	221	3% 48%22%9%19%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	6	
15	T	26	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32010 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1425	Total	C	N	O	S	0	0	0
			11197	7051	1958	2126	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8859	5609	1554	1641	55			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called NON TEMPLATE DNA 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP *GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	11	Total	C	N	O	P	0	0	0
			226	109	44	63	10			

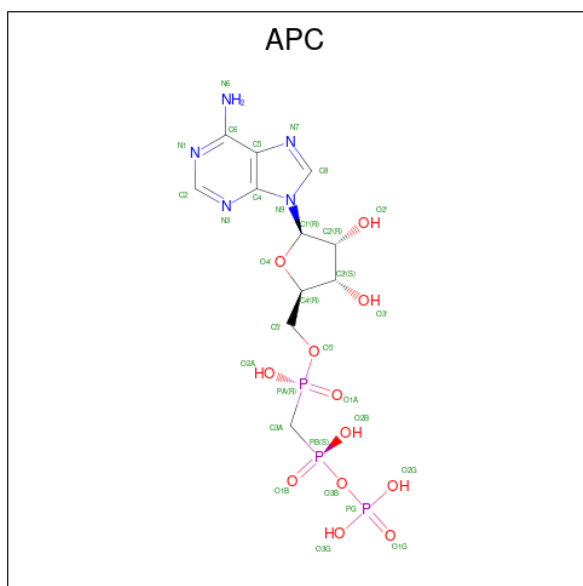
- Molecule 14 is a RNA chain called TRANSCRIPT RNA 5'-R(*CP*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	6	Total	C	N	O	P	0	0	0
			130	58	26	40	6			

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*DTP *TP*TP*CP*C BRU*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	20	Total	Br	C	N	O	P	0	0	0
			404	1	194	63	126	20			

- Molecule 16 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total 2	Zn 2	0	0
17	B	1	Total 1	Zn 1	0	0
17	C	1	Total 1	Zn 1	0	0
17	I	2	Total 2	Zn 2	0	0
17	J	1	Total 1	Zn 1	0	0
17	L	1	Total 1	Zn 1	0	0

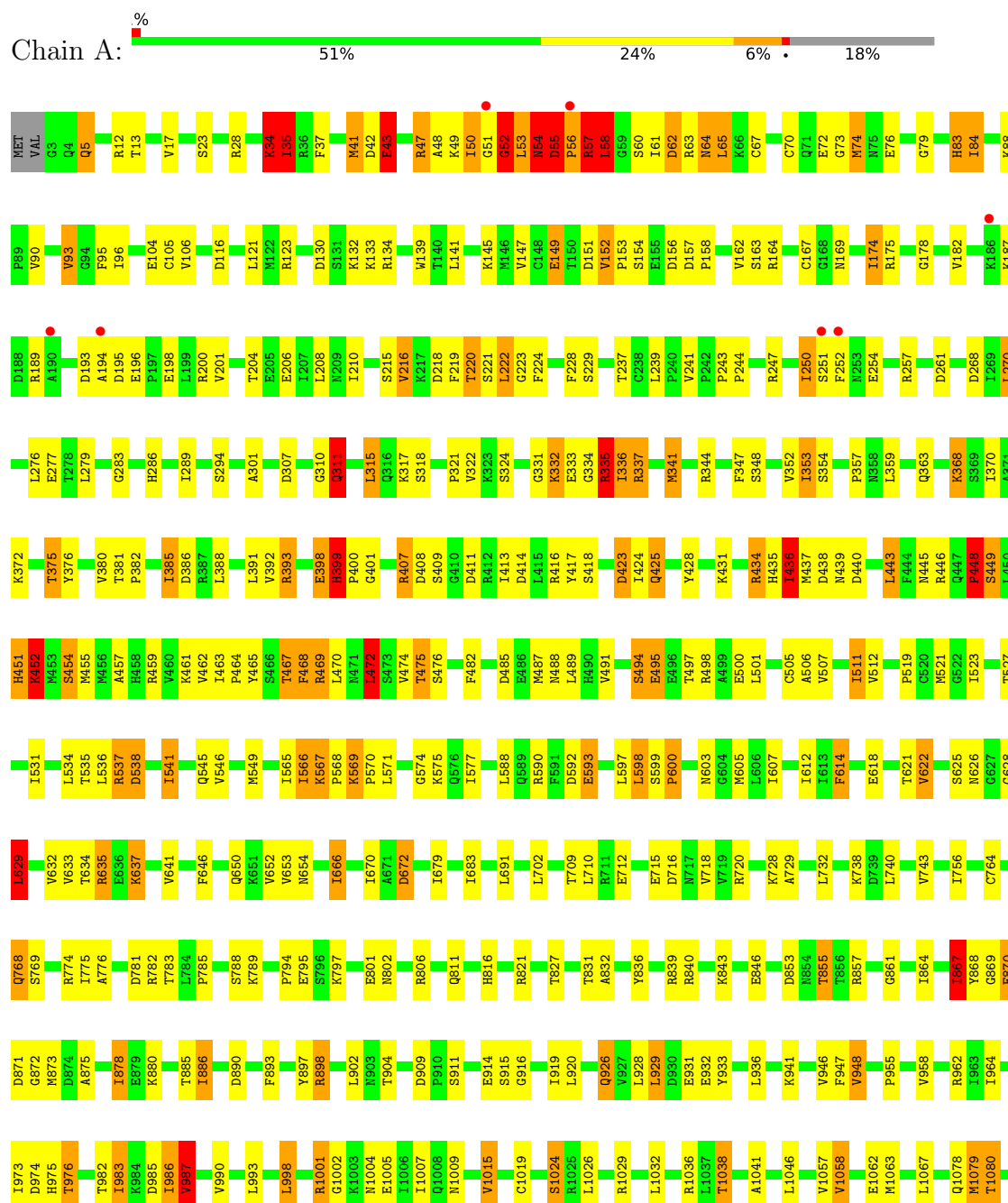
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

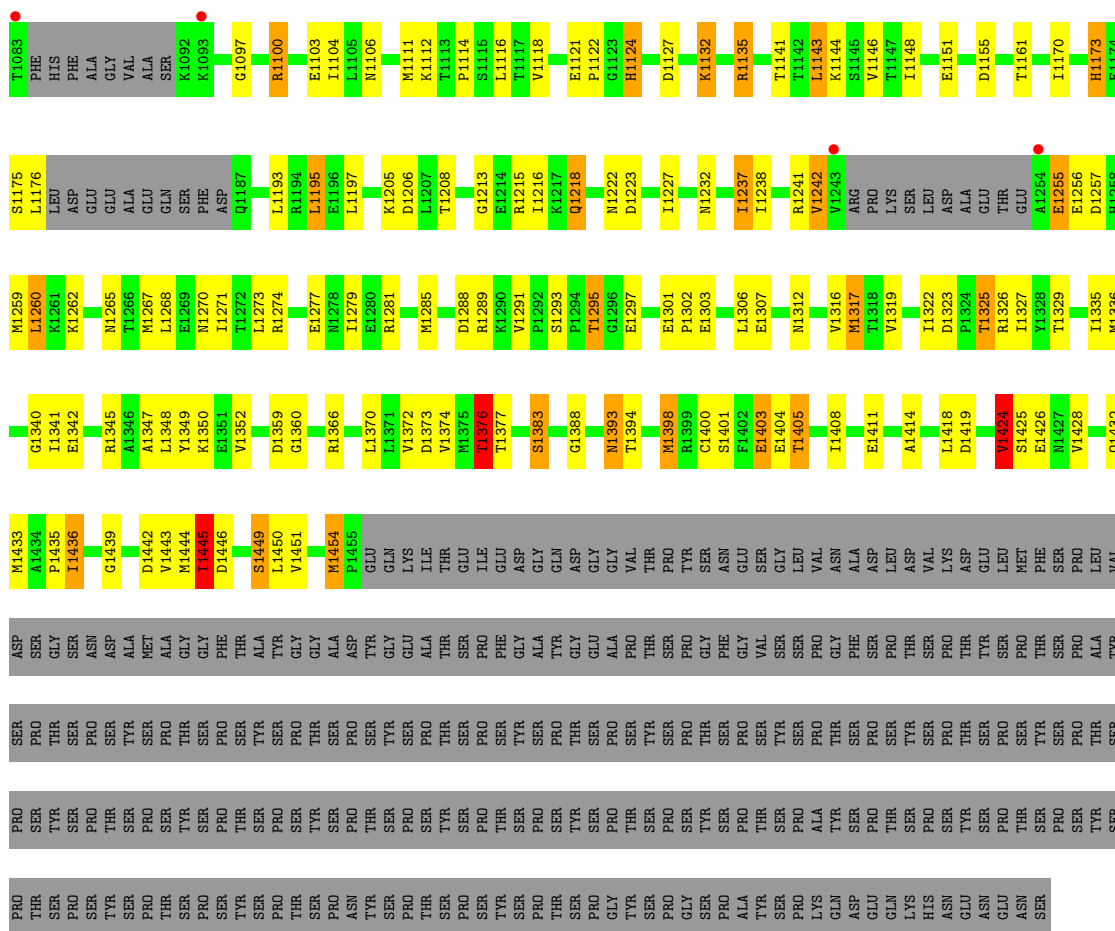
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total 1	Mg 1	0	0

3 Residue-property plots [i](#)

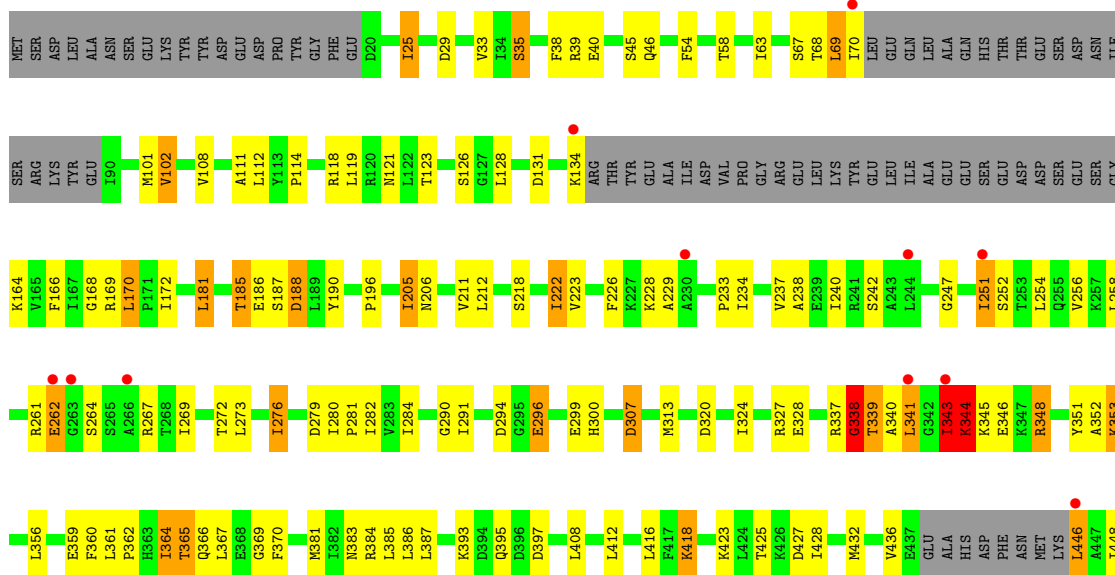
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

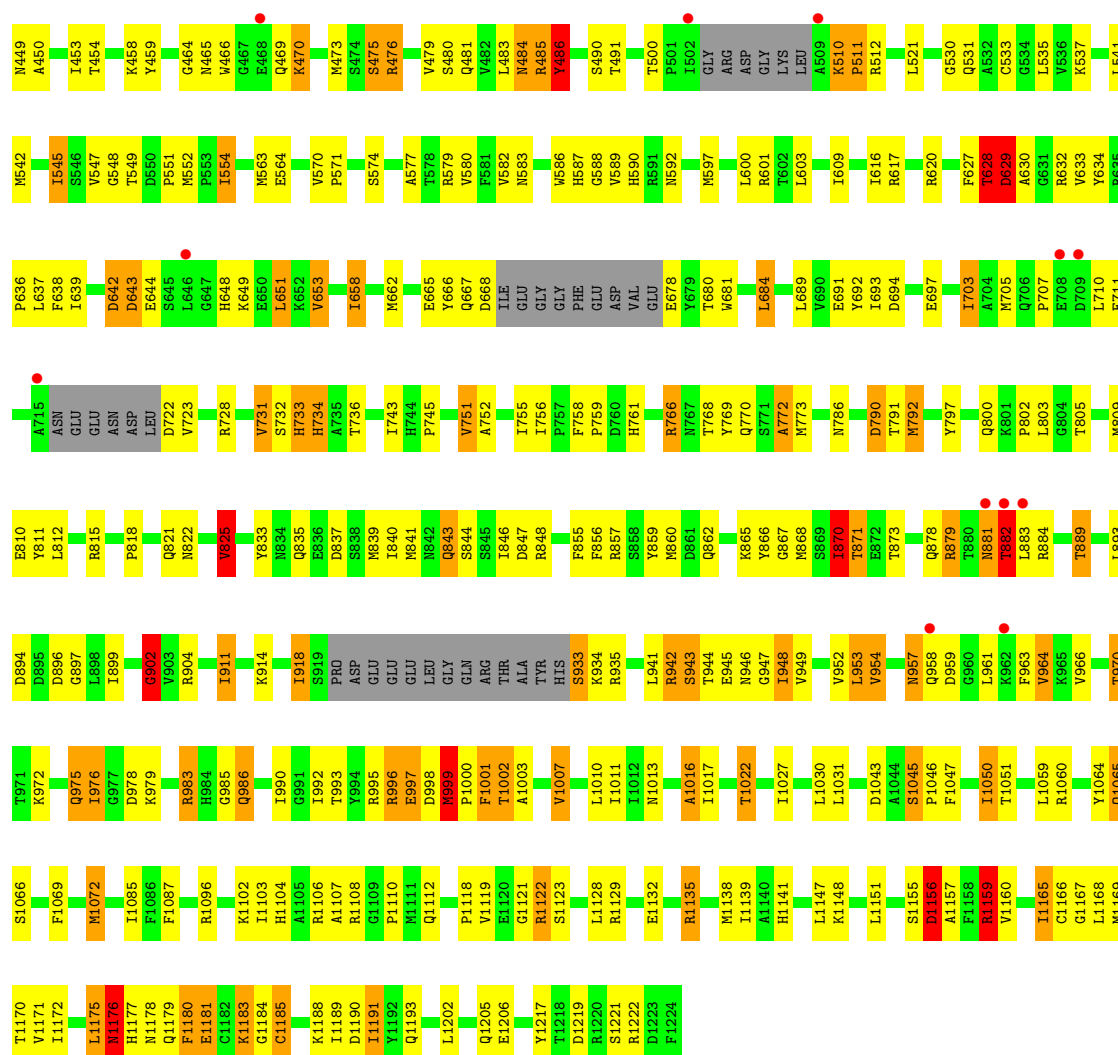
- Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



