



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:39 AM UTC

PDB ID : 4BBR / pdb_00004bbr
Title : Structure of RNA polymerase II-TFIIB complex
Authors : Sainsbury, S.; Niesser, J.; Cramer, P.
Deposited on : 2012-09-27
Resolution : 3.40 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:

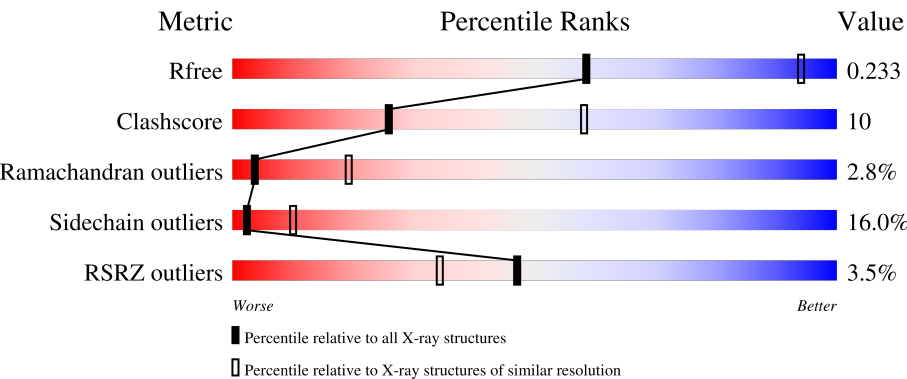
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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% 51%24%5%18%
2	B	1224	4% 60%27%6%6%
3	C	318	53%26%16%
4	D	221	5% 50%19%9%19%
5	E	215	3% 73%25%

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Mol	Chain	Length	Quality of chain
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 32800 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	1414	Total	C	N	O	S	0	0	0
			11123	7007	1945	2109	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1150	Total	C	N	O	S	0	0	0
			9095	5751	1598	1690	56			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 13 is a protein called TRANSCRIPTION INITIATION FACTOR IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	193	Total	C	N	O	S	0	0	0
			1396	862	246	274	14			

- 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		
14	M	1	Total	Zn	0	0
			1	1		

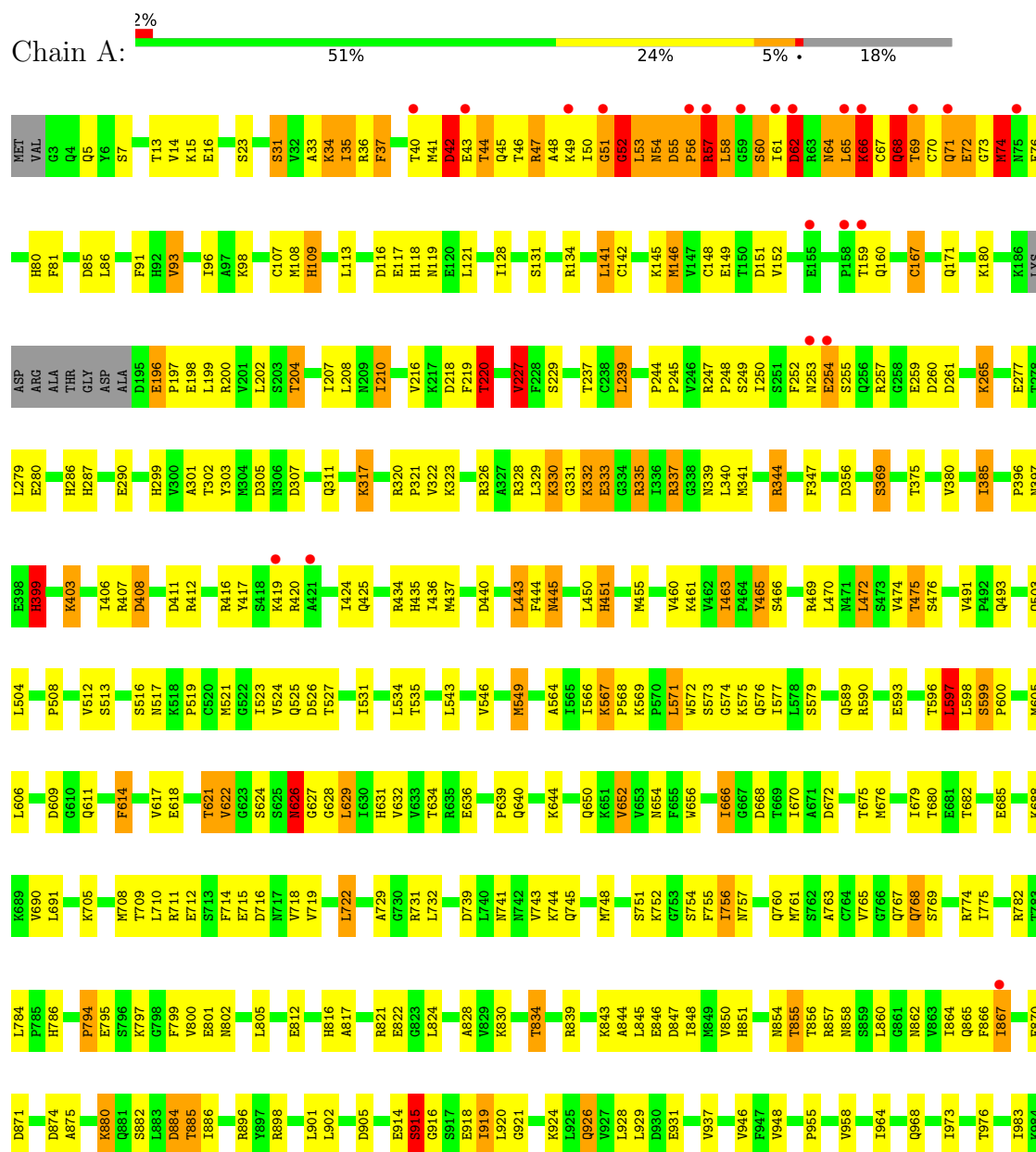
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

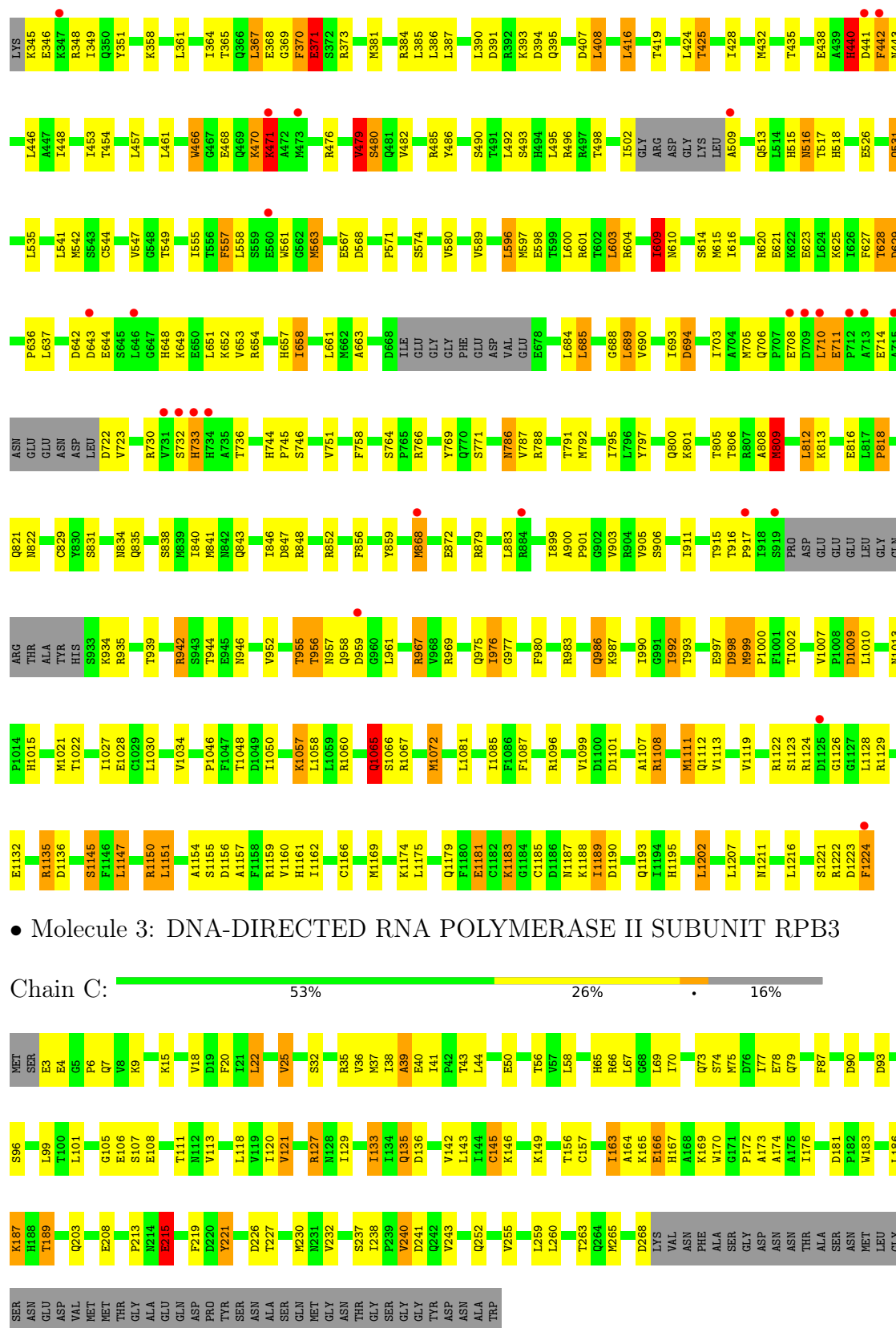
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Mg	0	0
			2	2		

