



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:47 PM UTC

PDB ID : 3S1Q / pdb_00003s1q
Title : RNA Polymerase II Initiation Complex with a 5-nt 3'-deoxy RNA soaked with ATP
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-16
Resolution : 3.30 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

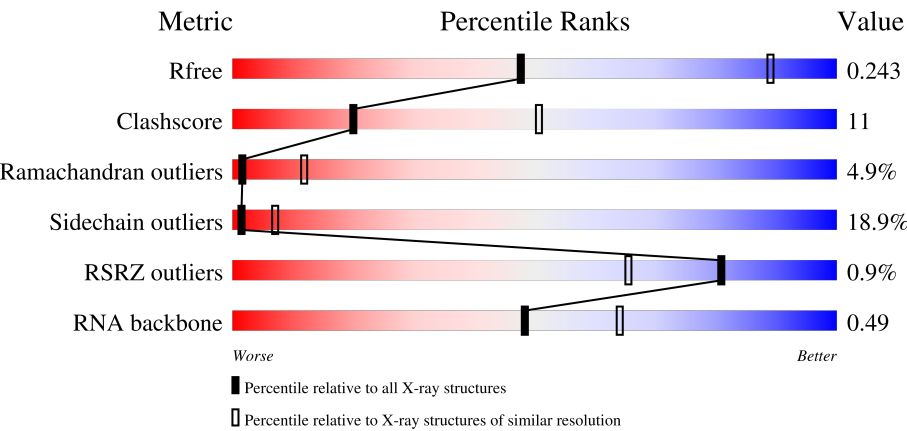
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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	1733	% 46% 26% 8% • 19%
2	B	1224	% 52% 30% 7% • 9%
3	C	318	49% 26% 7% • 16%
4	E	215	65% 31% •

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Mol	Chain	Length	Quality of chain
5	F	155	35%17%45%
6	H	146	% 51%34%6%9%
7	I	122	2% 64%29%...
8	J	70	41%33%16%7%
9	K	120	52%38%6%5%
10	L	70	4% 24%27%11%34%
11	R	5	40%60%
12	T	29	38%7%55%

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 28703 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	1405	Total	C	N	O	S	0	0	0
			11043	6965	1936	2081	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0	0
			8861	5610	1549	1647	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 polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	85	Total	C	N	O	S	0	0	0
			688	439	116	130	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	5	Total	C	N	O	P	0	0	0
			109	50	25	30	4			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	13	Total	C	N	O	P	0	0	0
			261	125	43	80	13			

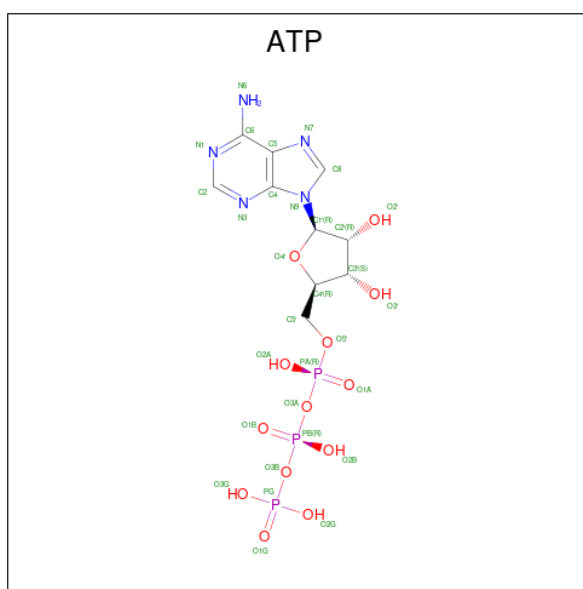
- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Mg	0	0
			2	2		

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

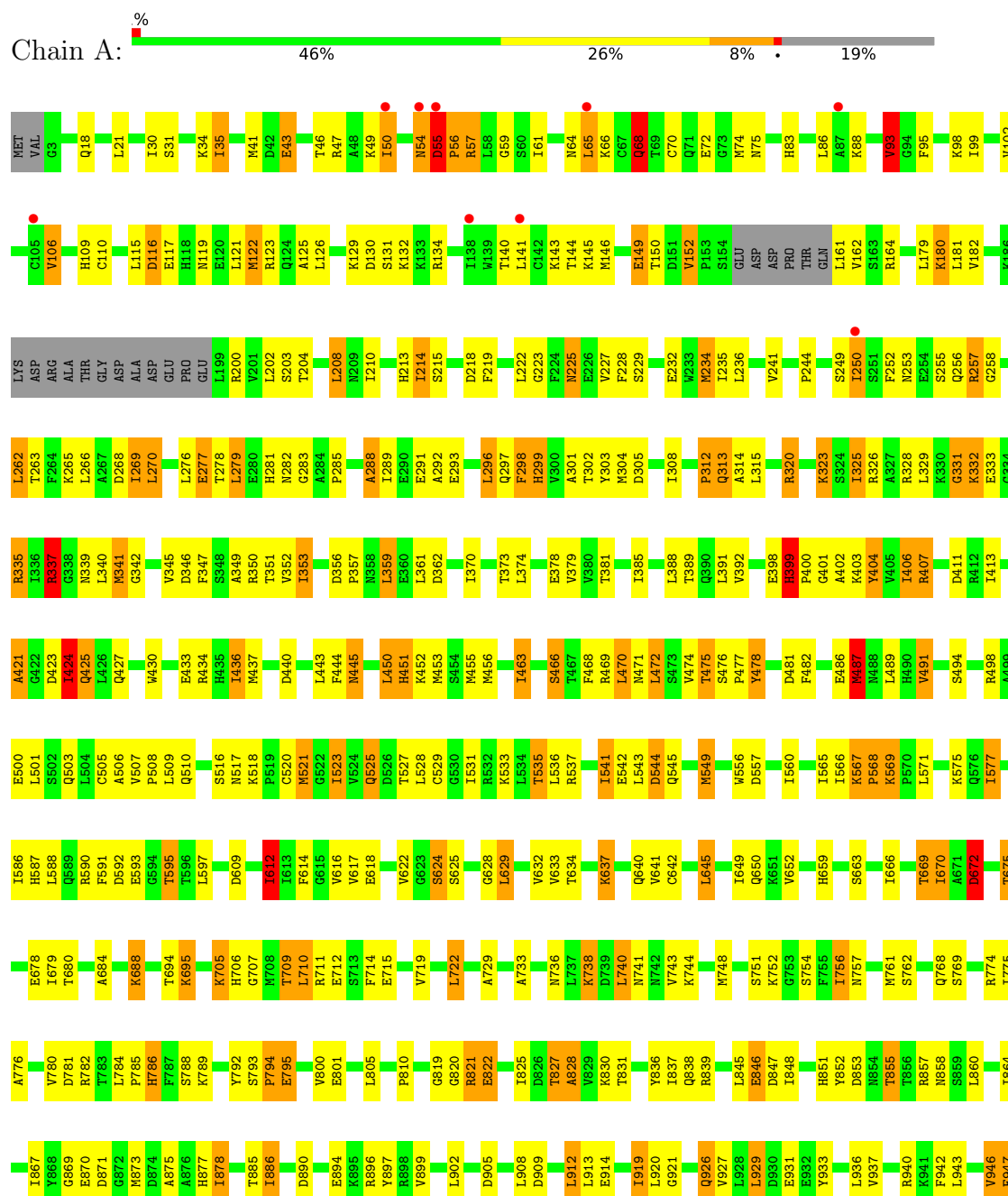


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

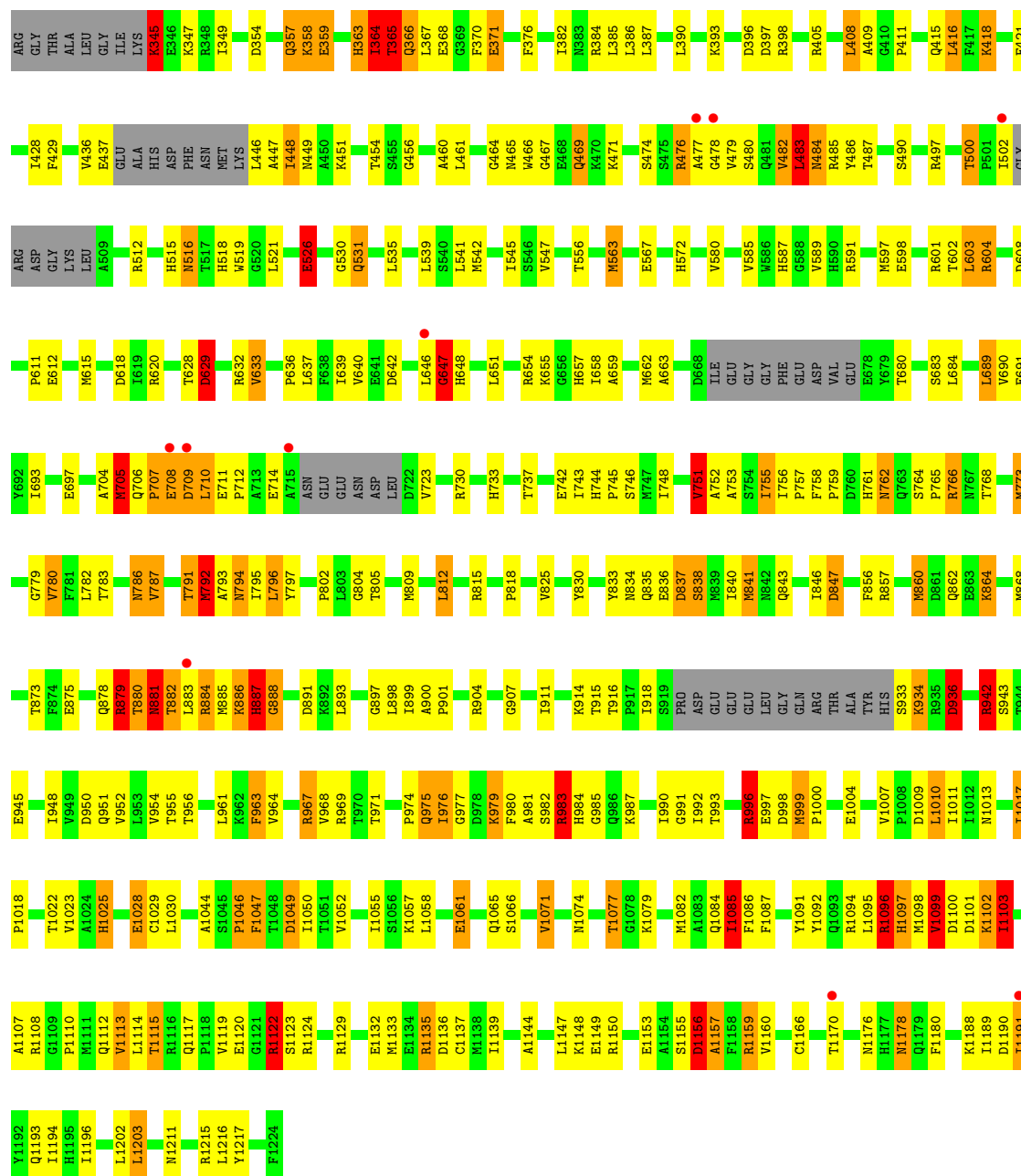
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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

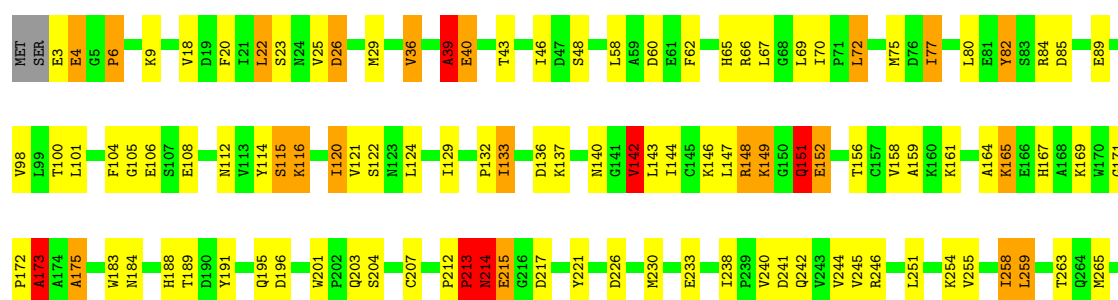


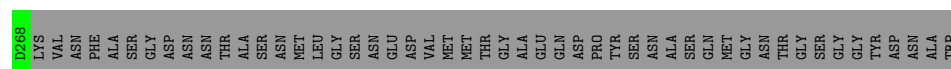




● Molecule 3: DNA-directed RNA polymerase II subunit RPB3

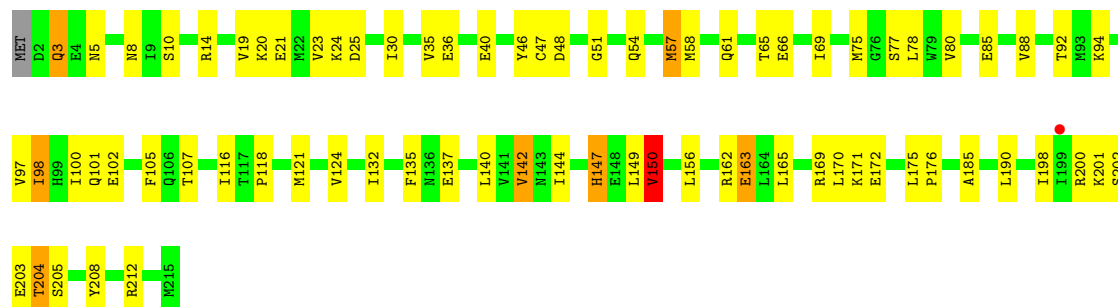
Chain C: 49% 26% 7% 16%





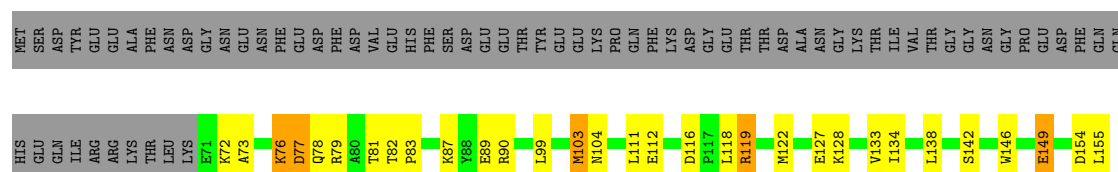
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 65% 31% .



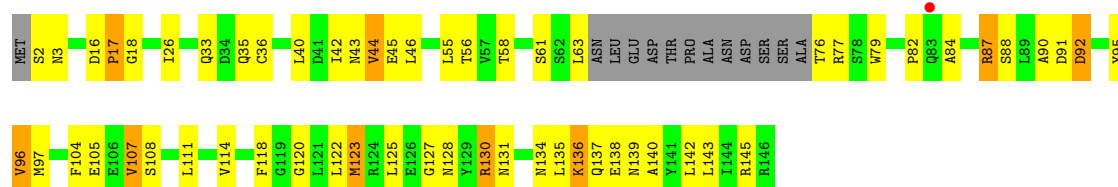
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 35% 17% . 45%



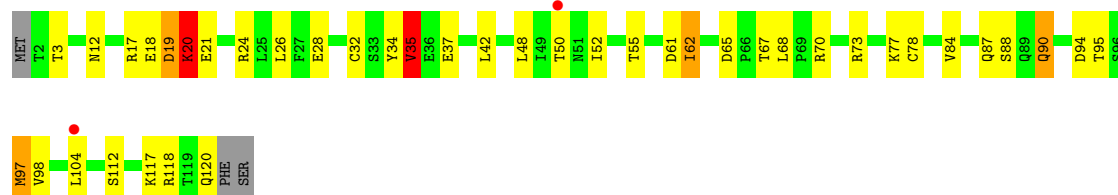
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 51% 34% 6% 9%

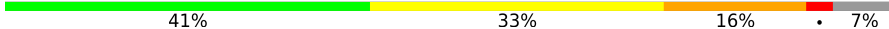


- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 2% 64% 29% . . .



