



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:22 AM UTC

PDB ID : 3S1R / pdb_00003s1r
Title : RNA Polymerase II Initiation Complex with a 5-nt 3'-deoxy RNA soaked with GTP
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-16
Resolution : 3.20 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

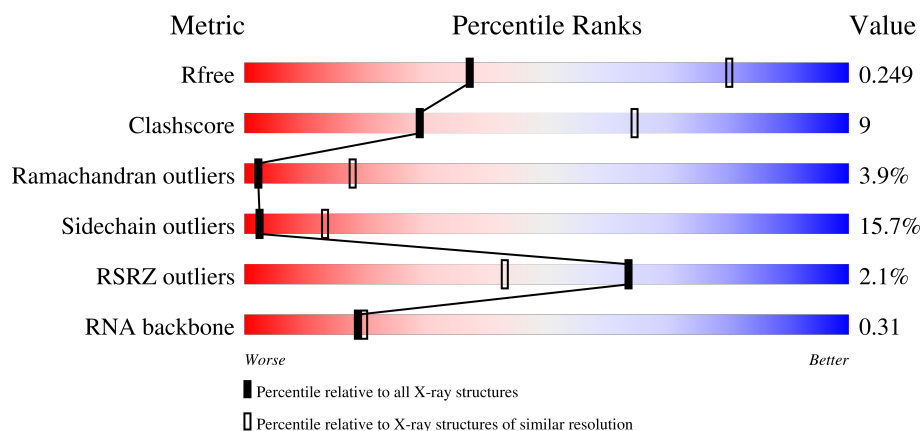
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	 2% 52% 23% 5% 19%
2	B	1224	 2% 58% 26% 6% 9%
3	C	318	 51% 25% 7% 16%
4	E	215	 66% 27% 6%

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	5	
12	T	29	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 28601 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	8	Total	C	N	O	P	0	0	0
			159	76	26	49	8			

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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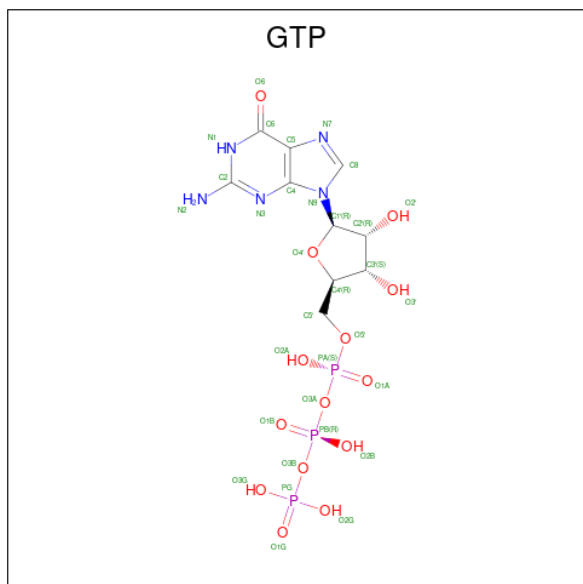
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	Zn	0	0
			1	1		
13	C	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	J	1	Total	Zn	0	0
			1	1		
13	L	1	Total	Zn	0	0
			1	1		

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 15 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

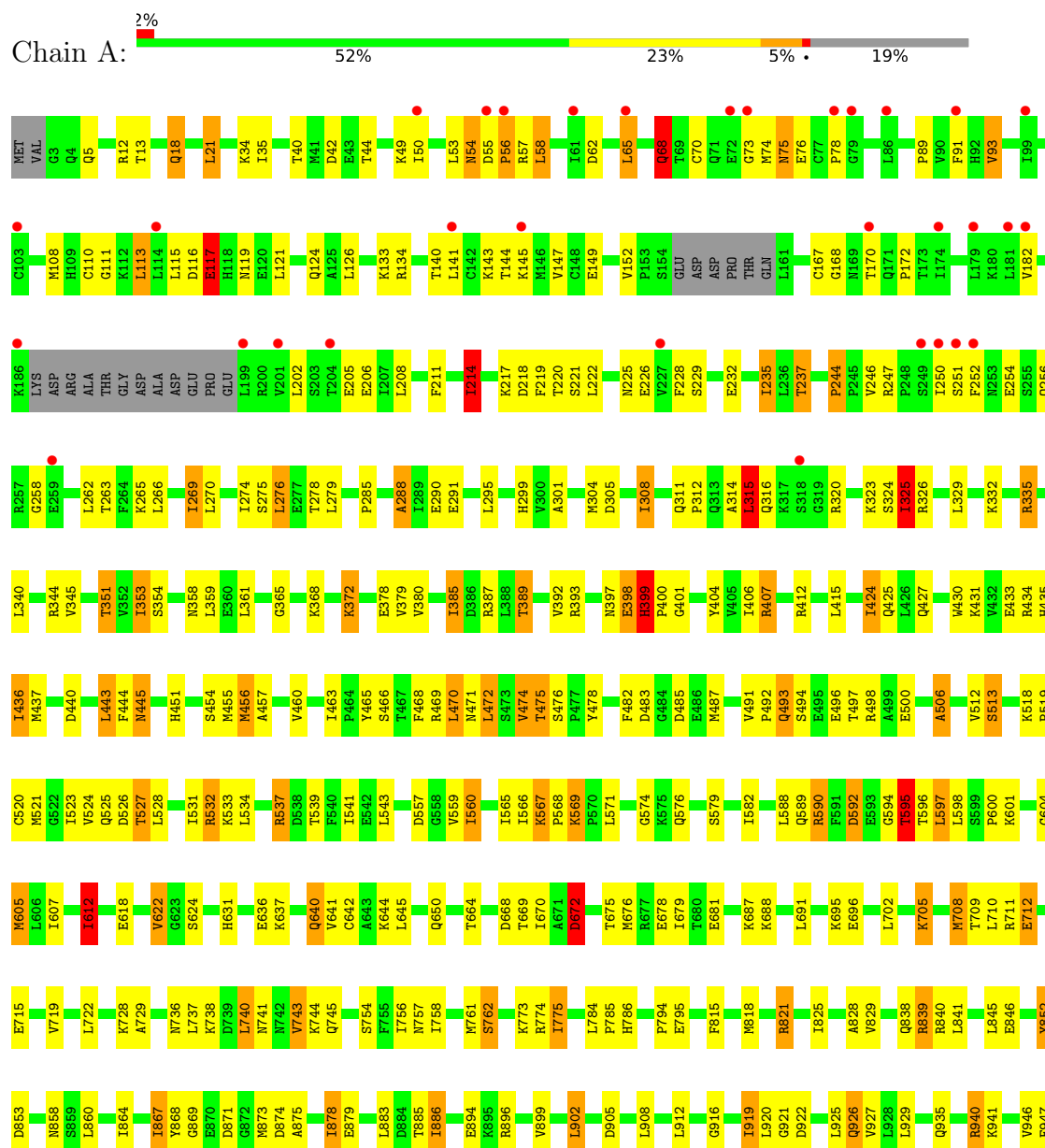


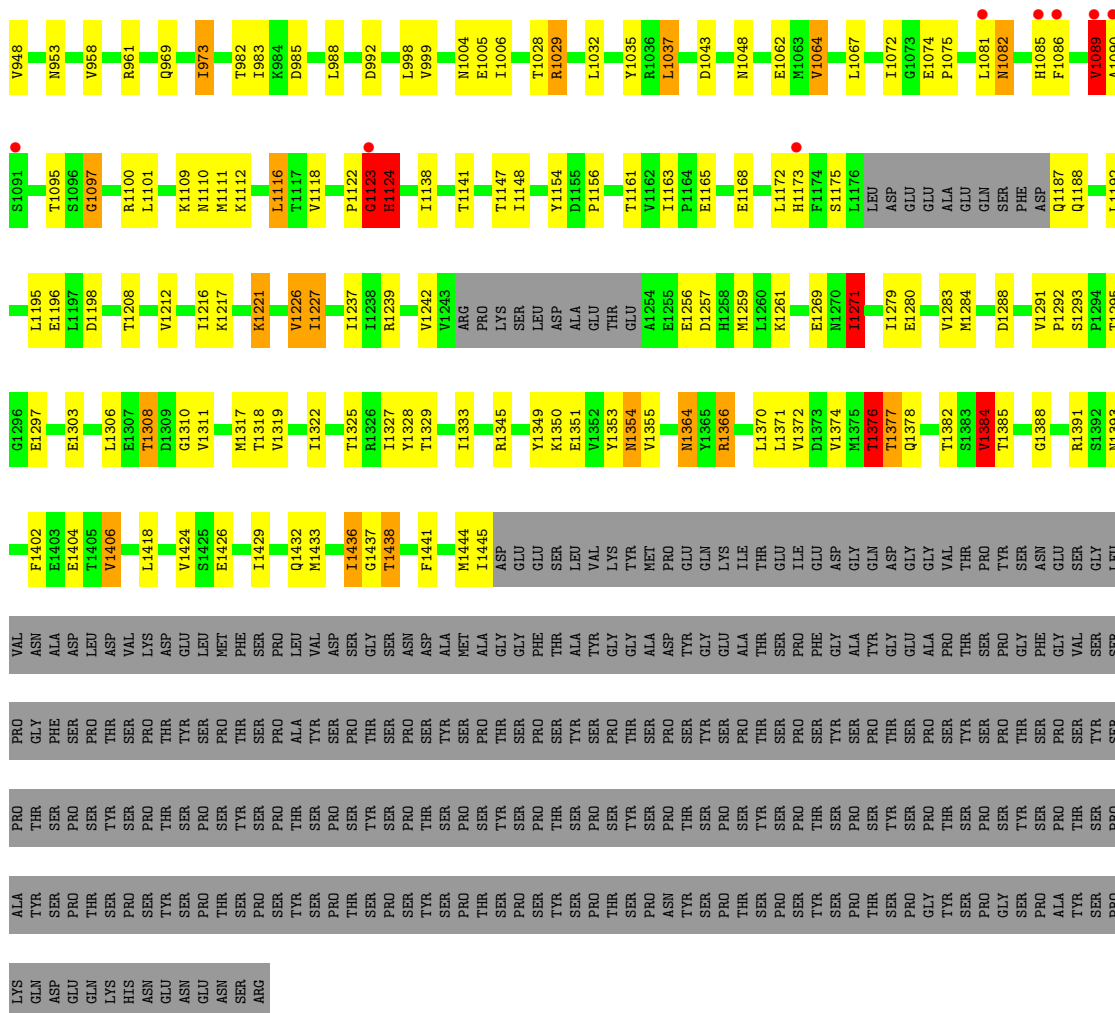
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	R	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

3 Residue-property plots

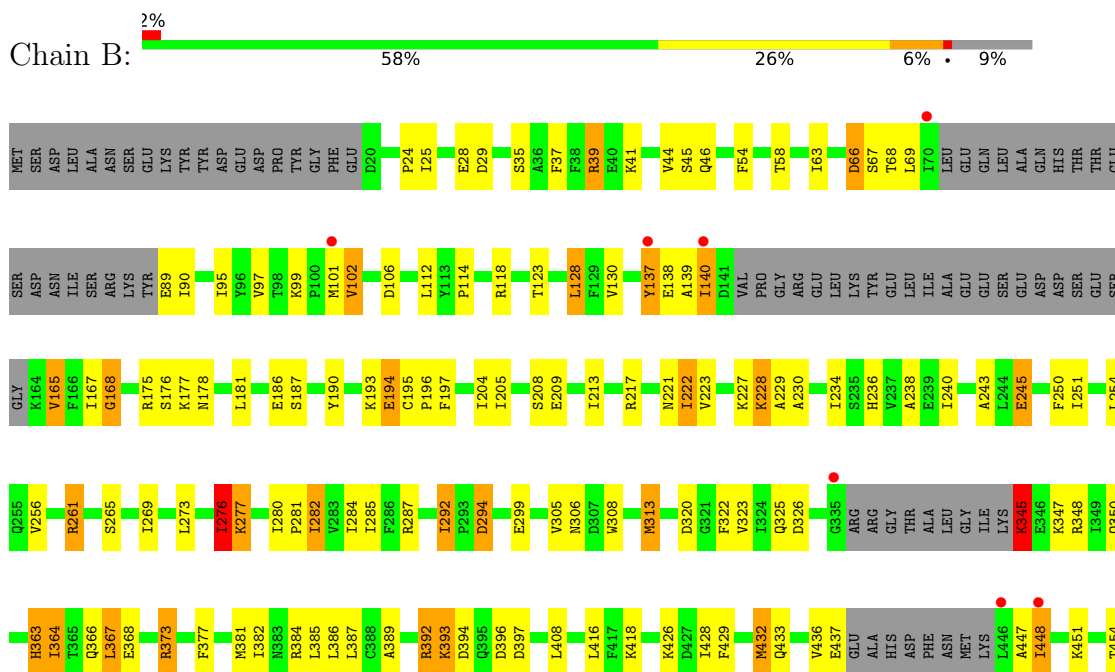
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