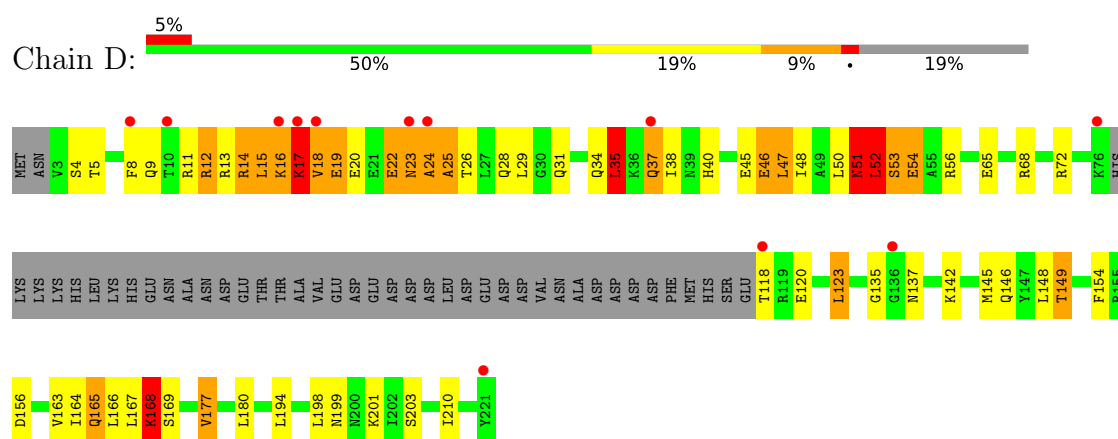
3 Residue-property plots

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.

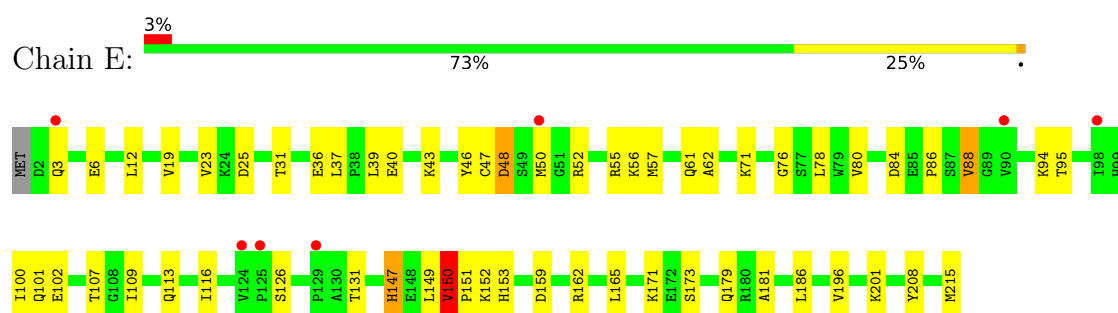
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



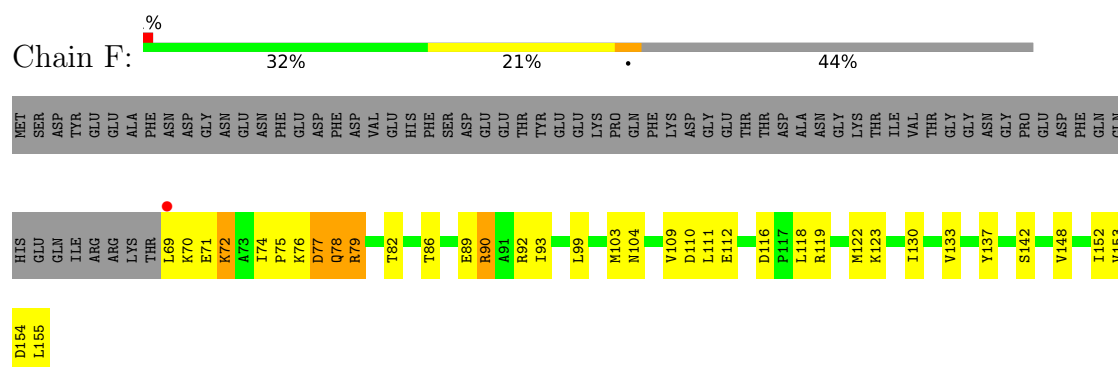




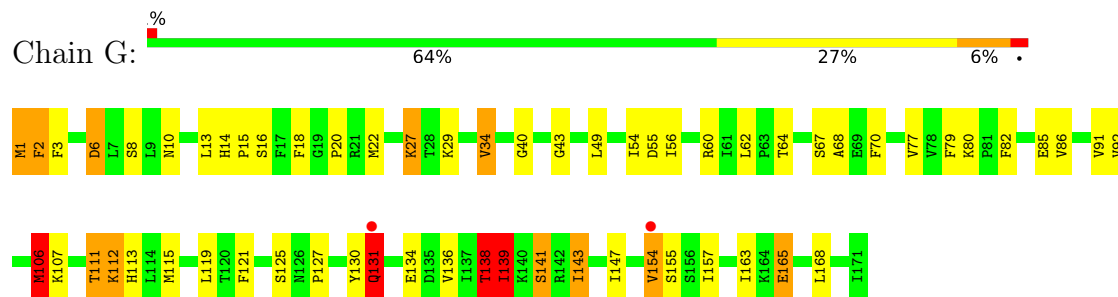
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



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

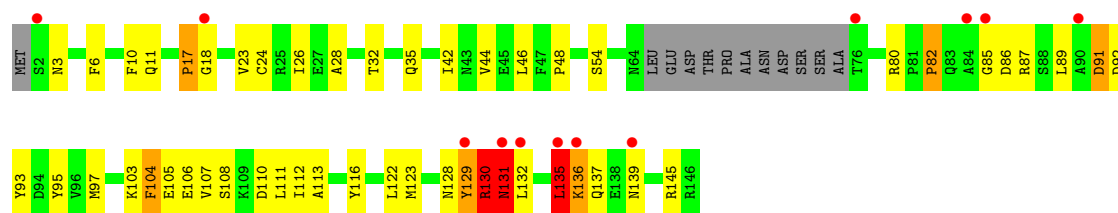


• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

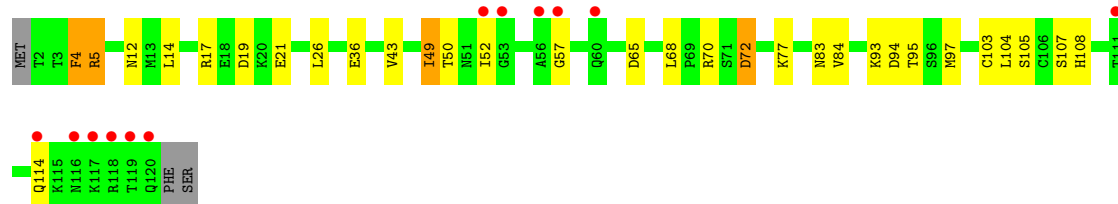


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3





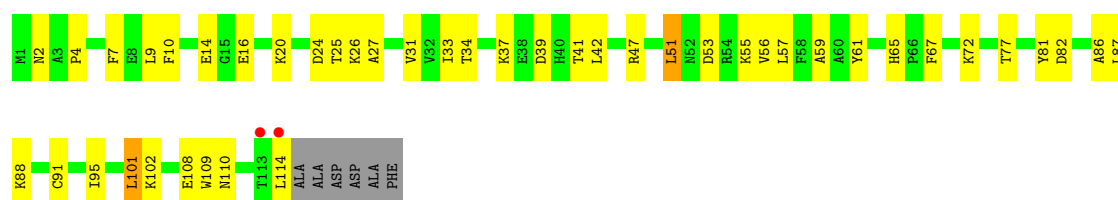
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



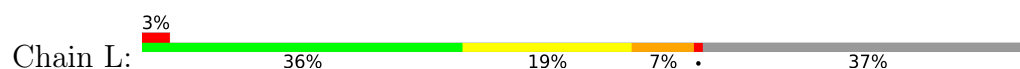
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



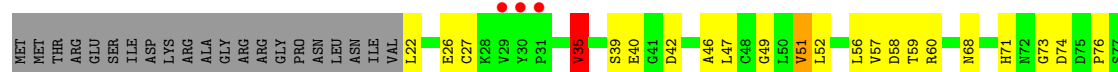
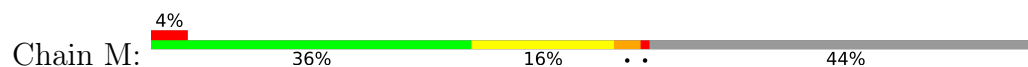
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