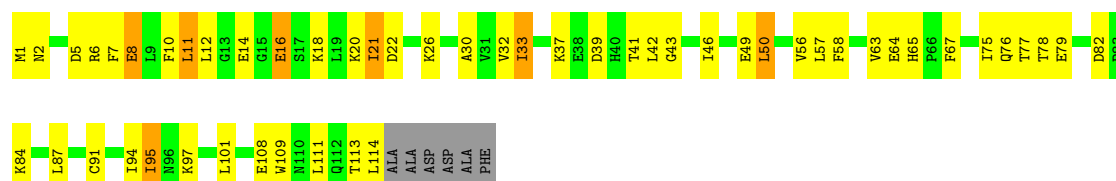
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 



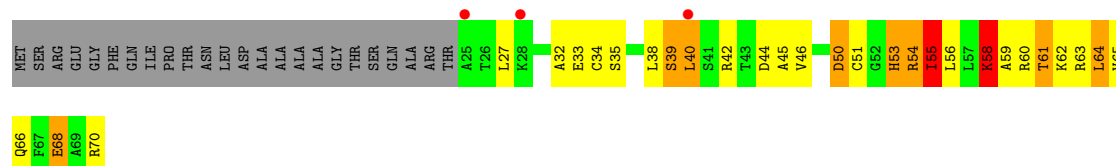
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 



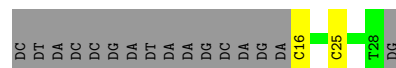
- Molecule 11: RNA (5'-R(*AP*GP*AP*GP*G)-3')

Chain R: 



- Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3')

Chain T: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.94Å 220.53Å 193.72Å 90.00° 98.48° 90.00°	Depositor
Resolution (Å)	29.67 – 3.30 29.67 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.67-3.30) 99.1 (29.67-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.31Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.176 , 0.229 0.192 , 0.243	Depositor DCC
R_{free} test set	4995 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	97.3	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 113.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28703	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: ATP, ZN, MG

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	0.88	3/11241 (0.0%)	1.56	142/15199 (0.9%)
2	B	0.92	4/9033 (0.0%)	1.53	115/12181 (0.9%)
3	C	0.84	2/2133 (0.1%)	1.48	26/2891 (0.9%)
4	E	0.81	0/1788	1.46	20/2406 (0.8%)
5	F	0.84	0/700	1.41	3/945 (0.3%)
6	H	0.83	0/1086	1.33	7/1470 (0.5%)
7	I	0.85	0/989	1.42	7/1331 (0.5%)
8	J	1.01	2/541 (0.4%)	1.71	10/727 (1.4%)
9	K	0.80	0/937	1.46	7/1265 (0.6%)
10	L	0.97	0/365	1.78	9/485 (1.9%)
11	R	0.50	0/123	1.07	0/191
12	T	0.48	0/290	1.38	3/444 (0.7%)
All	All	0.88	11/29226 (0.0%)	1.52	349/39535 (0.9%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1	MET	SD-CE	6.91	1.96	1.79
8	J	6	ARG	CA-C	6.80	1.61	1.52
2	B	563	MET	SD-CE	-6.31	1.63	1.79
1	A	487	MET	SD-CE	-6.27	1.63	1.79
2	B	705	MET	SD-CE	-5.97	1.64	1.79
1	A	213	HIS	CA-C	5.68	1.55	1.52
2	B	983	ARG	CA-C	5.56	1.60	1.52
3	C	175	ALA	CA-C	5.40	1.59	1.52
2	B	140	ILE	CA-C	5.35	1.59	1.52
3	C	40	GLU	CA-C	5.32	1.59	1.52
1	A	521	MET	SD-CE	-5.16	1.66	1.79