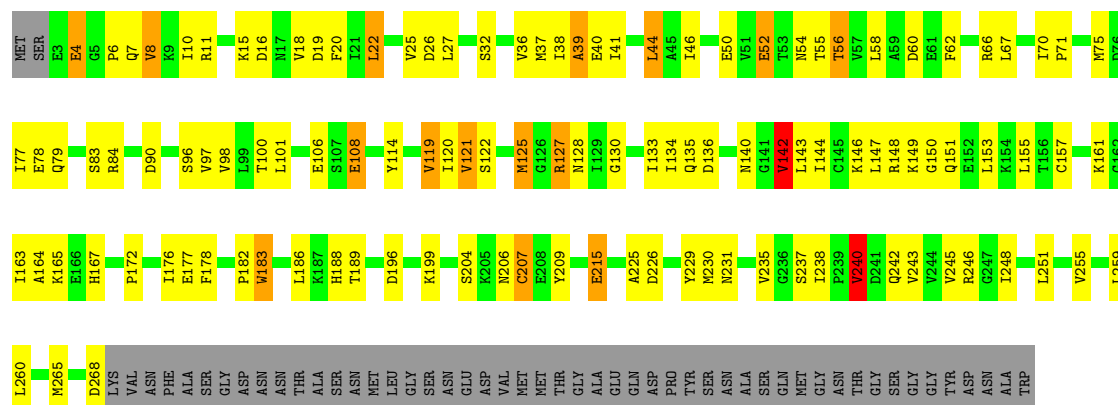


- Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2



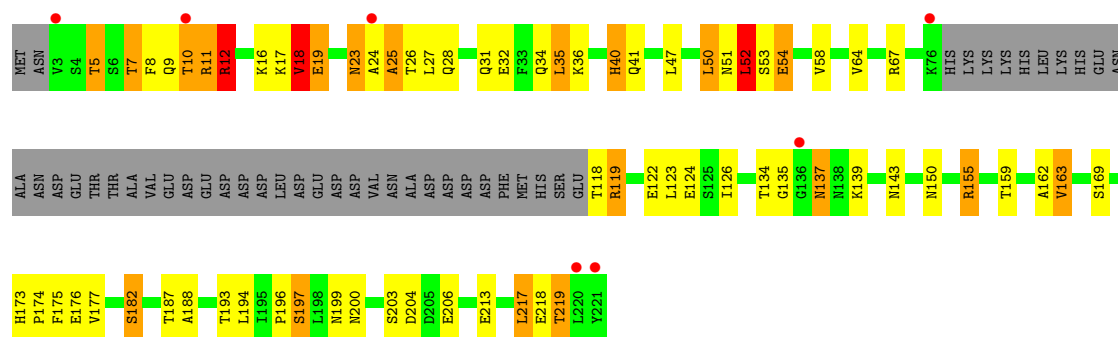


• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3



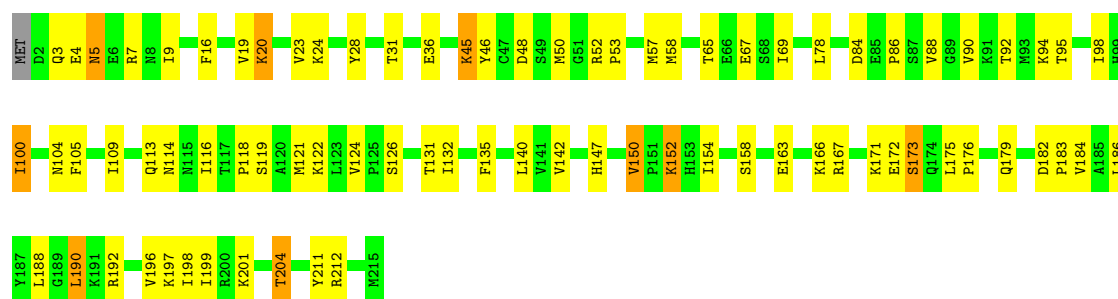
● Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4





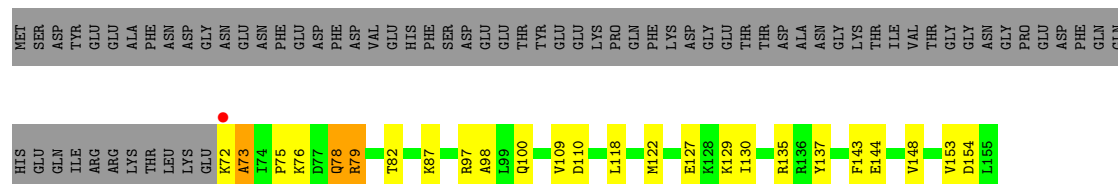
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E: 62% 33% .



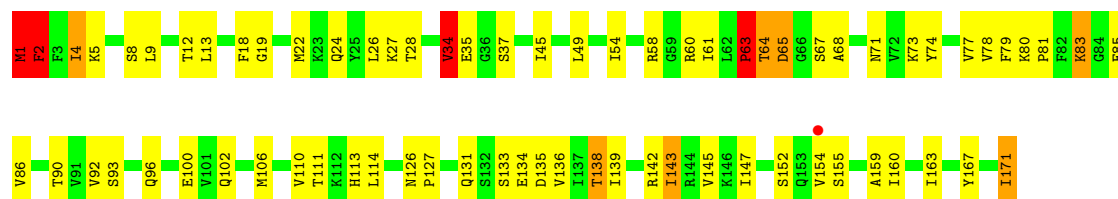
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F: 38% 14% 46% .



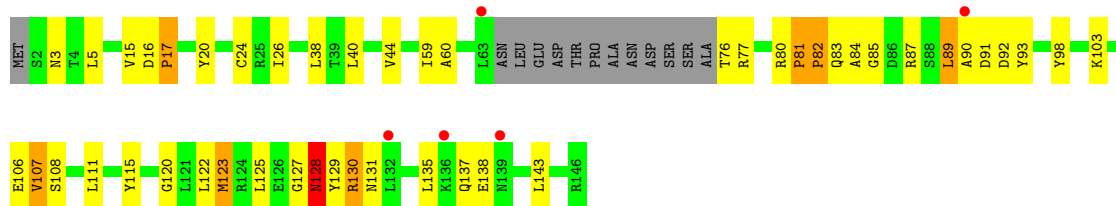
• Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G: 58% 36% . .



• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H: 3% 59% 27% 5% 9% .



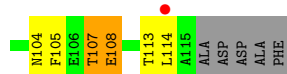
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



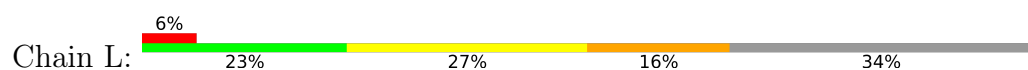
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



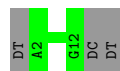
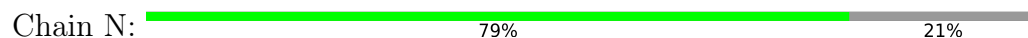
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



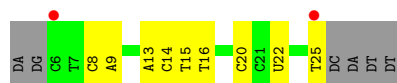
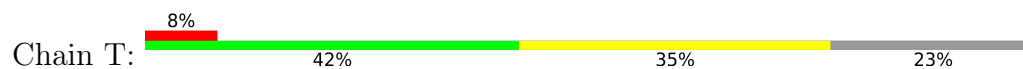
• Molecule 13: NON TEMPLATE DNA 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*TP)-3'



- Molecule 14: TRANSCRIPT RNA 5'-R(*CP*CP*AP*GP*GP*AP)-3'



- Molecule 15: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*DTP *TP*TP*CP*C
BRU*GP*GP*TP*CP*AP*TP*T)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.60Å 391.30Å 283.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.89 – 3.50 49.89 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.89-3.50) 98.1 (49.89-3.50)	Depositor EDS
R_{merge}	0.68	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.156 , 0.185 0.180 , 0.207	Depositor DCC
R_{free} test set	3255 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	110.5	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 123.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.036 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.037 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32010	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APC, BRU, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.92	10/11397 (0.1%)	1.58	149/15415 (1.0%)
2	B	0.89	3/9029 (0.0%)	1.50	120/12171 (1.0%)
3	C	0.84	0/2133	1.42	18/2891 (0.6%)
4	D	0.89	2/1444 (0.1%)	1.64	28/1935 (1.4%)
5	E	0.79	0/1788	1.43	18/2406 (0.7%)
6	F	0.94	2/691 (0.3%)	1.40	7/933 (0.8%)
7	G	0.90	1/1368 (0.1%)	1.43	9/1844 (0.5%)
8	H	0.88	1/1086 (0.1%)	1.44	12/1470 (0.8%)
9	I	0.81	0/989	1.36	9/1331 (0.7%)
10	J	0.89	1/541 (0.2%)	1.49	3/727 (0.4%)
11	K	0.81	0/938	1.46	10/1267 (0.8%)
12	L	0.90	0/365	1.51	2/485 (0.4%)
13	N	0.47	0/254	0.61	0/391
14	P	0.81	0/145	0.73	0/224
15	T	0.62	0/426	0.73	0/652
All	All	0.88	20/32594 (0.1%)	1.50	385/44142 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1	MET	C-N	7.88	1.44	1.33
1	A	54	ASN	CA-C	7.72	1.63	1.52
1	A	867	ILE	CG1-CD1	7.15	1.79	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	ARG	CA-C	6.45	1.61	1.52
4	D	24	ALA	CA-C	6.31	1.61	1.52
2	B	881	ASN	C-N	6.25	1.41	1.33
1	A	53	LEU	N-CA	6.24	1.53	1.45
1	A	1454	MET	CA-C	6.23	1.60	1.52
4	D	18	VAL	CA-C	6.02	1.60	1.52
1	A	52	GLY	C-N	5.87	1.41	1.33
6	F	122	MET	SD-CE	5.68	1.93	1.79
1	A	437	MET	SD-CE	5.68	1.93	1.79
10	J	49	MET	SD-CE	-5.58	1.65	1.79
1	A	1398	MET	SD-CE	5.54	1.93	1.79
2	B	948	ILE	CG1-CD1	5.37	1.72	1.51
2	B	882	THR	N-CA	5.30	1.52	1.46
1	A	55	ASP	CA-C	-5.09	1.46	1.52
8	H	15	VAL	C-N	5.05	1.38	1.33
6	F	153	VAL	CA-C	5.03	1.59	1.52
1	A	56	PRO	C-N	5.02	1.40	1.33