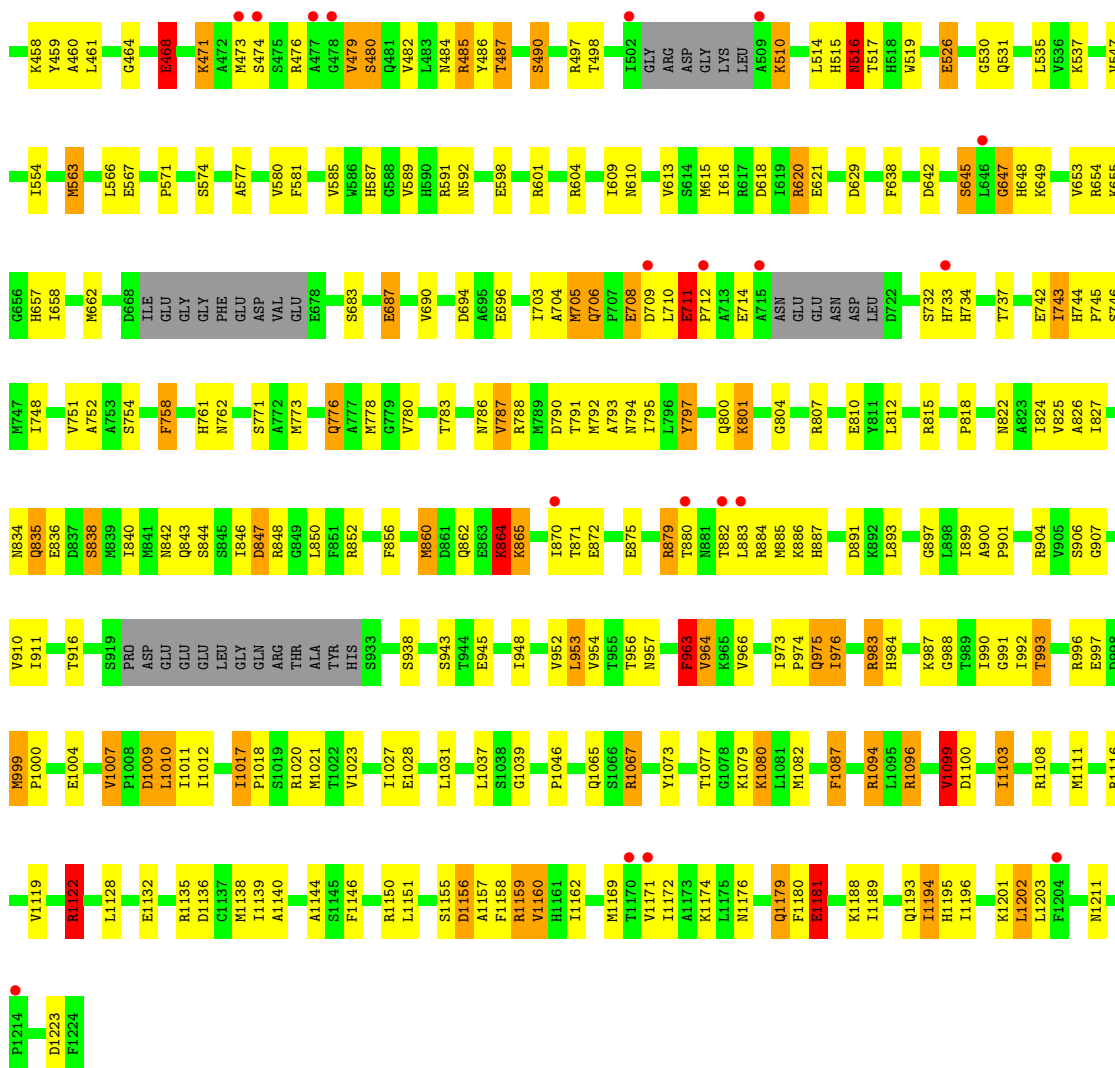
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



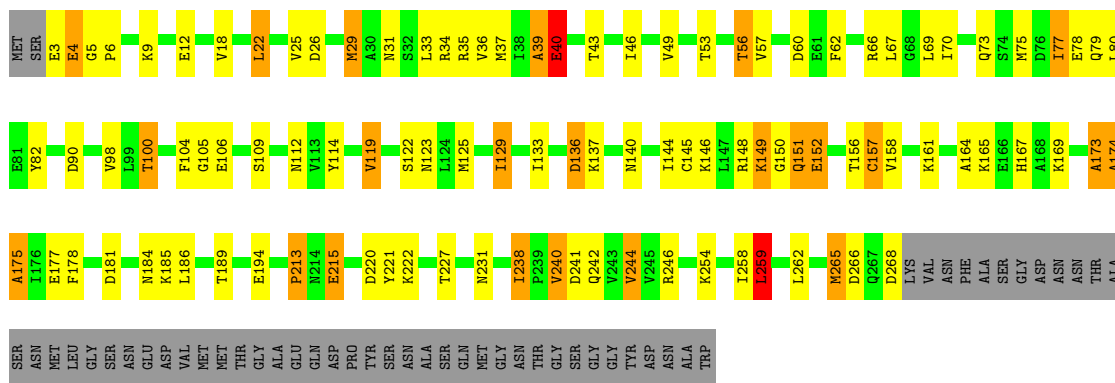


- Molecule 2: DNA-directed RNA polymerase II subunit RPB2



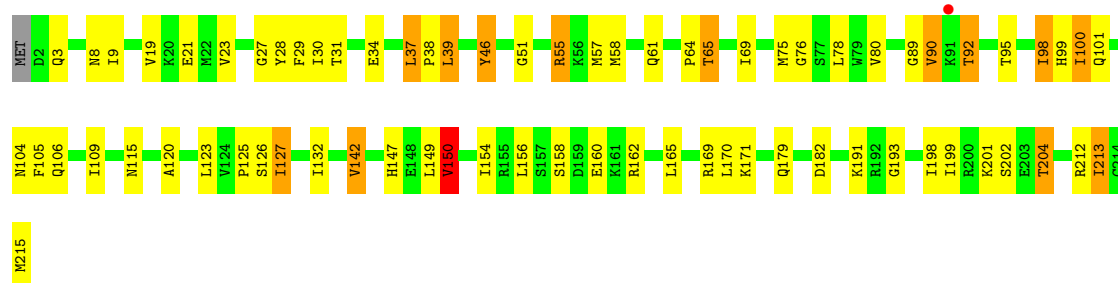


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

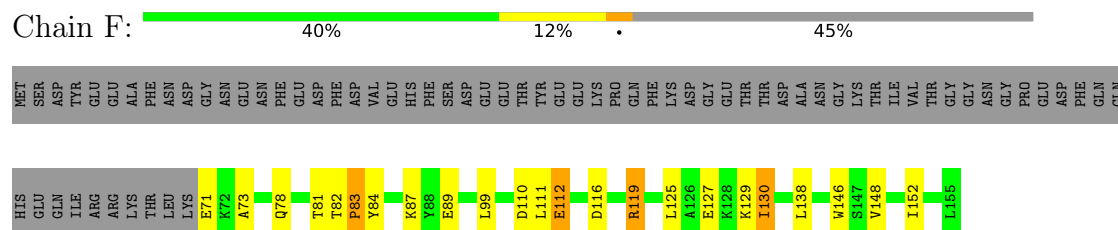


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

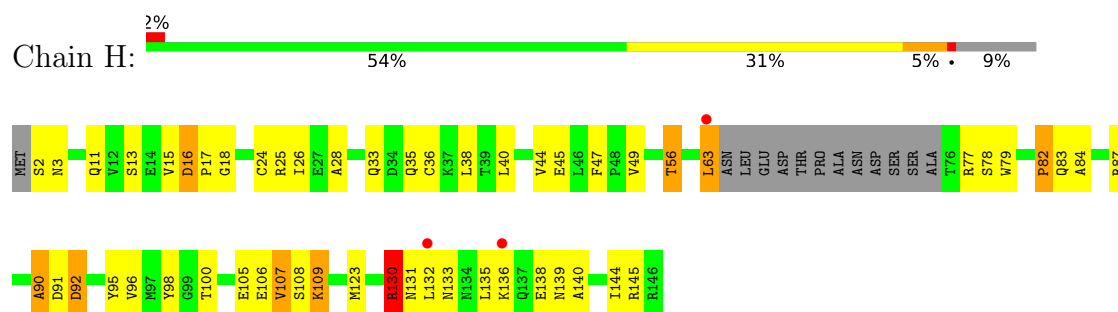




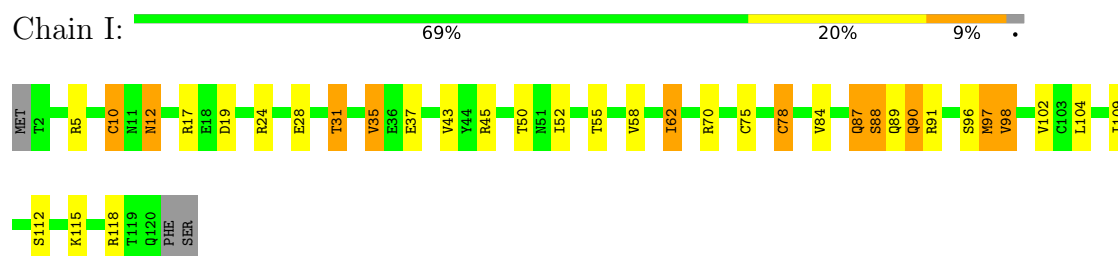
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



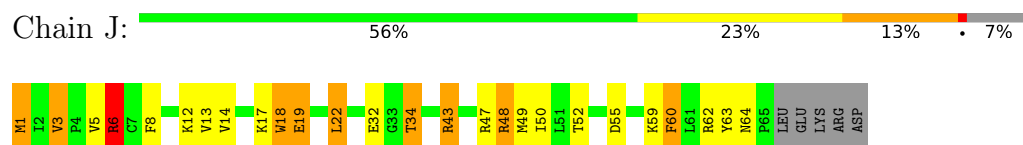
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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

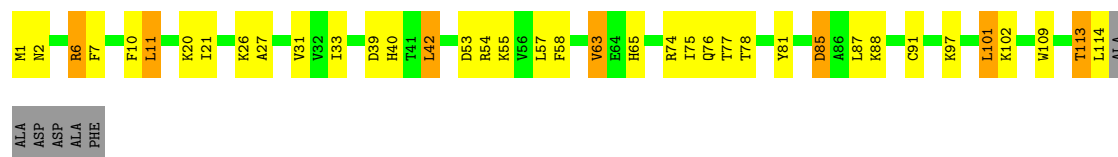


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

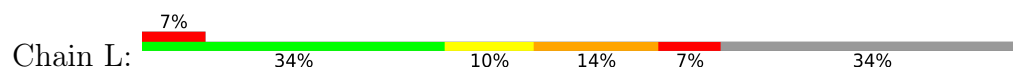


- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

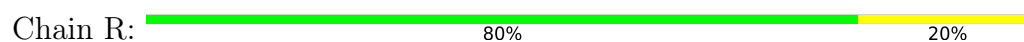




- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



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



- 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')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.67Å 221.32Å 193.21Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	29.97 – 3.20 29.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.97-3.20) 99.2 (29.97-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.18Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.177 , 0.226 0.201 , 0.249	Depositor DCC
R_{free} test set	5435 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 110.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28601	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: ZN, GTP, 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	0.87	4/11241 (0.0%)	1.50	94/15199 (0.6%)
2	B	0.90	7/9033 (0.1%)	1.49	91/12181 (0.7%)
3	C	0.84	1/2133 (0.0%)	1.45	24/2891 (0.8%)
4	E	0.79	0/1788	1.44	20/2406 (0.8%)
5	F	0.88	1/700 (0.1%)	1.38	5/945 (0.5%)
6	H	0.85	0/1086	1.40	17/1470 (1.2%)
7	I	0.85	0/989	1.45	9/1331 (0.7%)
8	J	0.92	1/541 (0.2%)	1.67	12/727 (1.7%)
9	K	0.77	0/937	1.40	8/1265 (0.6%)
10	L	0.97	0/365	1.89	13/485 (2.7%)
11	R	0.52	0/123	1.07	0/191
12	T	0.51	0/176	1.25	1/268 (0.4%)
All	All	0.87	14/29112 (0.0%)	1.48	294/39359 (0.7%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	563	MET	SD-CE	-7.97	1.59	1.79
1	A	315	LEU	CA-C	7.40	1.56	1.52
1	A	605	MET	SD-CE	-6.29	1.63	1.79
3	C	40	GLU	CA-C	6.10	1.60	1.52
1	A	256	GLN	CA-C	5.90	1.55	1.52
2	B	140	ILE	CA-C	5.60	1.59	1.52
1	A	867	ILE	CG1-CD1	5.58	1.73	1.51
8	J	6	ARG	CA-C	5.48	1.60	1.52
2	B	705	MET	SD-CE	-5.38	1.66	1.79
2	B	1196	ILE	CA-C	5.36	1.57	1.52
2	B	976	ILE	CA-C	-5.27	1.46	1.52
2	B	860	MET	SD-CE	5.09	1.92	1.79
5	F	129	LYS	C-N	5.07	1.37	1.33
2	B	69	LEU	CA-C	5.05	1.59	1.53