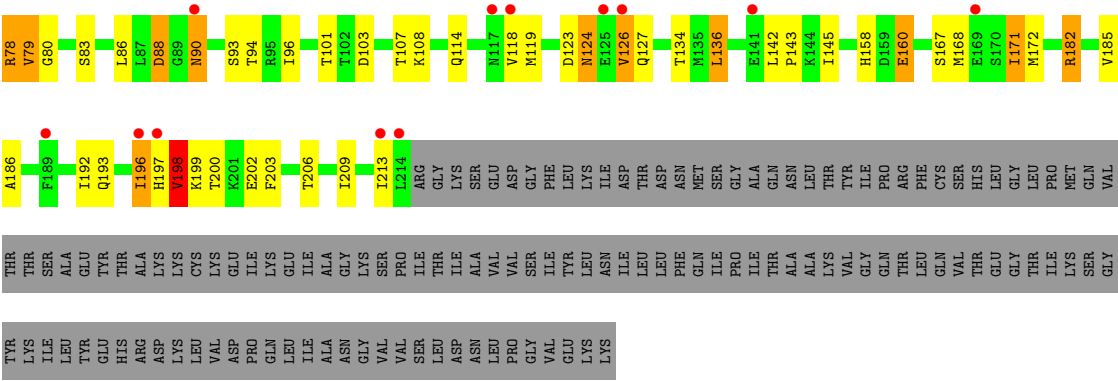


• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



• Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.44Å 386.76Å 254.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 3.40 49.41 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.41-3.40) 99.9 (49.41-3.40)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.174 , 0.211 0.195 , 0.233	Depositor DCC
R_{free} test set	2995 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 108.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.025 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.029 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32800	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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: MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.90	7/11322 (0.1%)	1.54	118/15312 (0.8%)
2	B	0.88	3/9271 (0.0%)	1.46	71/12505 (0.6%)
3	C	0.90	2/2133 (0.1%)	1.49	25/2891 (0.9%)
4	D	0.92	2/1444 (0.1%)	1.64	28/1935 (1.4%)
5	E	0.79	0/1788	1.41	8/2406 (0.3%)
6	F	0.88	0/717	1.39	3/967 (0.3%)
7	G	0.89	0/1368	1.44	19/1844 (1.0%)
8	H	0.83	0/1094	1.38	15/1481 (1.0%)
9	I	0.77	0/989	1.36	4/1331 (0.3%)
10	J	1.00	1/541 (0.2%)	1.65	4/727 (0.6%)
11	K	0.81	0/937	1.38	9/1265 (0.7%)
12	L	0.82	0/353	1.50	5/468 (1.1%)
13	M	0.89	0/1413	1.66	28/1916 (1.5%)
All	All	0.88	15/33370 (0.0%)	1.50	337/45048 (0.7%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	867	ILE	CG1-CD1	11.28	1.95	1.51
1	A	57	ARG	CA-C	10.85	1.67	1.52
1	A	549	MET	SD-CE	-7.57	1.60	1.79
4	D	24	ALA	CA-C	7.36	1.62	1.52
3	C	4	GLU	CA-C	6.82	1.55	1.52
1	A	54	ASN	CA-C	6.53	1.60	1.52
1	A	437	MET	SD-CE	6.40	1.95	1.79
3	C	133	ILE	CG1-CD1	-5.96	1.28	1.51
10	J	2	ILE	CA-C	5.81	1.60	1.52
1	A	676	MET	SD-CE	5.58	1.93	1.79
2	B	563	MET	SD-CE	-5.51	1.65	1.79
4	D	23	ASN	C-N	5.48	1.41	1.33
2	B	101	MET	SD-CE	5.31	1.92	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	732	SER	CA-C	5.11	1.59	1.52
1	A	52	GLY	C-N	5.02	1.40	1.33