All (385) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	THR	N-CA-C	-11.10	98.56	112.88
1	A	72	GLU	N-CA-C	10.53	122.71	111.03
1	A	1404	GLU	N-CA-C	9.83	124.89	113.19
1	A	54	ASN	CA-CB-CG	9.66	122.26	112.60
1	A	34	LYS	CA-C-N	9.39	138.61	121.70
1	A	34	LYS	C-N-CA	9.39	138.61	121.70
8	H	92	ASP	N-CA-C	-9.15	100.52	112.41
3	C	39	ALA	N-CA-C	9.14	125.20	112.04
7	G	34	VAL	N-CA-C	8.73	118.80	110.42
4	D	25	ALA	CA-C-N	8.47	135.81	122.60
4	D	25	ALA	C-N-CA	8.47	135.81	122.60
1	A	64	ASN	N-CA-C	-8.41	99.20	110.55
10	J	5	VAL	N-CA-C	-8.40	97.78	109.21
4	D	54	GLU	N-CA-C	-8.09	102.46	111.28
1	A	57	ARG	CA-C-N	7.88	136.60	121.54
1	A	57	ARG	C-N-CA	7.88	136.60	121.54
8	H	81	PRO	N-CA-C	7.84	120.27	110.70
4	D	188	ALA	N-CA-C	-7.68	102.88	111.71
2	B	945	GLU	N-CA-C	7.67	119.85	110.41
10	J	9	SER	N-CA-C	7.62	119.22	111.07
1	A	42	ASP	CA-CB-CG	7.58	120.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	PRO	CA-C-N	7.55	135.97	121.54
1	A	56	PRO	C-N-CA	7.55	135.97	121.54
1	A	998	LEU	N-CA-C	7.55	120.97	108.96
2	B	998	ASP	CA-CB-CG	7.54	120.14	112.60
1	A	1112	LYS	N-CA-C	7.48	119.21	111.14
2	B	628	THR	CA-C-N	7.44	135.75	121.54
2	B	628	THR	C-N-CA	7.44	135.75	121.54
1	A	399	HIS	N-CA-CB	7.43	123.60	110.37
2	B	1122	ARG	CA-C-N	7.41	131.09	120.79
2	B	1122	ARG	C-N-CA	7.41	131.09	120.79
3	C	135	GLN	CA-C-N	7.36	131.28	120.90
3	C	135	GLN	C-N-CA	7.36	131.28	120.90
2	B	338	GLY	CA-C-N	7.35	134.93	121.70
2	B	338	GLY	C-N-CA	7.35	134.93	121.70
2	B	694	ASP	CA-CB-CG	7.34	119.94	112.60
1	A	629	LEU	N-CA-C	-7.33	103.28	111.71
1	A	34	LYS	N-CA-C	-7.31	95.02	108.02
1	A	229	SER	N-CA-C	7.21	119.21	107.32
1	A	218	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	485	ASP	CA-CB-CG	7.14	119.74	112.60
1	A	70	CYS	CA-C-N	-7.13	111.25	122.65
1	A	70	CYS	C-N-CA	-7.13	111.25	122.65
1	A	219	PHE	CA-CB-CG	7.13	120.93	113.80
1	A	1445	ILE	N-CA-CB	7.07	119.47	110.99
8	H	129	TYR	N-CA-C	7.07	119.06	111.36
2	B	902	GLY	CA-C-N	7.01	130.93	120.69
2	B	902	GLY	C-N-CA	7.01	130.93	120.69
1	A	535	THR	N-CA-C	6.98	120.75	112.93
2	B	825	VAL	N-CA-C	6.93	117.82	108.11
2	B	1184	GLY	CA-C-N	6.91	134.73	121.54
2	B	1184	GLY	C-N-CA	6.91	134.73	121.54
2	B	366	GLN	N-CA-C	-6.89	104.77	113.72
2	B	479	VAL	N-CA-C	-6.85	104.17	110.82
1	A	472	LEU	N-CA-C	6.85	118.74	111.28
4	D	31	GLN	N-CA-C	-6.84	103.06	111.40
1	A	244	PRO	N-CA-C	6.82	119.02	110.70
5	E	171	LYS	N-CA-C	-6.77	99.93	110.42
1	A	35	ILE	N-CA-CB	6.77	123.00	111.50
2	B	102	VAL	N-CA-C	6.72	117.52	108.11
1	A	411	ASP	CA-C-N	6.69	130.21	120.71
1	A	411	ASP	C-N-CA	6.69	130.21	120.71
5	E	5	ASN	N-CA-C	-6.68	105.13	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	GLN	N-CA-C	6.67	124.55	109.81
2	B	736	THR	N-CA-C	-6.59	105.77	113.88
2	B	359	GLU	N-CA-C	6.59	119.80	111.69
3	C	60	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	1419	ASP	CA-C-N	6.58	129.39	120.38
1	A	1419	ASP	C-N-CA	6.58	129.39	120.38
2	B	1156	ASP	CA-C-N	6.57	134.09	121.54
2	B	1156	ASP	C-N-CA	6.57	134.09	121.54
2	B	703	ILE	N-CA-C	6.57	117.36	108.17
1	A	70	CYS	N-CA-C	-6.53	101.74	110.55
3	C	183	TRP	N-CA-C	-6.53	97.90	108.41
6	F	87	LYS	CA-C-N	6.45	129.44	120.29
6	F	87	LYS	C-N-CA	6.45	129.44	120.29
1	A	194	ALA	CA-C-N	6.45	133.30	121.70
1	A	194	ALA	C-N-CA	6.45	133.30	121.70
8	H	131	ASN	CA-CB-CG	6.44	119.04	112.60
2	B	1013	ASN	N-CA-C	6.41	117.73	109.72
1	A	897	TYR	N-CA-C	6.41	121.35	112.45
2	B	1016	ALA	CA-C-N	6.37	126.54	120.43
2	B	1016	ALA	C-N-CA	6.37	126.54	120.43
1	A	948	VAL	N-CA-C	6.36	117.87	110.62
1	A	250	ILE	CA-C-N	6.35	133.67	121.54
1	A	250	ILE	C-N-CA	6.35	133.67	121.54
2	B	427	ASP	N-CA-C	-6.34	105.56	113.55
2	B	188	ASP	CA-CB-CG	6.33	118.93	112.60
3	C	62	PHE	CA-C-N	6.31	128.59	120.70
3	C	62	PHE	C-N-CA	6.31	128.59	120.70
2	B	684	LEU	CA-C-N	6.30	128.72	120.28
2	B	684	LEU	C-N-CA	6.30	128.72	120.28
8	H	128	ASN	CA-C-N	6.29	129.22	120.29
8	H	128	ASN	C-N-CA	6.29	129.22	120.29
7	G	65	ASP	CA-CB-CG	6.28	118.88	112.60
2	B	1219	ASP	CA-CB-CG	6.27	118.87	112.60
2	B	944	THR	CA-C-N	6.24	132.79	121.06
2	B	944	THR	C-N-CA	6.24	132.79	121.06
1	A	832	ALA	CA-C-N	6.23	128.91	120.38
1	A	832	ALA	C-N-CA	6.23	128.91	120.38
2	B	465	ASN	CA-CB-CG	6.21	118.81	112.60
2	B	45	SER	CA-C-N	6.19	130.11	120.82
2	B	45	SER	C-N-CA	6.19	130.11	120.82
1	A	614	PHE	CA-CB-CG	6.17	119.97	113.80
3	C	40	GLU	N-CA-C	6.17	120.94	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	14	VAL	CB-CA-C	6.16	116.69	110.65
1	A	398	GLU	CA-C-O	-6.16	114.39	121.47
2	B	642	ASP	N-CA-C	-6.15	104.63	111.71
2	B	397	ASP	CA-CB-CG	6.13	118.73	112.60
2	B	651	LEU	CA-C-N	6.12	128.80	120.54
2	B	651	LEU	C-N-CA	6.12	128.80	120.54
1	A	1436	ILE	N-CA-CB	-6.11	102.98	111.41
2	B	186	GLU	CA-C-N	6.11	128.47	120.28
2	B	186	GLU	C-N-CA	6.11	128.47	120.28
11	K	107	THR	CB-CA-C	6.10	120.58	110.81
1	A	886	ILE	N-CA-C	6.10	116.57	110.23
1	A	718	VAL	CA-C-N	6.06	128.76	120.46
1	A	718	VAL	C-N-CA	6.06	128.76	120.46
1	A	1325	THR	N-CA-C	-6.06	106.43	113.88
6	F	154	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	54	ASN	CA-C-N	6.06	136.58	121.80
1	A	54	ASN	C-N-CA	6.06	136.58	121.80
11	K	113	THR	CB-CA-C	6.05	120.74	111.85
2	B	343	ILE	CA-C-N	6.04	133.09	121.54
2	B	343	ILE	C-N-CA	6.04	133.09	121.54
1	A	425	GLN	N-CA-C	6.02	118.59	107.99
1	A	743	VAL	N-CA-C	-6.02	104.76	110.42
1	A	1403	GLU	N-CA-C	6.01	123.61	110.80
7	G	4	ILE	N-CA-C	-6.01	99.76	108.17
9	I	93	LYS	CA-C-N	6.00	129.13	120.79
9	I	93	LYS	C-N-CA	6.00	129.13	120.79
1	A	423	ASP	CA-CB-CG	6.00	118.60	112.60
9	I	31	THR	N-CA-C	-6.00	106.50	113.88
2	B	296	GLU	N-CA-C	-5.96	104.72	112.23
1	A	672	ASP	CA-CB-CG	5.96	118.56	112.60
4	D	163	VAL	CA-C-N	5.96	128.62	120.46
4	D	163	VAL	C-N-CA	5.96	128.62	120.46
2	B	1121	GLY	CA-C-N	5.94	128.23	120.28
2	B	1121	GLY	C-N-CA	5.94	128.23	120.28
11	K	53	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	1424	VAL	CA-C-N	5.92	128.53	120.54
1	A	1424	VAL	C-N-CA	5.92	128.53	120.54
2	B	1001	PHE	N-CA-C	5.91	119.18	109.72
1	A	467	THR	CB-CA-C	-5.91	99.51	109.50
5	E	173	SER	CA-C-N	5.91	130.14	120.63
5	E	173	SER	C-N-CA	5.91	130.14	120.63
8	H	138	GLU	N-CA-C	-5.90	104.76	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	51	ASN	CA-CB-CG	5.89	118.50	112.60
2	B	752	ALA	N-CA-C	5.89	117.37	111.07
2	B	339	THR	CA-C-N	5.88	132.77	121.54
2	B	339	THR	C-N-CA	5.88	132.77	121.54
2	B	1135	ARG	N-CA-C	-5.88	104.78	111.07
1	A	239	LEU	N-CA-C	5.88	117.41	109.24
3	C	136	ASP	CA-CB-CG	5.86	118.46	112.60
2	B	976	ILE	N-CA-C	5.86	118.38	111.05
4	D	18	VAL	CA-C-N	5.84	132.22	121.70
4	D	18	VAL	C-N-CA	5.84	132.22	121.70
1	A	223	GLY	CA-C-N	5.84	132.69	121.54
1	A	223	GLY	C-N-CA	5.84	132.69	121.54
2	B	1102	LYS	CA-C-N	5.84	129.21	120.69
2	B	1102	LYS	C-N-CA	5.84	129.21	120.69
5	E	150	VAL	N-CA-C	5.82	112.86	107.56
9	I	83	ASN	CA-C-N	5.82	130.41	123.19
9	I	83	ASN	C-N-CA	5.82	130.41	123.19
7	G	2	PHE	CA-CB-CG	5.79	119.59	113.80
1	A	898	ARG	N-CA-C	5.79	118.65	109.96
2	B	1180	PHE	CA-CB-CG	-5.79	108.01	113.80
1	A	54	ASN	CB-CA-C	5.78	121.92	110.42
1	A	1350	LYS	CA-C-N	5.77	128.01	120.28
1	A	1350	LYS	C-N-CA	5.77	128.01	120.28
1	A	1376	THR	CB-CA-C	5.77	119.89	110.95
2	B	881	ASN	CA-C-N	5.74	128.23	120.65
2	B	881	ASN	C-N-CA	5.74	128.23	120.65
1	A	794	PRO	CA-C-N	5.73	127.96	120.28
1	A	794	PRO	C-N-CA	5.73	127.96	120.28
2	B	809	MET	CA-C-N	5.73	128.28	120.54
2	B	809	MET	C-N-CA	5.73	128.28	120.54
2	B	1159	ARG	N-CA-C	5.73	118.04	108.02
2	B	1085	ILE	N-CA-C	5.72	116.54	108.36
1	A	310	GLY	CA-C-N	5.71	135.74	121.80
1	A	310	GLY	C-N-CA	5.71	135.74	121.80
3	C	225	ALA	N-CA-C	5.71	118.05	108.23
2	B	818	PRO	N-CA-C	5.71	119.49	111.33
1	A	331	GLY	CA-C-N	5.70	132.42	121.54
1	A	331	GLY	C-N-CA	5.70	132.42	121.54
1	A	462	VAL	N-CA-CB	5.69	117.31	110.31
2	B	1222	ARG	N-CA-C	5.67	118.40	111.82
1	A	622	VAL	N-CA-CB	-5.67	104.80	112.22
1	A	537	ARG	CA-C-N	5.66	132.36	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	537	ARG	C-N-CA	5.66	132.36	121.54
1	A	1005	GLU	CB-CG-CD	5.66	122.22	112.60
1	A	710	LEU	N-CA-C	-5.66	105.19	111.36
1	A	1360	GLY	CA-C-N	5.64	130.37	121.56
1	A	1360	GLY	C-N-CA	5.64	130.37	121.56
1	A	592	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	646	PHE	CA-C-N	5.64	126.36	119.99
1	A	646	PHE	C-N-CA	5.64	126.36	119.99
1	A	452	LYS	N-CA-C	-5.63	105.22	111.36
3	C	142	VAL	N-CA-C	5.63	116.87	109.21
2	B	627	PHE	N-CA-C	5.60	117.99	108.02
4	D	35	LEU	N-CA-C	5.60	117.83	111.11
5	E	172	GLU	CA-C-N	5.59	128.57	120.79
5	E	172	GLU	C-N-CA	5.59	128.57	120.79
1	A	116	ASP	CA-C-N	5.57	128.52	120.38
1	A	116	ASP	C-N-CA	5.57	128.52	120.38
1	A	1001	ARG	N-CA-C	5.57	120.34	113.50
2	B	733	HIS	CA-C-N	5.56	129.49	120.60
2	B	733	HIS	C-N-CA	5.56	129.49	120.60
6	F	122	MET	CA-C-N	5.55	127.65	120.44
6	F	122	MET	C-N-CA	5.55	127.65	120.44
1	A	495	GLU	CA-C-N	5.55	130.06	120.58
1	A	495	GLU	C-N-CA	5.55	130.06	120.58
5	E	53	PRO	N-CA-C	5.55	119.17	110.80
1	A	468	PHE	CA-CB-CG	5.54	119.34	113.80
1	A	1237	ILE	N-CA-C	5.53	116.71	108.46
1	A	425	GLN	CA-C-N	5.53	128.96	121.05
1	A	425	GLN	C-N-CA	5.53	128.96	121.05
1	A	436	ILE	CA-CB-CG2	5.52	119.89	110.50
4	D	173	HIS	CB-CA-C	5.52	118.35	109.41
1	A	399	HIS	CA-CB-CG	-5.51	108.29	113.80
4	D	12	ARG	N-CA-C	5.51	118.10	108.52
1	A	23	SER	N-CA-C	-5.50	102.85	109.83
1	A	451	HIS	CB-CA-C	-5.50	100.73	109.80
1	A	710	LEU	CA-C-N	5.50	127.59	120.44
1	A	710	LEU	C-N-CA	5.50	127.59	120.44
1	A	5	GLN	N-CA-C	5.49	117.96	110.55
9	I	94	ASP	CA-C-N	5.49	132.02	121.54
9	I	94	ASP	C-N-CA	5.49	132.02	121.54
8	H	85	GLY	N-CA-C	-5.47	105.87	112.49
1	A	511	ILE	N-CA-CB	5.47	116.58	110.51
1	A	1205	LYS	N-CA-C	-5.46	107.18	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	3	ASN	N-CA-C	5.46	117.74	110.53
1	A	73	GLY	CA-C-N	5.46	131.97	121.54
1	A	73	GLY	C-N-CA	5.46	131.97	121.54
1	A	1005	GLU	N-CA-C	5.46	117.04	111.14
4	D	143	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	728	LYS	CA-C-N	5.45	127.59	120.28
1	A	728	LYS	C-N-CA	5.45	127.59	120.28
2	B	276	ILE	CA-C-N	5.44	128.35	120.79
2	B	276	ILE	C-N-CA	5.44	128.35	120.79
1	A	123	ARG	CA-C-N	5.43	128.00	120.29
1	A	123	ARG	C-N-CA	5.43	128.00	120.29
1	A	1097	GLY	CA-C-N	5.43	125.64	120.43
1	A	1097	GLY	C-N-CA	5.43	125.64	120.43
4	D	52	LEU	CA-C-N	5.41	131.88	121.54
4	D	52	LEU	C-N-CA	5.41	131.88	121.54
3	C	108	GLU	N-CA-C	-5.41	105.04	111.69
2	B	896	ASP	CA-CB-CG	5.41	118.01	112.60
5	E	95	THR	CA-C-N	5.40	127.95	120.29
5	E	95	THR	C-N-CA	5.40	127.95	120.29
2	B	307	ASP	CA-C-N	5.40	128.05	120.28
2	B	307	ASP	C-N-CA	5.40	128.05	120.28
1	A	222	LEU	N-CA-C	-5.39	103.57	110.53
9	I	9	ASP	CA-CB-CG	5.38	117.98	112.60
3	C	19	ASP	CA-CB-CG	5.38	117.98	112.60
2	B	1181	GLU	N-CA-C	5.38	122.26	110.80
2	B	999	MET	N-CA-C	5.37	117.49	110.08
2	B	918	ILE	N-CA-C	5.37	116.09	108.42
1	A	334	GLY	CA-C-N	5.36	131.78	121.54
1	A	334	GLY	C-N-CA	5.36	131.78	121.54
5	E	204	THR	CB-CA-C	5.35	118.49	110.08
1	A	846	GLU	CA-C-N	5.35	130.94	120.99
1	A	846	GLU	C-N-CA	5.35	130.94	120.99
2	B	484	ASN	CA-CB-CG	5.35	117.95	112.60
5	E	126	SER	N-CA-C	5.34	117.85	111.71
2	B	870	ILE	CA-C-N	5.34	128.67	120.82
2	B	870	ILE	C-N-CA	5.34	128.67	120.82
11	K	84	LYS	CA-C-N	5.34	127.43	120.28
11	K	84	LYS	C-N-CA	5.34	127.43	120.28
3	C	135	GLN	N-CA-C	-5.33	106.79	113.72
1	A	83	HIS	N-CA-C	5.33	116.94	108.79
1	A	1029	ARG	CA-C-N	5.32	127.72	120.54
1	A	1029	ARG	C-N-CA	5.32	127.72	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	ARG	N-CA-C	-5.32	105.38	111.07
11	K	32	VAL	N-CA-C	5.31	115.72	107.28
1	A	1127	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	55	ASP	N-CA-CB	5.30	119.80	110.37
2	B	1171	VAL	N-CA-C	5.30	116.24	109.30
2	B	418	LYS	CA-C-N	5.30	127.64	120.38
2	B	418	LYS	C-N-CA	5.30	127.64	120.38
1	A	1295	THR	CB-CA-C	5.29	120.17	110.11
2	B	629	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	646	PHE	N-CA-C	-5.29	105.21	110.97
2	B	222	ILE	CB-CA-C	5.29	118.45	110.63
3	C	207	CYS	CA-C-N	5.28	127.31	120.44
3	C	207	CYS	C-N-CA	5.28	127.31	120.44
2	B	1065	GLN	CB-CA-C	5.28	118.70	110.67
1	A	408	ASP	N-CA-C	-5.28	105.42	111.07
2	B	643	ASP	CA-C-N	5.27	131.61	121.54
2	B	643	ASP	C-N-CA	5.27	131.61	121.54
1	A	802	ASN	N-CA-C	5.26	118.27	110.48
1	A	1080	THR	CA-C-N	5.26	128.06	120.38
1	A	1080	THR	C-N-CA	5.26	128.06	120.38
2	B	1156	ASP	N-CA-C	5.25	121.99	110.80
9	I	52	ILE	N-CA-CB	5.24	117.76	111.31
6	F	100	GLN	CA-C-N	5.24	127.92	120.53
6	F	100	GLN	C-N-CA	5.24	127.92	120.53
2	B	790	ASP	CA-CB-CG	5.24	117.84	112.60
2	B	1087	PHE	CA-CB-CG	5.24	119.04	113.80
5	E	163	GLU	CB-CG-CD	5.24	121.50	112.60
2	B	1003	ALA	CA-C-N	5.23	128.97	120.60
2	B	1003	ALA	C-N-CA	5.23	128.97	120.60
8	H	137	GLN	CA-C-N	5.23	127.24	120.44
8	H	137	GLN	C-N-CA	5.23	127.24	120.44
2	B	69	LEU	CA-C-N	5.22	131.10	121.70
2	B	69	LEU	C-N-CA	5.22	131.10	121.70
8	H	131	ASN	N-CA-C	-5.22	105.67	111.36
1	A	195	ASP	CA-CB-CG	5.22	117.82	112.60
4	D	122	GLU	CA-C-N	5.21	127.25	120.28
4	D	122	GLU	C-N-CA	5.21	127.25	120.28
1	A	216	VAL	N-CA-CB	5.20	116.29	110.62
4	D	200	ASN	CA-C-N	5.20	127.77	120.28
4	D	200	ASN	C-N-CA	5.20	127.77	120.28
1	A	228	PHE	N-CA-C	5.18	118.76	112.23
1	A	1026	LEU	N-CA-C	5.18	119.10	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	947	PHE	CA-C-N	5.18	127.83	120.53
1	A	947	PHE	C-N-CA	5.18	127.83	120.53
1	A	1132	LYS	CA-C-N	5.17	127.17	120.44
1	A	1132	LYS	C-N-CA	5.17	127.17	120.44
4	D	26	THR	CA-C-N	5.17	129.69	122.08
4	D	26	THR	C-N-CA	5.17	129.69	122.08
1	A	268	ASP	CA-CB-CG	5.17	117.77	112.60
2	B	353	LYS	CA-C-N	5.16	127.20	120.28
2	B	353	LYS	C-N-CA	5.16	127.20	120.28
2	B	958	GLN	CA-C-N	5.16	131.22	122.65
2	B	958	GLN	C-N-CA	5.16	131.22	122.65
1	A	1161	THR	N-CA-C	5.16	117.90	109.59
2	B	294	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	17	VAL	N-CA-CB	5.14	118.32	111.64
1	A	931	GLU	CA-C-N	5.13	127.92	120.79
1	A	931	GLU	C-N-CA	5.13	127.92	120.79
4	D	124	GLU	CA-C-N	5.13	127.16	120.28
4	D	124	GLU	C-N-CA	5.13	127.16	120.28
2	B	511	PRO	N-CA-C	5.12	120.33	114.03
5	E	196	VAL	N-CA-CB	5.12	118.21	111.25
2	B	957	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	53	LEU	N-CA-CB	5.11	120.45	111.55
1	A	317	LYS	CA-C-N	5.11	131.30	121.54
1	A	317	LYS	C-N-CA	5.11	131.30	121.54
11	K	25	THR	CA-C-N	5.09	127.82	120.38
11	K	25	THR	C-N-CA	5.09	127.82	120.38
4	D	118	THR	CA-C-N	5.09	131.26	121.54
4	D	118	THR	C-N-CA	5.09	131.26	121.54
1	A	1411	GLU	CB-CG-CD	5.08	121.24	112.60
1	A	1205	LYS	CA-C-N	5.08	131.25	121.54
1	A	1205	LYS	C-N-CA	5.08	131.25	121.54
2	B	894	ASP	CA-CB-CG	5.08	117.68	112.60
2	B	600	LEU	CA-C-N	5.08	127.40	120.54
2	B	600	LEU	C-N-CA	5.08	127.40	120.54
2	B	339	THR	CB-CA-C	5.08	120.28	109.10
2	B	964	VAL	N-CA-C	5.08	116.03	108.46
2	B	1017	ILE	N-CA-CB	-5.08	107.12	110.52
11	K	53	ASP	CA-C-N	5.08	127.08	120.28
11	K	53	ASP	C-N-CA	5.08	127.08	120.28
5	E	20	LYS	CA-C-N	5.07	127.04	120.44
5	E	20	LYS	C-N-CA	5.07	127.04	120.44
2	B	228	LYS	CA-C-N	5.07	131.23	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	228	LYS	C-N-CA	5.07	131.23	121.54
12	L	56	LEU	N-CA-C	5.07	121.60	110.80
4	D	24	ALA	N-CA-C	5.06	121.59	110.80
2	B	943	SER	CA-C-N	5.06	127.02	120.44
2	B	943	SER	C-N-CA	5.06	127.02	120.44
7	G	64	THR	N-CA-C	5.06	118.71	112.54
1	A	637	LYS	N-CA-C	5.05	119.91	113.55
2	B	628	THR	N-CA-C	-5.05	106.97	113.23
3	C	243	VAL	N-CA-C	-5.05	105.62	110.72
2	B	978	ASP	CA-CB-CG	5.05	117.65	112.60
5	E	24	LYS	CA-C-N	5.04	127.04	120.28
5	E	24	LYS	C-N-CA	5.04	127.04	120.28
2	B	181	LEU	N-CA-C	5.04	117.51	111.71
2	B	486	TYR	N-CA-C	-5.04	106.82	113.12
2	B	320	ASP	CA-CB-CG	5.04	117.64	112.60
7	G	18	PHE	CA-CB-CG	5.04	118.83	113.80
1	A	1393	ASN	N-CA-C	5.03	118.30	112.97
7	G	63	PRO	N-CA-C	5.03	122.83	112.47
2	B	454	THR	CA-C-N	5.03	127.27	120.38
2	B	454	THR	C-N-CA	5.03	127.27	120.38
2	B	768	THR	CA-C-N	5.02	127.46	120.63
2	B	768	THR	C-N-CA	5.02	127.46	120.63
2	B	871	THR	N-CA-C	5.02	116.76	110.24
3	C	96	SER	N-CA-C	5.02	116.43	108.96
2	B	1017	ILE	N-CA-C	5.01	118.94	112.67
7	G	1	MET	CA-C-N	5.01	131.11	121.54
7	G	1	MET	C-N-CA	5.01	131.11	121.54
12	L	40	LEU	N-CA-C	5.00	117.55	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Peptide,Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11197	0	11257	236	0
2	B	8859	0	8901	196	0
3	C	2095	0	2051	58	0
4	D	1434	0	1460	28	0
5	E	1752	0	1776	34	0
6	F	679	0	701	11	0
7	G	1340	0	1357	40	0
8	H	1068	0	1040	21	0
9	I	971	0	927	10	0
10	J	532	0	542	14	0
11	K	920	0	929	22	0
12	L	363	0	386	15	0
13	N	226	0	126	0	0
14	P	130	0	66	1	0
15	T	404	0	227	6	0
16	A	31	0	14	2	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	32010	0	31760	614	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 10.