All (349) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	GLU	N-CA-C	-9.89	103.35	114.62
3	C	172	PRO	CA-C-N	9.02	138.77	121.54
3	C	172	PRO	C-N-CA	9.02	138.77	121.54
2	B	881	ASN	CA-C-N	8.96	133.02	120.29
2	B	881	ASN	C-N-CA	8.96	133.02	120.29
10	L	58	LYS	N-CA-C	8.95	122.00	111.71
8	J	18	TRP	N-CA-C	8.91	120.69	110.97
2	B	359	GLU	N-CA-C	8.82	120.90	111.28
8	J	5	VAL	N-CA-C	-8.81	98.08	109.80
5	F	87	LYS	CA-C-N	8.78	131.85	120.44
5	F	87	LYS	C-N-CA	8.78	131.85	120.44
2	B	1009	ASP	N-CA-C	-8.58	102.95	113.50
1	A	1084	PHE	CA-CB-CG	8.55	122.35	113.80
2	B	628	THR	CA-C-N	8.18	137.17	121.54
2	B	628	THR	C-N-CA	8.18	137.17	121.54
12	T	16	DC	P-O3'-C3'	8.08	132.32	120.20
1	A	117	GLU	CA-C-N	7.91	131.94	120.38
1	A	117	GLU	C-N-CA	7.91	131.94	120.38
1	A	999	VAL	N-CA-C	-7.85	105.42	111.62
2	B	37	PHE	N-CA-C	-7.83	99.71	110.35
1	A	1123	GLY	CA-C-N	7.82	135.78	121.70
1	A	1123	GLY	C-N-CA	7.82	135.78	121.70
1	A	1096	SER	N-CA-C	7.81	120.55	111.02
10	L	54	ARG	N-CA-C	7.67	122.32	113.19
1	A	466	SER	N-CA-C	7.57	122.54	113.16
1	A	1082	ASN	CA-C-N	7.43	135.07	121.70
1	A	1082	ASN	C-N-CA	7.43	135.07	121.70
2	B	140	ILE	CA-C-N	7.37	134.97	121.70
2	B	140	ILE	C-N-CA	7.37	134.97	121.70
2	B	363	HIS	N-CA-C	-7.36	101.07	110.19
1	A	491	VAL	N-CA-C	7.33	115.44	107.60
3	C	172	PRO	N-CA-C	-7.24	105.31	114.35
1	A	1093	LYS	CA-C-N	7.21	134.67	121.70
1	A	1093	LYS	C-N-CA	7.21	134.67	121.70
1	A	1095	THR	N-CA-C	7.21	123.26	111.37
1	A	541	ILE	N-CA-C	7.18	118.22	108.17
6	H	92	ASP	N-CA-C	-7.09	101.74	110.61
2	B	1087	PHE	CA-CB-CG	7.05	120.85	113.80
6	H	122	LEU	N-CA-C	7.05	120.94	109.59
10	L	62	LYS	CA-C-N	7.04	130.66	120.38
10	L	62	LYS	C-N-CA	7.04	130.66	120.38
1	A	54	ASN	CA-CB-CG	7.03	119.63	112.60
1	A	1083	THR	CA-C-N	7.03	134.35	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1083	THR	C-N-CA	7.03	134.35	121.70
1	A	827	THR	N-CA-C	-6.93	103.34	111.03
1	A	445	ASN	CA-CB-CG	6.92	119.52	112.60
1	A	794	PRO	CA-C-N	6.85	129.46	120.28
1	A	794	PRO	C-N-CA	6.85	129.46	120.28
2	B	322	PHE	CA-CB-CG	6.78	120.58	113.80
2	B	659	ALA	CA-C-N	6.75	129.66	120.54
2	B	659	ALA	C-N-CA	6.75	129.66	120.54
2	B	541	LEU	N-CA-C	6.75	122.45	111.37
3	C	136	ASP	CA-CB-CG	6.74	119.34	112.60
4	E	150	VAL	N-CA-C	6.72	114.20	107.55
3	C	133	ILE	N-CA-CB	6.70	118.55	110.31
3	C	89	GLU	N-CA-C	-6.69	99.75	109.59
2	B	647	GLY	CA-C-N	6.68	133.72	121.70
2	B	647	GLY	C-N-CA	6.68	133.72	121.70
2	B	1049	ASP	CA-C-N	6.66	129.49	120.63
2	B	1049	ASP	C-N-CA	6.66	129.49	120.63
2	B	847	ASP	CA-CB-CG	6.64	119.25	112.60
1	A	1424	VAL	CA-C-N	6.64	129.47	120.38
1	A	1424	VAL	C-N-CA	6.64	129.47	120.38
2	B	447	ALA	CA-C-N	6.63	131.66	123.17
2	B	447	ALA	C-N-CA	6.63	131.66	123.17
6	H	2	SER	CA-C-N	6.63	133.63	121.70
6	H	2	SER	C-N-CA	6.63	133.63	121.70
3	C	26	ASP	CA-CB-CG	6.61	119.21	112.60
3	C	39	ALA	CA-C-N	6.59	134.13	121.54
3	C	39	ALA	C-N-CA	6.59	134.13	121.54
3	C	204	SER	N-CA-C	6.59	119.06	110.43
2	B	56	ASP	CA-CB-CG	6.53	119.13	112.60
7	I	78	CYS	CA-C-N	-6.51	112.34	122.37
7	I	78	CYS	C-N-CA	-6.51	112.34	122.37
1	A	463	ILE	N-CA-C	6.49	116.24	108.45
2	B	618	ASP	CA-C-N	6.43	128.89	120.60
2	B	618	ASP	C-N-CA	6.43	128.89	120.60
3	C	40	GLU	N-CA-C	6.41	124.46	110.80
2	B	140	ILE	N-CA-C	6.41	116.89	110.23
2	B	1122	ARG	CA-C-N	6.40	128.76	120.44
2	B	1122	ARG	C-N-CA	6.40	128.76	120.44
2	B	887	HIS	CA-C-N	6.37	133.16	121.70
2	B	887	HIS	C-N-CA	6.37	133.16	121.70
1	A	244	PRO	N-CA-C	6.37	118.47	110.70
1	A	288	ALA	N-CA-C	-6.34	104.80	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	945	GLU	N-CA-C	6.32	119.75	110.59
4	E	172	GLU	CA-C-N	6.29	129.57	120.38
4	E	172	GLU	C-N-CA	6.29	129.57	120.38
8	J	60	PHE	CA-CB-CG	6.29	120.09	113.80
2	B	1004	GLU	N-CA-C	-6.29	105.43	113.23
8	J	64	ASN	N-CA-C	6.29	123.70	109.81
1	A	947	PHE	CA-C-N	6.28	129.38	120.53
1	A	947	PHE	C-N-CA	6.28	129.38	120.53
1	A	228	PHE	N-CA-C	6.26	121.06	112.04
1	A	1084	PHE	CA-C-N	6.26	132.96	121.70
1	A	1084	PHE	C-N-CA	6.26	132.96	121.70
2	B	222	ILE	CB-CA-C	6.24	118.64	110.91
1	A	99	ILE	N-CA-C	-6.22	104.44	110.42
1	A	421	ALA	CA-C-N	6.22	126.85	119.94
1	A	421	ALA	C-N-CA	6.22	126.85	119.94
1	A	1091	SER	CA-C-N	6.21	132.88	121.70
1	A	1091	SER	C-N-CA	6.21	132.88	121.70
7	I	62	ILE	N-CA-C	6.16	117.64	110.62
1	A	481	ASP	N-CA-C	-6.15	99.78	109.50
2	B	1071	VAL	N-CA-CB	6.15	117.23	110.53
1	A	1026	LEU	N-CA-C	6.13	119.50	112.57
1	A	152	VAL	N-CA-C	6.12	114.64	107.84
2	B	476	ARG	CA-C-N	6.12	133.23	121.54
2	B	476	ARG	C-N-CA	6.12	133.23	121.54
2	B	1013	ASN	CA-CB-CG	6.11	118.71	112.60
9	K	32	VAL	N-CA-C	6.11	115.14	106.53
1	A	236	LEU	N-CA-C	6.09	117.93	109.15
2	B	213	ILE	N-CA-C	6.09	117.15	108.93
1	A	1257	ASP	N-CA-C	6.09	121.41	111.37
2	B	881	ASN	CA-CB-CG	6.08	118.68	112.60
2	B	345	LYS	CA-C-N	6.07	132.63	121.70
2	B	345	LYS	C-N-CA	6.07	132.63	121.70
2	B	629	ASP	CA-CB-CG	6.07	118.67	112.60
2	B	834	ASN	CA-CB-CG	6.07	118.67	112.60
1	A	451	HIS	N-CA-CB	-6.06	100.24	110.49
1	A	1029	ARG	CA-C-N	6.06	128.40	120.28
1	A	1029	ARG	C-N-CA	6.06	128.40	120.28
1	A	1311	VAL	N-CA-C	6.04	117.18	108.48
1	A	249	SER	N-CA-C	6.02	113.72	108.78
2	B	99	LYS	N-CA-C	-6.01	102.30	110.36
6	H	91	ASP	CA-C-N	6.01	133.47	122.54
6	H	91	ASP	C-N-CA	6.01	133.47	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	786	ASN	CA-CB-CG	5.97	118.57	112.60
2	B	860	MET	N-CA-C	5.96	118.13	109.07
3	C	175	ALA	N-CA-C	5.92	119.04	110.28
1	A	337	ARG	N-CA-C	5.92	117.40	111.07
6	H	91	ASP	N-CA-C	5.90	119.09	109.06
3	C	60	ASP	CA-CB-CG	5.89	118.49	112.60
2	B	825	VAL	N-CA-C	5.89	116.36	108.11
1	A	537	ARG	CA-C-N	5.89	129.26	120.31
1	A	537	ARG	C-N-CA	5.89	129.26	120.31
2	B	1028	GLU	CB-CG-CD	5.88	122.61	112.60
1	A	249	SER	CA-C-N	5.87	132.54	121.97
1	A	249	SER	C-N-CA	5.87	132.54	121.97
3	C	230	MET	N-CA-C	5.85	119.09	109.72
1	A	1094	VAL	CA-C-N	5.85	129.59	120.82
1	A	1094	VAL	C-N-CA	5.85	129.59	120.82
1	A	897	TYR	N-CA-C	5.82	120.54	112.45
2	B	421	PHE	CA-C-N	5.81	128.00	120.44
2	B	421	PHE	C-N-CA	5.81	128.00	120.44
2	B	1135	ARG	CA-C-N	5.81	127.99	120.44
2	B	1135	ARG	C-N-CA	5.81	127.99	120.44
1	A	544	ASP	CA-C-N	5.80	128.52	120.63
1	A	544	ASP	C-N-CA	5.80	128.52	120.63
1	A	640	GLN	CA-C-N	5.79	128.39	120.46
1	A	640	GLN	C-N-CA	5.79	128.39	120.46
2	B	358	LYS	CA-C-N	5.79	128.04	120.28
2	B	358	LYS	C-N-CA	5.79	128.04	120.28
8	J	2	ILE	N-CA-C	5.79	121.38	109.34
1	A	203	SER	CA-C-N	5.79	128.31	120.44
1	A	203	SER	C-N-CA	5.79	128.31	120.44
1	A	399	HIS	N-CA-CB	5.78	120.65	110.37
1	A	890	ASP	CA-C-N	5.77	128.27	120.65
1	A	890	ASP	C-N-CA	5.77	128.27	120.65
4	E	163	GLU	CB-CG-CD	5.76	122.40	112.60
1	A	762	SER	N-CA-C	5.76	120.97	113.88
4	E	147	HIS	CA-C-N	5.76	128.79	120.79
4	E	147	HIS	C-N-CA	5.76	128.79	120.79
2	B	1085	ILE	N-CA-C	5.75	116.22	108.17
4	E	170	LEU	N-CA-C	5.73	119.31	110.42
10	L	40	LEU	CA-C-N	5.73	129.00	120.87
10	L	40	LEU	C-N-CA	5.73	129.00	120.87
1	A	622	VAL	N-CA-CB	-5.73	104.66	112.28
1	A	1089	VAL	CA-C-N	5.70	131.95	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1089	VAL	C-N-CA	5.70	131.95	121.70
1	A	710	LEU	N-CA-C	-5.70	105.07	111.28
1	A	800	VAL	CA-C-N	5.69	128.37	120.29
1	A	800	VAL	C-N-CA	5.69	128.37	120.29
1	A	864	ILE	N-CA-C	-5.69	106.16	111.45
2	B	180	TYR	CA-C-N	5.67	127.88	120.28
2	B	180	TYR	C-N-CA	5.67	127.88	120.28
1	A	1355	VAL	CA-C-N	5.67	128.20	120.77
1	A	1355	VAL	C-N-CA	5.67	128.20	120.77
1	A	99	ILE	CA-C-N	5.66	128.19	120.54
1	A	99	ILE	C-N-CA	5.66	128.19	120.54
1	A	520	CYS	N-CA-C	5.65	120.01	113.18
8	J	31	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	314	ALA	CA-C-N	5.63	129.54	121.71
1	A	314	ALA	C-N-CA	5.63	129.54	121.71
2	B	484	ASN	CA-CB-CG	5.62	118.22	112.60
2	B	879	ARG	CA-C-N	5.61	132.26	121.54
2	B	879	ARG	C-N-CA	5.61	132.26	121.54
2	B	230	ALA	N-CA-C	5.61	122.20	109.81
1	A	219	PHE	CA-CB-CG	5.60	119.40	113.80
2	B	397	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	858	ASN	CA-C-N	5.58	128.32	120.28
1	A	858	ASN	C-N-CA	5.58	128.32	120.28
4	E	25	ASP	CA-CB-CG	5.57	118.17	112.60
9	K	43	GLY	CA-C-N	5.57	127.74	120.28
9	K	43	GLY	C-N-CA	5.57	127.74	120.28
2	B	1007	VAL	N-CA-CB	-5.55	103.44	111.21
2	B	1013	ASN	N-CA-C	5.55	116.66	109.72
1	A	1063	MET	CA-C-N	5.53	131.92	121.97
1	A	1063	MET	C-N-CA	5.53	131.92	121.97
1	A	948	VAL	N-CA-C	5.53	116.92	110.62
1	A	557	ASP	CA-CB-CG	5.52	118.12	112.60
8	J	8	PHE	CA-CB-CG	5.52	119.32	113.80
2	B	535	LEU	N-CA-C	-5.52	106.60	113.55
7	I	97	MET	N-CA-C	-5.51	106.53	113.20
2	B	415	GLN	CA-C-N	5.51	127.92	120.65
2	B	415	GLN	C-N-CA	5.51	127.92	120.65
2	B	229	ALA	N-CA-C	5.51	117.98	110.55
7	I	19	ASP	CA-CB-CG	5.50	118.10	112.60
2	B	1029	CYS	CA-C-N	5.49	127.95	120.54
2	B	1029	CYS	C-N-CA	5.49	127.95	120.54
2	B	697	GLU	CA-C-N	5.48	127.89	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	697	GLU	C-N-CA	5.48	127.89	120.38
2	B	456	GLY	CA-C-N	5.48	127.88	120.65
2	B	456	GLY	C-N-CA	5.48	127.88	120.65
2	B	1114	LEU	CA-C-N	5.47	128.16	120.28
2	B	1114	LEU	C-N-CA	5.47	128.16	120.28
5	F	77	ASP	CA-CB-CG	5.47	118.07	112.60
2	B	39	ARG	N-CA-C	-5.46	105.72	112.38
2	B	54	PHE	CA-C-N	5.46	127.65	120.60
2	B	54	PHE	C-N-CA	5.46	127.65	120.60
2	B	1047	PHE	CB-CA-C	5.46	118.54	111.50
2	B	1086	PHE	N-CA-C	-5.45	101.31	109.15
12	T	25	DC	P-O5'-C5'	5.45	128.17	120.00
10	L	45	ALA	N-CA-C	5.44	116.05	108.00
2	B	916	THR	CB-CA-C	5.42	116.03	109.85
9	K	39	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	998	LEU	CA-C-N	5.41	128.90	123.16
1	A	998	LEU	C-N-CA	5.41	128.90	123.16
1	A	270	LEU	CA-C-N	5.41	127.79	120.38
1	A	270	LEU	C-N-CA	5.41	127.79	120.38
3	C	3	GLU	CA-C-N	5.41	131.87	121.54
3	C	3	GLU	C-N-CA	5.41	131.87	121.54
2	B	276	ILE	CA-C-N	5.41	131.87	121.54
2	B	276	ILE	C-N-CA	5.41	131.87	121.54
3	C	82	TYR	N-CA-C	-5.39	101.00	109.25
10	L	68	GLU	N-CA-C	-5.39	101.19	109.76
3	C	173	ALA	CA-C-N	5.39	131.83	121.54
3	C	173	ALA	C-N-CA	5.39	131.83	121.54
3	C	142	VAL	N-CA-C	-5.38	101.89	109.21
2	B	794	ASN	CA-CB-CG	5.37	117.97	112.60
2	B	1113	VAL	N-CA-C	5.36	115.50	110.30
1	A	218	ASP	CA-C-N	5.36	127.72	120.65
1	A	218	ASP	C-N-CA	5.36	127.72	120.65
3	C	4	GLU	N-CA-C	5.35	122.19	110.80
1	A	705	LYS	CA-C-N	5.35	131.75	121.54
1	A	705	LYS	C-N-CA	5.35	131.75	121.54
2	B	709	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	786	HIS	N-CA-C	-5.33	106.83	113.38
2	B	1103	ILE	N-CA-CB	5.32	117.07	110.05
4	E	171	LYS	N-CA-C	-5.32	101.49	109.95
7	I	78	CYS	N-CA-C	-5.31	101.50	109.79
1	A	370	ILE	N-CA-CB	5.29	116.74	110.55
2	B	602	THR	CA-C-N	5.29	127.31	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	THR	C-N-CA	5.29	127.31	120.44
1	A	659	HIS	CA-CB-CG	-5.29	108.52	113.80
1	A	985	ASP	CA-CB-CG	5.28	117.88	112.60
2	B	936	ASP	N-CA-C	5.28	122.05	110.80
8	J	47	ARG	CA-C-N	5.28	127.36	120.28
8	J	47	ARG	C-N-CA	5.28	127.36	120.28
1	A	624	SER	CA-C-N	5.28	128.21	120.71
1	A	624	SER	C-N-CA	5.28	128.21	120.71
4	E	48	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	836	TYR	N-CA-C	-5.28	105.44	111.14
7	I	48	LEU	N-CA-C	-5.28	105.97	112.72
1	A	612	ILE	N-CA-CB	5.24	116.24	110.53
1	A	1043	ASP	CA-C-N	5.24	127.73	120.29
1	A	1043	ASP	C-N-CA	5.24	127.73	120.29
2	B	418	LYS	CA-C-N	5.24	127.25	120.44
2	B	418	LYS	C-N-CA	5.24	127.25	120.44
9	K	113	THR	CA-C-N	5.24	131.13	121.70
9	K	113	THR	C-N-CA	5.24	131.13	121.70
2	B	140	ILE	CA-C-O	-5.23	115.97	121.41
1	A	291	GLU	N-CA-C	-5.23	106.40	112.89
1	A	523	ILE	CB-CA-C	5.23	117.20	111.08
1	A	592	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	320	ARG	CB-CA-C	5.22	115.73	109.31
4	E	203	GLU	CA-C-N	5.21	130.38	122.56
4	E	203	GLU	C-N-CA	5.21	130.38	122.56
3	C	196	ASP	N-CA-C	5.21	117.09	108.13
1	A	733	ALA	CA-C-N	5.21	128.63	120.82
1	A	733	ALA	C-N-CA	5.21	128.63	120.82
2	B	264	SER	CA-C-N	5.20	131.48	121.54
2	B	264	SER	C-N-CA	5.20	131.48	121.54
1	A	55	ASP	N-CA-C	5.18	121.27	109.81
3	C	121	VAL	N-CA-C	-5.18	108.46	113.53
1	A	776	ALA	N-CA-C	5.17	118.09	110.59
2	B	818	PRO	N-CA-C	5.17	118.47	111.22
1	A	123	ARG	N-CA-C	-5.17	105.33	111.69
4	E	40	GLU	CA-C-N	5.17	127.20	120.28
4	E	40	GLU	C-N-CA	5.17	127.20	120.28
2	B	1166	CYS	N-CA-C	5.16	117.64	111.71
1	A	1109	LYS	CA-C-N	5.16	130.96	123.12
1	A	1109	LYS	C-N-CA	5.16	130.96	123.12
2	B	136	THR	CA-C-N	5.16	131.39	121.54
2	B	136	THR	C-N-CA	5.16	131.39	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1085	HIS	CA-C-N	5.15	130.98	121.70
1	A	1085	HIS	C-N-CA	5.15	130.98	121.70
1	A	1146	VAL	N-CA-C	5.15	117.49	111.05
1	A	1292	PRO	N-CA-C	5.15	118.57	110.80
1	A	529	CYS	CA-C-N	5.14	125.66	120.00
1	A	529	CYS	C-N-CA	5.14	125.66	120.00
1	A	792	TYR	CA-C-N	5.14	128.47	120.60
1	A	792	TYR	C-N-CA	5.14	128.47	120.60
3	C	120	ILE	CA-C-N	5.13	127.87	121.71
3	C	120	ILE	C-N-CA	5.13	127.87	121.71
1	A	1148	ILE	N-CA-C	-5.12	106.08	110.74
10	L	55	ILE	N-CA-C	5.12	119.99	109.34
2	B	1061	GLU	N-CA-C	-5.12	105.70	111.28
4	E	5	ASN	N-CA-C	-5.12	105.78	112.23
1	A	250	ILE	N-CA-C	5.11	119.97	109.34
1	A	919	ILE	CB-CA-C	5.11	117.22	110.84
2	B	478	GLY	CA-C-N	5.10	131.16	121.97
2	B	478	GLY	C-N-CA	5.10	131.16	121.97
2	B	165	VAL	N-CA-C	5.10	115.43	107.99
2	B	971	THR	CB-CA-C	5.09	118.72	110.22
1	A	478	TYR	CA-C-N	5.09	129.84	122.36
1	A	478	TYR	C-N-CA	5.09	129.84	122.36
2	B	59	LEU	N-CA-C	5.09	116.51	111.07
1	A	525	GLN	CB-CA-C	-5.09	110.69	116.54
9	K	82	ASP	CA-CB-CG	5.08	117.68	112.60
4	E	162	ARG	CA-C-N	5.08	127.08	120.28
4	E	162	ARG	C-N-CA	5.08	127.08	120.28
1	A	614	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	399	HIS	CA-C-O	-5.05	113.24	120.16
8	J	5	VAL	CA-C-O	-5.05	116.39	121.59
2	B	787	VAL	N-CA-CB	-5.05	105.60	112.16
2	B	1055	ILE	CA-C-N	5.05	127.29	120.38
2	B	1055	ILE	C-N-CA	5.05	127.29	120.38
2	B	1025	HIS	CA-C-N	5.04	126.99	120.44
2	B	1025	HIS	C-N-CA	5.04	126.99	120.44
2	B	251	ILE	N-CA-C	5.03	114.82	107.37
2	B	663	ALA	N-CA-C	-5.03	105.88	111.36
2	B	364	ILE	CA-C-N	5.03	131.15	121.54
2	B	364	ILE	C-N-CA	5.03	131.15	121.54
1	A	1376	THR	CB-CA-C	5.03	120.42	110.42
3	C	213	PRO	N-CA-C	5.03	122.82	112.47
4	E	21	GLU	CA-C-N	5.02	127.32	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	21	GLU	C-N-CA	5.02	127.32	120.54
1	A	1393	ASN	CA-CB-CG	5.02	117.62	112.60
1	A	1361	SER	N-CA-C	5.02	117.01	110.43
12	T	16	DC	N1-C1'-C2'	5.02	121.03	113.50
1	A	1004	ASN	N-CA-C	5.02	116.58	110.41
1	A	1354	ASN	N-CA-C	5.02	117.48	111.71
1	A	445	ASN	N-CA-C	5.01	116.69	109.07
1	A	56	PRO	CA-C-N	5.01	131.10	121.54
1	A	56	PRO	C-N-CA	5.01	131.10	121.54
4	E	100	ILE	N-CA-C	5.01	115.73	110.62
1	A	116	ASP	CA-C-N	5.00	130.71	121.70
1	A	116	ASP	C-N-CA	5.00	130.71	121.70

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	A	11043	0	11133	293	0
2	B	8861	0	8884	228	0
3	C	2095	0	2051	58	0
4	E	1752	0	1776	39	0
5	F	688	0	707	10	0
6	H	1068	0	1040	21	0
7	I	971	0	927	13	0
8	J	532	0	542	22	0
9	K	919	0	929	28	0
10	L	363	0	386	14	0
11	R	109	0	55	2	0
12	T	261	0	148	0	0
13	A	2	0	0	0	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	31	0	12	5	0
All	All	28703	0	28590	651	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 11.