All (337) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	470	LYS	CA-C-N	9.56	138.91	121.70
2	B	470	LYS	C-N-CA	9.56	138.91	121.70
3	C	39	ALA	N-CA-C	9.45	124.14	112.23
2	B	371	GLU	N-CA-C	-9.25	100.38	112.68
4	D	26	THR	N-CA-C	-9.01	100.23	112.94
1	A	56	PRO	CA-C-N	8.86	138.47	121.54
1	A	56	PRO	C-N-CA	8.86	138.47	121.54
10	J	5	VAL	N-CA-C	-8.48	98.70	109.30
2	B	1122	ARG	CA-C-N	8.33	131.78	120.54
2	B	1122	ARG	C-N-CA	8.33	131.78	120.54
7	G	34	VAL	N-CA-C	8.26	118.18	110.42
12	L	58	LYS	N-CA-C	8.26	122.45	112.38
1	A	999	VAL	N-CA-C	-8.11	104.84	111.81
4	D	19	GLU	N-CA-C	7.84	119.90	111.36
1	A	219	PHE	CA-CB-CG	7.83	121.63	113.80
4	D	35	LEU	N-CA-C	7.78	120.66	111.71
1	A	1403	GLU	CA-C-N	-7.74	110.53	122.60
1	A	1403	GLU	C-N-CA	-7.74	110.53	122.60
13	M	42	ASP	CA-CB-CG	7.61	120.21	112.60
2	B	41	LYS	N-CA-C	7.60	119.35	111.14
1	A	332	LYS	N-CA-C	-7.58	96.93	108.67
7	G	55	ASP	CA-C-N	7.56	130.81	120.46
7	G	55	ASP	C-N-CA	7.56	130.81	120.46
2	B	1185	CYS	N-CA-C	-7.44	104.05	113.72
2	B	557	PHE	CA-CB-CG	7.41	121.21	113.80
4	D	51	ASN	CA-CB-CG	7.18	119.78	112.60
5	E	126	SER	N-CA-C	7.17	119.96	111.71
2	B	629	ASP	CA-CB-CG	7.13	119.73	112.60
9	I	4	PHE	CA-CB-CG	7.09	120.89	113.80
1	A	628	GLY	N-CA-C	7.04	120.02	111.93
1	A	42	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	1241	ARG	N-CA-C	7.00	122.25	113.43
1	A	1112	LYS	N-CA-C	6.99	119.55	111.02
6	F	71	GLU	N-CA-C	-6.98	104.92	113.50
13	M	71	HIS	CA-C-N	6.98	129.93	120.44
13	M	71	HIS	C-N-CA	6.98	129.93	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	43	LEU	N-CA-C	6.97	119.91	111.82
3	C	213	PRO	N-CA-C	6.96	122.68	113.57
1	A	1403	GLU	N-CA-C	6.95	125.59	110.80
4	D	38	ILE	N-CA-C	6.93	117.82	108.11
1	A	915	SER	CA-C-N	6.90	127.76	120.03
1	A	915	SER	C-N-CA	6.90	127.76	120.03
3	C	181	ASP	CA-CB-CG	6.87	119.47	112.60
2	B	368	GLU	N-CA-C	6.85	121.92	109.32
2	B	628	THR	CA-C-N	6.82	134.57	121.54
2	B	628	THR	C-N-CA	6.82	134.57	121.54
7	G	141	SER	N-CA-C	6.82	120.12	110.50
1	A	1406	VAL	N-CA-C	6.79	117.55	110.62
10	J	55	ASP	CA-CB-CG	6.78	119.38	112.60
2	B	509	ALA	CA-C-N	6.77	132.40	124.21
2	B	509	ALA	C-N-CA	6.77	132.40	124.21
13	M	71	HIS	N-CA-C	-6.76	105.97	114.56
4	D	24	ALA	CA-C-N	6.75	133.78	122.79
4	D	24	ALA	C-N-CA	6.75	133.78	122.79
2	B	1101	ASP	CA-CB-CG	6.73	119.33	112.60
1	A	227	VAL	N-CA-C	6.70	117.32	111.90
13	M	51	VAL	N-CA-CB	6.67	118.42	110.95
1	A	331	GLY	CA-C-N	6.61	131.84	121.99
1	A	331	GLY	C-N-CA	6.61	131.84	121.99
3	C	135	GLN	CA-C-N	6.61	130.14	120.82
3	C	135	GLN	C-N-CA	6.61	130.14	120.82
2	B	67	SER	CA-C-N	6.60	130.49	121.05
2	B	67	SER	C-N-CA	6.60	130.49	121.05
6	F	77	ASP	N-CA-C	-6.59	100.07	109.96
4	D	24	ALA	N-CA-C	6.55	124.75	110.80
6	F	110	ASP	CA-CB-CG	6.53	119.13	112.60
11	K	82	ASP	CA-CB-CG	6.51	119.11	112.60
2	B	628	THR	N-CA-C	-6.48	105.53	113.50
1	A	985	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	794	PRO	CA-C-N	6.46	129.18	120.65
1	A	794	PRO	C-N-CA	6.46	129.18	120.65
2	B	367	LEU	N-CA-C	6.43	118.85	109.07
1	A	117	GLU	N-CA-C	-6.42	105.42	113.18
5	E	150	VAL	N-CA-C	6.37	113.36	107.56
3	C	87	PHE	N-CA-C	6.36	119.20	111.82
1	A	54	ASN	CB-CA-C	6.36	117.62	109.80
2	B	1190	ASP	CA-CB-CG	6.35	118.95	112.60
2	B	230	ALA	N-CA-C	6.35	123.84	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	25	ALA	CA-C-N	6.34	132.14	122.37
4	D	25	ALA	C-N-CA	6.34	132.14	122.37
5	E	48	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	1405	THR	CA-C-N	6.26	129.04	120.46
1	A	1405	THR	C-N-CA	6.26	129.04	120.46
9	I	5	ARG	N-CA-C	6.25	119.72	109.85
13	M	124	ASN	CA-CB-CG	6.25	118.85	112.60
3	C	120	ILE	N-CA-CB	6.24	117.98	110.31
1	A	614	PHE	CA-CB-CG	6.21	120.01	113.80
10	J	14	VAL	CB-CA-C	6.19	116.72	110.65
2	B	694	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	54	ASN	CA-CB-CG	6.18	118.78	112.60
8	H	91	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	710	LEU	N-CA-C	-6.13	104.60	111.28
10	J	16	ASP	CA-CB-CG	6.13	118.73	112.60
4	D	17	LYS	CA-C-N	6.13	133.00	121.97
4	D	17	LYS	C-N-CA	6.13	133.00	121.97
1	A	244	PRO	N-CA-C	6.12	118.17	110.70
1	A	914	GLU	CA-C-N	6.11	130.37	120.60
1	A	914	GLU	C-N-CA	6.11	130.37	120.60
1	A	1063	MET	CA-C-N	6.08	132.91	121.97
1	A	1063	MET	C-N-CA	6.08	132.91	121.97
7	G	92	VAL	CB-CA-C	6.07	116.59	110.65
1	A	220	THR	CB-CA-C	6.04	120.81	110.79
12	L	68	GLU	CB-CG-CD	6.03	122.85	112.60
8	H	128	ASN	CA-C-N	6.03	133.05	121.54
8	H	128	ASN	C-N-CA	6.03	133.05	121.54
1	A	1222	ASN	N-CA-C	6.02	119.45	111.75
1	A	329	LEU	CA-C-N	6.01	133.02	121.54
1	A	329	LEU	C-N-CA	6.01	133.02	121.54
1	A	472	LEU	N-CA-C	6.01	118.79	111.82
1	A	1422	ARG	N-CA-C	-6.00	106.08	113.41
4	D	149	THR	CB-CA-C	6.00	120.75	110.79
7	G	27	LYS	CA-C-N	5.99	128.59	120.44
7	G	27	LYS	C-N-CA	5.99	128.59	120.44
1	A	513	SER	N-CA-C	5.96	117.58	110.07
3	C	227	THR	CA-C-N	5.96	131.41	123.00
3	C	227	THR	C-N-CA	5.96	131.41	123.00
3	C	226	ASP	N-CA-C	-5.94	100.31	109.52
4	D	52	LEU	N-CA-C	-5.93	102.68	110.33
4	D	9	GLN	N-CA-C	5.93	118.87	109.50
11	K	53	ASP	CA-CB-CG	5.92	118.53	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	250	PHE	CA-CB-CG	5.91	119.71	113.80
1	A	254	GLU	CB-CG-CD	5.91	122.65	112.60
1	A	23	SER	N-CA-C	-5.90	102.22	109.65
1	A	1223	ASP	N-CA-C	5.88	119.71	112.54
7	G	154	VAL	CA-C-N	5.86	132.73	121.54
7	G	154	VAL	C-N-CA	5.86	132.73	121.54
11	K	39	ASP	CA-C-N	5.85	128.40	120.38
11	K	39	ASP	C-N-CA	5.85	128.40	120.38
8	H	131	ASN	CA-CB-CG	5.84	118.44	112.60
3	C	221	TYR	CA-C-N	5.83	128.68	120.28
3	C	221	TYR	C-N-CA	5.83	128.68	120.28
8	H	92	ASP	N-CA-C	-5.83	104.84	112.41
13	M	108	LYS	CA-C-N	5.83	128.41	120.54
13	M	108	LYS	C-N-CA	5.83	128.41	120.54
8	H	87	ARG	N-CA-C	5.81	117.87	108.34
2	B	80	GLU	CA-C-N	5.80	132.13	121.70
2	B	80	GLU	C-N-CA	5.80	132.13	121.70
2	B	1183	LYS	N-CA-C	-5.79	102.33	110.50
13	M	68	ASN	CA-C-N	5.79	129.11	120.31
13	M	68	ASN	C-N-CA	5.79	129.11	120.31
7	G	18	PHE	CA-CB-CG	5.78	119.58	113.80
5	E	147	HIS	CA-C-N	5.78	130.38	121.19
5	E	147	HIS	C-N-CA	5.78	130.38	121.19
13	M	198	VAL	N-CA-C	5.77	116.17	107.75
1	A	317	LYS	CA-C-N	5.76	129.81	120.60
1	A	317	LYS	C-N-CA	5.76	129.81	120.60
2	B	1065	GLN	CA-C-N	5.75	132.51	121.54
2	B	1065	GLN	C-N-CA	5.75	132.51	121.54
7	G	2	PHE	CA-CB-CG	5.74	119.53	113.80
2	B	809	MET	CA-C-N	5.73	128.24	120.44
2	B	809	MET	C-N-CA	5.73	128.24	120.44
1	A	48	ALA	CA-C-N	5.73	128.90	120.82
1	A	48	ALA	C-N-CA	5.73	128.90	120.82
1	A	399	HIS	N-CA-CB	5.72	120.55	110.37
2	B	714	GLU	N-CA-C	5.72	118.88	110.30
1	A	408	ASP	CA-C-N	5.71	128.50	120.28
1	A	408	ASP	C-N-CA	5.71	128.50	120.28
2	B	693	ILE	N-CA-C	5.71	116.36	107.28
13	M	96	ILE	N-CA-C	-5.71	99.01	107.51
1	A	248	PRO	N-CA-C	5.70	120.28	111.21
8	H	104	PHE	CA-C-N	5.70	129.20	121.05
8	H	104	PHE	C-N-CA	5.70	129.20	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	76	GLY	N-CA-C	5.69	119.11	111.20
13	M	90	ASN	CA-CB-CG	5.68	118.28	112.60
2	B	232	SER	N-CA-C	5.67	116.12	109.60
1	A	1068	ALA	CA-C-N	5.66	127.80	120.44
1	A	1068	ALA	C-N-CA	5.66	127.80	120.44
13	M	171	ILE	N-CA-CB	5.65	117.80	110.57