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	647	GLY	CA-C-N	10.63	140.83	121.70
2	B	647	GLY	C-N-CA	10.63	140.83	121.70
10	L	50	ASP	CA-C-N	10.05	140.74	121.54
10	L	50	ASP	C-N-CA	10.05	140.74	121.54
10	L	58	LYS	N-CA-C	9.60	122.95	111.33
8	J	18	TRP	N-CA-C	9.10	120.80	111.07
2	B	976	ILE	N-CA-C	8.79	118.86	110.42
2	B	37	PHE	N-CA-C	-8.50	99.95	110.41
1	A	1123	GLY	CA-C-N	8.36	136.75	121.70
1	A	1123	GLY	C-N-CA	8.36	136.75	121.70
2	B	1009	ASP	N-CA-C	-8.34	103.24	113.41
6	H	92	ASP	N-CA-C	-8.33	100.61	113.02
2	B	347	LYS	CA-C-N	8.24	131.16	120.44
2	B	347	LYS	C-N-CA	8.24	131.16	120.44
1	A	445	ASN	CA-CB-CG	8.12	120.72	112.60
4	E	123	LEU	CA-C-N	8.09	126.80	120.33
4	E	123	LEU	C-N-CA	8.09	126.80	120.33
1	A	506	ALA	CA-C-N	7.93	128.04	120.43
1	A	506	ALA	C-N-CA	7.93	128.04	120.43
1	A	794	PRO	CA-C-N	7.84	130.63	120.44
1	A	794	PRO	C-N-CA	7.84	130.63	120.44
2	B	787	VAL	N-CA-C	-7.74	105.95	113.53
1	A	251	SER	CA-C-N	7.68	131.07	120.63
1	A	251	SER	C-N-CA	7.68	131.07	120.63
6	H	91	ASP	CA-C-N	7.65	134.25	122.08
6	H	91	ASP	C-N-CA	7.65	134.25	122.08
2	B	1087	PHE	CA-CB-CG	7.46	121.26	113.80
2	B	140	ILE	CA-C-N	7.41	135.04	121.70
2	B	140	ILE	C-N-CA	7.41	135.04	121.70
10	L	51	CYS	N-CA-C	-7.39	95.06	110.80
1	A	1097	GLY	CA-C-N	7.38	124.89	120.24
1	A	1097	GLY	C-N-CA	7.38	124.89	120.24
2	B	140	ILE	N-CA-C	7.33	117.41	110.30
2	B	99	LYS	N-CA-C	-7.30	100.58	110.36
1	A	1004	ASN	CA-C-N	7.19	129.92	120.28
1	A	1004	ASN	C-N-CA	7.19	129.92	120.28
3	C	173	ALA	N-CA-C	7.19	122.56	111.56
8	J	5	VAL	N-CA-C	-7.17	100.33	109.30
2	B	1007	VAL	CB-CA-C	7.06	116.25	109.33
1	A	466	SER	N-CA-C	7.00	121.82	113.28
2	B	24	PRO	CA-C-N	6.94	130.00	120.35
2	B	24	PRO	C-N-CA	6.94	130.00	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	853	ASP	CA-CB-CG	6.93	119.53	112.60
3	C	82	TYR	N-CA-C	-6.93	98.74	109.76
1	A	244	PRO	N-CA-C	6.89	119.10	110.70
8	J	17	LYS	N-CA-C	6.86	120.90	112.54
2	B	363	HIS	N-CA-C	-6.84	101.31	110.55
1	A	525	GLN	N-CA-C	6.70	118.49	108.31
2	B	516	ASN	CA-C-N	6.69	130.14	120.38
2	B	516	ASN	C-N-CA	6.69	130.14	120.38
3	C	175	ALA	N-CA-C	6.67	119.78	108.90
1	A	998	LEU	N-CA-C	6.65	120.51	109.46
2	B	436	VAL	N-CA-C	-6.62	106.54	112.90
1	A	864	ILE	N-CA-C	-6.58	106.57	111.90
2	B	345	LYS	CA-C-N	6.54	133.48	121.70
2	B	345	LYS	C-N-CA	6.54	133.48	121.70
2	B	1007	VAL	N-CA-CB	-6.54	104.64	111.64
1	A	1072	ILE	CA-C-N	6.54	127.19	119.94
1	A	1072	ILE	C-N-CA	6.54	127.19	119.94
6	H	138	GLU	N-CA-C	-6.53	104.58	112.54
2	B	711	GLU	N-CA-C	6.47	124.11	109.81
1	A	314	ALA	CA-C-N	6.45	129.38	121.64
1	A	314	ALA	C-N-CA	6.45	129.38	121.64
3	C	265	MET	CA-C-N	6.44	129.20	120.38
3	C	265	MET	C-N-CA	6.44	129.20	120.38
1	A	612	ILE	N-CA-CB	6.39	117.92	110.82
1	A	463	ILE	N-CA-C	6.31	116.03	108.45
1	A	474	VAL	CA-C-N	6.31	129.06	120.54
1	A	474	VAL	C-N-CA	6.31	129.06	120.54
2	B	322	PHE	CA-CB-CG	6.30	120.10	113.80
6	H	45	GLU	N-CA-C	-6.28	105.75	113.41
9	K	113	THR	CA-C-N	6.22	132.90	121.70
9	K	113	THR	C-N-CA	6.22	132.90	121.70
4	E	150	VAL	N-CA-C	6.20	113.69	107.55
10	L	49	LYS	CA-C-N	6.20	133.38	121.54
10	L	49	LYS	C-N-CA	6.20	133.38	121.54
10	L	26	THR	CA-C-N	6.20	129.93	120.82
10	L	26	THR	C-N-CA	6.20	129.93	120.82
2	B	165	VAL	N-CA-C	6.17	117.61	109.21
2	B	294	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	947	PHE	CA-C-N	6.16	129.21	120.53
1	A	947	PHE	C-N-CA	6.16	129.21	120.53
1	A	886	ILE	N-CA-C	6.15	117.71	111.00
10	L	68	GLU	N-CA-C	-6.14	101.43	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	695	LYS	CA-C-N	6.06	128.65	120.65
1	A	695	LYS	C-N-CA	6.06	128.65	120.65
6	H	2	SER	CA-C-N	6.03	132.55	121.70
6	H	2	SER	C-N-CA	6.03	132.55	121.70
2	B	694	ASP	CA-CB-CG	6.03	118.63	112.60
2	B	392	ARG	N-CA-C	-5.98	106.32	113.97
2	B	884	ARG	CA-C-N	5.97	129.77	120.75
2	B	884	ARG	C-N-CA	5.97	129.77	120.75
3	C	39	ALA	CA-C-N	5.97	132.95	121.54
3	C	39	ALA	C-N-CA	5.97	132.95	121.54
1	A	1311	VAL	N-CA-C	5.97	116.47	108.11
2	B	916	THR	CB-CA-C	5.96	116.50	109.47
1	A	1085	HIS	N-CA-C	-5.95	107.25	114.75
4	E	171	LYS	N-CA-C	-5.94	100.93	110.14
2	B	1194	ILE	N-CA-C	5.93	116.42	107.75
7	I	50	THR	N-CA-C	5.92	118.56	108.90
2	B	629	ASP	CA-CB-CG	5.92	118.52	112.60
7	I	112	SER	CA-C-N	5.89	129.20	120.90
7	I	112	SER	C-N-CA	5.89	129.20	120.90
4	E	92	THR	CA-C-N	5.87	128.06	120.44
4	E	92	THR	C-N-CA	5.87	128.06	120.44
3	C	60	ASP	CA-CB-CG	5.86	118.46	112.60
7	I	10	CYS	N-CA-C	5.86	117.66	111.28
2	B	482	VAL	N-CA-CB	5.84	117.95	110.13
2	B	69	LEU	N-CA-C	5.84	115.98	108.34
1	A	454	SER	N-CA-C	-5.82	106.18	113.28
3	C	136	ASP	CA-CB-CG	5.81	118.41	112.60
7	I	5	ARG	N-CA-C	5.80	119.14	110.14
1	A	922	ASP	N-CA-C	5.80	118.38	111.71
2	B	818	PRO	N-CA-C	5.79	120.38	111.57
4	E	27	GLY	CA-C-N	5.75	129.28	120.82
4	E	27	GLY	C-N-CA	5.75	129.28	120.82
3	C	40	GLU	N-CA-C	5.73	123.00	110.80
6	H	15	VAL	CB-CA-C	5.72	116.94	110.41
1	A	624	SER	CA-C-N	5.72	129.92	120.94
1	A	624	SER	C-N-CA	5.72	129.92	120.94
6	H	16	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	1004	ASN	N-CA-C	5.70	118.24	110.55
2	B	276	ILE	CA-C-N	5.69	132.41	121.54
2	B	276	ILE	C-N-CA	5.69	132.41	121.54
2	B	222	ILE	CB-CA-C	5.68	119.25	110.96
6	H	3	ASN	CA-C-N	5.68	129.86	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	3	ASN	C-N-CA	5.68	129.86	120.94
1	A	829	VAL	CA-C-N	5.67	128.20	120.54
1	A	829	VAL	C-N-CA	5.67	128.20	120.54
2	B	964	VAL	N-CA-C	5.67	116.91	108.46
1	A	1198	ASP	CA-C-N	5.67	128.15	120.38
1	A	1198	ASP	C-N-CA	5.67	128.15	120.38
3	C	259	LEU	CA-C-N	5.66	128.33	120.29
3	C	259	LEU	C-N-CA	5.66	128.33	120.29
1	A	537	ARG	CA-C-N	5.66	128.43	120.28
1	A	537	ARG	C-N-CA	5.66	128.43	120.28
2	B	645	SER	CA-C-N	5.66	129.74	120.63
2	B	645	SER	C-N-CA	5.66	129.74	120.63
5	F	130	ILE	N-CA-CB	5.65	117.98	111.31
2	B	864	LYS	CA-C-N	5.65	132.32	121.54
2	B	864	LYS	C-N-CA	5.65	132.32	121.54
3	C	78	GLU	CB-CG-CD	5.64	122.19	112.60
2	B	432	MET	CA-C-N	5.63	127.83	120.28
2	B	432	MET	C-N-CA	5.63	127.83	120.28
2	B	396	ASP	CA-C-N	5.63	130.44	121.66
2	B	396	ASP	C-N-CA	5.63	130.44	121.66
2	B	484	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	1257	ASP	N-CA-C	5.63	118.96	111.75
2	B	834	ASN	CA-CB-CG	5.62	118.22	112.60
2	B	276	ILE	N-CA-C	5.61	115.67	107.37
9	K	27	ALA	N-CA-C	5.60	116.94	109.83
1	A	399	HIS	N-CA-CB	5.59	120.32	110.37
2	B	1028	GLU	CB-CG-CD	5.59	122.10	112.60
3	C	34	ARG	CA-C-N	5.59	127.71	120.44
3	C	34	ARG	C-N-CA	5.59	127.71	120.44
1	A	708	MET	N-CA-C	5.58	118.55	109.06
2	B	490	SER	CA-C-N	5.58	128.01	120.65
2	B	490	SER	C-N-CA	5.58	128.01	120.65
1	A	314	ALA	N-CA-C	5.58	118.04	110.35
4	E	21	GLU	CA-C-N	5.58	128.01	120.65
4	E	21	GLU	C-N-CA	5.58	128.01	120.65
1	A	1404	GLU	CA-C-N	5.57	130.05	121.19
1	A	1404	GLU	C-N-CA	5.57	130.05	121.19
1	A	117	GLU	CA-C-N	5.57	128.51	120.38
1	A	117	GLU	C-N-CA	5.57	128.51	120.38
2	B	1004	GLU	N-CA-C	-5.57	106.33	113.23
1	A	1043	ASP	CA-C-N	5.56	127.73	120.28
1	A	1043	ASP	C-N-CA	5.56	127.73	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	62	LYS	CA-C-N	5.55	129.56	120.63
10	L	62	LYS	C-N-CA	5.55	129.56	120.63
2	B	230	ALA	N-CA-C	5.54	121.15	113.45
2	B	645	SER	N-CA-C	5.52	118.22	109.50
1	A	1376	THR	CB-CA-C	5.49	121.35	110.42
1	A	983	ILE	CA-C-N	5.47	127.55	120.44
1	A	983	ILE	C-N-CA	5.47	127.55	120.44
2	B	714	GLU	N-CA-C	5.46	117.69	109.23
7	I	52	ILE	N-CA-C	5.45	116.60	108.54
1	A	54	ASN	N-CA-C	5.43	116.79	107.28
8	J	8	PHE	CA-CB-CG	5.42	119.22	113.80
2	B	66	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	305	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	1271	ILE	N-CA-C	5.41	115.88	107.28
1	A	795	GLU	CB-CG-CD	5.40	121.78	112.60
1	A	1082	ASN	N-CA-C	5.40	118.12	107.98
2	B	186	GLU	CA-C-N	5.39	127.50	120.28
2	B	186	GLU	C-N-CA	5.39	127.50	120.28
2	B	535	LEU	N-CA-C	-5.39	106.39	113.12
9	K	53	ASP	CA-CB-CG	5.39	117.99	112.60
6	H	91	ASP	N-CA-C	5.37	118.19	109.06
2	B	1011	ILE	N-CA-CB	5.36	118.73	112.35
2	B	758	PHE	CA-C-O	-5.35	116.78	120.47
12	T	23	DC	P-O5'-C5'	5.35	128.02	120.00
2	B	229	ALA	CA-C-N	5.33	127.62	120.58
2	B	229	ALA	C-N-CA	5.33	127.62	120.58
1	A	948	VAL	N-CA-C	5.33	116.70	110.62
2	B	847	ASP	CA-CB-CG	5.32	117.92	112.60
8	J	60	PHE	CA-CB-CG	5.32	119.12	113.80
1	A	557	ASP	CA-CB-CG	5.31	117.91	112.60
2	B	963	PHE	CA-CB-CG	5.30	119.10	113.80
2	B	320	ASP	CA-CB-CG	5.30	117.90	112.60
8	J	19	GLU	CA-C-N	5.30	127.69	120.54
8	J	19	GLU	C-N-CA	5.30	127.69	120.54
1	A	451	HIS	CB-CA-C	-5.29	100.18	109.71
2	B	245	GLU	N-CA-C	5.29	119.22	112.34
2	B	368	GLU	N-CA-C	5.28	116.52	108.12
6	H	130	ARG	CA-C-N	5.28	131.63	121.54
6	H	130	ARG	C-N-CA	5.28	131.63	121.54
1	A	526	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	985	ASP	CA-CB-CG	5.28	117.88	112.60
2	B	326	ASP	CA-C-N	5.28	127.35	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	326	ASP	C-N-CA	5.28	127.35	120.28
4	E	115	ASN	N-CA-C	5.28	116.02	108.74
1	A	590	ARG	N-CA-C	5.27	119.20	111.34
3	C	3	GLU	CA-C-N	5.27	131.61	121.54
3	C	3	GLU	C-N-CA	5.27	131.61	121.54
8	J	22	LEU	CA-C-N	5.26	127.28	120.44
8	J	22	LEU	C-N-CA	5.26	127.28	120.44
2	B	609	ILE	N-CA-C	-5.25	100.92	108.48
2	B	842	ASN	CA-CB-CG	5.24	117.84	112.60
1	A	1090	ALA	CA-C-N	5.24	127.73	120.29
1	A	1090	ALA	C-N-CA	5.24	127.73	120.29
1	A	596	THR	CA-C-N	5.23	131.54	121.54
1	A	596	THR	C-N-CA	5.23	131.54	121.54
1	A	919	ILE	CB-CA-C	5.23	117.38	110.84
1	A	874	ASP	CA-C-N	5.22	128.00	120.38
1	A	874	ASP	C-N-CA	5.22	128.00	120.38
4	E	160	GLU	CA-C-N	5.22	127.23	120.44
4	E	160	GLU	C-N-CA	5.22	127.23	120.44
1	A	288	ALA	CA-C-N	5.21	128.49	122.35
1	A	288	ALA	C-N-CA	5.21	128.49	122.35
3	C	213	PRO	N-CA-C	5.20	120.43	114.03
1	A	398	GLU	N-CA-C	-5.20	101.98	110.20
4	E	90	VAL	CA-C-N	5.19	127.76	120.28
4	E	90	VAL	C-N-CA	5.19	127.76	120.28
1	A	708	MET	CA-C-N	5.19	128.22	120.90
1	A	708	MET	C-N-CA	5.19	128.22	120.90
3	C	177	GLU	N-CA-C	-5.19	102.00	110.20
3	C	178	PHE	CA-CB-CG	5.19	118.99	113.80
3	C	220	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	91	PHE	CA-CB-CG	5.18	118.98	113.80
2	B	957	ASN	CA-C-N	5.18	128.59	120.82
2	B	957	ASN	C-N-CA	5.18	128.59	120.82
7	I	78	CYS	CA-C-N	-5.18	112.57	122.61
7	I	78	CYS	C-N-CA	-5.18	112.57	122.61
10	L	59	ALA	CA-C-N	5.17	129.02	121.31
10	L	59	ALA	C-N-CA	5.17	129.02	121.31
2	B	708	GLU	CA-C-N	5.17	131.41	121.54
2	B	708	GLU	C-N-CA	5.17	131.41	121.54
4	E	202	SER	N-CA-C	5.16	117.38	109.07
8	J	34	THR	CA-C-N	5.16	127.50	120.54
8	J	34	THR	C-N-CA	5.16	127.50	120.54
9	K	2	ASN	CA-C-N	5.15	127.57	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	2	ASN	C-N-CA	5.15	127.57	120.67
7	I	87	GLN	N-CA-C	-5.14	102.86	110.48
1	A	1292	PRO	N-CA-C	5.13	118.55	110.80
4	E	39	LEU	CA-C-N	5.13	127.46	120.54
4	E	39	LEU	C-N-CA	5.13	127.46	120.54
5	F	83	PRO	CA-C-N	5.12	128.74	121.42
5	F	83	PRO	C-N-CA	5.12	128.74	121.42
1	A	485	ASP	CA-CB-CG	5.12	117.72	112.60
4	E	46	TYR	N-CA-C	5.12	118.55	112.72
2	B	1140	ALA	CA-C-N	5.10	129.24	120.72
2	B	1140	ALA	C-N-CA	5.10	129.24	120.72
2	B	44	VAL	CA-C-N	5.10	127.42	120.54
2	B	44	VAL	C-N-CA	5.10	127.42	120.54
2	B	581	PHE	CA-CB-CG	5.10	118.90	113.80
2	B	39	ARG	N-CA-C	-5.10	105.91	111.82
3	C	4	GLU	N-CA-C	5.08	121.63	110.80
5	F	87	LYS	CA-C-N	5.08	127.09	120.28
5	F	87	LYS	C-N-CA	5.08	127.09	120.28
1	A	1393	ASN	CA-CB-CG	5.07	117.67	112.60
4	E	150	VAL	N-CA-CB	5.05	117.27	111.31
1	A	351	THR	CA-C-N	5.05	127.26	120.50
1	A	351	THR	C-N-CA	5.05	127.26	120.50
3	C	150	GLY	CA-C-N	5.04	129.43	121.56
3	C	150	GLY	C-N-CA	5.04	129.43	121.56
6	H	82	PRO	CA-C-N	5.04	131.17	121.54
6	H	82	PRO	C-N-CA	5.04	131.17	121.54
2	B	106	ASP	CA-CB-CG	5.04	117.64	112.60
8	J	55	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	1226	VAL	N-CA-C	5.04	115.16	108.11
2	B	397	ASP	N-CA-C	5.03	116.39	109.15
1	A	1371	LEU	CA-C-N	5.02	127.08	120.60
1	A	1371	LEU	C-N-CA	5.02	127.08	120.60
1	A	940	ARG	CA-C-N	5.01	127.41	120.29
1	A	940	ARG	C-N-CA	5.01	127.41	120.29
1	A	1354	ASN	CA-C-N	5.01	126.97	120.56
1	A	1354	ASN	C-N-CA	5.01	126.97	120.56
6	H	105	GLU	CB-CG-CD	5.01	121.11	112.60
2	B	366	GLN	N-CA-C	-5.00	106.43	112.88
9	K	102	LYS	CA-C-N	5.00	126.94	120.44
9	K	102	LYS	C-N-CA	5.00	126.94	120.44
2	B	1122	ARG	CA-C-N	5.00	127.23	120.38
2	B	1122	ARG	C-N-CA	5.00	127.23	120.38