All (651) 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)
15:A:1736:ATP:H5'1	15:A:1736:ATP:H8	1.25	1.01
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.45	0.99
1:A:855:THR:HG21	1:A:857:ARG:HE	1.37	0.88
1:A:830:LYS:HG3	1:A:1098:VAL:HG11	1.55	0.87
1:A:525:GLN:HB2	2:B:835:GLN:HE21	1.43	0.84
15:A:1736:ATP:H5'1	15:A:1736:ATP:C8	2.13	0.83
2:B:996:ARG:HH22	3:C:173:ALA:HB1	1.41	0.83
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.58	0.83
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.62	0.81
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.46	0.81
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.60	0.81
1:A:869:GLY:O	4:E:204:THR:HG21	1.83	0.80
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.64	0.79
1:A:741:ASN:HD22	1:A:744:LYS:H	1.32	0.78
1:A:421:ALA:HA	1:A:424:ILE:HD11	1.68	0.75
2:B:797:TYR:O	8:J:1:MET:HG2	1.87	0.75
10:L:32:ALA:HB3	10:L:55:ILE:HG13	1.67	0.75
1:A:1004:ASN:HD21	1:A:1007:ILE:HD12	1.52	0.74
2:B:232:SER:HB3	2:B:261:ARG:HH22	1.52	0.73
2:B:744:HIS:CD2	2:B:746:SER:OG	2.41	0.73
1:A:756:ILE:HD12	1:A:756:ILE:H	1.53	0.73
2:B:604:ARG:HD3	2:B:611:PRO:HA	1.69	0.73
1:A:1123:GLY:CA	1:A:1124:HIS:HB2	2.19	0.72
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.72	0.71
2:B:705:MET:HE3	2:B:742:GLU:HG3	1.71	0.71
2:B:244:LEU:HD12	2:B:250:PHE:HB2	1.73	0.71
2:B:516:ASN:H	2:B:516:ASN:HD22	1.39	0.70
2:B:54:PHE:HA	2:B:58:THR:HB	1.72	0.70
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.40	0.70
1:A:106:VAL:HG11	1:A:214:ILE:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.72	0.70
2:B:563:MET:HE3	2:B:580:VAL:HB	1.73	0.70
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.73	0.69
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.73	0.69
3:C:214:ASN:HB3	3:C:217:ASP:HB2	1.73	0.69
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.28	0.68
1:A:469:ARG:NH2	2:B:991:GLY:O	2.27	0.68
2:B:38:PHE:HA	2:B:42:GLY:H	1.59	0.67
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.74	0.67
7:I:28:GLU:HB3	7:I:35:VAL:HG13	1.76	0.67
2:B:38:PHE:H	2:B:41:LYS:HB2	1.60	0.67
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.60	0.67
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.10	0.66
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.76	0.66
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.77	0.66
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.43	0.65
2:B:887:HIS:HA	2:B:888:GLY:O	1.96	0.65
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.78	0.65
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.77	0.65
1:A:709:THR:HB	1:A:712:GLU:H	1.61	0.65
2:B:63:ILE:O	2:B:67:SER:HB3	1.97	0.65
1:A:456:MET:HE3	1:A:510:GLN:HB2	1.79	0.65
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.78	0.65
2:B:887:HIS:HA	2:B:888:GLY:C	2.21	0.65
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.77	0.65
2:B:363:HIS:O	2:B:364:ILE:HB	1.96	0.65
1:A:399:HIS:O	1:A:401:GLY:N	2.30	0.64
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.78	0.64
1:A:466:SER:HB3	2:B:1103:ILE:HD13	1.79	0.64
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.79	0.64
2:B:1180:PHE:HB3	2:B:1191:ILE:HG21	1.79	0.64
1:A:57:ARG:HB3	1:A:68:GLN:H	1.63	0.64
2:B:843:GLN:HB2	2:B:993:THR:HB	1.79	0.64
1:A:378:GLU:OE2	1:A:434:ARG:HD3	1.97	0.63
8:J:28:ASP:HB3	8:J:30:LEU:HD12	1.79	0.63
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.80	0.63
1:A:827:THR:OG1	1:A:1083:THR:HG21	1.99	0.63
2:B:762:ASN:HD21	2:B:1022:THR:HA	1.62	0.63
1:A:140:THR:HA	1:A:143:LYS:HE3	1.80	0.63
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.81	0.63
1:A:855:THR:CG2	1:A:857:ARG:HE	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.13	0.63
2:B:211:VAL:HG23	2:B:483:LEU:HA	1.81	0.63
1:A:1080:THR:C	1:A:1082:ASN:H	2.06	0.62
4:E:185:ALA:HA	4:E:190:LEU:HD12	1.79	0.62
1:A:672:ASP:HB2	1:A:675:THR:HB	1.81	0.62
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.82	0.62
2:B:744:HIS:HD2	2:B:746:SER:H	1.47	0.62
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.81	0.62
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.80	0.62
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.80	0.62
1:A:853:ASP:OD2	1:A:855:THR:HG22	2.00	0.62
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.82	0.62
1:A:1154:TYR:CE2	1:A:1156:PRO:HG3	2.34	0.62
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.64	0.62
1:A:1083:THR:N	1:A:1084:PHE:O	2.33	0.61
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.65	0.61
1:A:349:ALA:HB3	1:A:489:LEU:HB3	1.82	0.61
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.41	0.61
1:A:567:LYS:HB3	6:H:96:VAL:H	1.64	0.61
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.83	0.60
1:A:1083:THR:HG23	1:A:1084:PHE:HB3	1.82	0.60
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.36	0.60
2:B:976:ILE:O	2:B:990:ILE:HB	2.00	0.60
1:A:1364:ASN:C	1:A:1364:ASN:HD22	2.10	0.60
1:A:278:THR:O	1:A:282:ASN:HB3	2.00	0.60
1:A:885:THR:O	1:A:940:ARG:HD3	2.01	0.60
2:B:313:MET:HE2	2:B:390:LEU:HG	1.83	0.60
2:B:773:MET:HE3	2:B:981:ALA:HB1	1.83	0.60
2:B:873:THR:O	2:B:914:LYS:HA	2.01	0.60
2:B:976:ILE:HG23	2:B:977:GLY:H	1.67	0.60
5:F:90:ARG:HD2	5:F:155:LEU:HD13	1.84	0.60
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.84	0.60
2:B:486:TYR:CZ	2:B:1096:ARG:HG2	2.36	0.59
1:A:304:MET:HG2	1:A:325:ILE:HD12	1.83	0.59
1:A:388:LEU:O	1:A:392:VAL:HG23	2.02	0.59
1:A:711:ARG:HA	7:I:97:MET:HE1	1.84	0.59
9:K:21:ILE:HG23	9:K:33:ILE:HG12	1.84	0.59
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.84	0.59
2:B:654:ARG:H	2:B:657:HIS:HD2	1.48	0.59
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.67	0.59
2:B:901:PRO:HD3	10:L:58:LYS:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLY:HA2	1:A:337:ARG:HG3	1.84	0.59
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.50	0.59
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.85	0.59
4:E:88:VAL:HB	4:E:116:ILE:HG12	1.84	0.59
3:C:115:SER:HB3	3:C:142:VAL:H	1.67	0.59
3:C:36:VAL:HG23	9:K:41:THR:HG21	1.85	0.59
2:B:975:GLN:O	2:B:990:ILE:HD12	2.03	0.58
3:C:82:TYR:HB3	3:C:84:ARG:HG2	1.85	0.58
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.85	0.58
1:A:466:SER:HB3	2:B:1103:ILE:CD1	2.33	0.58
1:A:709:THR:HG23	7:I:94:ASP:HA	1.84	0.58
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.84	0.58
1:A:587:HIS:HD2	1:A:966:ASN:HA	1.69	0.58
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.85	0.58
1:A:119:ASN:HB2	1:A:122:MET:HB2	1.83	0.58
1:A:830:LYS:HD3	1:A:1080:THR:HB	1.85	0.58
1:A:1325:THR:HA	4:E:147:HIS:HA	1.86	0.58
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.86	0.58
1:A:913:LEU:HD11	1:A:981:LEU:O	2.04	0.58
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.85	0.58
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.34	0.58
1:A:628:GLY:O	1:A:632:VAL:HG23	2.04	0.57
3:C:147:LEU:HD23	3:C:151:GLN:HB2	1.85	0.57
2:B:345:LYS:HA	2:B:347:LYS:H	1.69	0.57
1:A:152:VAL:HG23	1:A:162:VAL:HG23	1.85	0.57
2:B:563:MET:HE1	2:B:587:HIS:HB2	1.85	0.57
2:B:885:MET:HA	2:B:936:ASP:HB2	1.87	0.57
4:E:46:TYR:HD2	4:E:57:MET:HB3	1.69	0.57
2:B:516:ASN:H	2:B:516:ASN:ND2	2.02	0.57
1:A:179:LEU:HB3	1:A:297:GLN:HG2	1.87	0.57
1:A:347:PHE:H	2:B:1107:ALA:HA	1.69	0.57
10:L:53:HIS:HB3	10:L:55:ILE:CD1	2.35	0.57
1:A:1354:ASN:O	1:A:1358:SER:HB2	2.05	0.57
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.86	0.57
1:A:567:LYS:HE3	6:H:46:LEU:HB2	1.87	0.56
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.87	0.56
3:C:167:HIS:HD2	3:C:169:LYS:H	1.51	0.56
1:A:885:THR:HG23	1:A:1024:SER:HB2	1.86	0.56
15:A:1736:ATP:H5'2	11:R:10:G:H2'	1.87	0.56
2:B:950:ASP:HB3	2:B:967:ARG:HG3	1.87	0.56
1:A:1081:LEU:HD11	15:A:1736:ATP:C5	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.87	0.56
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.88	0.56
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.41	0.56
2:B:862:GLN:HB3	2:B:963:PHE:HB2	1.88	0.56
1:A:323:LYS:HE2	1:A:328:ARG:HE	1.70	0.56
3:C:251:LEU:O	3:C:255:VAL:HG23	2.06	0.56
2:B:955:THR:HG22	2:B:956:THR:H	1.71	0.56
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.88	0.56
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.31	0.56
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.38	0.56
4:E:19:VAL:O	4:E:23:VAL:HG23	2.04	0.56
10:L:55:ILE:HD13	10:L:55:ILE:H	1.69	0.56
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.87	0.55
2:B:542:MET:HE2	2:B:636:PRO:HG2	1.87	0.55
2:B:915:THR:HA	2:B:936:ASP:O	2.06	0.55
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.86	0.55
2:B:879:ARG:NH1	2:B:879:ARG:HA	2.21	0.55
2:B:654:ARG:H	2:B:657:HIS:CD2	2.24	0.55
1:A:256:GLN:HG2	1:A:257:ARG:HD2	1.89	0.55
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.21	0.55
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.88	0.55
5:F:72:LYS:HB3	5:F:142:SER:HA	1.89	0.55
2:B:1074:ASN:HB3	2:B:1077:THR:HG22	1.89	0.55
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.39	0.55
1:A:831:THR:HG21	1:A:1081:LEU:HD13	1.87	0.55
4:E:10:SER:O	4:E:14:ARG:HG3	2.06	0.55
3:C:148:ARG:H	3:C:151:GLN:HG3	1.72	0.55
1:A:423:ASP:CG	1:A:424:ILE:H	2.14	0.54
3:C:98:VAL:H	3:C:122:SER:HB2	1.71	0.54
1:A:1092:LYS:HB2	1:A:1096:SER:HB3	1.89	0.54
3:C:105:GLY:O	3:C:149:LYS:O	2.26	0.54
1:A:55:ASP:O	1:A:57:ARG:N	2.32	0.54
1:A:1030:ARG:O	1:A:1034:GLU:HB2	2.07	0.54
1:A:821:ARG:HD2	1:A:825:ILE:HD11	1.89	0.54
3:C:29:MET:HE1	9:K:97:LYS:HD3	1.90	0.54
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.88	0.54
2:B:706:GLN:H	2:B:710:LEU:HG	1.72	0.54
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.88	0.54
2:B:787:VAL:HG12	2:B:787:VAL:O	2.08	0.54
1:A:756:ILE:H	1:A:756:ILE:CD1	2.21	0.53
2:B:904:ARG:HG2	2:B:948:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1097:HIS:HB2	2:B:1102:LYS:HE3	1.90	0.53
6:H:114:VAL:HG22	6:H:125:LEU:HB3	1.89	0.53
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.90	0.53
2:B:755:ILE:HD13	2:B:809:MET:HG2	1.90	0.53
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.38	0.53
1:A:332:LYS:O	1:A:333:GLU:HG2	2.08	0.53
1:A:743:VAL:HG13	2:B:1018:PRO:HB3	1.91	0.53
2:B:237:VAL:HG22	2:B:257:LYS:HB3	1.90	0.53
1:A:86:LEU:HD12	1:A:296:LEU:HD21	1.90	0.53
1:A:297:GLN:C	1:A:299:HIS:H	2.17	0.53
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.91	0.53
5:F:76:LYS:HA	5:F:79:ARG:HH11	1.74	0.53
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.90	0.53
1:A:587:HIS:CD2	1:A:966:ASN:HA	2.43	0.52
2:B:216:GLU:HB3	2:B:500:THR:HG23	1.91	0.52
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.91	0.52
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.91	0.52
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.91	0.52
1:A:31:SER:HB2	1:A:83:HIS:HD2	1.73	0.52
1:A:518:LYS:HD2	1:A:624:SER:O	2.08	0.52
4:E:94:LYS:HA	4:E:97:VAL:HG22	1.92	0.52
1:A:351:THR:O	1:A:486:GLU:O	2.28	0.52
1:A:549:MET:HB3	1:A:577:ILE:HD13	1.91	0.52
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.90	0.52
5:F:116:ASP:HB3	5:F:119:ARG:HB2	1.92	0.52
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.92	0.52
3:C:120:ILE:HG21	3:C:124:LEU:HD21	1.91	0.52
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.90	0.52
1:A:886:ILE:HG13	1:A:943:LEU:HB3	1.90	0.52
1:A:1035:TYR:HB3	1:A:1037:LEU:HD23	1.92	0.52
2:B:597:MET:HG3	2:B:601:ARG:HH12	1.75	0.52
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.45	0.52
2:B:1110:PRO:HB2	2:B:1119:VAL:CG2	2.40	0.52
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.58	0.52
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.44	0.52
1:A:1075:PRO:O	1:A:1079:MET:HG2	2.10	0.52
2:B:70:ILE:H	2:B:429:PHE:HE1	1.57	0.51
2:B:1115:THR:HG23	2:B:1117:GLN:HB2	1.92	0.51
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.25	0.51
3:C:175:ALA:HB3	8:J:43:ARG:HE	1.75	0.51
1:A:1016:THR:HB	4:E:205:SER:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.92	0.51
1:A:341:MET:HB3	2:B:1132:GLU:HG2	1.93	0.51
2:B:563:MET:HA	2:B:589:VAL:O	2.10	0.51
6:H:104:PHE:CE1	6:H:136:LYS:HA	2.45	0.51
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.93	0.51
2:B:766:ARG:HG2	2:B:1022:THR:HG22	1.91	0.51
2:B:804:GLY:O	2:B:983:ARG:NH2	2.43	0.51
1:A:225:ASN:HB3	1:A:229:SER:H	1.75	0.51
2:B:792:MET:HE2	2:B:857:ARG:HG3	1.91	0.51
2:B:1215:ARG:HB2	2:B:1217:TYR:CE1	2.46	0.51
6:H:137:GLN:C	6:H:139:ASN:H	2.19	0.51
2:B:857:ARG:NH2	2:B:942:ARG:HE	2.09	0.51
2:B:955:THR:HG23	10:L:54:ARG:O	2.10	0.51
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.76	0.51
1:A:820:GLY:HA3	2:B:764:SER:OG	2.11	0.51
1:A:1035:TYR:CB	1:A:1037:LEU:HD23	2.41	0.51
1:A:179:LEU:HB2	1:A:180:LYS:HE2	1.92	0.51
1:A:361:LEU:HD12	1:A:471:ASN:HD22	1.75	0.51
1:A:406:ILE:HD11	1:A:433:GLU:HG3	1.92	0.51
2:B:791:THR:HG22	2:B:792:MET:HE3	1.92	0.51
6:H:58:THR:HB	6:H:143:LEU:HB2	1.93	0.51
1:A:528:LEU:HD23	1:A:751:SER:HA	1.93	0.50
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.46	0.50
1:A:1327:ILE:O	4:E:147:HIS:HE1	1.94	0.50
5:F:128:LYS:HD3	5:F:149:GLU:HA	1.93	0.50
1:A:402:ALA:CB	1:A:434:ARG:HA	2.42	0.50
3:C:39:ALA:HB1	3:C:165:LYS:HB2	1.92	0.50
1:A:1284:MET:HG3	1:A:1306:LEU:CD2	2.41	0.50
4:E:66:GLU:HA	4:E:69:ILE:HD12	1.93	0.50
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.46	0.50
1:A:830:LYS:HE3	1:A:1098:VAL:HB	1.94	0.50
3:C:98:VAL:H	3:C:122:SER:CB	2.25	0.50
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.94	0.50
1:A:663:SER:HB2	2:B:1085:ILE:HG13	1.94	0.50
1:A:472:LEU:O	1:A:475:THR:HB	2.12	0.49
1:A:575:LYS:HD2	6:H:120:GLY:HA3	1.93	0.49
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.94	0.49
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.93	0.49
8:J:36:LEU:HD11	8:J:51:LEU:HD13	1.94	0.49
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.77	0.49
1:A:629:LEU:O	1:A:633:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:GLU:HG3	4:E:198:ILE:HG21	1.93	0.49
2:B:1112:GLN:HB3	2:B:1115:THR:HG22	1.94	0.49
3:C:242:GLN:HG3	3:C:246:ARG:HH21	1.77	0.49
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.94	0.49
2:B:357:GLN:HG3	2:B:368:GLU:HA	1.95	0.49
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.27	0.49
1:A:981:LEU:HD12	1:A:981:LEU:H	1.77	0.49
2:B:1098:MET:HE3	2:B:1101:ASP:OD2	2.12	0.49
3:C:148:ARG:N	3:C:151:GLN:HG3	2.27	0.49
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.94	0.49
1:A:95:PHE:HB3	1:A:234:MET:HE3	1.95	0.49
1:A:252:PHE:HD1	1:A:253:ASN:H	1.60	0.49
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.42	0.49
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.95	0.49
3:C:184:ASN:ND2	3:C:189:THR:O	2.45	0.49
9:K:63:VAL:HG23	9:K:63:VAL:O	2.13	0.49
1:A:55:ASP:C	1:A:57:ARG:H	2.19	0.49
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.94	0.49
1:A:666:ILE:HG21	2:B:1030:LEU:HD22	1.95	0.49
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.78	0.49
6:H:33:GLN:HB2	6:H:36:CYS:HB3	1.95	0.49
1:A:781:ASP:HB2	1:A:789:LYS:HD3	1.95	0.49
3:C:18:VAL:CG2	9:K:109:TRP:HZ3	2.26	0.49
1:A:795:GLU:CD	1:A:795:GLU:H	2.21	0.48
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.95	0.48
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.46	0.48
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.95	0.48
1:A:810:PRO:HB2	2:B:519:TRP:HH2	1.78	0.48
2:B:840:ILE:O	2:B:1010:LEU:HA	2.14	0.48
2:B:847:ASP:O	3:C:65:HIS:HE1	1.96	0.48
3:C:66:ARG:NH2	8:J:3:VAL:O	2.43	0.48
9:K:5:ASP:HB2	9:K:8:GLU:OE2	2.12	0.48
11:R:6:A:H2'	11:R:7:G:H8	1.78	0.48
1:A:684:ALA:O	1:A:688:LYS:HG2	2.13	0.48
1:A:942:PHE:O	1:A:946:VAL:HG12	2.13	0.48
1:A:567:LYS:CE	6:H:46:LEU:HB2	2.43	0.48
1:A:586:ILE:N	1:A:609:ASP:O	2.47	0.48
2:B:515:HIS:H	2:B:518:HIS:CD2	2.31	0.48
4:E:116:ILE:HB	4:E:121:MET:HE2	1.94	0.48
2:B:707:PRO:HG2	2:B:708:GLU:HG3	1.95	0.48
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:879:ARG:HA	2:B:879:ARG:CZ	2.43	0.48
2:B:884:ARG:O	2:B:936:ASP:HB2	2.13	0.48
3:C:29:MET:HE2	9:K:94:ILE:HG23	1.95	0.48
1:A:456:MET:HE2	1:A:507:VAL:HA	1.95	0.48
1:A:825:ILE:CD1	2:B:512:ARG:HB3	2.44	0.48
10:L:61:THR:HB	10:L:63:ARG:H	1.78	0.48
1:A:474:VAL:HG23	1:A:521:MET:HE3	1.96	0.48