All (614) 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)
1:A:867:ILE:CG1	1:A:867:ILE:CD1	1.79	1.60
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.43	0.98
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.54	0.90
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.53	0.90
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.55	0.87
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.57	0.87
3:C:66:ARG:NH2	10:J:3:VAL:O	2.08	0.86
1:A:855:THR:HG21	1:A:857:ARG:HE	1.37	0.86
16:A:2455:APC:H8	16:A:2455:APC:H5'2	1.58	0.86
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.58	0.84
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.61	0.81
3:C:56:THR:HG22	3:C:58:LEU:H	1.44	0.81
1:A:53:LEU:HD23	1:A:54:ASN:HB3	1.63	0.80
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.46	0.80
12:L:28:LYS:HB2	12:L:39:SER:HA	1.64	0.80
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.67	0.77
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.67	0.77
2:B:563:MET:HE3	2:B:580:VAL:HB	1.67	0.76
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.67	0.76
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.69	0.75
1:A:348:SER:HB2	2:B:1128:LEU:HD12	1.68	0.74
2:B:638:PHE:HB3	2:B:651:LEU:HD21	1.69	0.74
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.68	0.74
4:D:176:GLU:OE2	4:D:197:SER:HB2	1.86	0.74
1:A:472:LEU:O	1:A:475:THR:HB	1.87	0.74
1:A:61:ILE:HG22	1:A:62:ASP:H	1.51	0.74
2:B:882:THR:HG21	2:B:935:ARG:HA	1.70	0.74
1:A:254:GLU:HB3	2:B:935:ARG:HH21	1.53	0.73
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.70	0.73
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.17	0.73
2:B:1172:ILE:HD11	2:B:1183:LYS:HE2	1.69	0.72
2:B:247:GLY:H	2:B:418:LYS:HZ1	1.37	0.72
7:G:111:THR:HG22	7:G:113:HIS:H	1.55	0.72
2:B:642:ASP:HA	2:B:649:LYS:HA	1.71	0.72
1:A:1445:ILE:HD11	7:G:68:ALA:CB	2.19	0.71
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.73	0.71
1:A:650:GLN:O	1:A:654:ASN:HB2	1.91	0.70
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.72	0.70
1:A:63:ARG:HA	1:A:74:MET:HG3	1.74	0.70
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.74	0.69
2:B:101:MET:HG2	2:B:111:ALA:HA	1.74	0.69
3:C:182:PRO:HB3	3:C:204:SER:HB3	1.73	0.69
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.56	0.69
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.57	0.69
1:A:1151:GLU:HG2	9:I:45:ARG:HG3	1.75	0.68
7:G:138:THR:HG22	7:G:139:ILE:H	1.57	0.68
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.74	0.68
3:C:55:THR:HB	3:C:151:GLN:HA	1.76	0.68
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.28	0.68
1:A:1079:MET:HE3	1:A:1359:ASP:HB2	1.76	0.67
3:C:100:THR:HG22	3:C:119:VAL:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1433:MET:CE	7:G:63:PRO:HB3	2.23	0.67
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.76	0.67
7:G:1:MET:SD	7:G:2:PHE:N	2.64	0.67
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.76	0.67
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	1.94	0.66
6:F:76:LYS:HA	6:F:79:ARG:CD	2.25	0.66
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.76	0.66
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.76	0.66
2:B:1175:LEU:O	2:B:1176:ASN:HB3	1.95	0.66
3:C:54:ASN:OD1	3:C:56:THR:HB	1.96	0.65
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.79	0.65
2:B:273:LEU:HD12	2:B:280:ILE:HD13	1.77	0.65
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.78	0.65
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.78	0.65
2:B:510:LYS:N	2:B:511:PRO:HD3	2.12	0.65
1:A:982:THR:HB	1:A:985:ASP:H	1.61	0.65
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.36	0.65
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.78	0.65
2:B:882:THR:HG1	2:B:935:ARG:N	1.95	0.65
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.79	0.65
2:B:705:MET:H	2:B:710:LEU:HD12	1.61	0.64
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.36	0.64
2:B:484:ASN:HB3	2:B:486:TYR:CE2	2.33	0.64
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.28	0.64
1:A:982:THR:H	1:A:985:ASP:HB2	1.63	0.64
1:A:629:LEU:O	1:A:633:VAL:HG23	1.96	0.64
2:B:563:MET:CE	2:B:580:VAL:HB	2.28	0.64
3:C:52:GLU:HA	12:L:64:LEU:HD21	1.78	0.64
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.81	0.63
1:A:315:LEU:HA	1:A:321:PRO:HA	1.80	0.63
5:E:176:PRO:O	5:E:212:ARG:HA	1.97	0.63
8:H:82:PRO:C	8:H:84:ALA:H	2.07	0.63
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.79	0.63
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.81	0.62
11:K:32:VAL:HG22	11:K:74:ARG:HG3	1.80	0.62
1:A:35:ILE:HG21	1:A:241:VAL:HG21	1.82	0.62
1:A:56:PRO:O	1:A:57:ARG:HG3	2.00	0.62
1:A:388:LEU:O	1:A:392:VAL:HG23	2.00	0.62
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.82	0.61
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.81	0.61
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.81	0.61
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.83	0.61
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.36	0.61
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.82	0.61
1:A:1445:ILE:HG13	7:G:61:ILE:HD11	1.82	0.61
2:B:296:GLU:O	2:B:300:HIS:HD2	1.83	0.61
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.33	0.61
1:A:332:LYS:H	1:A:337:ARG:HB3	1.67	0.60
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.84	0.60
1:A:1288:ASP:HA	1:A:1302:PRO:HB3	1.82	0.60
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.84	0.60
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.02	0.60
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.83	0.59
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.37	0.59
2:B:428:ILE:HG22	2:B:432:MET:HE2	1.85	0.59
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.66	0.59
1:A:446:ARG:HB2	1:A:487:MET:SD	2.42	0.59
2:B:825:VAL:HG13	2:B:1010:LEU:HB3	1.85	0.59
1:A:869:GLY:O	5:E:204:THR:HG21	2.02	0.58
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.02	0.58
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.84	0.58
12:L:27:LEU:HD22	12:L:37:LYS:HE3	1.84	0.58
1:A:105:CYS:SG	1:A:139:TRP:HA	2.44	0.58
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.85	0.58
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.18	0.58
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.69	0.58
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.83	0.58
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.85	0.58
2:B:1002:THR:HG22	2:B:1072:MET:HE2	1.86	0.57
1:A:449:SER:HA	1:A:454:SER:HB3	1.85	0.57
1:A:41:MET:HB3	1:A:49:LYS:HA	1.86	0.57
1:A:448:PRO:O	1:A:449:SER:HB2	2.04	0.57
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.86	0.57
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.87	0.57
1:A:855:THR:CG2	1:A:857:ARG:HE	2.13	0.57
1:A:885:THR:HG23	1:A:893:PHE:HE2	1.69	0.57
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.87	0.57
2:B:882:THR:CG2	2:B:935:ARG:HA	2.34	0.57
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.87	0.57
3:C:11:ARG:HH21	3:C:229:TYR:HD1	1.53	0.56
1:A:534:LEU:O	1:A:574:GLY:HA3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.88	0.56
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.86	0.56
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.88	0.56
11:K:7:PHE:O	11:K:11:LEU:HB2	2.05	0.56
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.71	0.56
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.87	0.56
2:B:815:ARG:HG3	2:B:815:ARG:HH11	1.71	0.56
7:G:34:VAL:O	7:G:37:SER:HB3	2.05	0.56
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.88	0.56
2:B:957:ASN:HB3	2:B:961:LEU:H	1.71	0.56
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.86	0.56
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.39	0.55
2:B:882:THR:C	2:B:884:ARG:H	2.14	0.55
5:E:188:LEU:HB2	5:E:190:LEU:HD23	1.88	0.55
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.53	0.55
3:C:143:LEU:HD21	3:C:146:LYS:HE2	1.88	0.55
1:A:216:VAL:O	1:A:220:THR:HB	2.05	0.55
2:B:1172:ILE:HD11	2:B:1183:LYS:CE	2.36	0.55
1:A:494:SER:HB3	1:A:497:THR:H	1.72	0.55
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.89	0.55
2:B:121:ASN:HD22	2:B:860:MET:HE2	1.71	0.55
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.72	0.55
2:B:590:HIS:HD2	2:B:592:ASN:H	1.53	0.55
2:B:597:MET:HG3	2:B:601:ARG:HH12	1.71	0.55
2:B:475:SER:O	2:B:476:ARG:HB3	2.07	0.54
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.89	0.54
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.88	0.54
2:B:1022:THR:HG23	2:B:1022:THR:O	2.08	0.54
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.89	0.54
2:B:902:GLY:O	12:L:65:VAL:HG11	2.08	0.54
3:C:163:ILE:HD12	3:C:165:LYS:HB2	1.89	0.54
1:A:134:ARG:HD2	1:A:221:SER:O	2.07	0.54
2:B:166:PHE:HZ	2:B:169:ARG:HG2	1.72	0.54
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.89	0.54
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.90	0.54
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.43	0.54
1:A:55:ASP:H	1:A:56:PRO:HD3	1.73	0.53
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.08	0.53
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.89	0.53
4:D:23:ASN:HA	4:D:28:GLN:O	2.08	0.53
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HB	1:A:712:GLU:H	1.73	0.53
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.90	0.53
1:A:1442:ASP:HB2	6:F:137:TYR:CE1	2.41	0.53
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.91	0.53
4:D:155:ARG:HB3	4:D:219:THR:HG21	1.90	0.53
1:A:54:ASN:HB2	1:A:247:ARG:HH12	1.74	0.53
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.91	0.53
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.74	0.53
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.90	0.53
1:A:1444:MET:HE3	6:F:135:ARG:HB2	1.89	0.53
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.09	0.53
2:B:899:ILE:HD12	2:B:911:ILE:HA	1.90	0.53
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.90	0.53
3:C:148:ARG:HG3	3:C:151:GLN:HG3	1.91	0.52
3:C:251:LEU:O	3:C:255:VAL:HG23	2.08	0.52
4:D:10:THR:HB	4:D:12:ARG:HH22	1.74	0.52
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.24	0.52
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.45	0.52
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.90	0.52
2:B:563:MET:HE1	2:B:587:HIS:HB2	1.91	0.52
2:B:843:GLN:HE21	11:K:6:ARG:HH21	1.57	0.52
1:A:376:TYR:CE1	1:A:498:ARG:HD2	2.44	0.52
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.39	0.52
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.91	0.52
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.92	0.52
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.92	0.52
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.91	0.52
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.91	0.52
1:A:565:ILE:O	1:A:570:PRO:HA	2.08	0.52
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.91	0.52
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.35	0.52
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.92	0.52
3:C:32:SER:O	3:C:36:VAL:HG23	2.10	0.52
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.58	0.52
1:A:449:SER:HA	1:A:454:SER:CB	2.40	0.52
2:B:918:ILE:HD13	2:B:935:ARG:HH12	1.74	0.52
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.75	0.52
1:A:332:LYS:H	1:A:337:ARG:CB	2.23	0.52
1:A:729:ALA:HA	1:A:732:LEU:HD12	1.91	0.52
7:G:143:ILE:HG22	7:G:145:VAL:HG23	1.91	0.52
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:HIS:CB	7:G:73:LYS:HE3	2.30	0.52
5:E:19:VAL:O	5:E:23:VAL:HG23	2.09	0.52
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.73	0.51
4:D:159:THR:O	4:D:163:VAL:HG23	2.10	0.51
8:H:89:LEU:C	8:H:91:ASP:H	2.18	0.51
1:A:149:GLU:HG2	1:A:152:VAL:HG23	1.92	0.51
2:B:1185:CYS:HA	4:D:17:LYS:HD3	1.91	0.51
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.91	0.51
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.93	0.51
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.93	0.51
10:J:8:PHE:H	10:J:49:MET:HE3	1.75	0.51
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.93	0.51
5:E:197:LYS:HD3	5:E:199:ILE:HD11	1.91	0.51
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.92	0.51
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.92	0.51
1:A:855:THR:HG21	1:A:857:ARG:NE	2.16	0.51
1:A:873:MET:C	1:A:1058:VAL:HG22	2.36	0.51
1:A:827:THR:O	1:A:831:THR:HB	2.11	0.51
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.93	0.51
7:G:8:SER:HB2	7:G:71:ASN:HD21	1.75	0.51
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.93	0.51
10:J:32:GLU:CD	10:J:32:GLU:H	2.18	0.51
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.93	0.50
2:B:1129:ARG:HG2	15:T:20:DC:H5"	1.92	0.50
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.45	0.50
3:C:206:ASN:HA	3:C:209:TYR:HD1	1.75	0.50
3:C:149:LYS:C	3:C:151:GLN:H	2.19	0.50
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.47	0.50
1:A:1132:LYS:HG2	1:A:1135:ARG:HH12	1.77	0.50
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.47	0.50
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.93	0.50
3:C:242:GLN:O	3:C:246:ARG:HB2	2.12	0.50
4:D:193:THR:HG21	7:G:167:TYR:HD2	1.76	0.50
10:J:6:ARG:H	10:J:14:VAL:H	1.57	0.50
2:B:35:SER:HA	2:B:811:TYR:HE1	1.77	0.50
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.94	0.50
1:A:62:ASP:HB3	1:A:64:ASN:O	2.11	0.50
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.94	0.50
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.45	0.50
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.93	0.50
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:LEU:HD11	2:B:273:LEU:HD23	1.93	0.50
1:A:53:LEU:HD23	1:A:54:ASN:N	2.26	0.49
4:D:5:THR:HG21	7:G:74:TYR:OH	2.12	0.49
1:A:52:GLY:N	1:A:56:PRO:HB3	2.27	0.49
1:A:1143:LEU:HD22	1:A:1267:MET:HB3	1.93	0.49
2:B:291:ILE:HD12	2:B:291:ILE:H	1.77	0.49
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.93	0.49
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.93	0.49
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.41	0.49
1:A:354:SER:O	1:A:469:ARG:HA	2.11	0.49
1:A:541:ILE:HG21	1:A:549:MET:HE2	1.94	0.49
2:B:276:ILE:HA	2:B:338:GLY:O	2.12	0.49
1:A:1323:ASP:CG	1:A:1326:ARG:HG3	2.37	0.49
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.13	0.49
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.94	0.49
3:C:148:ARG:H	3:C:151:GLN:HG3	1.77	0.49
1:A:928:LEU:HB3	1:A:987:VAL:HG11	1.94	0.49
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.77	0.49
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.78	0.49
2:B:486:TYR:HB3	2:B:1096:ARG:HD2	1.94	0.49
2:B:933:SER:O	2:B:935:ARG:N	2.46	0.49
4:D:5:THR:HG21	7:G:74:TYR:HH	1.78	0.49
1:A:716:ASP:O	1:A:720:ARG:HB2	2.13	0.49
2:B:953:LEU:HD11	12:L:55:ILE:HG22	1.95	0.49
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.78	0.49
1:A:35:ILE:HG22	1:A:84:ILE:HG23	1.94	0.48
1:A:88:LYS:HB2	1:A:276:LEU:HD21	1.95	0.48
1:A:341:MET:HE1	1:A:1425:SER:HB3	1.94	0.48
1:A:370:ILE:HD11	2:B:1103:ILE:HG13	1.95	0.48
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.94	0.48
2:B:841:MET:O	2:B:993:THR:HA	2.13	0.48
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.78	0.48
4:D:23:ASN:O	7:G:83:LYS:HG2	2.12	0.48
1:A:55:ASP:CG	1:A:55:ASP:O	2.55	0.48
16:A:2455:APC:H5'2	16:A:2455:APC:C8	2.38	0.48
2:B:577:ALA:HB1	2:B:589:VAL:HB	1.95	0.48
1:A:632:VAL:HG13	1:A:962:ARG:HD3	1.95	0.48
4:D:162:ALA:HB3	4:D:217:LEU:HD21	1.95	0.48
8:H:5:LEU:HB2	8:H:59:ILE:HG22	1.96	0.48
9:I:73:ARG:HH12	9:I:112:SER:HA	1.78	0.48
11:K:8:GLU:O	11:K:37:LYS:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.96	0.48
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.95	0.48
12:L:61:THR:HG22	12:L:63:ARG:H	1.79	0.48