1	A	652	VAL	N-CA-CB	5.64	117.03	110.65
2	B	108	VAL	N-CA-C	5.63	121.05	109.34
3	C	38	ILE	CA-C-N	5.63	130.25	120.68
3	C	38	ILE	C-N-CA	5.63	130.25	120.68
13	M	88	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	628	GLY	CA-C-N	5.62	132.28	121.54
1	A	628	GLY	C-N-CA	5.62	132.28	121.54
13	M	196	ILE	CA-C-N	5.62	132.27	121.54
13	M	196	ILE	C-N-CA	5.62	132.27	121.54
2	B	609	ILE	N-CA-CB	5.60	119.13	111.41
8	H	85	GLY	N-CA-C	-5.59	107.39	114.16
8	H	85	GLY	CA-C-N	5.58	132.20	121.54
8	H	85	GLY	C-N-CA	5.58	132.20	121.54
1	A	885	THR	CA-C-N	5.58	127.58	120.56
1	A	885	THR	C-N-CA	5.58	127.58	120.56
2	B	711	GLU	N-CA-C	5.57	122.12	109.81
3	C	78	GLU	CB-CG-CD	5.57	122.07	112.60
2	B	231	PRO	CA-C-N	5.56	128.58	120.51
2	B	231	PRO	C-N-CA	5.56	128.58	120.51
1	A	91	PHE	CA-CB-CG	5.56	119.36	113.80
2	B	998	ASP	CA-CB-CG	5.56	118.16	112.60
7	G	6	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	874	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	60	SER	CA-C-N	5.54	128.32	122.11
1	A	60	SER	C-N-CA	5.54	128.32	122.11
1	A	218	ASP	CA-CB-CG	5.54	118.14	112.60
3	C	136	ASP	CA-CB-CG	5.54	118.14	112.60
9	I	72	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	204	THR	CA-C-N	5.52	127.62	120.44
1	A	204	THR	C-N-CA	5.52	127.62	120.44
11	K	24	ASP	CA-C-N	5.52	127.68	120.28
11	K	24	ASP	C-N-CA	5.52	127.68	120.28
2	B	829	CYS	N-CA-C	-5.52	100.30	109.46
1	A	916	GLY	N-CA-C	5.51	119.56	112.83
7	G	40	GLY	CA-C-N	5.51	127.66	120.28
7	G	40	GLY	C-N-CA	5.51	127.66	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	751	SER	N-CA-C	5.51	117.36	111.36
2	B	1009	ASP	N-CA-C	-5.50	105.69	112.90
2	B	370	PHE	CA-CB-CG	5.50	119.30	113.80
13	M	78	ARG	CA-C-N	5.50	128.24	122.14
13	M	78	ARG	C-N-CA	5.50	128.24	122.14
2	B	190	TYR	CA-C-N	5.49	127.64	120.28
2	B	190	TYR	C-N-CA	5.49	127.64	120.28
13	M	160	GLU	N-CA-C	5.49	118.19	110.23
4	D	163	VAL	N-CA-C	-5.49	105.50	110.82
3	C	121	VAL	CB-CA-C	5.48	116.02	110.65
7	G	138	THR	CA-C-N	5.46	131.81	121.97
7	G	138	THR	C-N-CA	5.46	131.81	121.97
1	A	1260	LEU	N-CA-C	-5.46	105.41	111.36
1	A	491	VAL	N-CA-C	5.45	112.94	107.55
1	A	1437	GLY	CA-C-N	5.45	129.40	120.63
1	A	1437	GLY	C-N-CA	5.45	129.40	120.63
4	D	168	LYS	N-CA-C	5.44	119.54	113.01
1	A	627	GLY	N-CA-C	5.43	120.36	113.24
13	M	103	ASP	N-CA-C	-5.43	100.32	108.96
9	I	4	PHE	N-CA-C	5.43	118.08	109.50
1	A	463	ILE	N-CA-C	5.42	114.96	108.45
2	B	97	VAL	CB-CA-C	5.42	116.59	110.41
1	A	763	ALA	N-CA-C	5.42	119.41	111.34
8	H	82	PRO	N-CA-C	5.42	123.63	112.47
2	B	1166	CYS	N-CA-C	-5.41	101.72	110.32
1	A	55	ASP	N-CA-CB	5.39	119.97	110.37
13	M	79	VAL	N-CA-CB	-5.39	105.92	112.33
1	A	330	LYS	N-CA-C	5.38	122.27	110.80
2	B	479	VAL	N-CA-C	-5.38	101.78	108.89
2	B	568	ASP	CA-CB-CG	5.38	117.97	112.60
1	A	1416	ALA	CA-C-N	5.37	128.72	120.82
1	A	1416	ALA	C-N-CA	5.37	128.72	120.82
1	A	526	ASP	CA-CB-CG	5.35	117.95	112.60
2	B	407	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	1422	ARG	CA-C-N	5.34	125.04	119.92
1	A	1422	ARG	C-N-CA	5.34	125.04	119.92
2	B	346	GLU	CA-C-N	5.33	127.37	120.44
2	B	346	GLU	C-N-CA	5.33	127.37	120.44
3	C	174	ALA	N-CA-C	-5.33	101.75	109.31
5	E	47	CYS	N-CA-C	5.31	118.06	109.40
1	A	1111	MET	CA-C-N	5.31	128.17	120.79
1	A	1111	MET	C-N-CA	5.31	128.17	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	88	VAL	N-CA-C	5.31	114.91	107.37
1	A	142	CYS	N-CA-C	5.30	119.38	113.02
1	A	1143	LEU	N-CA-C	-5.30	105.67	111.82
2	B	1136	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	1120	LEU	N-CA-C	5.29	118.34	110.14
1	A	245	PRO	CA-C-N	5.29	129.01	120.55
1	A	245	PRO	C-N-CA	5.29	129.01	120.55
13	M	192	ILE	CA-C-N	5.29	127.37	120.28
13	M	192	ILE	C-N-CA	5.29	127.37	120.28
7	G	106	MET	N-CA-C	5.28	118.17	109.72
2	B	847	ASP	CA-CB-CG	5.27	117.87	112.60
13	M	127	GLN	N-CA-C	-5.26	106.81	113.18
1	A	436	ILE	N-CA-C	-5.26	102.27	109.37
1	A	1269	GLU	N-CA-C	5.24	118.78	112.38
2	B	470	LYS	CA-C-O	-5.24	114.89	121.02
1	A	411	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	450	LEU	N-CA-C	5.23	118.82	112.23
1	A	867	ILE	CB-CG1-CD1	5.23	124.78	113.80
1	A	627	GLY	CA-C-N	5.23	125.06	120.10
1	A	627	GLY	C-N-CA	5.23	125.06	120.10
2	B	1224	PHE	CA-CB-CG	5.23	119.03	113.80
2	B	1013	ASN	N-CA-C	5.22	116.65	110.07
3	C	183	TRP	N-CA-C	-5.21	100.67	108.96
4	D	46	GLU	CA-C-N	5.20	128.48	121.05
4	D	46	GLU	C-N-CA	5.20	128.48	121.05
1	A	53	LEU	N-CA-CB	5.20	119.27	110.49
1	A	57	ARG	CA-CB-CG	5.19	124.49	114.10
1	A	968	GLN	CA-C-N	5.19	127.95	120.38
1	A	968	GLN	C-N-CA	5.19	127.95	120.38
2	B	119	LEU	N-CA-C	5.19	117.02	111.36
1	A	998	LEU	N-CA-C	5.18	118.39	110.20
1	A	305	ASP	CA-CB-CG	5.17	117.77	112.60
2	B	955	THR	CA-C-N	5.17	131.26	122.37
2	B	955	THR	C-N-CA	5.17	131.26	122.37
1	A	37	PHE	N-CA-C	5.16	117.66	109.40
1	A	62	ASP	CA-CB-CG	5.16	117.75	112.60
1	A	1326	ARG	N-CA-C	5.15	119.62	113.23
8	H	128	ASN	CA-CB-CG	5.14	117.75	112.60
8	H	135	LEU	CA-C-N	5.14	131.37	121.54
8	H	135	LEU	C-N-CA	5.14	131.37	121.54
4	D	53	SER	CA-C-N	5.13	127.42	120.44
4	D	53	SER	C-N-CA	5.13	127.42	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	54	GLU	N-CA-C	-5.13	105.60	111.14
11	K	27	ALA	N-CA-C	5.13	116.35	109.83
4	D	163	VAL	CA-C-N	5.13	127.76	120.53
4	D	163	VAL	C-N-CA	5.13	127.76	120.53
7	G	131	GLN	N-CA-C	5.12	117.99	107.69
12	L	67	PHE	CA-C-N	5.11	129.40	122.19
12	L	67	PHE	C-N-CA	5.11	129.40	122.19
4	D	37	GLN	N-CA-C	5.10	117.87	110.17
1	A	640	GLN	CA-C-N	5.10	127.09	120.56
1	A	640	GLN	C-N-CA	5.10	127.09	120.56
7	G	56	ILE	N-CA-CB	-5.10	103.60	110.54
1	A	802	ASN	N-CA-C	5.10	117.11	110.53
4	D	22	GLU	N-CA-C	5.10	116.91	110.33
2	B	791	THR	N-CA-C	-5.09	100.78	108.67
2	B	818	PRO	N-CA-C	5.08	119.22	111.34
2	B	535	LEU	N-CA-C	-5.08	106.25	112.90
2	B	596	LEU	CA-C-N	5.07	127.03	120.44
2	B	596	LEU	C-N-CA	5.07	127.03	120.44
2	B	663	ALA	CA-C-N	5.07	127.50	120.29
2	B	663	ALA	C-N-CA	5.07	127.50	120.29
1	A	34	LYS	N-CA-C	5.07	116.88	111.36
4	D	165	GLN	CA-C-N	5.06	127.31	120.38
4	D	165	GLN	C-N-CA	5.06	127.31	120.38
3	C	255	VAL	CA-C-N	5.05	127.30	120.38
3	C	255	VAL	C-N-CA	5.05	127.30	120.38
11	K	88	LYS	CA-C-N	5.05	127.35	120.54
11	K	88	LYS	C-N-CA	5.05	127.35	120.54
1	A	119	ASN	CA-C-N	5.04	127.04	120.28
1	A	119	ASN	C-N-CA	5.04	127.04	120.28
3	C	215	GLU	CA-C-N	5.04	125.58	119.98
3	C	215	GLU	C-N-CA	5.04	125.58	119.98
1	A	96	ILE	CA-C-N	5.04	127.79	120.79
1	A	96	ILE	C-N-CA	5.04	127.79	120.79
2	B	609	ILE	CB-CA-C	5.03	118.08	110.63
1	A	1326	ARG	CA-C-N	5.03	128.03	120.69
1	A	1326	ARG	C-N-CA	5.03	128.03	120.69
13	M	35	VAL	N-CA-C	5.03	116.76	108.97
1	A	828	ALA	CA-C-N	5.03	127.08	120.60
1	A	828	ALA	C-N-CA	5.03	127.08	120.60
13	M	119	MET	CA-C-N	5.03	128.21	120.82
13	M	119	MET	C-N-CA	5.03	128.21	120.82
2	B	732	SER	N-CA-C	5.02	121.50	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	722	ASP	CA-C-N	5.02	131.00	121.97
2	B	722	ASP	C-N-CA	5.02	131.00	121.97
3	C	120	ILE	N-CA-C	-5.02	103.03	109.30
12	L	29	TYR	N-CA-C	5.01	117.03	109.41
1	A	817	ALA	CA-C-N	5.01	126.95	120.44
1	A	817	ALA	C-N-CA	5.01	126.95	120.44
3	C	96	SER	N-CA-C	5.00	115.90	108.60