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	1.95	0.48
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.28	0.48
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.48	0.48
1:A:276:LEU:HD11	1:A:292:ALA:HB1	1.96	0.48
2:B:35:SER:O	2:B:39:ARG:HB2	2.13	0.48
2:B:487:THR:HG23	2:B:490:SER:H	1.78	0.48
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.96	0.48
2:B:1110:PRO:HG2	2:B:1124:ARG:O	2.14	0.48
4:E:118:PRO:HA	4:E:121:MET:HB2	1.96	0.47
1:A:715:GLU:O	1:A:719:VAL:HG23	2.14	0.47
3:C:213:PRO:O	3:C:214:ASN:HB2	2.14	0.47
1:A:672:ASP:CG	1:A:736:ASN:HD21	2.23	0.47
1:A:709:THR:CG2	7:I:94:ASP:HA	2.43	0.47
2:B:68:THR:HA	2:B:90:ILE:O	2.14	0.47
7:I:97:MET:HE2	7:I:97:MET:HB2	1.79	0.47
8:J:1:MET:HB2	8:J:56:LEU:HD12	1.96	0.47
1:A:1088:GLY:HA2	1:A:1089:VAL:HA	1.71	0.47
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.31	0.47
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.54	0.47
2:B:358:LYS:HA	2:B:366:GLN:HG2	1.97	0.47
2:B:773:MET:HE3	2:B:981:ALA:CB	2.44	0.47
2:B:841:MET:HB3	2:B:846:ILE:HD11	1.96	0.47
3:C:191:TYR:HD2	3:C:201:TRP:CE2	2.32	0.47
9:K:79:GLU:CD	9:K:79:GLU:H	2.23	0.47
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.96	0.47
1:A:516:SER:C	1:A:518:LYS:H	2.23	0.47
2:B:881:ASN:HB3	2:B:933:SER:OG	2.15	0.47
6:H:130:ARG:HB3	6:H:134:ASN:HD21	1.80	0.47
8:J:36:LEU:HD13	8:J:47:ARG:HD2	1.95	0.47
9:K:65:HIS:CD2	9:K:67:PHE:H	2.32	0.47
1:A:642:CYS:O	1:A:645:LEU:HB3	2.15	0.47
4:E:24:LYS:HB3	4:E:30:ILE:HB	1.97	0.47
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.50	0.47
1:A:494:SER:O	1:A:498:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.44	0.47
2:B:545:ILE:HG13	2:B:633:VAL:HG13	1.96	0.47
7:I:73:ARG:HH12	7:I:112:SER:HA	1.80	0.47
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.80	0.47
10:L:68:GLU:C	10:L:70:ARG:H	2.23	0.47
1:A:262:LEU:HD11	1:A:325:ILE:HG12	1.97	0.46
1:A:456:MET:HE3	1:A:510:GLN:CB	2.44	0.46
1:A:472:LEU:HD21	2:B:835:GLN:HB3	1.97	0.46
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.56	0.46
1:A:1368:MET:O	1:A:1372:VAL:HG23	2.15	0.46
2:B:601:ARG:HA	2:B:615:MET:HE1	1.96	0.46
1:A:116:ASP:HB3	1:A:164:ARG:HH12	1.80	0.46
1:A:830:LYS:HG3	1:A:1098:VAL:CG1	2.37	0.46
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.50	0.46
2:B:1082:MET:HA	3:C:189:THR:HA	1.98	0.46
2:B:1110:PRO:HB2	2:B:1119:VAL:HG21	1.98	0.46
4:E:101:GLN:HG3	4:E:102:GLU:HG3	1.96	0.46
9:K:50:LEU:O	9:K:56:VAL:HG11	2.15	0.46
1:A:109:HIS:H	1:A:210:ILE:HD12	1.80	0.46
1:A:352:VAL:HB	2:B:1099:VAL:HG13	1.96	0.46
2:B:979:LYS:HD3	2:B:1095:LEU:HD12	1.97	0.46
3:C:66:ARG:HH21	8:J:4:PRO:HA	1.81	0.46
1:A:780:VAL:HG12	1:A:789:LYS:HE2	1.97	0.46
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	1.98	0.46
2:B:408:LEU:H	2:B:411:PRO:HG2	1.79	0.46
1:A:181:LEU:O	1:A:202:LEU:HB3	2.16	0.46
1:A:353:ILE:HG22	1:A:468:PHE:CB	2.45	0.46
1:A:757:ASN:HB3	1:A:761:MET:HE2	1.97	0.46
2:B:680:THR:O	2:B:683:SER:HB2	2.16	0.46
1:A:535:THR:HG22	1:A:575:LYS:HG2	1.98	0.46
1:A:695:LYS:HD2	1:A:695:LYS:HA	1.88	0.46
1:A:1205:LYS:O	1:A:1207:LEU:N	2.45	0.46
2:B:212:LEU:HD13	2:B:409:ALA:HA	1.98	0.46
2:B:955:THR:HG22	2:B:956:THR:N	2.31	0.46
2:B:1120:GLU:H	2:B:1124:ARG:HH21	1.64	0.46
4:E:94:LYS:O	4:E:98:ILE:HB	2.16	0.46
8:J:43:ARG:HG2	8:J:43:ARG:HH11	1.81	0.46
1:A:43:GLU:HG3	1:A:50:ILE:HG12	1.97	0.46
1:A:983:ILE:HD12	1:A:1028:THR:HG21	1.97	0.46
2:B:1058:LEU:O	2:B:1061:GLU:HB2	2.15	0.46
1:A:41:MET:HA	1:A:49:LYS:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.29	0.45
1:A:1080:THR:O	1:A:1082:ASN:N	2.46	0.45
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.98	0.45
3:C:65:HIS:O	3:C:69:LEU:HD12	2.16	0.45
4:E:98:ILE:HA	4:E:101:GLN:HG2	1.97	0.45
9:K:12:LEU:HD21	9:K:18:LYS:HG2	1.98	0.45
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.99	0.45
1:A:694:THR:HA	1:A:714:PHE:HE1	1.80	0.45
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.52	0.45
3:C:173:ALA:O	3:C:233:GLU:O	2.34	0.45
8:J:58:GLU:HA	8:J:61:LEU:HD12	1.97	0.45
1:A:1093:LYS:HG3	1:A:1359:ASP:HB2	1.98	0.45
6:H:118:PHE:HE1	6:H:123:MET:HB2	1.80	0.45
1:A:131:SER:HB3	1:A:223:GLY:CA	2.45	0.45
2:B:835:GLN:O	2:B:838:SER:HB2	2.17	0.45
3:C:151:GLN:H	3:C:151:GLN:HG2	1.25	0.45
8:J:4:PRO:O	8:J:14:VAL:HG23	2.15	0.45
1:A:947:PHE:HE2	1:A:1017:LEU:HD11	1.82	0.45
1:A:1081:LEU:HG	15:A:1736:ATP:H2'	1.99	0.45
2:B:114:PRO:HB3	2:B:174:LEU:HD21	1.99	0.45
2:B:841:MET:HG2	2:B:1010:LEU:HD12	1.99	0.45
2:B:1099:VAL:O	2:B:1103:ILE:HG12	2.17	0.45
7:I:18:GLU:HG2	7:I:20:LYS:H	1.82	0.45
1:A:279:LEU:HD22	1:A:289:ILE:HA	1.98	0.45
3:C:6:PRO:HB2	9:K:101:LEU:HD13	1.99	0.45
10:L:34:CYS:SG	10:L:34:CYS:O	2.75	0.45
1:A:1317:MET:HG3	4:E:142:VAL:HG21	1.99	0.45
2:B:744:HIS:HD2	2:B:746:SER:OG	1.96	0.45
2:B:900:ALA:HA	10:L:58:LYS:HD3	1.98	0.45
3:C:255:VAL:O	3:C:258:ILE:HG22	2.16	0.45
7:I:88:SER:C	7:I:90:GLN:H	2.25	0.45
1:A:41:MET:HE2	1:A:257:ARG:HG3	1.99	0.45
1:A:744:LYS:O	1:A:748:MET:HG3	2.17	0.45
1:A:946:VAL:HB	4:E:201:LYS:HD2	1.98	0.45
8:J:6:ARG:HG3	8:J:13:VAL:HG13	1.99	0.45
1:A:593:GLU:C	1:A:595:THR:H	2.25	0.45
2:B:44:VAL:HA	2:B:46:GLN:HE21	1.82	0.45
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.99	0.45
4:E:61:GLN:HG3	4:E:105:PHE:CE2	2.51	0.45
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.17	0.44
1:A:1353:TYR:C	1:A:1353:TYR:CD2	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:65:HIS:HD2	9:K:67:PHE:H	1.65	0.44
1:A:129:LYS:HA	1:A:134:ARG:HH21	1.82	0.44
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.99	0.44
1:A:1318:THR:HG22	4:E:142:VAL:HG22	1.99	0.44
2:B:125:SER:HB3	2:B:171:PRO:HA	1.98	0.44
2:B:751:VAL:HG22	2:B:812:LEU:HD22	1.98	0.44
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.99	0.44
3:C:259:LEU:HD13	9:K:91:CYS:HB2	1.99	0.44
4:E:147:HIS:HD2	4:E:149:LEU:HB2	1.82	0.44
8:J:24:LEU:HA	8:J:28:ASP:HB2	2.00	0.44
3:C:165:LYS:O	9:K:6:ARG:NH1	2.51	0.44
8:J:53:HIS:CE1	8:J:55:ASP:HB2	2.53	0.44
10:L:61:THR:HB	10:L:63:ARG:HB2	2.00	0.44
1:A:115:LEU:HD21	1:A:145:LYS:HG3	1.99	0.44
2:B:765:PRO:O	2:B:768:THR:N	2.50	0.44
2:B:880:THR:C	2:B:882:THR:H	2.26	0.44
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.52	0.44
1:A:1336:MET:HG3	1:A:1381:LEU:HD13	1.99	0.44
2:B:446:LEU:O	2:B:448:ILE:HD12	2.18	0.44
2:B:745:PRO:O	2:B:748:ILE:HG12	2.18	0.44
2:B:773:MET:SD	2:B:987:LYS:HG3	2.58	0.44
2:B:893:LEU:HD22	2:B:897:GLY:C	2.43	0.44
1:A:357:PRO:HD2	2:B:833:TYR:CE2	2.53	0.44
1:A:567:LYS:O	1:A:569:LYS:N	2.41	0.44
2:B:213:ILE:O	2:B:215:GLN:HG2	2.18	0.44
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.99	0.44
2:B:195:CYS:HA	2:B:196:PRO:HD3	1.92	0.44
1:A:98:LYS:O	1:A:102:VAL:HG23	2.18	0.43
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.99	0.43
1:A:1006:ILE:HD11	4:E:163:GLU:HG3	1.99	0.43
2:B:597:MET:HG3	2:B:601:ARG:NH1	2.32	0.43
2:B:637:LEU:HD12	2:B:693:ILE:HG13	2.00	0.43
2:B:757:PRO:CB	2:B:1044:ALA:HB1	2.48	0.43
4:E:202:SER:C	4:E:204:THR:H	2.26	0.43
1:A:456:MET:HB2	1:A:478:TYR:OH	2.18	0.43
1:A:877:HIS:HB3	1:A:1056:SER:HA	2.00	0.43
1:A:1430:LEU:O	2:B:1196:ILE:HG22	2.18	0.43
2:B:211:VAL:CG2	2:B:483:LEU:HA	2.47	0.43
2:B:836:GLU:O	2:B:837:ASP:HB2	2.18	0.43
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	2.00	0.43
1:A:434:ARG:NH2	1:A:440:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ASN:HD21	1:A:650:GLN:HE22	1.65	0.43
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.52	0.43
2:B:48:LEU:HD23	2:B:173:MET:SD	2.58	0.43
6:H:79:TRP:CH2	6:H:82:PRO:HD3	2.54	0.43
6:H:96:VAL:HG13	6:H:143:LEU:HG	1.99	0.43
1:A:528:LEU:O	1:A:531:ILE:HG22	2.18	0.43
1:A:575:LYS:HB3	1:A:612:ILE:CG1	2.49	0.43
1:A:782:ARG:NH1	1:A:785:PRO:HA	2.33	0.43
1:A:1264:GLU:HA	1:A:1267:MET:HE2	2.00	0.43
1:A:1376:THR:HG22	1:A:1377:THR:N	2.34	0.43
2:B:365:THR:HG21	2:B:370:PHE:HD1	1.83	0.43
9:K:30:ALA:HA	9:K:75:ILE:O	2.19	0.43
1:A:1316:VAL:O	1:A:1319:VAL:HB	2.18	0.43
4:E:20:LYS:HE3	4:E:35:VAL:HA	2.00	0.43
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.54	0.43
1:A:208:LEU:HG	1:A:235:ILE:HD11	2.01	0.43
1:A:587:HIS:CE1	1:A:969:GLN:HE21	2.37	0.43
1:A:852:TYR:O	5:F:81:THR:HG22	2.18	0.43
1:A:933:TYR:O	1:A:937:VAL:HG13	2.19	0.43
2:B:640:VAL:HG22	2:B:651:LEU:HG	2.01	0.43
4:E:176:PRO:O	4:E:212:ARG:HA	2.19	0.43
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.53	0.43
1:A:830:LYS:HD2	1:A:1094:VAL:HG23	2.01	0.43
1:A:35:ILE:HG13	1:A:241:VAL:HG21	2.01	0.43
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	2.01	0.43
1:A:1154:TYR:HB2	1:A:1191:TRP:CZ3	2.54	0.43
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.47	0.43
1:A:710:LEU:H	1:A:710:LEU:HD22	1.83	0.43
1:A:754:SER:H	1:A:757:ASN:HD22	1.67	0.43
1:A:851:HIS:HB2	1:A:855:THR:HG22	2.01	0.43
1:A:1141:THR:HG21	1:A:1205:LYS:HD3	2.01	0.43
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.52	0.43
6:H:40:LEU:HD21	6:H:142:LEU:HD21	2.00	0.43
2:B:753:ALA:HA	2:B:756:ILE:HD12	2.01	0.42
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.54	0.42
7:I:19:ASP:HB3	7:I:24:ARG:H	1.84	0.42
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.01	0.42
1:A:588:LEU:HD12	1:A:632:VAL:HG21	2.01	0.42
1:A:738:LYS:HD2	1:A:740:LEU:HD21	2.01	0.42
1:A:1390:ASN:O	1:A:1399:ARG:HD2	2.19	0.42
1:A:1428:VAL:HG21	2:B:1135:ARG:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:956:THR:HB	10:L:46:VAL:HG21	2.01	0.42
4:E:65:THR:O	4:E:69:ILE:HG13	2.20	0.42
8:J:1:MET:N	8:J:56:LEU:N	2.67	0.42
2:B:123:THR:HG23	2:B:205:ILE:HA	2.01	0.42
2:B:487:THR:HG22	2:B:490:SER:HB3	2.01	0.42
2:B:764:SER:HB3	2:B:765:PRO:HD3	2.01	0.42
3:C:148:ARG:HD3	8:J:61:LEU:O	2.18	0.42
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.55	0.42
4:E:97:VAL:HG23	4:E:98:ILE:HD12	2.01	0.42
1:A:64:ASN:C	1:A:66:LYS:H	2.26	0.42
1:A:353:ILE:HG21	1:A:487:MET:HB2	2.02	0.42
1:A:361:LEU:HD11	1:A:521:MET:HE2	2.01	0.42
1:A:404:TYR:HA	1:A:413:ILE:O	2.19	0.42
1:A:774:ARG:HH21	1:A:794:PRO:HA	1.83	0.42
1:A:1436:ILE:O	1:A:1437:GLY:C	2.62	0.42
2:B:54:PHE:HA	2:B:58:THR:CB	2.45	0.42
2:B:91:SER:HB3	2:B:133:LYS:HB2	2.01	0.42
2:B:857:ARG:HH21	2:B:942:ARG:HE	1.66	0.42
1:A:694:THR:HA	1:A:714:PHE:CE1	2.55	0.42
1:A:819:GLY:O	1:A:822:GLU:HB2	2.20	0.42
1:A:131:SER:CB	1:A:223:GLY:HA2	2.49	0.42
1:A:182:VAL:HG22	1:A:202:LEU:H	1.84	0.42
8:J:44:TYR:HA	8:J:47:ARG:HB2	2.00	0.42
1:A:55:ASP:H	1:A:56:PRO:HD3	1.85	0.42
1:A:121:LEU:HB3	1:A:141:LEU:HD22	2.00	0.42
1:A:506:ALA:HB3	1:A:509:LEU:HD12	2.01	0.42
1:A:670:ILE:HD12	2:B:1052:VAL:HG11	2.01	0.42
1:A:860:LEU:HD21	1:A:1394:THR:HA	2.02	0.42
1:A:877:HIS:CB	1:A:1056:SER:HA	2.50	0.42
1:A:1128:GLN:HG2	1:A:1304:TRP:NE1	2.35	0.42
1:A:1129:GLU:HA	1:A:1132:LYS:HE3	2.00	0.42
2:B:428:ILE:HG12	2:B:448:ILE:HG13	2.01	0.42
2:B:841:MET:HE2	2:B:1010:LEU:CD1	2.49	0.42
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	2.02	0.42
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.02	0.42
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.74	0.42
1:A:1366:ARG:HA	1:A:1369:ALA:HB3	2.02	0.42
2:B:1017:ILE:H	2:B:1018:PRO:CD	2.31	0.42
3:C:77:ILE:CD1	3:C:161:LYS:HG3	2.50	0.42
3:C:241:ASP:O	3:C:245:VAL:HG23	2.20	0.42
4:E:147:HIS:CD2	4:E:149:LEU:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:91:CYS:O	9:K:95:ILE:HG12	2.20	0.42
1:A:341:MET:HE1	1:A:1425:SER:HA	2.02	0.42
1:A:453:MET:HB3	1:A:477:PRO:HB2	2.02	0.42
1:A:871:ASP:CG	4:E:204:THR:HG23	2.45	0.42
7:I:32:CYS:SG	7:I:34:TYR:HB2	2.60	0.42
1:A:568:PRO:O	1:A:569:LYS:HB2	2.19	0.42
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.55	0.42
1:A:793:SER:HB2	1:A:795:GLU:OE2	2.19	0.41
2:B:293:PRO:HB2	2:B:296:GLU:HB2	2.02	0.41
3:C:20:PHE:HE1	3:C:22:LEU:HD13	1.84	0.41
1:A:342:GLY:HA3	2:B:1129:ARG:NH2	2.35	0.41
2:B:260:GLY:O	2:B:267:ARG:HD3	2.20	0.41
2:B:791:THR:HG22	2:B:792:MET:CE	2.50	0.41
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.56	0.41
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.54	0.41
4:E:124:VAL:HA	4:E:132:ILE:HD11	2.01	0.41
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.55	0.41
1:A:645:LEU:HD11	1:A:649:ILE:HD11	2.01	0.41
4:E:47:CYS:HB3	4:E:51:GLY:HA2	2.03	0.41
6:H:87:ARG:HH11	6:H:87:ARG:HA	1.84	0.41
1:A:302:THR:HA	1:A:305:ASP:O	2.21	0.41
2:B:29:ASP:HB3	2:B:658:ILE:HG13	2.03	0.41
2:B:1156:ASP:HB3	2:B:1157:ALA:H	1.65	0.41
3:C:171:GLY:C	3:C:173:ALA:H	2.22	0.41
6:H:42:ILE:HG23	6:H:95:TYR:HE1	1.85	0.41
10:L:55:ILE:HG12	10:L:56:LEU:H	1.85	0.41
1:A:870:GLU:HG2	4:E:208:TYR:CD1	2.56	0.41
2:B:364:ILE:HD13	2:B:585:VAL:HG13	2.02	0.41
2:B:899:ILE:HD11	2:B:911:ILE:HA	2.02	0.41
3:C:58:LEU:HD21	8:J:57:ILE:HD12	2.02	0.41
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.99	0.41
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.85	0.41
1:A:1080:THR:C	1:A:1082:ASN:N	2.76	0.41
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	2.02	0.41
2:B:193:LYS:HB3	2:B:787:VAL:HG11	2.02	0.41
2:B:256:VAL:HG12	2:B:385:LEU:HD22	2.02	0.41
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.50	0.41
1:A:345:VAL:HA	2:B:1155:SER:HB2	2.02	0.41
1:A:407:ARG:HD2	1:A:413:ILE:HD11	2.03	0.41
1:A:845:LEU:O	1:A:846:GLU:C	2.63	0.41
2:B:189:LEU:HB3	2:B:194:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HA	3:C:159:ALA:HA	2.02	0.41
9:K:16:GLU:OE2	9:K:37:LYS:NZ	2.53	0.41
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.73	0.41
2:B:46:GLN:H	2:B:46:GLN:HG3	1.71	0.41
2:B:313:MET:HE3	2:B:386:LEU:HD22	2.03	0.41
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.56	0.41
6:H:56:THR:HB	6:H:145:ARG:HB3	2.02	0.41
1:A:41:MET:HB3	1:A:49:LYS:HE3	2.03	0.41
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	2.01	0.41
1:A:912:LEU:HB3	1:A:1036:ARG:HH22	1.86	0.41
1:A:1086:PHE:HB2	1:A:1087:ALA:H	1.73	0.41
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.01	0.41
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.56	0.41
2:B:647:GLY:HA2	2:B:648:HIS:C	2.46	0.41
2:B:684:LEU:HA	2:B:689:LEU:HD12	2.01	0.41
2:B:843:GLN:HA	2:B:846:ILE:HD12	2.01	0.41
2:B:976:ILE:HG23	2:B:977:GLY:N	2.32	0.41
2:B:982:SER:HB3	2:B:1092:TYR:CZ	2.56	0.41
2:B:1100:ASP:OD1	2:B:1103:ILE:HD11	2.21	0.41
6:H:43:ASN:C	6:H:45:GLU:H	2.28	0.41
1:A:312:PRO:HB2	1:A:313:GLN:H	1.74	0.41
3:C:67:LEU:HA	3:C:70:ILE:HD12	2.02	0.41
3:C:72:LEU:HB3	3:C:132:PRO:HA	2.03	0.41
7:I:65:ASP:OD1	7:I:67:THR:OG1	2.36	0.41
1:A:425:GLN:H	1:A:425:GLN:NE2	2.19	0.40
1:A:963:ILE:HG22	1:A:1045:VAL:HG22	2.02	0.40
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.04	0.40
2:B:745:PRO:HB2	2:B:1047:PHE:CD1	2.56	0.40
2:B:780:VAL:HG11	8:J:56:LEU:HD13	2.03	0.40
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.22	0.40
3:C:62:PHE:O	3:C:66:ARG:HG3	2.21	0.40
9:K:42:LEU:HG	9:K:46:ILE:HD12	2.01	0.40
1:A:669:THR:HB	1:A:805:LEU:HD13	2.02	0.40
2:B:275:TYR:CD1	2:B:275:TYR:N	2.89	0.40
4:E:147:HIS:CD2	4:E:149:LEU:H	2.39	0.40
6:H:127:GLY:HA3	6:H:130:ARG:CZ	2.51	0.40
9:K:5:ASP:HB3	9:K:7:PHE:CE2	2.57	0.40
1:A:535:THR:HB	1:A:616:VAL:HG13	2.02	0.40
9:K:57:LEU:HD12	9:K:76:GLN:HG2	2.02	0.40
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	2.03	0.40
2:B:1149:GLU:HG2	2:B:1153:GLU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:33:ILE:HD13	9:K:87:LEU:HD22	2.04	0.40
1:A:31:SER:HB2	1:A:83:HIS:CD2	2.53	0.40
1:A:379:VAL:HG21	5:F:103:MET:HE3	2.04	0.40
2:B:53:GLN:HG2	2:B:547:VAL:HB	2.04	0.40
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.86	0.40
7:I:65:ASP:HB3	7:I:68:LEU:HD12	2.02	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 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	1395/1733 (80%)	1177 (84%)	149 (11%)	69 (5%)	1	12
2	B	1096/1224 (90%)	927 (85%)	110 (10%)	59 (5%)	1	10
3	C	264/318 (83%)	235 (89%)	19 (7%)	10 (4%)	2	16
4	E	212/215 (99%)	199 (94%)	11 (5%)	2 (1%)	14	43
5	F	83/155 (54%)	73 (88%)	7 (8%)	3 (4%)	2	17
6	H	129/146 (88%)	93 (72%)	24 (19%)	12 (9%)	0	3
7	I	117/122 (96%)	103 (88%)	10 (8%)	4 (3%)	3	18
8	J	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	3	19
9	K	112/120 (93%)	101 (90%)	8 (7%)	3 (3%)	4	22
10	L	44/70 (63%)	28 (64%)	7 (16%)	9 (20%)	0	0
All	All	3515/4173 (84%)	2991 (85%)	351 (10%)	173 (5%)	1	12