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.94	0.48
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.96	0.48
1:A:414:ASP:OD1	1:A:416:ARG:HB2	2.13	0.47
2:B:769:TYR:O	2:B:772:ALA:HB3	2.14	0.47
1:A:781:ASP:HB2	1:A:789:LYS:HG2	1.95	0.47
2:B:206:ASN:HD21	2:B:458:LYS:HD3	1.79	0.47
8:H:127:GLY:N	8:H:130:ARG:HH21	2.11	0.47
1:A:531:ILE:HD12	1:A:653:VAL:HG21	1.96	0.47
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.50	0.47
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.95	0.47
7:G:1:MET:CG	7:G:2:PHE:N	2.77	0.47
1:A:399:HIS:O	1:A:401:GLY:N	2.47	0.47
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.97	0.47
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.45	0.47
2:B:123:THR:HG23	2:B:205:ILE:HA	1.96	0.47
2:B:770:GLN:CD	2:B:983:ARG:HA	2.39	0.47
3:C:22:LEU:HD22	3:C:230:MET:HE1	1.95	0.47
1:A:511:ILE:HA	1:A:521:MET:HE3	1.97	0.47
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.96	0.47
3:C:98:VAL:H	3:C:122:SER:HB3	1.80	0.47
7:G:92:VAL:HG21	7:G:102:GLN:HB2	1.95	0.47
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.97	0.47
2:B:873:THR:O	2:B:914:LYS:HA	2.15	0.47
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.97	0.47
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.96	0.47
1:A:1215:ARG:HG3	1:A:1273:LEU:HA	1.97	0.47
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.15	0.47
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.96	0.47
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.80	0.47
2:B:121:ASN:ND2	2:B:860:MET:HE2	2.30	0.47
2:B:732:SER:HB2	2:B:734:HIS:ND1	2.30	0.47
2:B:986:GLN:OE1	2:B:1016:ALA:HB1	2.15	0.47
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.97	0.47
1:A:1015:VAL:HG13	1:A:1019:CYS:SG	2.56	0.46
2:B:1221:SER:HB3	4:D:12:ARG:HD2	1.97	0.46
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.96	0.46
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.97	0.46
1:A:457:ALA:O	1:A:507:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.97	0.46
1:A:495:GLU:HG3	6:F:98:ALA:HB1	1.97	0.46
1:A:567:LYS:HD3	1:A:569:LYS:H	1.80	0.46
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.98	0.46
2:B:1104:HIS:HB2	2:B:1122:ARG:HG3	1.98	0.46
8:H:80:ARG:HH11	8:H:87:ARG:HH22	1.62	0.46
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.96	0.46
1:A:448:PRO:O	1:A:449:SER:CB	2.64	0.46
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.51	0.46
11:K:35:PHE:O	11:K:70:ARG:HA	2.15	0.46
1:A:575:LYS:HD2	8:H:120:GLY:HA3	1.98	0.46
1:A:605:MET:HE2	1:A:607:ILE:HG13	1.97	0.46
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.98	0.46
7:G:93:SER:OG	7:G:100:GLU:HB2	2.16	0.46
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.81	0.46
4:D:52:LEU:HG	4:D:182:SER:HB3	1.97	0.46
4:D:54:GLU:O	4:D:58:VAL:HG23	2.16	0.46
2:B:383:ASN:O	2:B:387:LEU:HB2	2.16	0.46
2:B:551:PRO:HA	2:B:554:ILE:HD12	1.97	0.46
3:C:77:ILE:HG13	3:C:161:LYS:HE3	1.98	0.46
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.46	0.46
1:A:588:LEU:HD23	1:A:607:ILE:HD12	1.97	0.46
1:A:605:MET:CE	1:A:612:ILE:HG23	2.46	0.46
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.98	0.46
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.98	0.45
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.46	0.45
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.98	0.45
2:B:242:SER:OG	2:B:362:PRO:HD2	2.16	0.45
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.97	0.45
1:A:537:ARG:HB2	8:H:20:TYR:CE1	2.52	0.45
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.97	0.45
1:A:1442:ASP:HB3	1:A:1444:MET:HE1	1.98	0.45
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.97	0.45
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.99	0.45
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.98	0.45
2:B:803:LEU:HG	10:J:52:THR:HG21	1.98	0.45
2:B:446:LEU:HD12	2:B:448:ILE:HD11	1.98	0.45
4:D:150:ASN:HB3	7:G:142:ARG:NH2	2.31	0.45
15:T:25:DT:H5"	15:T:25:DT:H6	1.80	0.45
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.51	0.45
12:L:68:GLU:HB2	12:L:70:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1317:MET:HE2	5:E:142:VAL:HG11	1.97	0.45
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.98	0.45
2:B:343:ILE:O	2:B:344:LYS:HB2	2.16	0.45
5:E:182:ASP:O	5:E:186:LEU:HG	2.16	0.45
11:K:82:ASP:OD2	11:K:84:LYS:HB2	2.17	0.45
12:L:25:ALA:HB1	12:L:62:LYS:HZ3	1.81	0.45
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.16	0.45
2:B:865:LYS:HB2	2:B:961:LEU:HD21	1.98	0.45
2:B:947:GLY:HA2	2:B:970:THR:HG23	1.98	0.45
5:E:78:LEU:HD11	5:E:109:ILE:HG13	1.99	0.45
1:A:567:LYS:HA	1:A:569:LYS:N	2.31	0.45
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.98	0.45
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.99	0.45
7:G:81:PRO:HG3	7:G:106:MET:SD	2.57	0.45
1:A:43:GLU:CD	1:A:48:ALA:HB3	2.42	0.45
1:A:464:PRO:HD2	11:K:67:PHE:HD2	1.82	0.45
2:B:296:GLU:O	2:B:300:HIS:CD2	2.66	0.45
1:A:880:LYS:HA	1:A:955:PRO:HA	1.99	0.44
2:B:290:GLY:HA2	2:B:327:ARG:HD2	1.98	0.44
8:H:16:ASP:HA	8:H:17:PRO:HD3	1.85	0.44
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.99	0.44
2:B:758:PHE:CE2	2:B:1027:ILE:HG22	2.52	0.44
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.99	0.44
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.98	0.44
3:C:100:THR:HB	3:C:121:VAL:HG21	2.00	0.44
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.17	0.44
2:B:70:ILE:HD12	2:B:70:ILE:H	1.81	0.44
2:B:629:ASP:HB3	2:B:632:ARG:NE	2.31	0.44
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.99	0.44
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.99	0.44
10:J:1:MET:HG3	10:J:60:PHE:CE2	2.52	0.44
1:A:200:ARG:HH22	1:A:206:GLU:CD	2.25	0.44
1:A:452:LYS:HG2	2:B:1141:HIS:CE1	2.52	0.44
5:E:50:MET:HB3	5:E:52:ARG:HG3	2.00	0.44
5:E:197:LYS:HG3	5:E:211:TYR:CE2	2.52	0.44
1:A:867:ILE:CD1	1:A:867:ILE:CB	2.85	0.44
2:B:1165:ILE:O	2:B:1217:TYR:OH	2.32	0.44
3:C:71:PRO:HG3	10:J:13:VAL:HG11	2.00	0.44
8:H:82:PRO:O	8:H:84:ALA:N	2.47	0.44
1:A:439:ASN:HD21	1:A:459:ARG:HE	1.65	0.44
1:A:1148:ILE:HG23	9:I:49:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:510:LYS:N	2:B:511:PRO:CD	2.81	0.44
2:B:810:GLU:HA	2:B:815:ARG:NH1	2.33	0.44
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.91	0.44
7:G:142:ARG:HB3	7:G:171:ILE:HD12	2.00	0.44
7:G:147:ILE:HG23	7:G:159:ALA:HB1	2.00	0.44
1:A:1446:ASP:HB3	1:A:1449:SER:HG	1.80	0.44
2:B:1050:ILE:H	2:B:1050:ILE:HG13	1.63	0.44
1:A:151:ASP:HA	1:A:163:SER:HA	2.00	0.44
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.99	0.44
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.00	0.44
5:E:5:ASN:HD21	5:E:52:ARG:HE	1.66	0.44
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.77	0.44
10:J:7:CYS:HA	10:J:49:MET:HG2	2.00	0.44
4:D:5:THR:HG23	7:G:9:LEU:HB2	2.00	0.44
11:K:5:ASP:HB2	11:K:8:GLU:HG3	1.98	0.44
1:A:182:VAL:HB	1:A:201:VAL:HG23	2.00	0.43
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.86	0.43
3:C:142:VAL:HG22	10:J:15:GLY:HA3	2.00	0.43
1:A:104:GLU:HG2	1:A:174:ILE:HD12	2.00	0.43
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.83	0.43
2:B:1106:ARG:NH1	2:B:1110:PRO:HD2	2.33	0.43
3:C:77:ILE:C	3:C:79:GLN:H	2.26	0.43
1:A:49:LYS:HE2	1:A:61:ILE:H	1.82	0.43
1:A:857:ARG:HD3	1:A:861:GLY:O	2.18	0.43
3:C:6:PRO:HB2	11:K:101:LEU:HD23	2.00	0.43
3:C:11:ARG:HD3	3:C:209:TYR:CE2	2.53	0.43
3:C:114:TYR:CD1	3:C:140:ASN:HB3	2.53	0.43
4:D:50:LEU:HD11	7:G:4:ILE:HG13	2.01	0.43
1:A:443:LEU:HD23	1:A:501:LEU:HD22	2.00	0.43
1:A:932:GLU:O	1:A:936:LEU:HG	2.19	0.43
2:B:128:LEU:HD21	2:B:170:LEU:CB	2.48	0.43
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.53	0.43
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.83	0.43
1:A:55:ASP:N	1:A:56:PRO:HD3	2.33	0.43
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.47	0.43
1:A:929:LEU:HD21	1:A:983:ILE:HG12	2.00	0.43
2:B:291:ILE:HD12	2:B:291:ILE:N	2.32	0.43
1:A:598:LEU:HB2	8:H:115:TYR:HE2	1.84	0.43
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.18	0.43
2:B:800:GLN:HB2	2:B:821:GLN:HA	2.00	0.43
2:B:954:VAL:HG21	12:L:29:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.01	0.43
2:B:666:TYR:C	2:B:668:ASP:H	2.26	0.43
2:B:693:ILE:HG23	2:B:697:GLU:HB3	2.01	0.43
5:E:4:GLU:HB3	5:E:7:ARG:NE	2.31	0.43
2:B:39:ARG:NE	2:B:665:GLU:HG2	2.33	0.43
5:E:46:TYR:CE1	5:E:58:MET:HA	2.54	0.43
1:A:546:VAL:HG13	1:A:577:ILE:HG21	2.00	0.43
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.19	0.43
2:B:893:LEU:HD22	2:B:897:GLY:C	2.44	0.43
2:B:1175:LEU:O	2:B:1176:ASN:CB	2.65	0.43
2:B:344:LYS:O	2:B:348:ARG:HD2	2.18	0.43
2:B:485:ARG:NH1	2:B:491:THR:HG21	2.34	0.43
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.84	0.43
1:A:49:LYS:NZ	1:A:60:SER:HA	2.34	0.42
1:A:628:GLY:O	1:A:632:VAL:HG23	2.19	0.42
1:A:1443:VAL:HG12	7:G:61:ILE:HD13	2.01	0.42
8:H:107:VAL:O	8:H:111:LEU:HB2	2.19	0.42
14:P:5:C:H2'	14:P:6:C:C6	2.54	0.42
2:B:542:MET:HE3	2:B:636:PRO:HG2	2.01	0.42
15:T:15:DT:H2'	15:T:16:DT:C6	2.54	0.42
1:A:53:LEU:HD12	1:A:270:LEU:HD23	2.01	0.42
1:A:354:SER:HA	1:A:482:PHE:CD1	2.54	0.42
1:A:776:ALA:O	1:A:783:THR:HG22	2.18	0.42
1:A:974:ASP:C	1:A:976:THR:H	2.27	0.42
2:B:548:GLY:HA3	2:B:630:ALA:HB2	2.00	0.42
2:B:792:MET:HG2	2:B:855:PHE:CZ	2.53	0.42
2:B:997:GLU:CD	2:B:997:GLU:H	2.28	0.42
7:G:126:ASN:HA	7:G:127:PRO:HA	1.88	0.42
15:T:13:DA:H2''	15:T:14:DC:O4'	2.20	0.42
1:A:885:THR:OG1	1:A:1024:SER:HB2	2.19	0.42
2:B:281:PRO:HD2	2:B:284:ILE:HD13	2.01	0.42
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.02	0.42
2:B:882:THR:O	2:B:884:ARG:N	2.52	0.42
2:B:35:SER:HA	2:B:811:TYR:CE1	2.53	0.42
3:C:37:MET:HA	3:C:41:ILE:HD12	2.01	0.42
1:A:152:VAL:HG22	1:A:153:PRO:HD2	2.01	0.42
1:A:774:ARG:CZ	1:A:797:LYS:HB2	2.49	0.42
2:B:512:ARG:CZ	2:B:535:LEU:HD11	2.50	0.42
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.20	0.42
1:A:35:ILE:HA	1:A:52:GLY:O	2.20	0.42
1:A:538:ASP:H	8:H:20:TYR:HE1	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:ASP:C	1:A:911:SER:H	2.28	0.42
1:A:1285:MET:HG3	1:A:1307:GLU:HG3	2.00	0.42
2:B:634:TYR:CD2	2:B:692:TYR:HB3	2.55	0.42
2:B:792:MET:HA	2:B:856:PHE:O	2.20	0.42
1:A:64:ASN:O	1:A:65:LEU:HB3	2.19	0.42
1:A:336:ILE:HG21	1:A:1401:SER:HA	2.02	0.42
1:A:347:PHE:H	2:B:1107:ALA:HA	1.85	0.42
1:A:1143:LEU:HD21	1:A:1195:LEU:HD13	2.01	0.42
2:B:126:SER:HB2	2:B:172:ILE:HD11	2.02	0.42
2:B:542:MET:HB3	2:B:636:PRO:HD2	2.02	0.42
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.55	0.42
2:B:185:THR:HG23	2:B:188:ASP:CG	2.45	0.42
2:B:459:TYR:CE2	2:B:470:LYS:HG3	2.54	0.42
2:B:658:ILE:HG23	2:B:662:MET:HE2	2.02	0.42
1:A:417:TYR:O	1:A:418:SER:C	2.62	0.42
1:A:840:ARG:NH2	1:A:1106:ASN:ND2	2.67	0.42
4:D:135:GLY:C	4:D:137:ASN:H	2.28	0.42
15:T:8:DC:H2'	15:T:9:DA:C8	2.55	0.42
1:A:382:PRO:HG3	1:A:428:TYR:CZ	2.55	0.41
3:C:114:TYR:HB3	3:C:140:ASN:O	2.20	0.41
3:C:125:MET:HB2	3:C:127:ARG:NE	2.35	0.41
5:E:3:GLN:HE22	5:E:5:ASN:HD22	1.68	0.41
1:A:359:LEU:HD22	1:A:363:GLN:HG3	2.02	0.41
4:D:7:THR:HB	4:D:8:PHE:H	1.45	0.41
15:T:13:DA:H4'	15:T:14:DC:OP1	2.20	0.41
2:B:848:ARG:HD2	10:J:8:PHE:O	2.19	0.41
7:G:27:LYS:HE2	7:G:54:ILE:HB	2.01	0.41
1:A:512:VAL:HA	1:A:519:PRO:HA	2.03	0.41
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.01	0.41
1:A:1173:HIS:HB3	1:A:1227:ILE:HG23	2.03	0.41
2:B:38:PHE:HZ	2:B:541:LEU:HB3	1.85	0.41
2:B:345:LYS:HA	2:B:348:ARG:CD	2.50	0.41
2:B:351:TYR:HB3	2:B:352:ALA:N	2.35	0.41
2:B:1043:ASP:OD2	2:B:1045:SER:HB2	2.20	0.41
2:B:1110:PRO:HG2	2:B:1119:VAL:HG21	2.03	0.41
5:E:23:VAL:HG12	5:E:28:TYR:HB2	2.03	0.41
7:G:110:VAL:HG11	7:G:163:ILE:HG12	2.02	0.41
9:I:118:ARG:HB3	9:I:119:THR:H	1.69	0.41
10:J:8:PHE:H	10:J:49:MET:CE	2.33	0.41
1:A:599:SER:HA	1:A:600:PRO:HD3	1.83	0.41
1:A:1400:CYS:HA	1:A:1408:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.54	0.41
1:A:488:ASN:HD22	2:B:1128:LEU:HD13	1.85	0.41
1:A:872:GLY:O	1:A:1057:VAL:HG13	2.20	0.41
1:A:1335:ILE:HG21	1:A:1347:ALA:HB2	2.02	0.41
2:B:168:GLY:H	2:B:450:ALA:HB1	1.86	0.41
2:B:464:GLY:HA2	2:B:480:SER:HB3	2.02	0.41
2:B:847:ASP:HB3	3:C:167:HIS:CE1	2.55	0.41
5:E:118:PRO:O	5:E:122:LYS:HG2	2.21	0.41
9:I:7:CYS:SG	9:I:10:CYS:HB2	2.59	0.41
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.21	0.41
1:A:1450:LEU:HD22	7:G:19:GLY:O	2.21	0.41
2:B:365:THR:HG21	2:B:370:PHE:HB2	2.02	0.41
2:B:530:GLY:H	2:B:533:CYS:HB2	1.85	0.41
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.56	0.41
1:A:336:ILE:CG2	1:A:1401:SER:HA	2.50	0.41
1:A:567:LYS:HA	1:A:568:PRO:C	2.46	0.41
1:A:840:ARG:NH2	1:A:1106:ASN:HD21	2.18	0.41
2:B:33:VAL:HG23	2:B:658:ILE:HD11	2.03	0.41
3:C:4:GLU:OE1	11:K:104:ASN:ND2	2.53	0.41
3:C:84:ARG:CZ	11:K:11:LEU:HD11	2.50	0.41
5:E:94:LYS:HE2	5:E:98:ILE:HD11	2.02	0.41
5:E:152:LYS:H	5:E:152:LYS:HG3	1.67	0.41
11:K:82:ASP:OD1	11:K:83:PRO:HD2	2.21	0.41
1:A:41:MET:HA	1:A:50:ILE:HB	2.02	0.41
1:A:79:GLY:HA3	1:A:243:PRO:HG3	2.03	0.41
1:A:157:ASP:HA	1:A:158:PRO:HD3	1.96	0.41
1:A:352:VAL:HG12	1:A:467:THR:HG22	2.02	0.41
2:B:564:GLU:O	2:B:588:GLY:HA3	2.21	0.41
2:B:1169:MET:HB2	2:B:1169:MET:HE3	1.79	0.41
4:D:7:THR:CG2	7:G:5:LYS:HZ2	2.34	0.41
5:E:16:PHE:CE2	5:E:20:LYS:HE2	2.56	0.41
12:L:47:ARG:HG3	12:L:54:ARG:HG3	2.03	0.41
1:A:200:ARG:NH2	1:A:206:GLU:OE1	2.50	0.40
1:A:206:GLU:O	1:A:210:ILE:HG12	2.21	0.40
1:A:709:THR:HG23	9:I:94:ASP:HA	2.02	0.40
1:A:1038:THR:HG23	1:A:1041:ALA:HB2	2.03	0.40
1:A:1215:ARG:O	1:A:1218:GLN:HG2	2.21	0.40
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.57	0.40
3:C:100:THR:HG22	3:C:119:VAL:CG2	2.48	0.40
7:G:1:MET:HE3	7:G:79:PHE:CE2	2.56	0.40
1:A:1444:MET:HG3	7:G:58:ARG:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:HG13	2:B:112:LEU:HD22	2.04	0.40
2:B:756:ILE:O	2:B:759:PRO:HD3	2.20	0.40
2:B:766:ARG:NH1	2:B:769:TYR:HD2	2.19	0.40
2:B:1059:LEU:HG	2:B:1064:TYR:HB2	2.04	0.40
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.36	0.40
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.80	0.40
4:D:25:ALA:HB1	4:D:196:PRO:HD2	2.04	0.40
8:H:93:TYR:CG	8:H:143:LEU:HB3	2.56	0.40
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.03	0.40
1:A:637:LYS:HB3	1:A:641:VAL:HG11	2.03	0.40
2:B:54:PHE:HA	2:B:58:THR:HB	2.03	0.40
2:B:69:LEU:HD11	2:B:425:THR:HG23	2.02	0.40
2:B:481:GLN:HE21	2:B:481:GLN:HB3	1.74	0.40
2:B:710:LEU:HA	2:B:733:HIS:HB3	2.03	0.40
1:A:368:LYS:HE2	1:A:399:HIS:HB2	2.03	0.40
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.55	0.40
1:A:986:ILE:O	1:A:990:VAL:HG23	2.22	0.40
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.20	0.40
2:B:328:GLU:H	2:B:328:GLU:CD	2.29	0.40
2:B:728:ARG:HH12	2:B:1047:PHE:HA	1.87	0.40
2:B:773:MET:CE	2:B:985:GLY:HA2	2.51	0.40
2:B:975:GLN:O	2:B:990:ILE:HD12	2.21	0.40
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.03	0.40
1:A:870:GLU:HB2	5:E:204:THR:CG2	2.52	0.40
1:A:946:VAL:HG22	5:E:201:LYS:HD2	2.03	0.40
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.21	0.40
3:C:15:LYS:O	3:C:240:VAL:HG22	2.20	0.40
3:C:153:LEU:HD11	3:C:155:LEU:HD23	2.04	0.40
11:K:10:PHE:CD2	11:K:11:LEU:HD13	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	1417/1732 (82%)	1225 (86%)	135 (10%)	57 (4%)	2	19
2	B	1095/1224 (90%)	951 (87%)	92 (8%)	52 (5%)	2	17
3	C	264/318 (83%)	237 (90%)	20 (8%)	7 (3%)	4	27
4	D	174/221 (79%)	153 (88%)	11 (6%)	10 (6%)	1	13
5	E	212/215 (99%)	196 (92%)	12 (6%)	4 (2%)	6	33
6	F	82/155 (53%)	77 (94%)	4 (5%)	1 (1%)	10	41
7	G	169/171 (99%)	156 (92%)	9 (5%)	4 (2%)	4	29
8	H	129/146 (88%)	104 (81%)	17 (13%)	8 (6%)	1	12
9	I	117/122 (96%)	93 (80%)	19 (16%)	5 (4%)	2	18
10	J	63/70 (90%)	53 (84%)	7 (11%)	3 (5%)	2	16
11	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
12	L	44/70 (63%)	24 (54%)	12 (27%)	8 (18%)	0	1
All	All	3879/4564 (85%)	3377 (87%)	343 (9%)	159 (4%)	2	19