There are no chirality outliers.

There are no planarity outliers.

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	11043	0	11133	217	0
2	B	8861	0	8884	184	0
3	C	2095	0	2051	48	0
4	E	1752	0	1776	32	0
5	F	688	0	707	6	0
6	H	1068	0	1040	17	0
7	I	971	0	927	17	0
8	J	532	0	542	23	0
9	K	919	0	929	19	0
10	L	363	0	386	11	0
11	R	109	0	55	0	0
12	T	159	0	91	2	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
15	R	32	0	12	0	0
All	All	28601	0	28533	496	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 9.

All (496) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:VAL:HG21	8:J:60:PHE:HB3	1.27	1.11
2:B:800:GLN:HB2	8:J:52:THR:HG22	1.19	1.08
2:B:862:GLN:HB3	2:B:963:PHE:HB2	1.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1094:ARG:HH11	2:B:1094:ARG:HG2	1.26	1.00
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.47	0.96
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.06	0.91
1:A:869:GLY:O	4:E:204:THR:HG21	1.70	0.91
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.51	0.90
1:A:567:LYS:HB3	6:H:96:VAL:H	1.35	0.90
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.53	0.89
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.37	0.88
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.63	0.79
1:A:741:ASN:HD22	1:A:744:LYS:H	1.26	0.79
2:B:848:ARG:HH22	2:B:996:ARG:NH1	1.80	0.79
2:B:54:PHE:HA	2:B:58:THR:HB	1.64	0.79
2:B:801:LYS:O	8:J:52:THR:HG23	1.83	0.79
2:B:654:ARG:H	2:B:657:HIS:HD2	1.29	0.77
2:B:1094:ARG:HG2	2:B:1094:ARG:NH1	1.99	0.76
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.34	0.74
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.69	0.74
2:B:451:LYS:HA	2:B:454:THR:HB	1.70	0.73
2:B:744:HIS:HD2	2:B:746:SER:H	1.35	0.73
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.22	0.72
7:I:28:GLU:HB3	7:I:35:VAL:HG13	1.72	0.72
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.54	0.72
3:C:56:THR:HG21	3:C:145:CYS:SG	2.30	0.72
2:B:1094:ARG:HH11	2:B:1094:ARG:CG	2.01	0.72
3:C:57:VAL:HG21	8:J:60:PHE:CB	2.14	0.71
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.53	0.71
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.71	0.70
1:A:1082:ASN:HB2	1:A:1097:GLY:HA3	1.74	0.70
2:B:1100:ASP:HA	2:B:1103:ILE:HG12	1.74	0.69
2:B:762:ASN:HD21	2:B:984:HIS:HD2	1.39	0.69
2:B:363:HIS:O	2:B:364:ILE:HB	1.91	0.69
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.58	0.69
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.75	0.68
8:J:48:ARG:O	8:J:52:THR:HB	1.93	0.68
1:A:709:THR:HB	1:A:712:GLU:HB2	1.75	0.68
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.75	0.68
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.75	0.68
2:B:825:VAL:HG23	2:B:1010:LEU:HB3	1.75	0.68
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.77	0.67
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.75	0.67
3:C:98:VAL:H	3:C:122:SER:HB2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.75	0.67
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.40	0.67
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.77	0.67
2:B:25:ILE:HG13	2:B:29:ASP:HB2	1.75	0.67
1:A:472:LEU:HD21	2:B:835:GLN:HB3	1.76	0.67
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.79	0.66
2:B:800:GLN:HB2	8:J:52:THR:CG2	2.11	0.66
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.24	0.65
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.77	0.65
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.11	0.65
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.78	0.65
2:B:515:HIS:HD2	2:B:517:THR:H	1.44	0.65
2:B:864:LYS:HG2	2:B:865:LYS:H	1.63	0.64
1:A:469:ARG:NH2	2:B:991:GLY:O	2.31	0.64
6:H:33:GLN:HB2	6:H:36:CYS:HB3	1.79	0.63
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.79	0.63
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.31	0.63
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.80	0.63
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.82	0.62
2:B:428:ILE:HG12	2:B:448:ILE:HG12	1.82	0.62
1:A:399:HIS:O	1:A:401:GLY:N	2.32	0.62
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.81	0.62
1:A:899:VAL:HB	1:A:929:LEU:HD22	1.81	0.62
1:A:1123:GLY:CA	1:A:1124:HIS:HB2	2.28	0.62
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.35	0.61
1:A:705:LYS:HE2	1:A:705:LYS:H	1.65	0.61
4:E:55:ARG:HA	4:E:58:MET:HG3	1.82	0.61
1:A:57:ARG:HA	1:A:68:GLN:HB3	1.83	0.61
1:A:1173:HIS:HB2	1:A:1227:ILE:HG23	1.82	0.61
1:A:711:ARG:HA	7:I:97:MET:HE1	1.83	0.61
1:A:378:GLU:OE2	1:A:434:ARG:HD3	2.00	0.61
1:A:754:SER:H	1:A:757:ASN:HD22	1.46	0.61
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.81	0.61
2:B:516:ASN:H	2:B:516:ASN:HD22	1.49	0.61
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.84	0.60
1:A:566:ILE:HD11	6:H:98:TYR:HB2	1.82	0.60
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.28	0.60
1:A:56:PRO:HB2	1:A:57:ARG:HH21	1.67	0.60
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.84	0.60
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.83	0.60
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:LEU:HD11	1:A:521:MET:HE2	1.83	0.60
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.84	0.59
2:B:835:GLN:O	2:B:838:SER:HB2	2.01	0.59
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.83	0.59
1:A:709:THR:HG22	1:A:711:ARG:H	1.67	0.59
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.83	0.59
8:J:3:VAL:CG1	8:J:18:TRP:HB2	2.29	0.59
1:A:569:LYS:HG2	1:A:571:LEU:HD13	1.84	0.59
1:A:669:THR:O	1:A:762:SER:HB3	2.03	0.59
2:B:563:MET:HE3	2:B:580:VAL:HB	1.85	0.59
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.68	0.59
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.03	0.59
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.85	0.59
2:B:783:THR:HG21	8:J:59:LYS:HB3	1.83	0.58
2:B:953:LEU:O	2:B:964:VAL:HG23	2.03	0.58
1:A:1154:TYR:CE2	1:A:1156:PRO:HG3	2.38	0.58
6:H:40:LEU:HD13	6:H:123:MET:HG3	1.86	0.58
1:A:1377:THR:HA	4:E:212:ARG:NH2	2.19	0.58
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.86	0.57
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.17	0.57
1:A:818:MET:HG3	2:B:514:LEU:HD23	1.85	0.57
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.86	0.57
1:A:434:ARG:HH21	1:A:437:MET:HB2	1.68	0.57
3:C:173:ALA:O	3:C:174:ALA:HB3	2.04	0.57
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.87	0.57
6:H:47:PHE:HB2	6:H:95:TYR:HD1	1.70	0.57
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.04	0.57
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.38	0.57
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.40	0.57
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.87	0.57
1:A:839:ARG:HH21	1:A:1402:PHE:HA	1.70	0.56
2:B:618:ASP:OD2	2:B:621:GLU:HB2	2.05	0.56
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.87	0.56
2:B:95:ILE:HD11	2:B:128:LEU:HB3	1.87	0.56
2:B:223:VAL:HG21	2:B:381:MET:HG2	1.88	0.56
5:F:116:ASP:HB3	5:F:119:ARG:HB2	1.87	0.56
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.85	0.56
1:A:670:ILE:HG13	2:B:1067:ARG:HH11	1.70	0.56
6:H:47:PHE:HB2	6:H:95:TYR:CD1	2.40	0.56
1:A:595:THR:HG21	1:A:604:GLY:HA3	1.87	0.56
2:B:601:ARG:HA	2:B:615:MET:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:HD12	1:A:235:ILE:HD13	1.86	0.56
3:C:31:ASN:O	3:C:35:ARG:HG3	2.06	0.56
12:T:22:DT:H2''	12:T:23:DC:H5'	1.88	0.56
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.14	0.55
2:B:705:MET:H	2:B:710:LEU:HG	1.71	0.55
1:A:494:SER:O	1:A:498:ARG:HG3	2.06	0.55
7:I:88:SER:C	7:I:90:GLN:H	2.14	0.55
10:L:38:LEU:HD21	10:L:48:CYS:HA	1.88	0.55
1:A:225:ASN:HD22	1:A:228:PHE:H	1.53	0.55
2:B:900:ALA:CB	10:L:61:THR:HG23	2.32	0.55
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.88	0.55
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.87	0.55
1:A:474:VAL:HG23	1:A:521:MET:HE3	1.88	0.55
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.89	0.55
7:I:88:SER:HB2	7:I:90:GLN:HB2	1.89	0.55
10:L:38:LEU:HD22	10:L:56:LEU:HD21	1.88	0.55
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.42	0.54
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.42	0.54
4:E:147:HIS:CD2	4:E:149:LEU:HB2	2.42	0.54
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.21	0.54
2:B:35:SER:O	2:B:39:ARG:HB2	2.08	0.54
3:C:262:LEU:HD11	9:K:87:LEU:HD23	1.89	0.54
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.38	0.54
1:A:40:THR:HG22	1:A:49:LYS:HD2	1.90	0.54
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.90	0.54
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.90	0.54
2:B:243:ALA:HB2	2:B:251:ILE:HD13	1.89	0.53
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.43	0.53
1:A:1325:THR:HA	4:E:147:HIS:HA	1.90	0.53
2:B:429:PHE:HA	2:B:432:MET:HE3	1.91	0.53
1:A:211:PHE:HA	1:A:214:ILE:HD11	1.91	0.53
1:A:1148:ILE:HB	1:A:1196:GLU:HG3	1.91	0.53
2:B:843:GLN:HB2	2:B:993:THR:HB	1.90	0.53
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.74	0.53
4:E:154:ILE:HD13	4:E:199:ILE:HD12	1.92	0.52
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.92	0.52
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.89	0.52
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.74	0.52
2:B:848:ARG:NH2	2:B:996:ARG:NH1	2.54	0.52
1:A:406:ILE:HG12	1:A:412:ARG:HG2	1.92	0.52
2:B:486:TYR:OH	2:B:1096:ARG:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:19:VAL:O	4:E:23:VAL:HG23	2.10	0.52
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.74	0.52
2:B:563:MET:HE1	2:B:587:HIS:HB2	1.92	0.52
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.90	0.52
3:C:148:ARG:H	3:C:151:GLN:HG3	1.75	0.52
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.45	0.52
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.91	0.52
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.45	0.52
4:E:147:HIS:CD2	4:E:149:LEU:H	2.27	0.52
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.92	0.51
2:B:428:ILE:HG22	2:B:432:MET:HE2	1.92	0.51
2:B:563:MET:HA	2:B:589:VAL:O	2.09	0.51
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.92	0.51
2:B:1122:ARG:HG2	12:T:23:DC:OP1	2.10	0.51
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.36	0.51
4:E:179:GLN:O	4:E:182:ASP:HB2	2.11	0.51
2:B:864:LYS:HB2	2:B:871:THR:HG23	1.92	0.51
3:C:167:HIS:HD2	3:C:169:LYS:H	1.58	0.51
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.93	0.51
7:I:10:CYS:SG	7:I:31:THR:HB	2.50	0.51
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.45	0.51
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	1.92	0.51
9:K:40:HIS:CE1	9:K:63:VAL:HG11	2.45	0.51
1:A:108:MET:HE3	1:A:172:PRO:HD2	1.93	0.51
1:A:472:LEU:O	1:A:475:THR:HB	2.10	0.51
1:A:775:ILE:HG21	1:A:815:PHE:CE2	2.46	0.51
2:B:377:PHE:CE2	2:B:381:MET:HE2	2.46	0.51
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.75	0.51
2:B:345:LYS:HG2	2:B:348:ARG:HD3	1.92	0.51
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.46	0.51
2:B:577:ALA:HB1	2:B:589:VAL:HB	1.92	0.50
2:B:1181:GLU:HB2	2:B:1188:LYS:HG2	1.93	0.50
3:C:175:ALA:HB3	8:J:43:ARG:HH21	1.76	0.50
1:A:741:ASN:ND2	1:A:744:LYS:H	2.03	0.50
4:E:31:THR:OG1	4:E:34:GLU:HB2	2.11	0.50
3:C:69:LEU:O	8:J:6:ARG:HD2	2.10	0.50
1:A:113:LEU:HD23	1:A:218:ASP:HB3	1.94	0.50
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.45	0.50
2:B:904:ARG:HG2	2:B:948:ILE:HG12	1.94	0.50
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.94	0.50
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.77	0.50
2:B:516:ASN:H	2:B:516:ASN:ND2	2.08	0.50
1:A:78:PRO:HB3	2:B:1201:LYS:HD2	1.92	0.50
1:A:821:ARG:HG3	1:A:825:ILE:CD1	2.41	0.49
1:A:738:LYS:HD3	1:A:740:LEU:HD21	1.93	0.49
3:C:73:GLN:HA	3:C:133:ILE:HD11	1.94	0.49
1:A:5:GLN:HE22	2:B:1176:ASN:HD22	1.60	0.49
1:A:372:LYS:HG2	1:A:435:HIS:CD2	2.48	0.49
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.95	0.49
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.46	0.49
9:K:85:ASP:HA	9:K:88:LYS:HG2	1.94	0.49
1:A:121:LEU:HA	1:A:124:GLN:HB2	1.94	0.49
3:C:33:LEU:HG	3:C:37:MET:HE3	1.95	0.49
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.47	0.49
2:B:620:ARG:HH21	7:I:89:GLN:HE22	1.61	0.49
2:B:910:VAL:HG11	2:B:938:SER:HB3	1.95	0.48
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.60	0.48
1:A:1035:TYR:HB3	1:A:1037:LEU:HD13	1.95	0.48
3:C:39:ALA:HB1	3:C:165:LYS:HB2	1.96	0.48
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.96	0.48
2:B:797:TYR:HB2	2:B:852:ARG:O	2.14	0.48
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.95	0.48
6:H:28:ALA:HB3	6:H:38:LEU:HB3	1.95	0.48
1:A:140:THR:HA	1:A:143:LYS:HE3	1.94	0.48
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.78	0.48
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.95	0.48
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.96	0.48
10:L:61:THR:HB	10:L:63:ARG:H	1.78	0.48
1:A:534:LEU:O	1:A:574:GLY:HA3	2.13	0.48
3:C:46:ILE:HG23	3:C:157:CYS:HB2	1.94	0.48
10:L:40:LEU:HB3	10:L:44:ASP:HB2	1.96	0.48
1:A:21:LEU:HD12	1:A:229:SER:HB2	1.95	0.48