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	11123	0	11184	252	0
2	B	9095	0	9055	194	0
3	C	2095	0	2051	44	0
4	D	1434	0	1460	27	0
5	E	1752	0	1776	20	0
6	F	705	0	731	20	0
7	G	1340	0	1357	34	0
8	H	1076	0	1046	23	0
9	I	971	0	927	12	0
10	J	532	0	542	28	0
11	K	919	0	929	26	0
12	L	351	0	374	14	0
13	M	1396	0	1312	21	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
14	J	1	0	0	0	0
14	L	1	0	0	0	0
14	M	1	0	0	0	0
15	A	2	0	0	0	0
All	All	32800	0	32744	623	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (623) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ILE:CG1	1:A:867:ILE:CD1	1.95	1.41
2:B:515:HIS:HD2	2:B:517:THR:H	1.04	0.93
11:K:65:HIS:HD2	11:K:67:PHE:H	1.09	0.92
2:B:955:THR:HG22	2:B:956:THR:H	1.33	0.90
12:L:61:THR:HB	12:L:63:ARG:HG3	1.53	0.90
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.54	0.89
2:B:470:LYS:HB2	2:B:471:LYS:HB2	1.53	0.88
2:B:515:HIS:CD2	2:B:517:THR:H	1.93	0.85
1:A:57:ARG:O	1:A:68:GLN:HG2	1.77	0.84
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.44	0.83
1:A:855:THR:HG21	1:A:857:ARG:HE	1.43	0.83
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.60	0.82
7:G:1:MET:CE	7:G:80:LYS:H	1.93	0.81
7:G:138:THR:HG22	7:G:139:ILE:H	1.45	0.81
2:B:986:GLN:HE22	2:B:1022:THR:HG21	1.46	0.80
3:C:73:GLN:HE21	3:C:75:MET:H	1.32	0.78
8:H:130:ARG:H	8:H:130:ARG:HD3	1.47	0.78
1:A:406:ILE:HG12	1:A:412:ARG:HG3	1.65	0.78
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.65	0.77
6:F:155:LEU:HD12	6:F:155:LEU:H	1.51	0.76
1:A:1329:THR:HG22	1:A:1331:SER:H	1.50	0.75
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.67	0.75
1:A:56:PRO:O	1:A:57:ARG:HD2	1.87	0.74
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.69	0.74
4:D:145:MET:O	4:D:149:THR:HG22	1.86	0.74
2:B:303:TYR:HD1	2:B:571:PRO:HB3	1.52	0.74
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	1.87	0.74
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.69	0.74
1:A:880:LYS:HE3	1:A:955:PRO:HG3	1.68	0.74
2:B:601:ARG:HA	2:B:615:MET:HE1	1.70	0.73
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.53	0.72
11:K:65:HIS:CD2	11:K:67:PHE:H	2.00	0.72
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.69	0.72
1:A:35:ILE:HA	1:A:52:GLY:O	1.89	0.72
1:A:216:VAL:O	1:A:220:THR:HB	1.90	0.72
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.71	0.71
2:B:955:THR:HG22	2:B:956:THR:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.73	0.70
8:H:129:TYR:H	8:H:129:TYR:HD1	1.37	0.70
2:B:486:TYR:HA	2:B:1096:ARG:HH22	1.56	0.70
2:B:438:GLU:HG3	2:B:440:HIS:HB2	1.72	0.70
7:G:1:MET:HE3	7:G:80:LYS:H	1.56	0.70
13:M:193:GLN:HA	13:M:198:VAL:HB	1.74	0.70
6:F:74:ILE:HD11	6:F:142:SER:HB3	1.74	0.70
7:G:1:MET:CE	7:G:2:PHE:H	2.04	0.69
7:G:1:MET:HE1	7:G:79:PHE:HA	1.74	0.69
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.75	0.69
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.74	0.68
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.74	0.68
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.73	0.68
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.76	0.68
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.75	0.68
13:M:203:PHE:HA	13:M:206:THR:HG22	1.76	0.68
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.75	0.68
2:B:516:ASN:H	2:B:516:ASN:HD22	1.42	0.67
1:A:1284:MET:HE2	1:A:1306:LEU:HD21	1.77	0.67
1:A:741:ASN:HD22	1:A:744:LYS:H	1.42	0.67
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.59	0.67
1:A:1120:LEU:HD13	1:A:1125:ALA:HA	1.78	0.66
1:A:709:THR:HB	1:A:712:GLU:H	1.61	0.66
2:B:86:ARG:HG2	2:B:138:GLU:HG3	1.77	0.66
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.30	0.66
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.30	0.66
2:B:236:HIS:HD2	2:B:258:LEU:HD23	1.59	0.66
1:A:567:LYS:HG3	1:A:568:PRO:HA	1.76	0.66
2:B:235:SER:HA	2:B:261:ARG:HH21	1.60	0.66
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.77	0.65
1:A:503:GLN:NE2	6:F:90:ARG:HH21	1.93	0.65
2:B:744:HIS:HD2	2:B:746:SER:H	1.45	0.65
1:A:108:MET:H	1:A:171:GLN:HE22	1.44	0.65
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.79	0.65
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.78	0.65
3:C:163:ILE:HD12	3:C:165:LYS:HB2	1.79	0.65
8:H:6:PHE:HD1	8:H:130:ARG:HG2	1.61	0.64
2:B:900:ALA:HB3	12:L:61:THR:HG22	1.80	0.64
1:A:65:LEU:HD23	1:A:71:GLN:HB3	1.78	0.64
1:A:60:SER:HB2	1:A:67:CYS:HB2	1.80	0.64
2:B:542:MET:HB3	2:B:636:PRO:HD2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:ILE:HG12	1:A:1260:LEU:HD23	1.80	0.63
4:D:52:LEU:HB3	4:D:148:LEU:HD23	1.81	0.63
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.81	0.63
2:B:515:HIS:H	2:B:518:HIS:CD2	2.16	0.63
2:B:955:THR:CG2	2:B:956:THR:H	2.10	0.63
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.80	0.63
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.82	0.62
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.81	0.62
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.81	0.62
2:B:64:CYS:HA	2:B:67:SER:HB3	1.80	0.62
7:G:115:MET:HG2	7:G:119:LEU:HD23	1.81	0.61
2:B:104:GLU:HG3	12:L:54:ARG:NH1	2.15	0.61
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.82	0.61
8:H:131:ASN:HD22	8:H:132:LEU:H	1.47	0.61
2:B:801:LYS:O	10:J:52:THR:HG23	2.00	0.61
5:E:50:MET:HE2	5:E:52:ARG:HH21	1.63	0.61
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.63	0.61
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.83	0.61
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.33	0.61
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.82	0.61
2:B:705:MET:H	2:B:710:LEU:HG	1.66	0.60
12:L:28:LYS:HB2	12:L:39:SER:HA	1.83	0.60
7:G:1:MET:HE1	7:G:80:LYS:H	1.66	0.60
2:B:70:ILE:HG22	2:B:89:GLU:HG2	1.83	0.60
2:B:240:ILE:HG21	2:B:381:MET:HE1	1.84	0.60
2:B:901:PRO:HD3	12:L:58:LYS:HB3	1.82	0.60
2:B:868:MET:HE3	13:M:182:ARG:HG2	1.83	0.60
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.84	0.60
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.84	0.59
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.84	0.59
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.82	0.59
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.84	0.59
9:I:103:CYS:O	9:I:107:SER:HA	2.02	0.59
2:B:165:VAL:HG11	2:B:448:ILE:HD13	1.82	0.59
2:B:90:ILE:HD11	2:B:134:LYS:HZ3	1.66	0.59
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.84	0.59
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.35	0.59
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.85	0.59
1:A:854:ASN:HB2	1:A:1000:LEU:HD21	1.85	0.59
1:A:67:CYS:C	1:A:68:GLN:HG3	2.28	0.58
1:A:229:SER:HB3	1:A:1416:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:72:LYS:HB2	6:F:142:SER:HA	1.84	0.58
4:D:35:LEU:HA	4:D:47:LEU:HB2	1.85	0.58
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.86	0.58
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.69	0.58
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.85	0.58
2:B:1188:LYS:H	2:B:1189:ILE:HD12	1.69	0.58
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.85	0.58
6:F:119:ARG:HA	6:F:122:MET:HE2	1.84	0.57
1:A:549:MET:CE	1:A:656:TRP:HD1	2.17	0.57
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.86	0.57
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.86	0.57
6:F:77:ASP:O	6:F:78:GLN:HB2	2.04	0.57
2:B:915:THR:O	2:B:917:PRO:HD3	2.04	0.57
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.87	0.57
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.35	0.57
7:G:1:MET:SD	7:G:2:PHE:N	2.67	0.57