All (159) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	58	LEU
1	A	169	ASN
1	A	189	ARG
1	A	251	SER
1	A	286	HIS
1	A	311	GLN
1	A	318	SER
1	A	448	PRO
1	A	449	SER
1	A	1122	PRO
1	A	1175	SER
1	A	1206	ASP
2	B	229	ALA
2	B	340	ALA
2	B	344	LYS
2	B	367	LEU
2	B	731	VAL
2	B	751	VAL
2	B	879	ARG
2	B	943	SER
2	B	1046	PRO

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Mol	Chain	Res	Type
2	B	1066	SER
2	B	1157	ALA
2	B	1181	GLU
3	C	215	GLU
3	C	237	SER
4	D	18	VAL
4	D	119	ARG
4	D	199	ASN
5	E	48	ASP
8	H	90	ALA
9	I	95	THR
10	J	6	ARG
12	L	56	LEU
12	L	60	ARG
1	A	52	GLY
1	A	55	ASP
1	A	57	ARG
1	A	76	GLU
1	A	167	CYS
1	A	178	GLY
1	A	257	ARG
1	A	332	LYS
1	A	335	ARG
1	A	465	TYR
1	A	775	ILE
1	A	1403	GLU
1	A	1405	THR
2	B	67	SER
2	B	262	GLU
2	B	307	ASP
2	B	343	ILE
2	B	369	GLY
2	B	473	MET
2	B	629	ASP
2	B	643	ASP
2	B	667	GLN
2	B	707	PRO
2	B	711	GLU
2	B	772	ALA
2	B	792	MET
2	B	867	GLY
2	B	883	LEU