1:A:335:ARG:HD3	2:B:1202:LEU:HD12	1.94	0.48
1:A:885:THR:O	1:A:940:ARG:HD2	2.12	0.48
7:I:19:ASP:HB2	7:I:24:ARG:HG3	1.95	0.48
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.95	0.48
1:A:1318:THR:HG22	4:E:142:VAL:HG22	1.95	0.48
1:A:58:LEU:HD23	1:A:244:PRO:HD3	1.95	0.48
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.96	0.48
2:B:882:THR:HG23	2:B:885:MET:HE3	1.96	0.48
2:B:879:ARG:HH12	2:B:885:MET:HG3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:80:VAL:HG22	4:E:109:ILE:HD12	1.95	0.47
1:A:89:PRO:HB3	1:A:237:THR:HG23	1.96	0.47
4:E:147:HIS:HD2	4:E:149:LEU:H	1.62	0.47
3:C:37:MET:HE2	3:C:244:VAL:HA	1.96	0.47
1:A:274:ILE:C	1:A:276:LEU:H	2.23	0.47
1:A:761:MET:HG3	2:B:1021:MET:HG3	1.95	0.47
1:A:775:ILE:HG21	1:A:815:PHE:CD2	2.50	0.47
1:A:858:ASN:HD21	1:A:860:LEU:HD12	1.78	0.47
1:A:1353:TYR:CD2	1:A:1353:TYR:C	2.93	0.47
1:A:605:MET:HE2	1:A:607:ILE:HG13	1.97	0.47
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.97	0.47
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.97	0.47
2:B:190:TYR:CD1	8:J:62:ARG:HG2	2.50	0.47
1:A:404:TYR:HB2	1:A:433:GLU:HG3	1.97	0.47
2:B:901:PRO:HD3	10:L:58:LYS:HB3	1.96	0.47
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.96	0.47
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.45	0.47
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.45	0.47
1:A:456:MET:HB2	1:A:478:TYR:OH	2.15	0.47
2:B:822:ASN:HD22	8:J:52:THR:CG2	2.26	0.47
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.81	0.46
2:B:910:VAL:CG1	2:B:938:SER:HB3	2.44	0.46
3:C:104:PHE:CD1	3:C:152:GLU:HG3	2.46	0.46
5:F:83:PRO:HG2	5:F:84:TYR:CD1	2.50	0.46
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.97	0.46
1:A:1116:LEU:HD13	1:A:1329:THR:HB	1.97	0.46
2:B:273:LEU:HD12	2:B:280:ILE:HG13	1.97	0.46
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.45	0.46
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.96	0.46
3:C:185:LYS:HG2	3:C:213:PRO:HG3	1.97	0.46
4:E:125:PRO:O	4:E:127:ILE:N	2.47	0.46
2:B:308:TRP:CH2	7:I:45:ARG:HD3	2.50	0.46
2:B:387:LEU:HD23	2:B:393:LYS:HD3	1.97	0.46
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.80	0.46
3:C:22:LEU:HD11	9:K:101:LEU:HD21	1.98	0.46
4:E:98:ILE:HA	4:E:101:GLN:HG2	1.98	0.46
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.96	0.46
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.97	0.46
2:B:487:THR:H	2:B:490:SER:HB3	1.81	0.46
6:H:56:THR:HB	6:H:145:ARG:HB3	1.97	0.46
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:610:ASN:HB3	2:B:613:VAL:HG23	1.97	0.46
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.51	0.46
1:A:672:ASP:HB2	1:A:675:THR:OG1	2.16	0.46
1:A:672:ASP:CG	1:A:736:ASN:HD21	2.24	0.46
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.98	0.46
2:B:778:MET:HG2	2:B:794:ASN:HB3	1.96	0.46
2:B:864:LYS:H	2:B:872:GLU:HB2	1.80	0.46
2:B:1099:VAL:HB	2:B:1103:ILE:HD11	1.98	0.46
4:E:65:THR:O	4:E:69:ILE:HG12	2.16	0.46
1:A:89:PRO:HG2	1:A:205:GLU:HG2	1.98	0.46
1:A:528:LEU:O	1:A:531:ILE:HG22	2.16	0.46
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.97	0.46
1:A:512:VAL:HA	1:A:519:PRO:HA	1.98	0.45
2:B:704:ALA:HB1	2:B:710:LEU:HB3	1.98	0.45
1:A:761:MET:CG	2:B:1021:MET:HG3	2.46	0.45
1:A:1116:LEU:HB2	1:A:1308:THR:CG2	2.47	0.45
4:E:165:LEU:HD23	4:E:170:LEU:HB2	1.98	0.45
7:I:96:SER:C	7:I:98:VAL:H	2.24	0.45
1:A:116:ASP:HA	1:A:117:GLU:HA	1.77	0.45
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.65	0.45
1:A:559:VAL:HG13	6:H:78:SER:HA	1.97	0.45
1:A:711:ARG:NH2	7:I:87:GLN:OE1	2.49	0.45
4:E:89:GLY:O	4:E:120:ALA:HB2	2.17	0.45
1:A:34:LYS:HE2	1:A:57:ARG:HH22	1.81	0.45
1:A:523:ILE:HG23	1:A:527:THR:HB	1.98	0.45
3:C:123:ASN:HD22	3:C:125:MET:HG3	1.80	0.45
2:B:68:THR:HA	2:B:90:ILE:O	2.17	0.45
2:B:654:ARG:H	2:B:657:HIS:CD2	2.20	0.45
3:C:181:ASP:OD2	3:C:184:ASN:HA	2.17	0.45
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.97	0.45
2:B:683:SER:O	2:B:687:GLU:HB2	2.17	0.45
3:C:258:ILE:HG13	9:K:42:LEU:HD21	1.99	0.45
1:A:18:GLN:HE21	1:A:1418:LEU:HB2	1.80	0.45
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.52	0.45
2:B:758:PHE:CZ	2:B:1031:LEU:HD22	2.51	0.45
2:B:1037:LEU:O	8:J:47:ARG:NH1	2.50	0.45
3:C:173:ALA:O	3:C:174:ALA:CB	2.65	0.45
9:K:113:THR:O	9:K:114:LEU:HB2	2.17	0.45
1:A:560:ILE:HB	6:H:79:TRP:HB3	1.99	0.44
1:A:1095:THR:HG21	1:A:1112:LYS:HB3	1.98	0.44
1:A:75:ASN:HA	2:B:1116:ARG:NH1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:TYR:HB3	2:B:140:ILE:HD11	1.99	0.44
2:B:732:SER:O	2:B:734:HIS:N	2.50	0.44
4:E:28:TYR:HA	4:E:64:PRO:HA	1.99	0.44
1:A:579:SER:HA	1:A:582:ILE:HD12	1.98	0.44
2:B:195:CYS:HA	2:B:196:PRO:HD3	1.92	0.44
3:C:6:PRO:HB3	3:C:25:VAL:HG22	1.99	0.44
7:I:102:VAL:HG22	7:I:109:ILE:HG12	1.99	0.44
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.82	0.44
1:A:1116:LEU:HB2	1:A:1308:THR:HG21	1.99	0.44
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.52	0.44
1:A:115:LEU:HD11	1:A:145:LYS:HG3	2.00	0.44
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.99	0.44
1:A:358:ASN:HB2	9:K:65:HIS:HD2	1.82	0.44
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.97	0.44
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.32	0.44
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.99	0.44
1:A:696:GLU:HG2	1:A:702:LEU:HD23	1.99	0.44
2:B:209:GLU:CD	2:B:485:ARG:HH21	2.26	0.44
2:B:804:GLY:O	2:B:983:ARG:NH2	2.51	0.44
2:B:1082:MET:HA	3:C:189:THR:HA	1.99	0.44
4:E:193:GLY:HA2	4:E:213:ILE:HD11	2.00	0.44
6:H:82:PRO:O	6:H:84:ALA:N	2.51	0.44
6:H:130:ARG:HA	6:H:133:ASN:HD21	1.83	0.44
1:A:1328:TYR:OH	1:A:1351:GLU:OE1	2.31	0.44
2:B:256:VAL:HG12	2:B:385:LEU:HD22	1.99	0.44
2:B:893:LEU:HD22	2:B:897:GLY:C	2.43	0.44
9:K:55:LYS:HB2	9:K:81:TYR:CE1	2.53	0.44
1:A:167:CYS:SG	1:A:168:GLY:N	2.91	0.44
1:A:246:VAL:HA	2:B:1202:LEU:HD21	1.99	0.44
1:A:325:ILE:H	1:A:325:ILE:HG13	1.69	0.44
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.99	0.44
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.18	0.44
2:B:900:ALA:HA	10:L:58:LYS:HD3	1.99	0.44
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.47	0.44
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	2.00	0.44
2:B:824:ILE:HG12	8:J:48:ARG:NH2	2.33	0.44
1:A:74:MET:C	1:A:76:GLU:H	2.26	0.43
1:A:708:MET:HE1	1:A:1089:VAL:HG12	2.00	0.43
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.58	0.43
2:B:773:MET:O	2:B:776:GLN:HB2	2.17	0.43
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:VAL:HG22	3:C:157:CYS:HB3	1.99	0.43
1:A:567:LYS:CB	1:A:568:PRO:CD	2.93	0.43
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	2.00	0.43
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.53	0.43
1:A:925:LEU:HD23	1:A:925:LEU:HA	1.90	0.43
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.83	0.43
2:B:282:ILE:HA	2:B:285:ILE:HD12	2.00	0.43
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.58	0.43
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.83	0.43
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.99	0.43
6:H:44:VAL:HG23	6:H:49:VAL:H	1.82	0.43
8:J:1:MET:SD	8:J:60:PHE:HE2	2.42	0.43
1:A:642:CYS:O	1:A:645:LEU:HB3	2.18	0.43
3:C:26:ASP:OD2	3:C:29:MET:HB2	2.18	0.43
1:A:534:LEU:HA	1:A:539:THR:HG21	2.00	0.43
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.67	0.43
2:B:976:ILE:O	2:B:990:ILE:O	2.36	0.43
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.83	0.43
2:B:860:MET:HE3	2:B:860:MET:HB3	1.92	0.43
1:A:365:GLY:HA3	1:A:469:ARG:HB2	2.01	0.43
3:C:238:ILE:HG23	3:C:242:GLN:HB2	2.00	0.43
10:L:55:ILE:H	10:L:55:ILE:HG12	1.65	0.43
2:B:526:GLU:HG3	2:B:771:SER:HB3	2.01	0.42
4:E:29:PHE:HB2	4:E:65:THR:HG23	2.00	0.42
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.96	0.42
1:A:1271:ILE:HD13	1:A:1271:ILE:HA	1.97	0.42
1:A:182:VAL:HA	1:A:202:LEU:HB3	2.00	0.42
1:A:247:ARG:HB3	1:A:262:LEU:HB3	2.02	0.42
1:A:440:ASP:O	1:A:460:VAL:HG23	2.19	0.42
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.73	0.42
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.85	0.42
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.54	0.42
2:B:745:PRO:O	2:B:748:ILE:HG12	2.19	0.42
4:E:37:LEU:HA	4:E:38:PRO:HD3	1.96	0.42
7:I:58:VAL:HG11	7:I:109:ILE:HD11	2.02	0.42
1:A:589:GLN:HB3	1:A:961:ARG:HH22	1.85	0.42
2:B:228:LYS:O	2:B:261:ARG:NH2	2.51	0.42
2:B:956:THR:HB	10:L:46:VAL:HG21	2.00	0.42
2:B:975:GLN:O	2:B:990:ILE:HD12	2.19	0.42
2:B:1158:PHE:HD2	2:B:1160:VAL:HG22	1.84	0.42
1:A:93:VAL:HG22	1:A:304:MET:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:LEU:HB2	2:B:276:ILE:HG22	2.01	0.42
3:C:66:ARG:NH2	8:J:3:VAL:O	2.43	0.42
1:A:351:THR:OG1	2:B:1103:ILE:CD1	2.68	0.42
1:A:594:GLY:HA3	1:A:601:LYS:HE2	2.01	0.42
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.54	0.42
2:B:459:TYR:CD2	2:B:468:GLU:HA	2.55	0.42
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.85	0.42
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.20	0.42
9:K:57:LEU:HB2	9:K:76:GLN:HG2	2.01	0.42
9:K:77:THR:HB	9:K:81:TYR:HB3	2.02	0.42
1:A:1217:LYS:O	1:A:1221:LYS:HA	2.20	0.41
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	2.01	0.41
2:B:827:ILE:HA	2:B:1012:ILE:O	2.20	0.41
3:C:100:THR:HG22	3:C:119:VAL:HG13	2.00	0.41
3:C:167:HIS:CD2	3:C:169:LYS:HG2	2.55	0.41
9:K:39:ASP:HB2	9:K:40:HIS:H	1.71	0.41
1:A:345:VAL:HG12	2:B:1155:SER:HB2	2.02	0.41
2:B:620:ARG:NH2	7:I:89:GLN:HE22	2.18	0.41
1:A:134:ARG:HD3	1:A:221:SER:O	2.21	0.41
1:A:380:VAL:CG1	1:A:385:ILE:HD12	2.50	0.41
2:B:377:PHE:HE2	2:B:381:MET:HE2	1.85	0.41
1:A:841:LEU:HD12	1:A:1384:VAL:HG11	2.01	0.41
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.56	0.41
4:E:23:VAL:HG12	4:E:28:TYR:HB2	2.02	0.41
4:E:76:GLY:HA3	4:E:106:GLN:HB2	2.01	0.41
5:F:130:ILE:HB	5:F:148:VAL:HG11	2.03	0.41
7:I:75:CYS:O	7:I:78:CYS:O	2.38	0.41
7:I:97:MET:HE2	7:I:97:MET:HB2	1.63	0.41
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.03	0.41
1:A:491:VAL:O	1:A:493:GLN:NE2	2.54	0.41
1:A:600:PRO:HA	6:H:25:ARG:NH1	2.35	0.41
3:C:259:LEU:HD22	9:K:91:CYS:HB3	2.01	0.41
4:E:9:ILE:HG22	4:E:39:LEU:HD11	2.02	0.41
4:E:198:ILE:HD13	4:E:212:ARG:HG3	2.02	0.41
1:A:1216:ILE:HG22	1:A:1226:VAL:HG21	2.02	0.41
2:B:282:ILE:HD13	2:B:382:ILE:HD13	2.02	0.41
2:B:313:MET:HE2	2:B:386:LEU:HD22	2.01	0.41
1:A:527:THR:HG21	1:A:650:GLN:HA	2.02	0.41
1:A:902:LEU:HG	1:A:926:GLN:HG3	2.03	0.41
1:A:1111:MET:HE2	1:A:1111:MET:HB3	1.99	0.41
3:C:62:PHE:O	3:C:66:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:HB3	1:A:316:GLN:H	1.79	0.41
1:A:353:ILE:HG22	1:A:468:PHE:HB2	2.01	0.41
1:A:361:LEU:HD12	1:A:471:ASN:HD22	1.85	0.41
1:A:513:SER:HB3	1:A:520:CYS:HB3	2.03	0.41
1:A:588:LEU:HB3	1:A:607:ILE:HD12	2.02	0.41
1:A:786:HIS:CE1	2:B:742:GLU:OE1	2.68	0.41
1:A:839:ARG:HB2	1:A:839:ARG:HH11	1.85	0.41
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	2.11	0.41
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.03	0.41
2:B:1162:ILE:HG12	2:B:1194:ILE:HG12	2.02	0.41
3:C:36:VAL:HG23	3:C:40:GLU:HB2	2.03	0.41
3:C:105:GLY:O	3:C:149:LYS:O	2.37	0.41
7:I:62:ILE:HG12	7:I:84:VAL:HG21	2.03	0.41
1:A:392:VAL:HG13	1:A:415:LEU:HD11	2.04	0.41
1:A:483:ASP:HA	2:B:988:GLY:HA2	2.03	0.41
1:A:567:LYS:O	1:A:568:PRO:C	2.64	0.41
2:B:706:GLN:O	2:B:710:LEU:HB2	2.21	0.41
1:A:496:GLU:H	1:A:496:GLU:HG2	1.78	0.40
1:A:592:ASP:H	1:A:595:THR:HG21	1.85	0.40
2:B:1039:GLY:O	8:J:32:GLU:HB2	2.21	0.40
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.57	0.40
6:H:63:LEU:HB2	6:H:90:ALA:H	1.86	0.40
9:K:7:PHE:HA	9:K:10:PHE:CZ	2.55	0.40
1:A:640:GLN:CD	1:A:640:GLN:H	2.30	0.40
2:B:563:MET:HE1	2:B:587:HIS:CB	2.51	0.40
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.21	0.40
3:C:73:GLN:O	3:C:129:ILE:HA	2.21	0.40
8:J:48:ARG:HD2	8:J:49:MET:HE2	2.03	0.40
1:A:389:THR:O	1:A:393:ARG:HG2	2.22	0.40
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	2.02	0.40
2:B:123:THR:HG23	2:B:205:ILE:HA	2.03	0.40
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.56	0.40
4:E:100:ILE:HG13	4:E:105:PHE:HB2	2.03	0.40
1:A:387:ARG:HD2	1:A:437:MET:HE1	2.04	0.40
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.03	0.40
1:A:737:LEU:HD11	1:A:758:ILE:HG23	2.03	0.40
1:A:852:TYR:O	5:F:81:THR:HG22	2.21	0.40
4:E:46:TYR:HD2	4:E:57:MET:HB3	1.86	0.40
1:A:113:LEU:HD21	1:A:222:LEU:HD13	2.03	0.40
1:A:351:THR:OG1	2:B:1103:ILE:HD13	2.21	0.40
1:A:358:ASN:HB2	9:K:65:HIS:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.22	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%)	1205 (86%)	137 (10%)	53 (4%)	2	18
2	B	1096/1224 (90%)	958 (87%)	90 (8%)	48 (4%)	2	15
3	C	264/318 (83%)	238 (90%)	19 (7%)	7 (3%)	4	25
4	E	212/215 (99%)	185 (87%)	22 (10%)	5 (2%)	4	28
5	F	83/155 (54%)	75 (90%)	6 (7%)	2 (2%)	4	28
6	H	129/146 (88%)	102 (79%)	18 (14%)	9 (7%)	1	6
7	I	117/122 (96%)	101 (86%)	14 (12%)	2 (2%)	7	35
8	J	63/70 (90%)	55 (87%)	7 (11%)	1 (2%)	7	36
9	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
10	L	44/70 (63%)	27 (61%)	7 (16%)	10 (23%)	0	0
All	All	3515/4173 (84%)	3053 (87%)	325 (9%)	137 (4%)	2	18