2:B:125:SER:HA	2:B:171:PRO:HA	1.86	0.57
5:E:62:ALA:HB3	5:E:78:LEU:HB3	1.86	0.57
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.86	0.57
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.35	0.57
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.70	0.57
2:B:324:ILE:HG13	2:B:329:THR:HG22	1.86	0.57
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.70	0.56
1:A:1329:THR:HG22	1:A:1331:SER:N	2.20	0.56
2:B:171:PRO:HG2	2:B:461:LEU:HD12	1.87	0.56
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.87	0.56
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.37	0.56
2:B:486:TYR:CA	2:B:1096:ARG:HH22	2.17	0.56
4:D:123:LEU:HD11	4:D:146:GLN:HG2	1.86	0.56
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.87	0.56
1:A:64:ASN:H	1:A:74:MET:HE1	1.71	0.56
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.87	0.56
4:D:8:PHE:CZ	4:D:37:GLN:HB2	2.41	0.56
7:G:131:GLN:HG3	7:G:136:VAL:HG22	1.87	0.56
1:A:227:VAL:HG12	4:D:15:LEU:HD23	1.88	0.56
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.89	0.56
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.06	0.56
2:B:614:SER:HB3	2:B:627:PHE:HB2	1.87	0.56
3:C:32:SER:O	3:C:36:VAL:HG23	2.05	0.56
1:A:69:THR:HG22	2:B:1174:LYS:HD3	1.88	0.55
1:A:589:GLN:HG3	1:A:606:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.88	0.55
1:A:590:ARG:HH21	1:A:621:THR:HG23	1.72	0.55
1:A:672:ASP:OD1	1:A:675:THR:HB	2.06	0.55
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.71	0.55
1:A:524:VAL:HG12	1:A:525:GLN:N	2.22	0.55
2:B:797:TYR:O	10:J:1:MET:HG2	2.06	0.55
1:A:472:LEU:O	1:A:475:THR:HB	2.06	0.55
1:A:858:ASN:ND2	1:A:862:ASN:HB2	2.22	0.55
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.89	0.55
2:B:557:PHE:O	2:B:561:TRP:HD1	1.90	0.55
1:A:650:GLN:O	1:A:654:ASN:HB2	2.06	0.55
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.72	0.55
2:B:291:ILE:HG23	2:B:296:GLU:HB3	1.89	0.55
1:A:58:LEU:HD22	1:A:80:HIS:O	2.08	0.55
2:B:822:ASN:HD22	10:J:52:THR:HG21	1.71	0.55
5:E:19:VAL:O	5:E:23:VAL:HG23	2.06	0.55
7:G:1:MET:HE2	7:G:3:PHE:CD1	2.42	0.55
1:A:399:HIS:O	1:A:435:HIS:CD2	2.59	0.54
1:A:866:PHE:HB3	1:A:867:ILE:HD12	1.89	0.54
2:B:856:PHE:CE1	2:B:969:ARG:HG3	2.42	0.54
1:A:754:SER:H	1:A:757:ASN:ND2	2.05	0.54
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.89	0.54
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.54	0.54
2:B:443:ASN:HD22	2:B:446:LEU:H	1.54	0.54
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.88	0.54
1:A:1292:PRO:HA	1:A:1298:TYR:HA	1.89	0.54
2:B:110:HIS:NE2	12:L:54:ARG:NH1	2.55	0.54
8:H:104:PHE:CE1	8:H:136:LYS:HA	2.43	0.54
10:J:6:ARG:H	10:J:14:VAL:H	1.56	0.54
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.08	0.54
3:C:15:LYS:NZ	3:C:135:GLN:HG2	2.22	0.54
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.42	0.54
1:A:714:PHE:O	1:A:718:VAL:HG23	2.08	0.54
2:B:786:ASN:HA	2:B:967:ARG:HH22	1.73	0.54
13:M:35:VAL:HG22	13:M:46:ALA:HB2	1.89	0.54
1:A:1120:LEU:CD1	1:A:1125:ALA:HA	2.38	0.54
2:B:102:VAL:HG23	2:B:112:LEU:HD22	1.88	0.54
2:B:654:ARG:H	2:B:657:HIS:HD2	1.56	0.54
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.06	0.54
1:A:503:GLN:HE22	6:F:90:ARG:HH21	1.55	0.54
7:G:1:MET:HE2	7:G:2:PHE:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:HB2	1:A:57:ARG:HH12	1.72	0.53
3:C:66:ARG:CZ	10:J:2:ILE:HG23	2.38	0.53
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.88	0.53
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.89	0.53
1:A:1266:THR:HG23	1:A:1270:ASN:HD22	1.74	0.53
2:B:653:VAL:HG22	2:B:689:LEU:HB2	1.91	0.53
2:B:1147:LEU:HD22	2:B:1151:LEU:CD2	2.38	0.53
1:A:42:ASP:C	1:A:44:THR:H	2.17	0.53
1:A:46:THR:HG22	1:A:47:ARG:H	1.72	0.53
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.89	0.53
1:A:412:ARG:HH12	2:B:1108:ARG:HD2	1.74	0.53
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.90	0.53
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.91	0.53
1:A:839:ARG:NH2	1:A:1402:PHE:HA	2.23	0.53
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.21	0.53
8:H:135:LEU:HB3	8:H:137:GLN:HG2	1.91	0.53
1:A:417:TYR:HB2	13:M:49:GLY:HA2	1.90	0.53
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.91	0.53
5:E:179:GLN:HB3	5:E:215:MET:HE3	1.91	0.53
7:G:14:HIS:CD2	7:G:16:SER:H	2.27	0.53
11:K:65:HIS:HD2	11:K:67:PHE:N	1.93	0.53
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	1.91	0.52
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.91	0.52
1:A:711:ARG:HE	9:I:97:MET:HG3	1.74	0.52
1:A:596:THR:C	1:A:598:LEU:H	2.16	0.52
1:A:1005:GLU:HG3	1:A:1009:ASN:HD21	1.74	0.52
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.74	0.52
1:A:534:LEU:O	1:A:574:GLY:HA3	2.08	0.52
2:B:72:GLU:HB3	2:B:87:LYS:HG2	1.90	0.52
2:B:280:ILE:HG13	2:B:333:PHE:HE1	1.74	0.52
2:B:303:TYR:CD1	2:B:571:PRO:HB3	2.40	0.52
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.90	0.52
1:A:1400:CYS:HB2	1:A:1405:THR:HA	1.91	0.52
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.92	0.52
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.91	0.52
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.91	0.52
4:D:8:PHE:HD2	7:G:6:ASP:HB2	1.74	0.52
1:A:851:HIS:HB2	1:A:855:THR:HG22	1.92	0.52
4:D:51:ASN:O	4:D:54:GLU:HB3	2.09	0.52
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.49	0.52
1:A:56:PRO:O	1:A:57:ARG:CD	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:136:LEU:HD21	13:M:196:ILE:HB	1.92	0.52
3:C:66:ARG:NH2	10:J:3:VAL:O	2.40	0.52
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.92	0.52
1:A:1129:GLU:HA	1:A:1132:LYS:HD2	1.92	0.51
2:B:1111:MET:HE3	13:M:57:VAL:HG13	1.93	0.51
4:D:12:ARG:HD3	4:D:14:ARG:HG2	1.92	0.51
1:A:332:LYS:O	1:A:333:GLU:HB2	2.10	0.51
7:G:125:SER:HB2	7:G:131:GLN:HE22	1.75	0.51
4:D:14:ARG:C	4:D:16:LYS:H	2.18	0.51
1:A:42:ASP:C	1:A:44:THR:N	2.69	0.51
1:A:1116:LEU:N	1:A:1308:THR:HG22	2.19	0.51
2:B:335:GLY:HA3	2:B:348:ARG:HB2	1.91	0.51
2:B:424:LEU:HD22	2:B:453:ILE:HD11	1.92	0.51
1:A:347:PHE:CE1	2:B:1107:ALA:HB1	2.46	0.51
1:A:535:THR:O	1:A:575:LYS:HE2	2.11	0.51
1:A:709:THR:HG23	9:I:94:ASP:HA	1.92	0.51
1:A:915:SER:O	1:A:919:ILE:HB	2.11	0.51
10:J:6:ARG:HG3	10:J:13:VAL:HA	1.93	0.51
1:A:524:VAL:HG12	1:A:525:GLN:H	1.75	0.51
1:A:847:ASP:HB3	1:A:1398:MET:HE1	1.92	0.51
2:B:900:ALA:HA	12:L:58:LYS:HD3	1.93	0.51
2:B:957:ASN:HD21	2:B:961:LEU:HD12	1.75	0.51
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.09	0.51
2:B:361:LEU:HB3	2:B:364:ILE:HD12	1.93	0.50
13:M:114:GLN:O	13:M:118:VAL:HG23	2.10	0.50
2:B:486:TYR:HB3	2:B:1096:ARG:HH12	1.76	0.50
2:B:806:THR:HB	2:B:809:MET:HG3	1.92	0.50
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.93	0.50
3:C:37:MET:HA	3:C:41:ILE:HD12	1.92	0.50
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.51	0.50
1:A:42:ASP:O	1:A:44:THR:N	2.37	0.50
1:A:822:GLU:HG3	2:B:513:GLN:HE21	1.76	0.50
3:C:22:LEU:HD22	3:C:230:MET:HE1	1.91	0.50
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.26	0.50
1:A:146:MET:HA	1:A:171:GLN:HB2	1.93	0.50
1:A:1387:HIS:HA	1:A:1391:ARG:HG3	1.92	0.50
1:A:31:SER:HA	1:A:81:PHE:O	2.11	0.50
1:A:1188:GLN:HG2	1:A:1243:VAL:HG12	1.94	0.50
2:B:597:MET:HE1	2:B:615:MET:HB3	1.94	0.50
2:B:642:ASP:HA	2:B:649:LYS:HA	1.93	0.50
2:B:685:LEU:HD12	2:B:690:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ILE:HG21	2:B:333:PHE:CD1	2.47	0.50
10:J:1:MET:H1	10:J:56:LEU:HB2	1.77	0.50
1:A:1433:MET:HE2	2:B:1145:SER:OG	2.11	0.49
5:E:19:VAL:HG11	5:E:80:VAL:HG11	1.93	0.49
1:A:626:ASN:O	1:A:631:HIS:HD2	1.95	0.49