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Mol	Chain	Res	Type
2	B	1069	PHE
2	B	1155	SER
2	B	1156	ASP
2	B	1176	ASN
2	B	1185	CYS
2	B	1190	ASP
4	D	11	ARG
4	D	16	LYS
4	D	53	SER
5	E	45	LYS
8	H	83	GLN
8	H	128	ASN
9	I	88	SER
12	L	39	SER
1	A	43	GLU
1	A	74	MET
1	A	156	ASP
1	A	164	ARG
1	A	975	HIS
1	A	1079	MET
2	B	338	GLY
2	B	341	LEU
2	B	449	ASN
2	B	889	THR
2	B	902	GLY
2	B	942	ARG
2	B	1167	GLY
4	D	52	LEU
4	D	169	SER
4	D	174	PRO
4	D	218	GLU
5	E	36	GLU
7	G	63	PRO
7	G	154	VAL
8	H	60	ALA
8	H	81	PRO
8	H	82	PRO
9	I	89	GLN
10	J	17	LYS
12	L	53	HIS
12	L	59	ALA
1	A	224	PHE

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Mol	Chain	Res	Type
1	A	399	HIS
1	A	409	SER
1	A	569	LYS
1	A	593	GLU
1	A	870	GLU
1	A	1255	GLU
1	A	1281	ARG
1	A	1377	THR
2	B	68	THR
2	B	282	ILE
2	B	466	TRP
2	B	476	ARG
3	C	78	GLU
7	G	2	PHE
7	G	67	SER
8	H	17	PRO
9	I	23	ASN
10	J	2	ILE
12	L	26	THR
1	A	196	GLU
1	A	250	ILE
1	A	336	ILE
1	A	600	PRO
1	A	635	ARG
1	A	958	VAL
1	A	986	ILE
1	A	1124	HIS
1	A	1242	VAL
2	B	353	LYS
2	B	1108	ARG
3	C	56	THR
3	C	90	ASP
6	F	73	ALA
8	H	108	SER
9	I	105	SER
12	L	45	ALA
1	A	54	ASN
1	A	283	GLY
1	A	916	GLY
2	B	648	HIS
5	E	90	VAL
1	A	35	ILE

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Mol	Chain	Res	Type
2	B	108	VAL
2	B	251	ILE
2	B	870	ILE
3	C	150	GLY
3	C	240	VAL
12	L	52	GLY
2	B	510	LYS
1	A	987	VAL
2	B	364	ILE
1	A	400	PRO
1	A	567	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	1243/1519 (82%)	1033 (83%)	210 (17%)	2	13
2	B	966/1061 (91%)	817 (85%)	149 (15%)	2	16
3	C	234/274 (85%)	201 (86%)	33 (14%)	3	18
4	D	160/200 (80%)	124 (78%)	36 (22%)	1	5
5	E	196/197 (100%)	171 (87%)	25 (13%)	4	21
6	F	74/137 (54%)	65 (88%)	9 (12%)	5	22
7	G	152/152 (100%)	126 (83%)	26 (17%)	2	12
8	H	117/128 (91%)	106 (91%)	11 (9%)	8	31
9	I	113/116 (97%)	103 (91%)	10 (9%)	9	32
10	J	60/65 (92%)	49 (82%)	11 (18%)	2	10
11	K	99/102 (97%)	83 (84%)	16 (16%)	2	14
12	L	40/57 (70%)	28 (70%)	12 (30%)	0	2
All	All	3454/4008 (86%)	2906 (84%)	548 (16%)	2	14

All (548) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	THR
1	A	28	ARG
1	A	34	LYS
1	A	41	MET
1	A	43	GLU
1	A	47	ARG
1	A	50	ILE
1	A	54	ASN
1	A	58	LEU
1	A	62	ASP
1	A	65	LEU
1	A	67	CYS
1	A	84	ILE
1	A	90	VAL
1	A	93	VAL
1	A	96	ILE
1	A	106	VAL
1	A	121	LEU
1	A	132	LYS
1	A	141	LEU
1	A	145	LYS
1	A	147	VAL
1	A	149	GLU
1	A	152	VAL
1	A	174	ILE
1	A	175	ARG
1	A	193	ASP
1	A	204	THR
1	A	208	LEU
1	A	215	SER
1	A	220	THR
1	A	222	LEU
1	A	237	THR
1	A	252	PHE
1	A	261	ASP
1	A	270	LEU
1	A	277	GLU
1	A	279	LEU
1	A	289	ILE
1	A	294	SER
1	A	307	ASP
1	A	311	GLN

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Mol	Chain	Res	Type
1	A	315	LEU
1	A	322	VAL
1	A	324	SER
1	A	333	GLU
1	A	335	ARG
1	A	337	ARG
1	A	341	MET
1	A	353	ILE
1	A	368	LYS
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	386	ASP
1	A	393	ARG
1	A	398	GLU
1	A	407	ARG
1	A	423	ASP
1	A	424	ILE
1	A	425	GLN
1	A	431	LYS
1	A	434	ARG
1	A	436	ILE
1	A	438	ASP
1	A	443	LEU
1	A	448	PRO
1	A	451	HIS
1	A	452	LYS
1	A	454	SER
1	A	461	LYS
1	A	463	ILE
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	494	SER
1	A	500	GLU
1	A	505	CYS
1	A	523	ILE
1	A	527	THR

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Mol	Chain	Res	Type
1	A	536	LEU
1	A	538	ASP
1	A	541	ILE
1	A	545	GLN
1	A	566	ILE
1	A	571	LEU
1	A	593	GLU
1	A	597	LEU
1	A	598	LEU
1	A	603	ASN
1	A	618	GLU
1	A	622	VAL
1	A	625	SER
1	A	626	ASN
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	652	VAL
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	691	LEU
1	A	702	LEU
1	A	738	LYS
1	A	740	LEU
1	A	756	ILE
1	A	764	CYS
1	A	768	GLN
1	A	769	SER
1	A	782	ARG
1	A	788	SER
1	A	795	GLU
1	A	806	ARG
1	A	811	GLN
1	A	821	ARG
1	A	839	ARG
1	A	855	THR
1	A	864	ILE
1	A	867	ILE
1	A	878	ILE
1	A	886	ILE
1	A	890	ASP

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Mol	Chain	Res	Type
1	A	904	THR
1	A	914	GLU
1	A	915	SER
1	A	919	ILE
1	A	920	LEU
1	A	926	GLN
1	A	929	LEU
1	A	941	LYS
1	A	948	VAL
1	A	964	ILE
1	A	973	ILE
1	A	976	THR
1	A	983	ILE
1	A	987	VAL
1	A	998	LEU
1	A	1001	ARG
1	A	1009	ASN
1	A	1015	VAL
1	A	1024	SER
1	A	1038	THR
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1078	GLN
1	A	1080	THR
1	A	1100	ARG
1	A	1103	GLU
1	A	1116	LEU
1	A	1121	GLU
1	A	1124	HIS
1	A	1135	ARG
1	A	1141	THR
1	A	1143	LEU
1	A	1146	VAL
1	A	1170	ILE
1	A	1173	HIS
1	A	1176	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1222	ASN
1	A	1223	ASP

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Mol	Chain	Res	Type
1	A	1232	ASN
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1256	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1265	ASN
1	A	1270	ASN
1	A	1274	ARG
1	A	1277	GLU
1	A	1279	ILE
1	A	1289	ARG
1	A	1291	VAL
1	A	1293	SER
1	A	1295	THR
1	A	1297	GLU
1	A	1301	GLU
1	A	1303	GLU
1	A	1317	MET
1	A	1319	VAL
1	A	1322	ILE
1	A	1325	THR
1	A	1327	ILE
1	A	1329	THR
1	A	1336	MET
1	A	1341	ILE
1	A	1376	THR
1	A	1383	SER
1	A	1393	ASN
1	A	1394	THR
1	A	1398	MET
1	A	1405	THR
1	A	1418	LEU
1	A	1424	VAL
1	A	1426	GLU
1	A	1432	GLN
1	A	1445	ILE
1	A	1449	SER
1	A	1451	VAL
1	A	1454	MET
2	B	25	ILE

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Mol	Chain	Res	Type
2	B	35	SER
2	B	40	GLU
2	B	46	GLN
2	B	63	ILE
2	B	118	ARG
2	B	119	LEU
2	B	134	LYS
2	B	170	LEU
2	B	185	THR
2	B	187	SER
2	B	205	ILE
2	B	218	SER
2	B	222	ILE
2	B	223	VAL
2	B	237	VAL
2	B	240	ILE
2	B	251	ILE
2	B	252	SER
2	B	261	ARG
2	B	262	GLU
2	B	264	SER
2	B	267	ARG
2	B	272	THR
2	B	279	ASP
2	B	313	MET
2	B	324	ILE
2	B	337	ARG
2	B	339	THR
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	346	GLU
2	B	348	ARG
2	B	361	LEU
2	B	364	ILE
2	B	365	THR
2	B	384	ARG
2	B	393	LYS
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	436	VAL

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Mol	Chain	Res	Type
2	B	446	LEU
2	B	453	ILE
2	B	469	GLN
2	B	470	LYS
2	B	475	SER
2	B	485	ARG
2	B	486	TYR
2	B	490	SER
2	B	500	THR
2	B	531	GLN
2	B	537	LYS
2	B	545	ILE
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	554	ILE
2	B	570	VAL
2	B	574	SER
2	B	582	VAL
2	B	603	LEU
2	B	609	ILE
2	B	616	ILE
2	B	617	ARG
2	B	620	ARG
2	B	628	THR
2	B	637	LEU
2	B	644	GLU
2	B	653	VAL
2	B	658	ILE
2	B	678	GLU
2	B	680	THR
2	B	722	ASP
2	B	723	VAL
2	B	731	VAL
2	B	734	HIS
2	B	743	ILE
2	B	755	ILE
2	B	766	ARG
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	797	TYR

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Mol	Chain	Res	Type
2	B	825	VAL
2	B	835	GLN
2	B	837	ASP
2	B	839	MET
2	B	843	GLN
2	B	844	SER
2	B	857	ARG
2	B	868	MET
2	B	871	THR
2	B	878	GLN
2	B	879	ARG
2	B	881	ASN
2	B	882	THR
2	B	889	THR
2	B	911	ILE
2	B	933	SER
2	B	934	LYS
2	B	942	ARG
2	B	946	ASN
2	B	953	LEU
2	B	954	VAL
2	B	959	ASP
2	B	964	VAL
2	B	970	THR
2	B	972	LYS
2	B	975	GLN
2	B	976	ILE
2	B	979	LYS
2	B	983	ARG
2	B	986	GLN
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1022	THR
2	B	1031	LEU
2	B	1045	SER
2	B	1050	ILE
2	B	1051	THR
2	B	1060	ARG
2	B	1065	GLN

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Mol	Chain	Res	Type
2	B	1072	MET
2	B	1112	GLN
2	B	1123	SER
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1165	ILE
2	B	1168	LEU
2	B	1170	THR
2	B	1175	LEU
2	B	1176	ASN
2	B	1177	HIS
2	B	1178	ASN
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1189	ILE
2	B	1191	ILE
2	B	1202	LEU
3	C	4	GLU
3	C	7	GLN
3	C	8	VAL
3	C	16	ASP
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	44	LEU
3	C	50	GLU
3	C	52	GLU
3	C	83	SER
3	C	101	LEU
3	C	106	GLU
3	C	108	GLU
3	C	119	VAL
3	C	120	ILE
3	C	121	VAL
3	C	125	MET
3	C	127	ARG

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Mol	Chain	Res	Type
3	C	133	ILE
3	C	134	ILE
3	C	142	VAL
3	C	189	THR
3	C	215	GLU
3	C	226	ASP
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	260	LEU
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	7	THR
4	D	9	GLN
4	D	10	THR
4	D	11	ARG
4	D	12	ARG
4	D	18	VAL
4	D	19	GLU
4	D	23	ASN
4	D	27	LEU
4	D	32	GLU
4	D	34	GLN
4	D	35	LEU
4	D	36	LYS
4	D	40	HIS
4	D	41	GLN
4	D	47	LEU
4	D	50	LEU
4	D	52	LEU
4	D	64	VAL
4	D	67	ARG
4	D	119	ARG
4	D	123	LEU
4	D	126	ILE
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	155	ARG
4	D	177	VAL

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Mol	Chain	Res	Type
4	D	182	SER
4	D	187	THR
4	D	197	SER
4	D	204	ASP
4	D	213	GLU
4	D	217	LEU
4	D	219	THR
5	E	9	ILE
5	E	31	THR
5	E	45	LYS
5	E	57	MET
5	E	65	THR
5	E	67	GLU
5	E	69	ILE
5	E	84	ASP
5	E	92	THR
5	E	100	ILE
5	E	104	ASN
5	E	114	ASN
5	E	119	SER
5	E	121	MET
5	E	131	THR
5	E	152	LYS
5	E	154	ILE
5	E	158	SER
5	E	166	LYS
5	E	173	SER
5	E	175	LEU
5	E	179	GLN
5	E	184	VAL
5	E	190	LEU
5	E	192	ARG
6	F	72	LYS
6	F	78	GLN
6	F	79	ARG
6	F	82	THR
6	F	109	VAL
6	F	110	ASP
6	F	118	LEU
6	F	127	GLU
6	F	129	LYS
7	G	1	MET

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Mol	Chain	Res	Type
7	G	12	THR
7	G	13	LEU
7	G	22	MET
7	G	24	GLN
7	G	26	LEU
7	G	28	THR
7	G	34	VAL
7	G	35	GLU
7	G	60	ARG
7	G	64	THR
7	G	65	ASP
7	G	80	LYS
7	G	83	LYS
7	G	90	THR
7	G	96	GLN
7	G	114	LEU
7	G	133	SER
7	G	134	GLU
7	G	135	ASP
7	G	138	THR
7	G	143	ILE
7	G	152	SER
7	G	155	SER
7	G	160	ILE
7	G	171	ILE
8	H	26	ILE
8	H	76	THR
8	H	77	ARG
8	H	89	LEU
8	H	103	LYS
8	H	106	GLU
8	H	107	VAL
8	H	123	MET
8	H	128	ASN
8	H	130	ARG
8	H	135	LEU
9	I	8	ARG
9	I	31	THR
9	I	42	LEU
9	I	50	THR
9	I	55	THR
9	I	74	GLU

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Mol	Chain	Res	Type
9	I	83	ASN
9	I	84	VAL
9	I	94	ASP
9	I	120	GLN
10	J	2	ILE
10	J	3	VAL
10	J	12	LYS
10	J	13	VAL
10	J	14	VAL
10	J	19	GLU
10	J	25	LEU
10	J	42	LYS
10	J	48	ARG
10	J	52	THR
10	J	56	LEU
11	K	1	MET
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	33	ILE
11	K	34	THR
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	79	GLU
11	K	101	LEU
11	K	107	THR
11	K	108	GLU
11	K	114	LEU
12	L	27	LEU
12	L	33	GLU
12	L	38	LEU
12	L	42	ARG
12	L	50	ASP
12	L	54	ARG
12	L	55	ILE
12	L	58	LYS
12	L	60	ARG
12	L	61	THR
12	L	64	LEU