All (173) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLN

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Mol	Chain	Res	Type
1	A	215	SER
1	A	250	ILE
1	A	312	PRO
1	A	556	TRP
1	A	569	LYS
1	A	672	ASP
1	A	978	PRO
1	A	1206	ASP
1	A	1377	THR
1	A	1394	THR
2	B	67	SER
2	B	168	GLY
2	B	230	ALA
2	B	265	SER
2	B	451	LYS
2	B	474	SER
2	B	477	ALA
2	B	479	VAL
2	B	712	PRO
2	B	880	THR
2	B	883	LEU
2	B	888	GLY
2	B	936	ASP
2	B	976	ILE
2	B	1156	ASP
2	B	1178	ASN
3	C	4	GLU
3	C	40	GLU
3	C	173	ALA
3	C	213	PRO
3	C	214	ASN
3	C	215	GLU
8	J	2	ILE
8	J	6	ARG
9	K	16	GLU
10	L	53	HIS
10	L	55	ILE
1	A	54	ASN
1	A	65	LEU
1	A	200	ARG
1	A	214	ILE
1	A	255	SER

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Mol	Chain	Res	Type
1	A	331	GLY
1	A	385	ILE
1	A	399	HIS
1	A	411	ASP
1	A	487	MET
1	A	775	ILE
1	A	1005	GLU
1	A	1094	VAL
1	A	1123	GLY
1	A	1124	HIS
1	A	1221	LYS
1	A	1359	ASP
1	A	1378	GLN
1	A	1393	ASN
1	A	1437	GLY
2	B	137	TYR
2	B	277	LYS
2	B	371	GLU
2	B	449	ASN
2	B	629	ASP
2	B	647	GLY
2	B	707	PRO
2	B	751	VAL
2	B	864	LYS
2	B	881	ASN
2	B	884	ARG
2	B	887	HIS
2	B	907	GLY
2	B	943	SER
2	B	996	ARG
2	B	1099	VAL
2	B	1176	ASN
5	F	73	ALA
6	H	61	SER
6	H	90	ALA
6	H	131	ASN
6	H	135	LEU
10	L	35	SER
10	L	39	SER
10	L	50	ASP
10	L	51	CYS
1	A	110	CYS