All (137) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	65	LEU
1	A	119	ASN
1	A	399	HIS
1	A	424	ILE
1	A	567	LYS

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Mol	Chain	Res	Type
1	A	597	LEU
1	A	846	GLU
1	A	1123	GLY
1	A	1221	LYS
1	A	1378	GLN
1	A	1437	GLY
2	B	137	TYR
2	B	476	ARG
2	B	510	LYS
2	B	648	HIS
2	B	709	ASP
2	B	712	PRO
2	B	733	HIS
2	B	751	VAL
2	B	1046	PRO
2	B	1156	ASP
3	C	40	GLU
3	C	215	GLU
3	C	227	THR
4	E	126	SER
5	F	73	ALA
6	H	83	GLN
6	H	131	ASN
7	I	91	ARG
8	J	6	ARG
10	L	50	ASP
1	A	68	GLN
1	A	250	ILE
1	A	312	PRO
1	A	332	LYS
1	A	385	ILE
1	A	672	ASP
1	A	1124	HIS
1	A	1188	GLN
1	A	1377	THR
2	B	67	SER
2	B	138	GLU
2	B	168	GLY
2	B	176	SER
2	B	277	LYS
2	B	364	ILE
2	B	480	SER

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Mol	Chain	Res	Type
2	B	531	GLN
2	B	708	GLU
2	B	891	ASP
2	B	1171	VAL
2	B	1181	GLU
3	C	174	ALA
6	H	90	ALA
7	I	115	LYS
10	L	49	LYS
10	L	51	CYS
10	L	64	LEU
1	A	42	ASP
1	A	308	ILE
1	A	324	SER
1	A	592	ASP
1	A	595	THR
1	A	1089	VAL
2	B	250	PHE
2	B	367	LEU
2	B	468	GLU
2	B	792	MET
2	B	864	LYS
2	B	865	LYS
2	B	879	ARG
2	B	887	HIS
2	B	974	PRO
2	B	1157	ALA
2	B	1180	PHE
2	B	1223	ASP
3	C	4	GLU
4	E	3	GLN
4	E	99	HIS
5	F	112	GLU
6	H	18	GLY
6	H	108	SER
10	L	40	LEU
1	A	53	LEU
1	A	56	PRO
1	A	110	CYS
1	A	111	GLY
1	A	149	GLU
1	A	214	ILE

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Mol	Chain	Res	Type
1	A	275	SER
1	A	569	LYS
1	A	852	TYR
2	B	474	SER
2	B	943	SER
2	B	1017	ILE
3	C	90	ASP
4	E	51	GLY
6	H	109	LYS
6	H	136	LYS
6	H	140	ALA
10	L	47	ARG
10	L	55	ILE
10	L	56	LEU
1	A	217	LYS
1	A	400	PRO
1	A	576	GLN
1	A	916	GLY
1	A	958	VAL
1	A	1376	THR
2	B	139	ALA
2	B	1099	VAL
10	L	46	VAL
10	L	59	ALA
1	A	543	LEU
1	A	1028	THR
2	B	177	LYS
2	B	447	ALA
2	B	471	LYS
4	E	37	LEU
1	A	73	GLY
1	A	258	GLY
1	A	325	ILE
2	B	647	GLY
3	C	5	GLY
1	A	35	ILE
1	A	1122	PRO
1	A	1388	GLY
2	B	592	ASN
2	B	479	VAL
2	B	711	GLU
2	B	907	GLY