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Mol	Chain	Res	Type
12	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	118	HIS
1	A	339	ASN
1	A	390	GLN
1	A	394	ASN
1	A	399	HIS
1	A	425	GLN
1	A	439	ASN
1	A	479	ASN
1	A	488	ASN
1	A	545	GLN
1	A	548	ASN
1	A	603	ASN
1	A	811	GLN
1	A	851	HIS
1	A	854	ASN
1	A	969	GLN
1	A	994	GLN
1	A	1009	ASN
1	A	1082	ASN
1	A	1106	ASN
1	A	1203	ASN
1	A	1265	ASN
1	A	1270	ASN
1	A	1312	ASN
1	A	1387	HIS
1	A	1390	ASN
1	A	1393	ASN
2	B	46	GLN
2	B	53	GLN
2	B	206	ASN
2	B	300	HIS
2	B	325	GLN
2	B	465	ASN
2	B	469	GLN
2	B	481	GLN
2	B	572	HIS

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Mol	Chain	Res	Type
2	B	573	GLN
2	B	587	HIS
2	B	590	HIS
2	B	592	ASN
2	B	667	GLN
2	B	686	ASN
2	B	767	ASN
2	B	770	GLN
2	B	794	ASN
2	B	843	GLN
2	B	862	GLN
2	B	975	GLN
2	B	1025	HIS
2	B	1040	ASN
2	B	1084	GLN
2	B	1093	GLN
2	B	1112	GLN
2	B	1117	GLN
2	B	1176	ASN
2	B	1177	HIS
2	B	1205	GLN
3	C	73	GLN
3	C	135	GLN
3	C	151	GLN
3	C	214	ASN
3	C	242	GLN
3	C	264	GLN
4	D	37	GLN
5	E	5	ASN
5	E	8	ASN
5	E	54	GLN
5	E	101	GLN
7	G	71	ASN
7	G	102	GLN
8	H	11	GLN
8	H	33	GLN
8	H	35	GLN
8	H	52	GLN
8	H	131	ASN
9	I	12	ASN
9	I	51	ASN
9	I	83	ASN

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Mol	Chain	Res	Type
9	I	89	GLN
9	I	108	HIS
9	I	114	GLN
11	K	29	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
15	BRU	T	22	14,15	18,21,22	1.28	2 (11%)	25,30,33	1.96	9 (36%)

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
15	BRU	T	22	14,15	-	0/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C1'-N1	-3.05	1.40	1.48
15	T	22	BRU	C2-N3	-2.77	1.33	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	O4'-C1'-N1	4.90	116.57	107.86
15	T	22	BRU	C5-C4-N3	4.59	118.62	113.34
15	T	22	BRU	C6-C5-C4	-2.96	117.67	120.67
15	T	22	BRU	C4-N3-C2	-2.89	123.56	127.34
15	T	22	BRU	O4-C4-C5	-2.50	122.61	125.80
15	T	22	BRU	O2-C2-N3	-2.38	117.10	121.49
15	T	22	BRU	N3-C2-N1	2.36	117.97	114.89
15	T	22	BRU	BR-C5-C4	2.21	120.57	118.02
15	T	22	BRU	C2'-C1'-N1	-2.10	108.57	113.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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
16	APC	A	2455	-	29,33,33	3.07	10 (34%)	44,52,52	2.45	13 (29%)

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
16	APC	A	2455	-	-	5/19/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	2455	APC	PB-O3B	10.02	1.69	1.58
16	A	2455	APC	PA-O1A	5.86	1.65	1.51
16	A	2455	APC	PB-O2B	5.69	1.70	1.56
16	A	2455	APC	PG-O1G	5.57	1.67	1.50
16	A	2455	APC	PG-O2G	4.37	1.71	1.54
16	A	2455	APC	C5-N7	-4.33	1.31	1.39
16	A	2455	APC	C6-N1	-2.93	1.27	1.35
16	A	2455	APC	C8-N9	-2.56	1.33	1.37
16	A	2455	APC	C2-N1	-2.11	1.30	1.33
16	A	2455	APC	O3'-C3'	2.10	1.48	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	2455	APC	C5-C4-N3	-8.08	115.59	126.72
16	A	2455	APC	N3-C4-N9	5.08	135.80	127.17
16	A	2455	APC	C4-C5-N7	-4.88	105.00	110.58
16	A	2455	APC	N3-C2-N1	-4.82	121.28	128.58
16	A	2455	APC	C5-N7-C8	4.46	110.47	103.45
16	A	2455	APC	C2-N3-C4	4.34	122.43	111.83
16	A	2455	APC	O3'-C3'-C2'	3.26	122.26	111.82
16	A	2455	APC	PB-O3B-PG	-3.10	121.35	132.45
16	A	2455	APC	O3G-PG-O3B	2.72	113.76	104.64
16	A	2455	APC	C5-C4-N9	2.56	108.60	105.81
16	A	2455	APC	C5'-C4'-C3'	-2.32	106.86	115.21
16	A	2455	APC	O2'-C2'-C3'	2.23	118.96	111.82
16	A	2455	APC	O2'-C2'-C1'	2.06	117.19	110.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	2455	APC	C5'-O5'-PA-O1A

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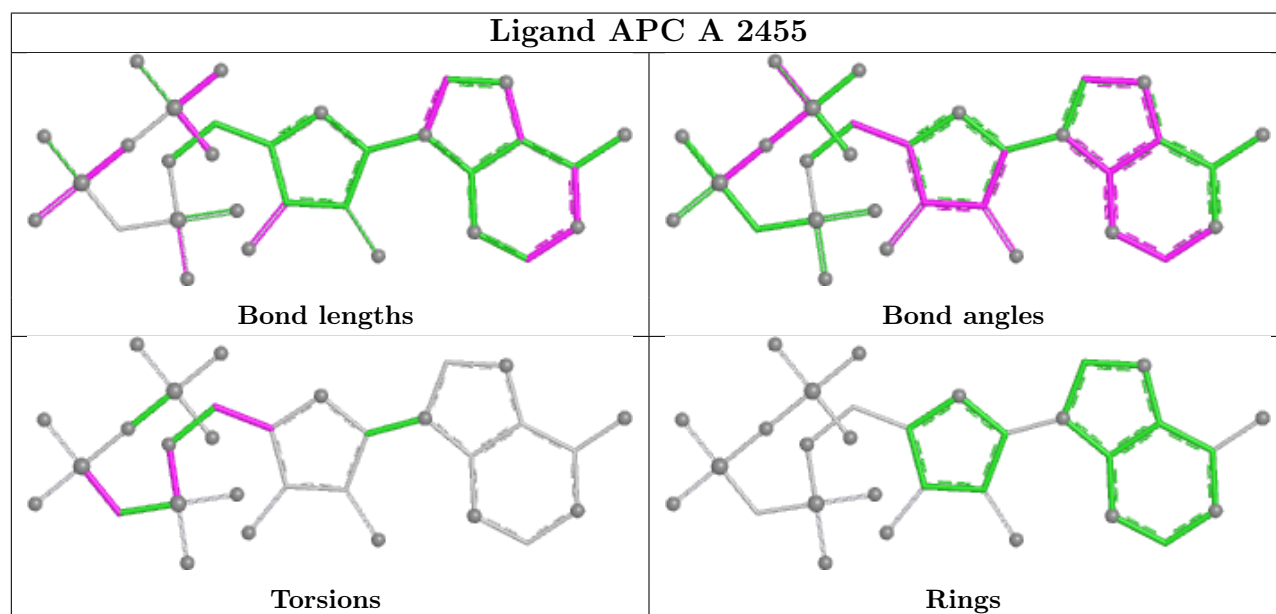
Mol	Chain	Res	Type	Atoms
16	A	2455	APC	C3'-C4'-C5'-O5'
16	A	2455	APC	O4'-C4'-C5'-O5'
16	A	2455	APC	PA-C3A-PB-O2B
16	A	2455	APC	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	2455	APC	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	5.45
1	B	351:TYR	C	352:ALA	N	3.24

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	1425/1732 (82%)	-0.29	11 (0%) 82 60	58, 110, 173, 226	0
2	B	1115/1224 (91%)	-0.07	23 (2%) 63 38	68, 123, 181, 210	0
3	C	266/318 (83%)	-0.47	0 100 100	81, 110, 148, 178	0
4	D	178/221 (80%)	-0.11	7 (3%) 43 23	85, 121, 175, 193	0
5	E	214/215 (99%)	-0.24	0 100 100	91, 148, 190, 200	0
6	F	84/155 (54%)	-0.58	1 (1%) 76 52	68, 92, 125, 138	0
7	G	171/171 (100%)	-0.28	1 (0%) 85 65	82, 109, 145, 167	0
8	H	133/146 (91%)	0.18	5 (3%) 44 24	121, 153, 184, 218	0
9	I	119/122 (97%)	0.03	1 (0%) 82 60	120, 158, 195, 213	0
10	J	65/70 (92%)	-0.40	2 (3%) 51 29	90, 106, 145, 161	0
11	K	115/120 (95%)	-0.56	1 (0%) 81 58	79, 110, 141, 156	0
12	L	46/70 (65%)	0.53	4 (8%) 16 10	100, 180, 195, 199	0
13	N	11/14 (78%)	0.67	0 100 100	181, 210, 266, 271	0
14	P	6/6 (100%)	-0.41	1 (16%) 4 4	91, 95, 119, 147	0
15	T	19/26 (73%)	0.41	2 (10%) 11 8	84, 141, 264, 267	0
All	All	3967/4610 (86%)	-0.21	59 (1%) 72 47	58, 117, 182, 271	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	509	ALA	8.0
1	A	1243	VAL	4.5
8	H	63	LEU	4.5
2	B	446	LEU	4.4
12	L	27	LEU	4.1
4	D	24	ALA	4.0
2	B	708	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
6	F	72	LYS	3.8
2	B	502	ILE	3.6
4	D	221	TYR	3.5
2	B	962	LYS	3.5
8	H	136	LYS	3.3
1	A	251	SER	3.2
8	H	139	ASN	3.2
2	B	262	GLU	3.1
2	B	882	THR	3.1
2	B	70	ILE	3.0
2	B	883	LEU	3.0
1	A	252	PHE	2.8
1	A	56	PRO	2.8
15	T	6	DC	2.7
2	B	715	ALA	2.7
12	L	28	LYS	2.7
2	B	709	ASP	2.7
15	T	25	DT	2.7
1	A	186	LYS	2.6
1	A	1093	LYS	2.5
9	I	47	GLU	2.5
2	B	134	LYS	2.5
11	K	114	LEU	2.5
2	B	343	ILE	2.5
8	H	90	ALA	2.5
14	P	5	C	2.4
4	D	3	VAL	2.4
4	D	220	LEU	2.4
1	A	190	ALA	2.4
12	L	26	THR	2.4
2	B	263	GLY	2.3
2	B	230	ALA	2.3
12	L	25	ALA	2.3
10	J	65	PRO	2.3
2	B	341	LEU	2.3
2	B	251	ILE	2.3
7	G	154	VAL	2.3
1	A	1083	THR	2.2
8	H	132	LEU	2.2
4	D	136	GLY	2.2
4	D	76	LYS	2.1
2	B	266	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	10	THR	2.1
2	B	958	GLN	2.1
10	J	64	ASN	2.1
1	A	194	ALA	2.1
2	B	646	LEU	2.0
2	B	881	ASN	2.0
1	A	51	GLY	2.0
2	B	244	LEU	2.0
2	B	468	GLU	2.0
1	A	1254	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	BRU	T	22	20/21	0.97	0.06	86,97,107,113	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

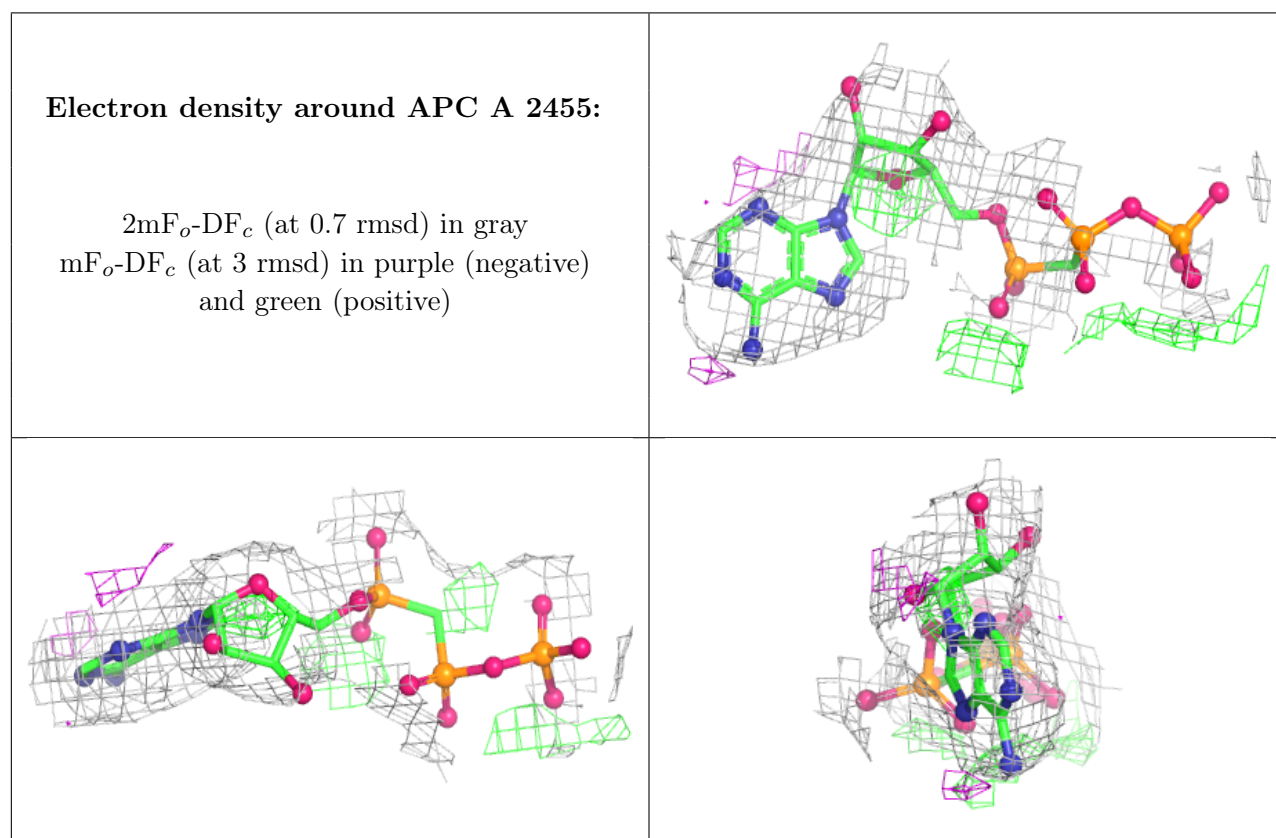
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	APC	A	2455	31/31	0.93	0.09	112,115,143,144	0
17	ZN	I	1122	1/1	0.99	0.03	201,201,201,201	0
17	ZN	L	1071	1/1	0.99	0.04	211,211,211,211	0
18	MG	A	2458	1/1	0.99	0.03	86,86,86,86	0
17	ZN	C	1269	1/1	1.00	0.02	93,93,93,93	0
17	ZN	I	1121	1/1	1.00	0.03	134,134,134,134	0
17	ZN	A	2456	1/1	1.00	0.03	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	ZN	J	1066	1/1	1.00	0.03	95,95,95,95	0
17	ZN	A	2457	1/1	1.00	0.02	74,74,74,74	0
17	ZN	B	2225	1/1	1.00	0.03	81,81,81,81	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.