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Mol	Chain	Res	Type
1	A	258	GLY
1	A	298	PHE
1	A	517	ASN
1	A	707	GLY
1	A	846	GLU
1	A	1064	VAL
1	A	1081	LEU
2	B	467	GLY
2	B	484	ASN
2	B	705	MET
2	B	792	MET
2	B	837	ASP
2	B	886	LYS
2	B	891	ASP
2	B	934	LYS
3	C	165	LYS
4	E	3	GLN
4	E	36	GLU
6	H	44	VAL
7	I	77	LYS
9	K	26	LYS
1	A	57	ARG
1	A	72	GLU
1	A	125	ALA
1	A	149	GLU
1	A	404	TYR
1	A	567	LYS
1	A	591	PHE
1	A	706	HIS
1	A	828	ALA
1	A	1084	PHE
1	A	1175	SER
1	A	1376	THR
2	B	139	ALA
2	B	365	THR
2	B	469	GLN
2	B	483	LEU
2	B	531	GLN
2	B	974	PRO
2	B	1017	ILE
2	B	1046	PRO
2	B	1096	ARG

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Mol	Chain	Res	Type
2	B	1097	HIS
2	B	1157	ALA
3	C	151	GLN
5	F	154	ASP
6	H	77	ARG
6	H	84	ALA
6	H	107	VAL
7	I	3	THR
7	I	20	LYS
10	L	64	LEU
1	A	35	ILE
1	A	55	ASP
1	A	130	ASP
1	A	132	LYS
1	A	283	GLY
1	A	350	ARG
1	A	424	ILE
1	A	958	VAL
1	A	973	ILE
1	A	1255	GLU
1	A	1388	GLY
2	B	526	GLU
2	B	704	ALA
2	B	942	ARG
3	C	39	ALA
5	F	78	GLN
6	H	17	PRO
6	H	18	GLY
6	H	140	ALA
7	I	35	VAL
9	K	64	GLU
10	L	33	GLU
10	L	59	ALA
1	A	400	PRO
1	A	1093	LYS
1	A	1395	GLY
2	B	737	THR
6	H	128	ASN
2	B	482	VAL
1	A	93	VAL
1	A	568	PRO
1	A	1384	VAL

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Mol	Chain	Res	Type
2	B	1023	VAL
1	A	59	GLY
2	B	364	ILE
3	C	6	PRO

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	1225/1520 (81%)	980 (80%)	245 (20%)	1	6
2	B	967/1061 (91%)	790 (82%)	177 (18%)	2	7
3	C	234/274 (85%)	192 (82%)	42 (18%)	2	8
4	E	196/197 (100%)	173 (88%)	23 (12%)	5	20
5	F	75/137 (55%)	59 (79%)	16 (21%)	1	5
6	H	117/128 (91%)	98 (84%)	19 (16%)	2	11
7	I	113/116 (97%)	91 (80%)	22 (20%)	1	6
8	J	60/65 (92%)	44 (73%)	16 (27%)	0	2
9	K	99/102 (97%)	82 (83%)	17 (17%)	2	10
10	L	40/57 (70%)	26 (65%)	14 (35%)	0	1
All	All	3126/3657 (86%)	2535 (81%)	591 (19%)	1	7

All (591) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	21	LEU
1	A	30	ILE
1	A	34	LYS
1	A	43	GLU
1	A	46	THR
1	A	47	ARG
1	A	50	ILE
1	A	55	ASP

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Mol	Chain	Res	Type
1	A	61	ILE
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS
1	A	74	MET
1	A	75	ASN
1	A	88	LYS
1	A	93	VAL
1	A	106	VAL
1	A	122	MET
1	A	126	LEU
1	A	144	THR
1	A	146	MET
1	A	149	GLU
1	A	150	THR
1	A	161	LEU
1	A	180	LYS
1	A	204	THR
1	A	208	LEU
1	A	222	LEU
1	A	225	ASN
1	A	227	VAL
1	A	232	GLU
1	A	234	MET
1	A	257	ARG
1	A	262	LEU
1	A	263	THR
1	A	265	LYS
1	A	266	LEU
1	A	268	ASP
1	A	269	ILE
1	A	270	LEU
1	A	277	GLU
1	A	279	LEU
1	A	281	HIS
1	A	293	GLU
1	A	296	LEU
1	A	298	PHE
1	A	299	HIS
1	A	303	TYR
1	A	308	ILE
1	A	313	GLN

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Mol	Chain	Res	Type
1	A	315	LEU
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	326	ARG
1	A	332	LYS
1	A	335	ARG
1	A	337	ARG
1	A	341	MET
1	A	353	ILE
1	A	359	LEU
1	A	373	THR
1	A	381	THR
1	A	389	THR
1	A	391	LEU
1	A	398	GLU
1	A	403	LYS
1	A	406	ILE
1	A	407	ARG
1	A	424	ILE
1	A	425	GLN
1	A	436	ILE
1	A	437	MET
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	455	MET
1	A	463	ILE
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	487	MET
1	A	500	GLU
1	A	501	LEU
1	A	505	CYS
1	A	523	ILE
1	A	527	THR
1	A	533	LYS
1	A	535	THR
1	A	536	LEU

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Mol	Chain	Res	Type
1	A	541	ILE
1	A	542	GLU
1	A	543	LEU
1	A	544	ASP
1	A	545	GLN
1	A	549	MET
1	A	560	ILE
1	A	566	ILE
1	A	571	LEU
1	A	577	ILE
1	A	590	ARG
1	A	595	THR
1	A	597	LEU
1	A	612	ILE
1	A	618	GLU
1	A	625	SER
1	A	629	LEU
1	A	634	THR
1	A	637	LYS
1	A	645	LEU
1	A	652	VAL
1	A	669	THR
1	A	670	ILE
1	A	672	ASP
1	A	675	THR
1	A	678	GLU
1	A	680	THR
1	A	688	LYS
1	A	695	LYS
1	A	705	LYS
1	A	709	THR
1	A	722	LEU
1	A	738	LYS
1	A	740	LEU
1	A	752	LYS
1	A	756	ILE
1	A	768	GLN
1	A	769	SER
1	A	788	SER
1	A	795	GLU
1	A	801	GLU
1	A	821	ARG

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Mol	Chain	Res	Type
1	A	822	GLU
1	A	837	ILE
1	A	838	GLN
1	A	839	ARG
1	A	847	ASP
1	A	848	ILE
1	A	855	THR
1	A	867	ILE
1	A	878	ILE
1	A	886	ILE
1	A	894	GLU
1	A	896	ARG
1	A	905	ASP
1	A	908	LEU
1	A	909	ASP
1	A	912	LEU
1	A	914	GLU
1	A	919	ILE
1	A	920	LEU
1	A	926	GLN
1	A	927	VAL
1	A	929	LEU
1	A	931	GLU
1	A	936	LEU
1	A	946	VAL
1	A	953	ASN
1	A	973	ILE
1	A	981	LEU
1	A	982	THR
1	A	983	ILE
1	A	999	VAL
1	A	1001	ARG
1	A	1005	GLU
1	A	1006	ILE
1	A	1009	ASN
1	A	1012	ARG
1	A	1024	SER
1	A	1025	ARG
1	A	1030	ARG
1	A	1033	GLN
1	A	1037	LEU
1	A	1048	ASN

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Mol	Chain	Res	Type
1	A	1052	GLN
1	A	1062	GLU
1	A	1067	LEU
1	A	1077	THR
1	A	1078	GLN
1	A	1081	LEU
1	A	1084	PHE
1	A	1086	PHE
1	A	1089	VAL
1	A	1093	LYS
1	A	1118	VAL
1	A	1124	HIS
1	A	1128	GLN
1	A	1129	GLU
1	A	1130	GLN
1	A	1133	LEU
1	A	1134	ILE
1	A	1143	LEU
1	A	1147	THR
1	A	1170	ILE
1	A	1176	LEU
1	A	1205	LYS
1	A	1221	LYS
1	A	1224	LEU
1	A	1227	ILE
1	A	1231	ASP
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1257	ASP
1	A	1261	LYS
1	A	1262	LYS
1	A	1264	GLU
1	A	1271	ILE
1	A	1283	VAL
1	A	1284	MET
1	A	1288	ASP
1	A	1297	GLU
1	A	1299	VAL
1	A	1308	THR
1	A	1322	ILE
1	A	1327	ILE

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Mol	Chain	Res	Type
1	A	1333	ILE
1	A	1335	ILE
1	A	1350	LYS
1	A	1351	GLU
1	A	1354	ASN
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1376	THR
1	A	1381	LEU
1	A	1382	THR
1	A	1384	VAL
1	A	1385	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1394	THR
1	A	1398	MET
1	A	1403	GLU
1	A	1406	VAL
1	A	1411	GLU
1	A	1422	ARG
1	A	1424	VAL
1	A	1425	SER
1	A	1426	GLU
1	A	1438	THR
1	A	1445	ILE
2	B	26	THR
2	B	28	GLU
2	B	44	VAL
2	B	46	GLN
2	B	56	ASP
2	B	62	ILE
2	B	63	ILE
2	B	66	ASP
2	B	70	ILE
2	B	89	GLU
2	B	94	LYS
2	B	97	VAL
2	B	101	MET
2	B	102	VAL
2	B	128	LEU
2	B	136	THR

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Mol	Chain	Res	Type
2	B	175	ARG
2	B	178	ASN
2	B	185	THR
2	B	194	GLU
2	B	218	SER
2	B	234	ILE
2	B	240	ILE
2	B	249	ARG
2	B	254	LEU
2	B	257	LYS
2	B	262	GLU
2	B	272	THR
2	B	273	LEU
2	B	277	LYS
2	B	292	ILE
2	B	296	GLU
2	B	311	LEU
2	B	315	LYS
2	B	323	VAL
2	B	325	GLN
2	B	345	LYS
2	B	349	ILE
2	B	354	ASP
2	B	357	GLN
2	B	359	GLU
2	B	365	THR
2	B	366	GLN
2	B	367	LEU
2	B	371	GLU
2	B	376	PHE
2	B	382	ILE
2	B	384	ARG
2	B	387	LEU
2	B	393	LYS
2	B	396	ASP
2	B	398	ARG
2	B	405	ARG
2	B	408	LEU
2	B	416	LEU
2	B	418	LYS
2	B	436	VAL
2	B	437	GLU

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Mol	Chain	Res	Type
2	B	448	ILE
2	B	454	THR
2	B	465	ASN
2	B	469	GLN
2	B	471	LYS
2	B	476	ARG
2	B	482	VAL
2	B	483	LEU
2	B	485	ARG
2	B	500	THR
2	B	502	ILE
2	B	516	ASN
2	B	521	LEU
2	B	526	GLU
2	B	531	GLN
2	B	539	LEU
2	B	556	THR
2	B	567	GLU
2	B	572	HIS
2	B	591	ARG
2	B	598	GLU
2	B	603	LEU
2	B	604	ARG
2	B	612	GLU
2	B	620	ARG
2	B	633	VAL
2	B	642	ASP
2	B	646	LEU
2	B	655	LYS
2	B	689	LEU
2	B	690	VAL
2	B	708	GLU
2	B	709	ASP
2	B	710	LEU
2	B	711	GLU
2	B	714	GLU
2	B	723	VAL
2	B	730	ARG
2	B	733	HIS
2	B	743	ILE
2	B	751	VAL
2	B	755	ILE

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Mol	Chain	Res	Type
2	B	762	ASN
2	B	766	ARG
2	B	773	MET
2	B	780	VAL
2	B	786	ASN
2	B	791	THR
2	B	792	MET
2	B	794	ASN
2	B	795	ILE
2	B	796	LEU
2	B	812	LEU
2	B	815	ARG
2	B	838	SER
2	B	841	MET
2	B	860	MET
2	B	864	LYS
2	B	868	MET
2	B	875	GLU
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	886	LYS
2	B	898	LEU
2	B	918	ILE
2	B	934	LYS
2	B	942	ARG
2	B	951	GLN
2	B	954	VAL
2	B	961	LEU
2	B	963	PHE
2	B	964	VAL
2	B	967	ARG
2	B	968	VAL
2	B	975	GLN
2	B	979	LYS
2	B	983	ARG
2	B	996	ARG
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1010	LEU
2	B	1028	GLU

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Mol	Chain	Res	Type
2	B	1049	ASP
2	B	1050	ILE
2	B	1057	LYS
2	B	1065	GLN
2	B	1066	SER
2	B	1071	VAL
2	B	1077	THR
2	B	1085	ILE
2	B	1096	ARG
2	B	1099	VAL
2	B	1102	LYS
2	B	1103	ILE
2	B	1113	VAL
2	B	1115	THR
2	B	1122	ARG
2	B	1123	SER
2	B	1133	MET
2	B	1137	CYS
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1170	THR
2	B	1178	ASN
2	B	1188	LYS
2	B	1189	ILE
2	B	1190	ASP
2	B	1191	ILE
2	B	1194	ILE
2	B	1202	LEU
2	B	1203	LEU
2	B	1211	ASN
2	B	1216	LEU
3	C	9	LYS
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	36	VAL
3	C	43	THR

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Mol	Chain	Res	Type
3	C	48	SER
3	C	72	LEU
3	C	75	MET
3	C	77	ILE
3	C	80	LEU
3	C	85	ASP
3	C	100	THR
3	C	101	LEU
3	C	106	GLU
3	C	108	GLU
3	C	115	SER
3	C	116	LYS
3	C	129	ILE
3	C	133	ILE
3	C	137	LYS
3	C	142	VAL
3	C	148	ARG
3	C	149	LYS
3	C	151	GLN
3	C	152	GLU
3	C	156	THR
3	C	188	HIS
3	C	195	GLN
3	C	203	GLN
3	C	214	ASN
3	C	215	GLU
3	C	226	ASP
3	C	238	ILE
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	258	ILE
3	C	259	LEU
3	C	263	THR
3	C	265	MET
4	E	3	GLN
4	E	8	ASN
4	E	54	GLN
4	E	57	MET
4	E	58	MET
4	E	75	MET
4	E	77	SER

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Mol	Chain	Res	Type
4	E	78	LEU
4	E	80	VAL
4	E	85	GLU
4	E	92	THR
4	E	98	ILE
4	E	107	THR
4	E	137	GLU
4	E	142	VAL
4	E	144	ILE
4	E	150	VAL
4	E	156	LEU
4	E	165	LEU
4	E	169	ARG
4	E	175	LEU
4	E	200	ARG
4	E	204	THR
5	F	76	LYS
5	F	77	ASP
5	F	82	THR
5	F	99	LEU
5	F	103	MET
5	F	104	ASN
5	F	111	LEU
5	F	112	GLU
5	F	118	LEU
5	F	119	ARG
5	F	122	MET
5	F	127	GLU
5	F	133	VAL
5	F	134	ILE
5	F	138	LEU
5	F	149	GLU
6	H	3	ASN
6	H	26	ILE
6	H	35	GLN
6	H	44	VAL
6	H	55	LEU
6	H	63	LEU
6	H	76	THR
6	H	87	ARG
6	H	88	SER
6	H	92	ASP

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Mol	Chain	Res	Type
6	H	96	VAL
6	H	105	GLU
6	H	107	VAL
6	H	108	SER
6	H	111	LEU
6	H	123	MET
6	H	130	ARG
6	H	136	LYS
6	H	138	GLU
7	I	17	ARG
7	I	20	LYS
7	I	21	GLU
7	I	26	LEU
7	I	35	VAL
7	I	37	GLU
7	I	42	LEU
7	I	50	THR
7	I	52	ILE
7	I	55	THR
7	I	61	ASP
7	I	62	ILE
7	I	70	ARG
7	I	84	VAL
7	I	87	GLN
7	I	90	GLN
7	I	95	THR
7	I	98	VAL
7	I	104	LEU
7	I	117	LYS
7	I	118	ARG
7	I	120	GLN
8	J	2	ILE
8	J	3	VAL
8	J	7	CYS
8	J	9	SER
8	J	13	VAL
8	J	19	GLU
8	J	22	LEU
8	J	26	GLN
8	J	28	ASP
8	J	30	LEU
8	J	31	ASP