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Mol	Chain	Res	Type
2	B	1119	VAL
6	H	107	VAL
1	A	973	ILE
1	A	1384	VAL
1	A	775	ILE

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%)	1025 (84%)	200 (16%)	2	12
2	B	967/1061 (91%)	824 (85%)	143 (15%)	3	15
3	C	234/274 (85%)	197 (84%)	37 (16%)	2	13
4	E	196/197 (100%)	171 (87%)	25 (13%)	4	20
5	F	75/137 (55%)	63 (84%)	12 (16%)	2	13
6	H	117/128 (91%)	98 (84%)	19 (16%)	2	12
7	I	113/116 (97%)	98 (87%)	15 (13%)	4	19
8	J	60/65 (92%)	50 (83%)	10 (17%)	2	11
9	K	99/102 (97%)	82 (83%)	17 (17%)	2	10
10	L	40/57 (70%)	26 (65%)	14 (35%)	0	0
All	All	3126/3657 (86%)	2634 (84%)	492 (16%)	2	13

All (492) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	THR
1	A	18	GLN
1	A	21	LEU
1	A	44	THR
1	A	50	ILE
1	A	58	LEU
1	A	62	ASP

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Mol	Chain	Res	Type
1	A	65	LEU
1	A	68	GLN
1	A	75	ASN
1	A	93	VAL
1	A	113	LEU
1	A	117	GLU
1	A	126	LEU
1	A	133	LYS
1	A	141	LEU
1	A	144	THR
1	A	147	VAL
1	A	152	VAL
1	A	170	THR
1	A	206	GLU
1	A	214	ILE
1	A	219	PHE
1	A	220	THR
1	A	226	GLU
1	A	232	GLU
1	A	235	ILE
1	A	237	THR
1	A	252	PHE
1	A	254	GLU
1	A	263	THR
1	A	265	LYS
1	A	266	LEU
1	A	269	ILE
1	A	270	LEU
1	A	276	LEU
1	A	278	THR
1	A	279	LEU
1	A	290	GLU
1	A	291	GLU
1	A	295	LEU
1	A	308	ILE
1	A	311	GLN
1	A	315	LEU
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	329	LEU
1	A	335	ARG

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Mol	Chain	Res	Type
1	A	344	ARG
1	A	353	ILE
1	A	354	SER
1	A	359	LEU
1	A	368	LYS
1	A	372	LYS
1	A	389	THR
1	A	397	ASN
1	A	398	GLU
1	A	407	ARG
1	A	424	ILE
1	A	425	GLN
1	A	427	GLN
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	455	MET
1	A	456	MET
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	493	GLN
1	A	500	GLU
1	A	513	SER
1	A	518	LYS
1	A	524	VAL
1	A	527	THR
1	A	532	ARG
1	A	537	ARG
1	A	541	ILE
1	A	560	ILE
1	A	590	ARG
1	A	595	THR
1	A	597	LEU
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	636	GLU
1	A	640	GLN
1	A	644	LYS

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Mol	Chain	Res	Type
1	A	664	THR
1	A	672	ASP
1	A	676	MET
1	A	678	GLU
1	A	681	GLU
1	A	687	LYS
1	A	688	LYS
1	A	691	LEU
1	A	705	LYS
1	A	710	LEU
1	A	712	GLU
1	A	719	VAL
1	A	722	LEU
1	A	728	LYS
1	A	740	LEU
1	A	743	VAL
1	A	756	ILE
1	A	762	SER
1	A	773	LYS
1	A	821	ARG
1	A	838	GLN
1	A	839	ARG
1	A	867	ILE
1	A	878	ILE
1	A	879	GLU
1	A	883	LEU
1	A	886	ILE
1	A	894	GLU
1	A	896	ARG
1	A	902	LEU
1	A	905	ASP
1	A	908	LEU
1	A	912	LEU
1	A	919	ILE
1	A	920	LEU
1	A	926	GLN
1	A	927	VAL
1	A	935	GLN
1	A	941	LYS
1	A	953	ASN
1	A	969	GLN
1	A	973	ILE

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Mol	Chain	Res	Type
1	A	982	THR
1	A	988	LEU
1	A	992	ASP
1	A	999	VAL
1	A	1005	GLU
1	A	1006	ILE
1	A	1029	ARG
1	A	1032	LEU
1	A	1037	LEU
1	A	1048	ASN
1	A	1062	GLU
1	A	1064	VAL
1	A	1067	LEU
1	A	1081	LEU
1	A	1086	PHE
1	A	1089	VAL
1	A	1109	LYS
1	A	1110	ASN
1	A	1116	LEU
1	A	1124	HIS
1	A	1141	THR
1	A	1147	THR
1	A	1165	GLU
1	A	1168	GLU
1	A	1172	LEU
1	A	1175	SER
1	A	1187	GLN
1	A	1195	LEU
1	A	1227	ILE
1	A	1237	ILE
1	A	1242	VAL
1	A	1256	GLU
1	A	1259	MET
1	A	1261	LYS
1	A	1269	GLU
1	A	1271	ILE
1	A	1279	ILE
1	A	1280	GLU
1	A	1283	VAL
1	A	1284	MET
1	A	1288	ASP
1	A	1291	VAL

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Mol	Chain	Res	Type
1	A	1293	SER
1	A	1295	THR
1	A	1297	GLU
1	A	1303	GLU
1	A	1308	THR
1	A	1327	ILE
1	A	1333	ILE
1	A	1350	LYS
1	A	1354	ASN
1	A	1364	ASN
1	A	1366	ARG
1	A	1376	THR
1	A	1382	THR
1	A	1384	VAL
1	A	1385	THR
1	A	1391	ARG
1	A	1406	VAL
1	A	1426	GLU
1	A	1432	GLN
1	A	1433	MET
1	A	1436	ILE
1	A	1438	THR
1	A	1444	MET
1	A	1445	ILE
2	B	28	GLU
2	B	41	LYS
2	B	45	SER
2	B	46	GLN
2	B	63	ILE
2	B	66	ASP
2	B	89	GLU
2	B	97	VAL
2	B	101	MET
2	B	102	VAL
2	B	128	LEU
2	B	130	VAL
2	B	165	VAL
2	B	167	ILE
2	B	175	ARG
2	B	178	ASN
2	B	187	SER
2	B	194	GLU

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Mol	Chain	Res	Type
2	B	208	SER
2	B	217	ARG
2	B	221	ASN
2	B	222	ILE
2	B	228	LYS
2	B	234	ILE
2	B	240	ILE
2	B	245	GLU
2	B	261	ARG
2	B	265	SER
2	B	276	ILE
2	B	277	LYS
2	B	282	ILE
2	B	292	ILE
2	B	305	VAL
2	B	306	ASN
2	B	313	MET
2	B	323	VAL
2	B	325	GLN
2	B	345	LYS
2	B	350	GLN
2	B	367	LEU
2	B	373	ARG
2	B	384	ARG
2	B	392	ARG
2	B	393	LYS
2	B	394	ASP
2	B	408	LEU
2	B	418	LYS
2	B	426	LYS
2	B	433	GLN
2	B	437	GLU
2	B	448	ILE
2	B	458	LYS
2	B	461	LEU
2	B	468	GLU
2	B	471	LYS
2	B	473	MET
2	B	479	VAL
2	B	485	ARG
2	B	487	THR
2	B	498	THR

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Mol	Chain	Res	Type
2	B	510	LYS
2	B	516	ASN
2	B	526	GLU
2	B	537	LYS
2	B	547	VAL
2	B	554	ILE
2	B	567	GLU
2	B	574	SER
2	B	591	ARG
2	B	598	GLU
2	B	604	ARG
2	B	616	ILE
2	B	620	ARG
2	B	642	ASP
2	B	645	SER
2	B	649	LYS
2	B	653	VAL
2	B	655	LYS
2	B	687	GLU
2	B	690	VAL
2	B	696	GLU
2	B	706	GLN
2	B	711	GLU
2	B	737	THR
2	B	743	ILE
2	B	776	GLN
2	B	780	VAL
2	B	786	ASN
2	B	791	THR
2	B	795	ILE
2	B	797	TYR
2	B	801	LYS
2	B	807	ARG
2	B	810	GLU
2	B	815	ARG
2	B	835	GLN
2	B	838	SER
2	B	844	SER
2	B	850	LEU
2	B	870	ILE
2	B	875	GLU
2	B	880	THR

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Mol	Chain	Res	Type
2	B	883	LEU
2	B	886	LYS
2	B	906	SER
2	B	945	GLU
2	B	953	LEU
2	B	954	VAL
2	B	963	PHE
2	B	973	ILE
2	B	975	GLN
2	B	983	ARG
2	B	987	LYS
2	B	993	THR
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1010	LEU
2	B	1020	ARG
2	B	1065	GLN
2	B	1067	ARG
2	B	1080	LYS
2	B	1094	ARG
2	B	1096	ARG
2	B	1099	VAL
2	B	1103	ILE
2	B	1108	ARG
2	B	1111	MET
2	B	1122	ARG
2	B	1128	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1172	ILE
2	B	1179	GLN
2	B	1181	GLU
2	B	1189	ILE
2	B	1195	HIS
2	B	1202	LEU
2	B	1203	LEU
2	B	1211	ASN
3	C	9	LYS

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Mol	Chain	Res	Type
3	C	12	GLU
3	C	22	LEU
3	C	29	MET
3	C	40	GLU
3	C	43	THR
3	C	53	THR
3	C	56	THR
3	C	75	MET
3	C	77	ILE
3	C	79	GLN
3	C	80	LEU
3	C	100	THR
3	C	106	GLU
3	C	109	SER
3	C	119	VAL
3	C	129	ILE
3	C	136	ASP
3	C	137	LYS
3	C	149	LYS
3	C	151	GLN
3	C	152	GLU
3	C	156	THR
3	C	157	CYS
3	C	186	LEU
3	C	194	GLU
3	C	215	GLU
3	C	222	LYS
3	C	231	ASN
3	C	238	ILE
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	259	LEU
3	C	265	MET
3	C	266	ASP
3	C	268	ASP
4	E	8	ASN
4	E	30	ILE
4	E	55	ARG
4	E	61	GLN
4	E	65	THR
4	E	75	MET

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Mol	Chain	Res	Type
4	E	78	LEU
4	E	90	VAL
4	E	92	THR
4	E	95	THR
4	E	98	ILE
4	E	100	ILE
4	E	104	ASN
4	E	127	ILE
4	E	132	ILE
4	E	142	VAL
4	E	150	VAL
4	E	156	LEU
4	E	158	SER
4	E	162	ARG
4	E	169	ARG
4	E	191	LYS
4	E	204	THR
4	E	213	ILE
4	E	215	MET
5	F	71	GLU
5	F	78	GLN
5	F	82	THR
5	F	99	LEU
5	F	110	ASP
5	F	111	LEU
5	F	112	GLU
5	F	119	ARG
5	F	125	LEU
5	F	127	GLU
5	F	138	LEU
5	F	152	ILE
6	H	11	GLN
6	H	13	SER
6	H	24	CYS
6	H	26	ILE
6	H	35	GLN
6	H	56	THR
6	H	63	LEU
6	H	77	ARG
6	H	87	ARG
6	H	92	ASP
6	H	100	THR

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Mol	Chain	Res	Type
6	H	106	GLU
6	H	107	VAL
6	H	109	LYS
6	H	130	ARG
6	H	132	LEU
6	H	135	LEU
6	H	139	ASN
6	H	144	ILE
7	I	12	ASN
7	I	17	ARG
7	I	31	THR
7	I	35	VAL
7	I	37	GLU
7	I	43	VAL
7	I	55	THR
7	I	62	ILE
7	I	70	ARG
7	I	88	SER
7	I	90	GLN
7	I	97	MET
7	I	98	VAL
7	I	104	LEU
7	I	118	ARG
8	J	1	MET
8	J	3	VAL
8	J	12	LYS
8	J	13	VAL
8	J	19	GLU
8	J	22	LEU
8	J	34	THR
8	J	43	ARG
8	J	48	ARG
8	J	64	ASN
9	K	1	MET
9	K	6	ARG
9	K	11	LEU
9	K	20	LYS
9	K	21	ILE
9	K	26	LYS
9	K	31	VAL
9	K	33	ILE
9	K	42	LEU

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Mol	Chain	Res	Type
9	K	54	ARG
9	K	63	VAL
9	K	74	ARG
9	K	75	ILE
9	K	78	THR
9	K	85	ASP
9	K	97	LYS
9	K	101	LEU
10	L	26	THR
10	L	27	LEU
10	L	28	LYS
10	L	38	LEU
10	L	44	ASP
10	L	46	VAL
10	L	48	CYS
10	L	50	ASP
10	L	51	CYS
10	L	55	ILE
10	L	58	LYS
10	L	62	LYS
10	L	64	LEU
10	L	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	64	ASN
1	A	71	GLN
1	A	225	ASN
1	A	253	ASN
1	A	286	HIS
1	A	287	HIS
1	A	306	ASN
1	A	339	ASN
1	A	390	GLN
1	A	394	ASN
1	A	427	GLN
1	A	445	ASN
1	A	471	ASN
1	A	503	GLN
1	A	517	ASN

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Mol	Chain	Res	Type
1	A	626	ASN
1	A	631	HIS
1	A	640	GLN
1	A	659	HIS
1	A	660	ASN
1	A	717	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	786	HIS
1	A	903	ASN
1	A	965	GLN
1	A	1070	GLN
1	A	1082	ASN
1	A	1140	HIS
1	A	1211	GLN
1	A	1222	ASN
1	A	1265	ASN
1	A	1364	ASN
1	A	1378	GLN
2	B	47	GLN
2	B	121	ASN
2	B	178	ASN
2	B	206	ASN
2	B	215	GLN
2	B	224	GLN
2	B	309	GLN
2	B	350	GLN
2	B	363	HIS
2	B	465	ASN
2	B	484	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	734	HIS
2	B	744	HIS
2	B	822	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1097	HIS
2	B	1117	GLN