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Mol	Chain	Res	Type
8	J	43	ARG
8	J	48	ARG
8	J	56	LEU
8	J	59	LYS
8	J	64	ASN
9	K	1	MET
9	K	2	ASN
9	K	8	GLU
9	K	11	LEU
9	K	14	GLU
9	K	20	LYS
9	K	21	ILE
9	K	22	ASP
9	K	33	ILE
9	K	50	LEU
9	K	77	THR
9	K	78	THR
9	K	84	LYS
9	K	95	ILE
9	K	108	GLU
9	K	111	LEU
9	K	114	LEU
10	L	27	LEU
10	L	38	LEU
10	L	39	SER
10	L	40	LEU
10	L	42	ARG
10	L	44	ASP
10	L	50	ASP
10	L	55	ILE
10	L	58	LYS
10	L	60	ARG
10	L	61	THR
10	L	64	LEU
10	L	65	VAL
10	L	66	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	68	GLN

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Mol	Chain	Res	Type
1	A	71	GLN
1	A	83	HIS
1	A	124	GLN
1	A	253	ASN
1	A	306	ASN
1	A	313	GLN
1	A	339	ASN
1	A	390	GLN
1	A	427	GLN
1	A	451	HIS
1	A	471	ASN
1	A	503	GLN
1	A	517	ASN
1	A	525	GLN
1	A	545	GLN
1	A	587	HIS
1	A	589	GLN
1	A	631	HIS
1	A	660	ASN
1	A	723	ASN
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	877	HIS
1	A	906	HIS
1	A	926	GLN
1	A	965	GLN
1	A	966	ASN
1	A	969	GLN
1	A	972	HIS
1	A	1004	ASN
1	A	1008	GLN
1	A	1009	ASN
1	A	1033	GLN
1	A	1078	GLN
1	A	1140	HIS
1	A	1171	GLN
1	A	1173	HIS
1	A	1203	ASN

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Mol	Chain	Res	Type
1	A	1265	ASN
1	A	1364	ASN
1	A	1393	ASN
2	B	46	GLN
2	B	53	GLN
2	B	103	ASN
2	B	215	GLN
2	B	366	GLN
2	B	499	ASN
2	B	516	ASN
2	B	518	HIS
2	B	573	GLN
2	B	587	HIS
2	B	657	HIS
2	B	706	GLN
2	B	744	HIS
2	B	762	ASN
2	B	776	GLN
2	B	834	ASN
2	B	835	GLN
2	B	842	ASN
2	B	862	GLN
2	B	887	HIS
2	B	984	HIS
2	B	1015	HIS
2	B	1025	HIS
2	B	1040	ASN
2	B	1097	HIS
2	B	1161	HIS
2	B	1195	HIS
2	B	1205	GLN
3	C	17	ASN
3	C	65	HIS
3	C	112	ASN
3	C	123	ASN
3	C	151	GLN
3	C	167	HIS
3	C	231	ASN
3	C	242	GLN
4	E	54	GLN
4	E	147	HIS
6	H	83	GLN

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Mol	Chain	Res	Type
6	H	133	ASN
6	H	134	ASN
7	I	108	HIS
7	I	116	ASN
8	J	53	HIS
8	J	64	ASN
9	K	29	ASN
9	K	65	HIS
9	K	76	GLN
9	K	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	3/5 (60%)	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 10 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
15	ATP	A	1736	13	32,33,33	1.47	7 (21%)	48,52,52	1.37	8 (16%)

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	ATP	A	1736	13	-	6/22/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1736	ATP	PA-O3A	3.65	1.63	1.59
15	A	1736	ATP	PB-O3A	3.64	1.63	1.59
15	A	1736	ATP	C2-N1	2.43	1.38	1.33
15	A	1736	ATP	PB-O1B	2.38	1.59	1.50
15	A	1736	ATP	C2-N3	2.13	1.37	1.33
15	A	1736	ATP	C5-C4	2.07	1.42	1.39
15	A	1736	ATP	PB-O3B	-2.05	1.57	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1736	ATP	O3'-C3'-C2'	3.31	122.43	111.82
15	A	1736	ATP	O4'-C1'-N9	3.19	114.22	108.09
15	A	1736	ATP	O3A-PA-O1A	2.87	119.35	110.70
15	A	1736	ATP	O3'-C3'-C4'	2.47	118.19	111.08
15	A	1736	ATP	O3G-PG-O3B	2.43	112.78	104.64
15	A	1736	ATP	C1'-N9-C8	2.38	132.37	127.09
15	A	1736	ATP	O2A-PA-O3A	-2.15	101.46	107.27
15	A	1736	ATP	O4'-C1'-C2'	-2.07	102.18	106.62

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	1736	ATP	PB-O3B-PG-O3G
15	A	1736	ATP	C5'-O5'-PA-O3A
15	A	1736	ATP	PB-O3B-PG-O2G
15	A	1736	ATP	C4'-C5'-O5'-PA

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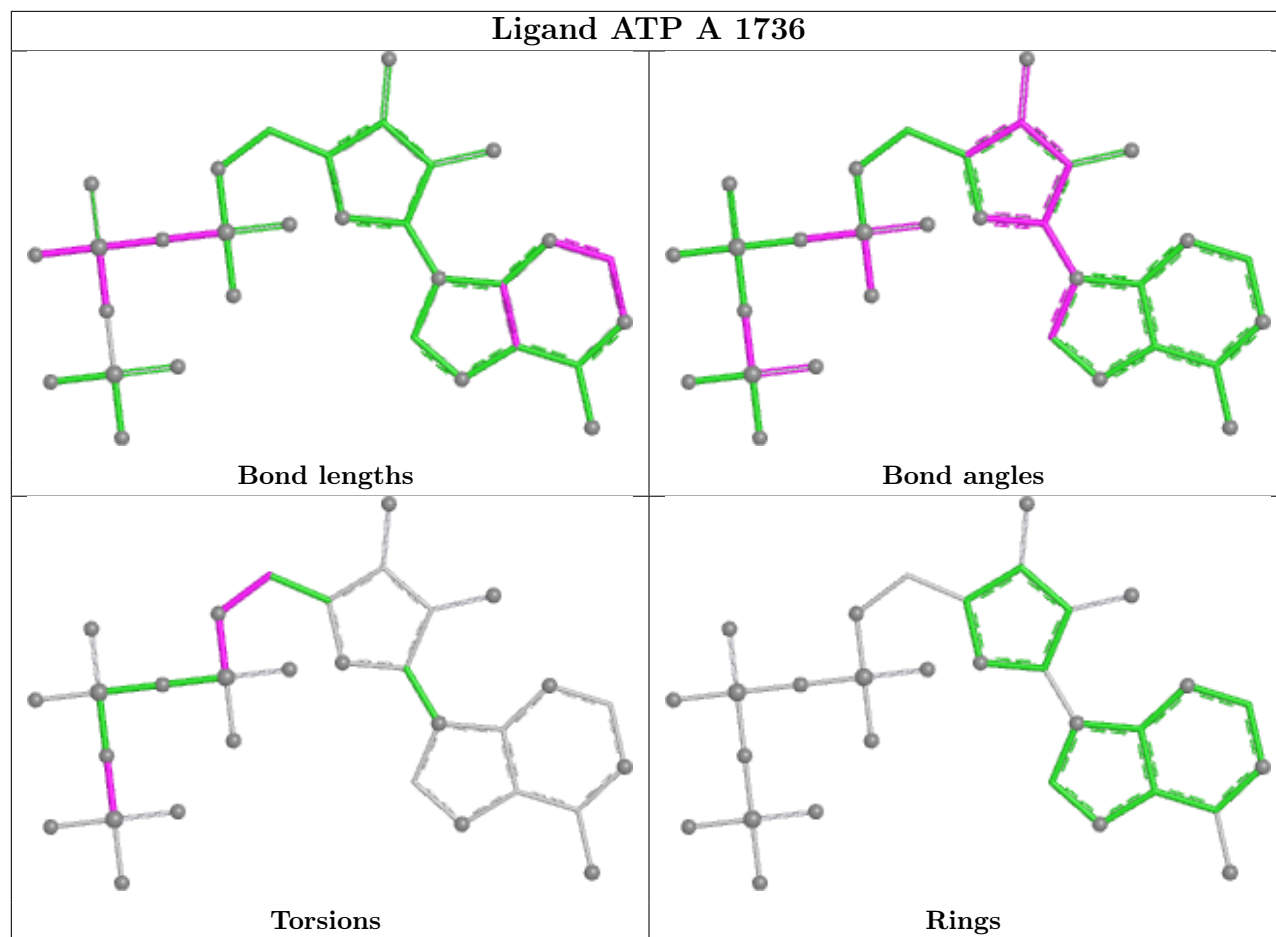
Mol	Chain	Res	Type	Atoms
15	A	1736	ATP	C5'-O5'-PA-O1A
15	A	1736	ATP	PB-O3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1736	ATP	5	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	1405/1733 (81%)	-0.12	13 (0%) 81 65	78, 133, 223, 254	0
2	B	1114/1224 (91%)	-0.13	11 (0%) 79 63	71, 115, 183, 241	0
3	C	266/318 (83%)	-0.29	0 100 100	87, 113, 153, 215	0
4	E	214/215 (99%)	-0.23	1 (0%) 87 76	102, 159, 206, 216	0
5	F	85/155 (54%)	-0.30	0 100 100	109, 139, 178, 196	0
6	H	133/146 (91%)	0.04	1 (0%) 82 68	131, 172, 202, 222	0
7	I	119/122 (97%)	-0.10	2 (1%) 69 50	93, 138, 185, 200	0
8	J	65/70 (92%)	-0.34	0 100 100	81, 104, 136, 151	0
9	K	114/120 (95%)	-0.32	0 100 100	87, 123, 150, 175	0
10	L	46/70 (65%)	0.30	3 (6%) 25 17	99, 155, 188, 214	0
11	R	5/5 (100%)	0.02	0 100 100	148, 153, 180, 183	0
12	T	13/29 (44%)	0.16	0 100 100	150, 170, 237, 245	0
All	All	3579/4207 (85%)	-0.14	31 (0%) 81 65	71, 128, 208, 254	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1086	PHE	4.7
2	B	715	ALA	3.5
2	B	708	GLU	3.2
4	E	199	ILE	3.2
2	B	478	GLY	3.1
7	I	104	LEU	3.1
2	B	477	ALA	3.0
1	A	65	LEU	3.0
2	B	335	GLY	2.9
2	B	883	LEU	2.8
1	A	105	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	502	ILE	2.7
1	A	1108	ALA	2.7
1	A	138	ILE	2.6
2	B	1191	ILE	2.5
1	A	1085	HIS	2.5
1	A	250	ILE	2.4
2	B	646	LEU	2.4
1	A	55	ASP	2.4
6	H	83	GLN	2.4
10	L	25	ALA	2.3
10	L	40	LEU	2.3
1	A	87	ALA	2.3
1	A	1087	ALA	2.3
7	I	50	THR	2.3
1	A	54	ASN	2.2
2	B	1170	THR	2.1
1	A	50	ILE	2.1
1	A	141	LEU	2.1
10	L	28	LYS	2.0
2	B	709	ASP	2.0

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

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

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.

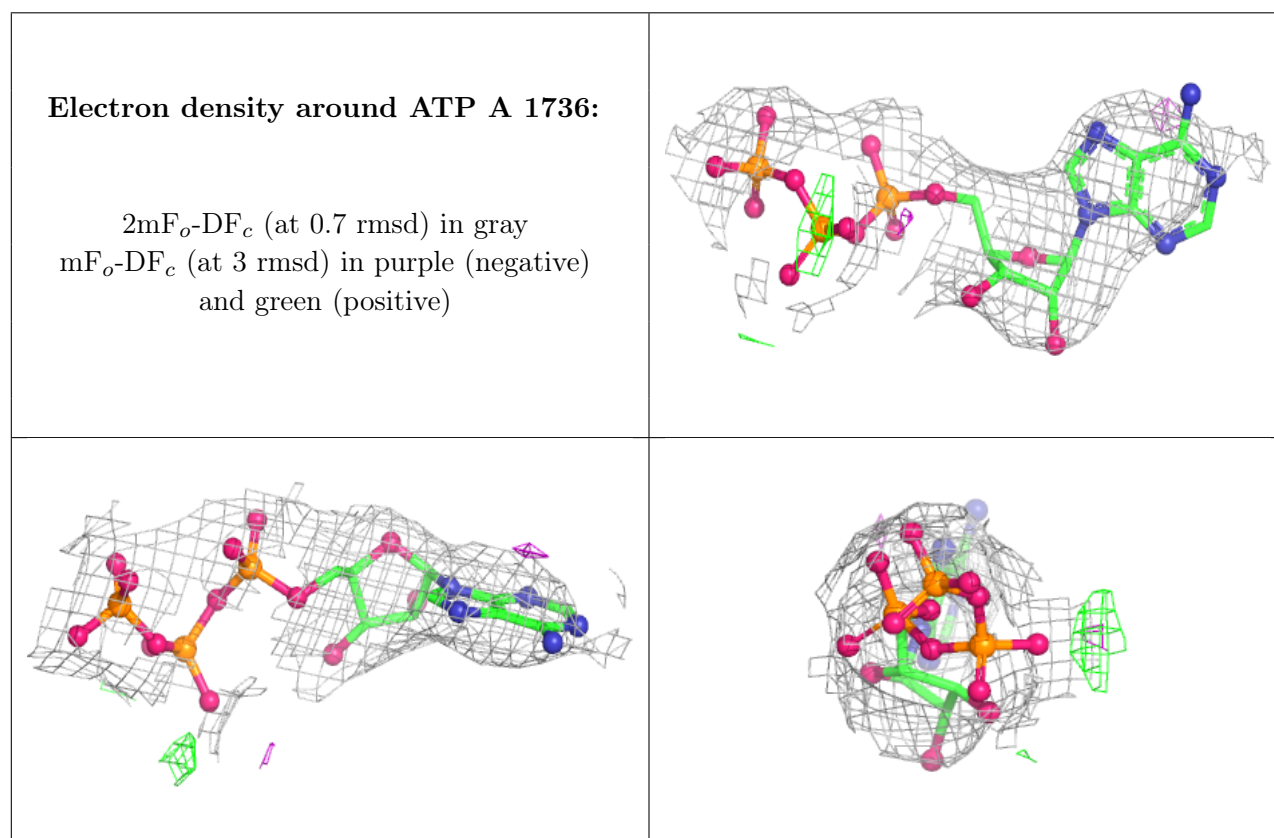
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	ZN	A	1734	1/1	0.84	0.09	300,300,300,300	0
15	ATP	A	1736	31/31	0.89	0.10	162,165,195,197	0
14	ZN	B	1307	1/1	0.93	0.06	221,221,221,221	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	MG	A	2002	1/1	0.95	0.05	131,131,131,131	0
14	ZN	A	1735	1/1	0.96	0.04	198,198,198,198	0
14	ZN	C	319	1/1	0.99	0.02	113,113,113,113	0
14	ZN	I	203	1/1	0.99	0.02	134,134,134,134	0
14	ZN	I	204	1/1	0.99	0.02	112,112,112,112	0
14	ZN	J	101	1/1	0.99	0.04	102,102,102,102	0
14	ZN	L	105	1/1	0.99	0.02	142,142,142,142	0
13	MG	A	2001	1/1	0.99	0.06	102,102,102,102	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 ⓘ

There are no such residues in this entry.