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Mol	Chain	Res	Type
2	B	1141	HIS
2	B	1161	HIS
2	B	1176	ASN
2	B	1211	ASN
3	C	24	ASN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	112	ASN
3	C	123	ASN
3	C	151	GLN
3	C	167	HIS
3	C	214	ASN
3	C	242	GLN
3	C	264	GLN
3	C	267	GLN
4	E	54	GLN
4	E	61	GLN
4	E	63	ASN
4	E	113	GLN
4	E	146	HIS
4	E	147	HIS
6	H	33	GLN
6	H	83	GLN
6	H	128	ASN
6	H	131	ASN
6	H	133	ASN
7	I	12	ASN
7	I	23	ASN
7	I	89	GLN
7	I	120	GLN
8	J	23	ASN
9	K	89	ASN
9	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	3/5 (60%)	1 (33%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	8	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
15	GTP	R	100	-	33,34,34	1.96	3 (9%)	50,54,54	1.66	10 (20%)

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	GTP	R	100	-	-	2/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	R	100	GTP	PA-O3A	6.05	1.66	1.59
15	R	100	GTP	PB-O3A	5.86	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	R	100	GTP	PB-O3B	5.05	1.65	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	R	100	GTP	C2-N3-C4	5.12	121.12	112.30
15	R	100	GTP	C5-C4-N3	-5.08	120.30	128.39
15	R	100	GTP	N9-C4-N3	3.85	133.66	125.95
15	R	100	GTP	C8-N7-C5	2.98	109.57	104.26
15	R	100	GTP	C6-C5-N7	2.70	135.19	130.29
15	R	100	GTP	C2-N1-C6	-2.59	120.41	125.11
15	R	100	GTP	C4-C5-N7	-2.55	106.62	110.67
15	R	100	GTP	C3'-C2'-C1'	-2.09	97.51	101.46
15	R	100	GTP	C5-C6-N1	2.07	118.52	113.25
15	R	100	GTP	PA-O5'-C5'	-2.02	109.76	121.35

There are no chirality outliers.

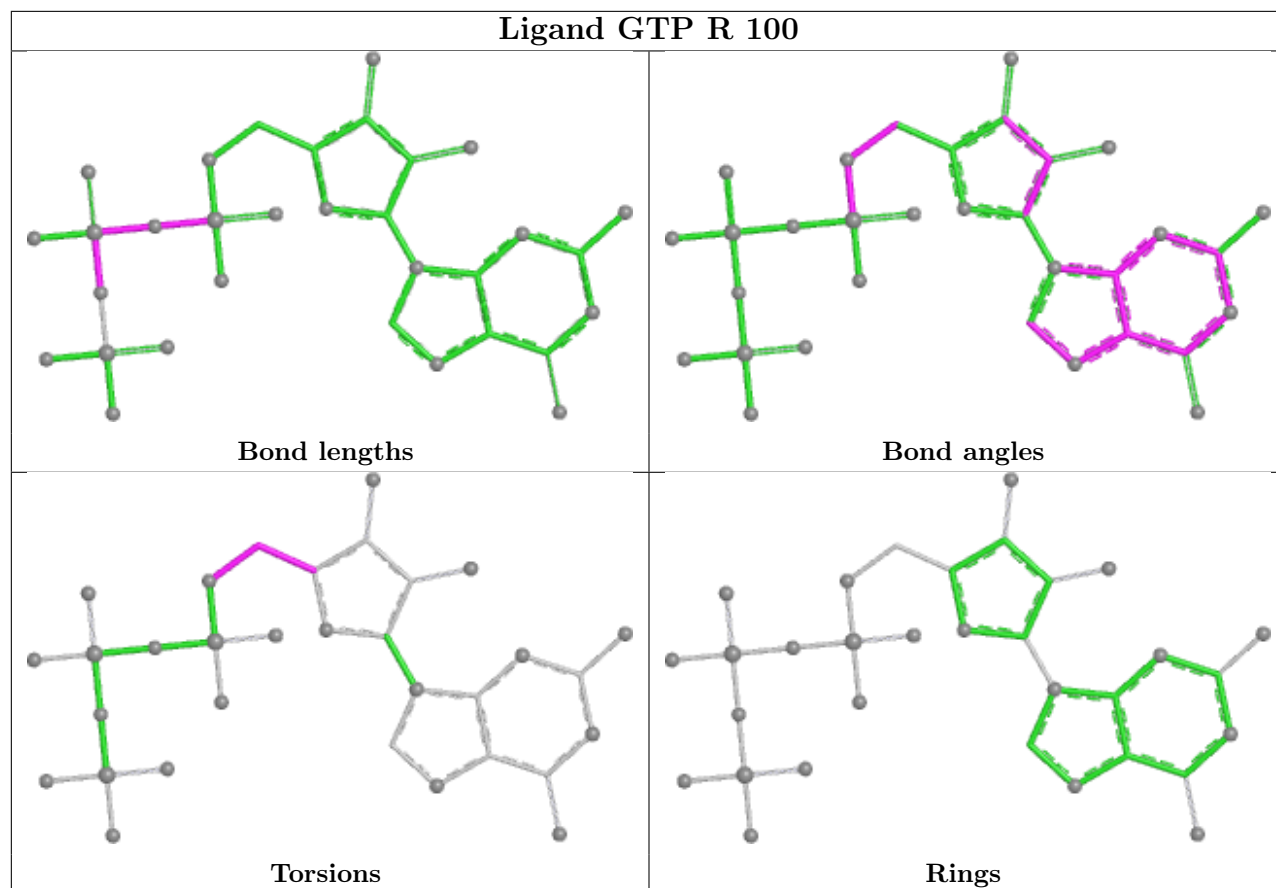
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	R	100	GTP	C4'-C5'-O5'-PA
15	R	100	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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%)	0.05	40 (2%) 55 35	49, 97, 192, 214	0
2	B	1114/1224 (91%)	-0.04	26 (2%) 61 41	48, 84, 152, 204	0
3	C	266/318 (83%)	-0.29	0 100 100	58, 81, 117, 175	0
4	E	214/215 (99%)	0.03	1 (0%) 87 76	69, 124, 172, 182	0
5	F	85/155 (54%)	-0.17	0 100 100	73, 103, 140, 156	0
6	H	133/146 (91%)	0.33	3 (2%) 61 41	97, 131, 163, 178	0
7	I	119/122 (97%)	0.05	0 100 100	61, 101, 141, 156	0
8	J	65/70 (92%)	-0.40	0 100 100	55, 73, 107, 123	0
9	K	114/120 (95%)	-0.24	0 100 100	59, 91, 118, 133	0
10	L	46/70 (65%)	0.58	5 (10%) 10 7	70, 116, 147, 156	0
11	R	5/5 (100%)	1.25	0 100 100	202, 206, 209, 212	0
12	T	8/29 (27%)	1.38	1 (12%) 8 6	169, 178, 191, 196	0
All	All	3574/4207 (84%)	-0.00	76 (2%) 63 43	48, 94, 180, 214	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	5.9
1	A	1089	VAL	5.1
1	A	73	GLY	4.6
1	A	1081	LEU	4.6
2	B	882	THR	4.5
10	L	27	LEU	4.5
1	A	65	LEU	4.3
1	A	250	ILE	4.0
2	B	715	ALA	3.9
1	A	179	LEU	3.9
2	B	335	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	709	ASP	3.5
2	B	477	ALA	3.2
1	A	79	GLY	3.0
2	B	733	HIS	3.0
6	H	63	LEU	2.9
2	B	1214	PRO	2.9
2	B	140	ILE	2.9
2	B	478	GLY	2.9
2	B	1204	PHE	2.9
12	T	19	DT	2.9
1	A	1091	SER	2.8
1	A	249	SER	2.8
1	A	1173	HIS	2.7
2	B	1171	VAL	2.7
6	H	132	LEU	2.7
1	A	55	ASP	2.6
2	B	1170	THR	2.6
1	A	86	LEU	2.5
1	A	50	ILE	2.5
2	B	70	ILE	2.5
1	A	141	LEU	2.5
1	A	78	PRO	2.5
6	H	136	LYS	2.5
1	A	201	VAL	2.5
2	B	101	MET	2.4
1	A	199	LEU	2.4
1	A	91	PHE	2.4
1	A	61	ILE	2.4
2	B	870	ILE	2.4
2	B	474	SER	2.4
2	B	646	LEU	2.3
1	A	182	VAL	2.3
10	L	25	ALA	2.3
2	B	509	ALA	2.3
10	L	45	ALA	2.3
1	A	186	LYS	2.3
10	L	55	ILE	2.2
1	A	72	GLU	2.2
1	A	114	LEU	2.2
2	B	446	LEU	2.2
1	A	259	GLU	2.2
1	A	1090	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1123	GLY	2.2
1	A	181	LEU	2.2
1	A	170	THR	2.1
1	A	145	LYS	2.1
1	A	318	SER	2.1
1	A	251	SER	2.1
2	B	137	TYR	2.1
10	L	26	THR	2.1
1	A	227	VAL	2.1
1	A	99	ILE	2.1
1	A	1086	PHE	2.1
1	A	1085	HIS	2.0
2	B	880	THR	2.0
2	B	712	PRO	2.0
2	B	473	MET	2.0
1	A	204	THR	2.0
1	A	103	CYS	2.0
1	A	252	PHE	2.0
1	A	56	PRO	2.0
4	E	91	LYS	2.0
1	A	174	ILE	2.0
2	B	448	ILE	2.0
2	B	502	ILE	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](#)

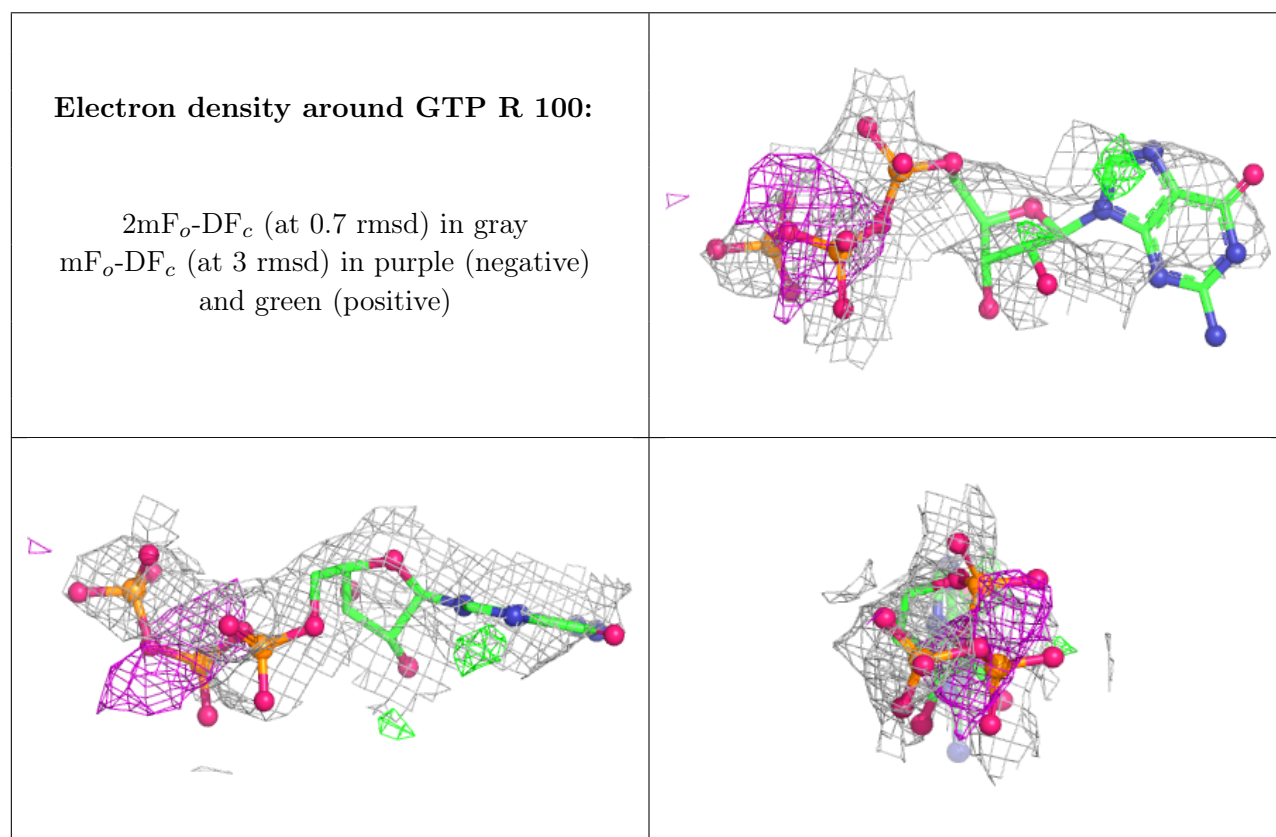
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	GTP	R	100	32/32	0.48	0.17	249,251,254,256	0
13	ZN	A	1734	1/1	0.90	0.08	289,289,289,289	0
13	ZN	A	1735	1/1	0.95	0.07	176,176,176,176	0
13	ZN	B	1307	1/1	0.97	0.04	183,183,183,183	0
13	ZN	J	101	1/1	0.99	0.04	78,78,78,78	0
14	MG	A	2001	1/1	0.99	0.05	60,60,60,60	0
13	ZN	I	203	1/1	0.99	0.02	102,102,102,102	0
13	ZN	L	105	1/1	1.00	0.02	99,99,99,99	0
13	ZN	I	204	1/1	1.00	0.02	82,82,82,82	0
13	ZN	C	319	1/1	1.00	0.03	89,89,89,89	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.