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.94	0.49
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.94	0.49
10:J:36:LEU:HD11	10:J:51:LEU:HD13	1.94	0.49
2:B:209:GLU:OE1	2:B:788:ARG:NH2	2.43	0.49
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.45	0.49
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.10	0.49
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.47	0.49
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.94	0.49
2:B:744:HIS:CD2	2:B:746:SER:H	2.26	0.49
3:C:73:GLN:NE2	3:C:75:MET:H	2.06	0.49
1:A:321:PRO:HD2	13:M:73:GLY:HA3	1.94	0.49
1:A:1317:MET:HE1	1:A:1339:LEU:HD21	1.93	0.49
2:B:70:ILE:CG2	2:B:89:GLU:HG2	2.42	0.49
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.95	0.49
5:E:56:LYS:HE2	5:E:84:ASP:H	1.77	0.49
1:A:332:LYS:HB2	1:A:337:ARG:CZ	2.43	0.48
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.93	0.48
13:M:123:ASP:HA	13:M:126:VAL:HB	1.95	0.48
1:A:34:LYS:H	1:A:57:ARG:HH11	1.60	0.48
2:B:373:ARG:HG3	2:B:567:GLU:HG2	1.95	0.48
6:F:118:LEU:O	6:F:122:MET:HG3	2.13	0.48
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.95	0.48
8:H:6:PHE:CD1	8:H:130:ARG:HG2	2.46	0.48
10:J:1:MET:H1	10:J:56:LEU:N	2.11	0.48
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.95	0.48
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.96	0.48
13:M:199:LYS:HB2	13:M:202:GLU:HB3	1.95	0.48
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.96	0.48
2:B:648:HIS:CD2	2:B:649:LYS:H	2.31	0.48
3:C:101:LEU:HB2	3:C:118:LEU:HD23	1.96	0.48
6:F:76:LYS:O	6:F:79:ARG:HD3	2.13	0.48
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.94	0.48
1:A:86:LEU:HD11	1:A:239:LEU:HD13	1.96	0.48
1:A:715:GLU:O	1:A:719:VAL:HG23	2.14	0.48
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.96	0.48
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:LEU:HD11	11:K:101:LEU:HD21	1.96	0.48
2:B:515:HIS:HD2	2:B:517:THR:N	1.89	0.48
1:A:121:LEU:HB2	1:A:141:LEU:HD21	1.95	0.47
1:A:180:LYS:HA	1:A:180:LYS:HE2	1.96	0.47
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.95	0.47
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.96	0.47
1:A:1387:HIS:HB3	1:A:1391:ARG:NH2	2.29	0.47
10:J:1:MET:N	10:J:56:LEU:N	2.61	0.47
12:L:31:CYS:O	12:L:35:SER:HA	2.14	0.47
2:B:956:THR:HA	2:B:961:LEU:O	2.13	0.47
7:G:111:THR:C	7:G:113:HIS:H	2.23	0.47
1:A:51:GLY:C	1:A:56:PRO:HB3	2.39	0.47
1:A:287:HIS:HA	1:A:290:GLU:CD	2.40	0.47
2:B:25:ILE:HG21	2:B:658:ILE:HD13	1.97	0.47
2:B:54:PHE:HA	2:B:58:THR:HB	1.97	0.47
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.50	0.47
5:E:80:VAL:HG22	5:E:109:ILE:HB	1.97	0.47
1:A:66:LYS:NZ	1:A:68:GLN:H	2.13	0.47
1:A:416:ARG:HH22	13:M:40:GLU:HG2	1.78	0.47
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.97	0.47
2:B:44:VAL:HA	2:B:46:GLN:HE21	1.80	0.47
2:B:603:LEU:HB3	2:B:609:ILE:HG23	1.95	0.47
1:A:320:ARG:NH2	13:M:80:GLY:O	2.47	0.47
2:B:470:LYS:CB	2:B:471:LYS:HB2	2.37	0.47
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.79	0.47
3:C:241:ASP:HB3	11:K:109:TRP:CD2	2.49	0.47
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.95	0.47
2:B:327:ARG:HH22	2:B:371:GLU:HG2	1.80	0.47
2:B:818:PRO:HG2	10:J:54:VAL:HG21	1.96	0.47
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.96	0.47
6:F:154:ASP:H	6:F:155:LEU:HD12	1.79	0.47
8:H:95:TYR:HE2	8:H:97:MET:HE2	1.79	0.47
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.97	0.47
7:G:1:MET:HE2	7:G:2:PHE:N	2.29	0.46
1:A:756:ILE:HG22	1:A:760:GLN:HE21	1.80	0.46
2:B:273:LEU:HD23	2:B:274:PRO:HD2	1.98	0.46
2:B:493:SER:OG	2:B:526:GLU:OE2	2.32	0.46
3:C:142:VAL:HG11	10:J:5:VAL:HG13	1.97	0.46
6:F:155:LEU:H	6:F:155:LEU:CD1	2.25	0.46
10:J:53:HIS:HE1	10:J:55:ASP:OD1	1.99	0.46
1:A:1079:MET:HE3	1:A:1098:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:MET:HE3	2:B:580:VAL:HB	1.97	0.46
2:B:1150:ARG:HA	2:B:1154:ALA:HB3	1.98	0.46
1:A:1031:VAL:HA	1:A:1035:TYR:HD2	1.80	0.46
4:D:17:LYS:HD2	4:D:18:VAL:H	1.81	0.46
1:A:440:ASP:O	1:A:460:VAL:HG23	2.15	0.46
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.51	0.46
2:B:294:ASP:H	9:I:12:ASN:HD22	1.61	0.46
2:B:333:PHE:O	2:B:337:ARG:HD2	2.14	0.46
3:C:187:LYS:HG3	3:C:219:PHE:CE1	2.50	0.46
1:A:579:SER:HB3	1:A:611:GLN:HA	1.97	0.46
2:B:516:ASN:H	2:B:516:ASN:ND2	2.10	0.46
8:H:130:ARG:HD3	8:H:130:ARG:N	2.24	0.46
1:A:568:PRO:HB2	3:C:221:TYR:CE2	2.51	0.46
2:B:106:ASP:HA	13:M:186:ALA:HB3	1.96	0.46
2:B:468:GLU:HB2	2:B:471:LYS:HD3	1.96	0.46
2:B:1009:ASP:OD2	10:J:48:ARG:NH2	2.48	0.46
11:K:56:VAL:HA	11:K:77:THR:HG22	1.97	0.46
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.16	0.46
2:B:338:GLY:HA3	2:B:351:TYR:HE2	1.80	0.46
2:B:1072:MET:HE1	2:B:1087:PHE:HB2	1.97	0.46
1:A:33:ALA:HA	1:A:57:ARG:HD3	1.98	0.46
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.98	0.46
1:A:915:SER:HB2	1:A:919:ILE:HD13	1.97	0.46
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.46	0.46
2:B:652:LYS:HD2	2:B:688:GLY:O	2.15	0.46
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.46	0.46
1:A:761:MET:HG3	2:B:1021:MET:HG2	1.97	0.46
1:A:1327:ILE:O	5:E:147:HIS:HE1	1.99	0.46
6:F:99:LEU:O	6:F:103:MET:HG2	2.16	0.46
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.97	0.45
7:G:106:MET:HG2	7:G:107:LYS:N	2.30	0.45
1:A:68:GLN:O	1:A:70:CYS:N	2.45	0.45
3:C:6:PRO:HB2	11:K:101:LEU:HG	1.98	0.45
7:G:115:MET:HG3	7:G:163:ILE:HD11	1.98	0.45
1:A:344:ARG:HD2	2:B:1119:VAL:O	2.16	0.45
1:A:508:PRO:HB2	1:A:639:PRO:HB2	1.98	0.45
1:A:845:LEU:HA	1:A:848:ILE:CD1	2.47	0.45
2:B:435:THR:HG23	2:B:442:PHE:HD1	1.81	0.45
1:A:521:MET:C	1:A:624:SER:HB3	2.42	0.45
1:A:567:LYS:NZ	8:H:91:ASP:HA	2.32	0.45
1:A:731:ARG:HG3	1:A:755:PHE:CE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1454:MET:HE3	7:G:20:PRO:HD3	1.97	0.45
2:B:313:MET:HE2	2:B:390:LEU:HG	1.99	0.45
2:B:816:GLU:C	2:B:818:PRO:HD3	2.41	0.45
7:G:91:VAL:CG2	7:G:143:ILE:HD13	2.46	0.45
11:K:7:PHE:C	11:K:9:LEU:H	2.24	0.45
13:M:143:PRO:HG3	13:M:185:VAL:HG21	1.98	0.45
1:A:1148:ILE:HA	9:I:49:ILE:HD12	1.97	0.45
2:B:800:GLN:CB	10:J:52:THR:HG22	2.47	0.45
2:B:1081:LEU:O	3:C:189:THR:HG23	2.17	0.45
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.98	0.45
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.97	0.45
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.98	0.45
1:A:109:HIS:H	1:A:210:ILE:HG12	1.82	0.45
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.64	0.45
2:B:211:VAL:O	2:B:480:SER:HA	2.16	0.45
2:B:903:VAL:HG23	12:L:61:THR:HG21	1.99	0.45
2:B:283:VAL:HG13	2:B:297:ILE:HD13	1.99	0.45
1:A:356:ASP:OD2	1:A:469:ARG:HD3	2.17	0.44
7:G:27:LYS:HE2	7:G:54:ILE:HB	2.00	0.44
1:A:416:ARG:NH2	13:M:40:GLU:HG2	2.32	0.44
1:A:705:LYS:NZ	1:A:716:ASP:OD2	2.51	0.44
1:A:708:MET:HG2	1:A:712:GLU:HB3	1.99	0.44
1:A:786:HIS:HA	2:B:703:ILE:O	2.17	0.44
1:A:856:THR:HB	1:A:865:GLN:HB2	1.99	0.44
4:D:52:LEU:O	4:D:53:SER:CB	2.65	0.44
1:A:34:LYS:H	1:A:57:ARG:NH1	2.15	0.44
1:A:323:LYS:HE3	13:M:76:PRO:HA	1.99	0.44
11:K:16:GLU:OE1	11:K:37:LYS:HE3	2.17	0.44
1:A:564:ALA:N	1:A:576:GLN:HE22	2.16	0.44
1:A:754:SER:H	1:A:757:ASN:HD22	1.65	0.44
1:A:850:VAL:CG2	1:A:1064:VAL:HG21	2.45	0.44
4:D:17:LYS:HD2	4:D:18:VAL:HG13	2.00	0.44
7:G:165:GLU:HG2	7:G:168:LEU:HD12	2.00	0.44
1:A:745:GLN:HA	1:A:748:MET:HE3	1.98	0.44
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.99	0.44
1:A:71:GLN:O	1:A:73:GLY:N	2.51	0.44
1:A:1107:VAL:HG13	1:A:1332:PHE:HE1	1.83	0.44
2:B:1002:THR:HG22	2:B:1072:MET:HE2	2.00	0.44
5:E:12:LEU:HD21	5:E:55:ARG:HH21	1.83	0.44
1:A:512:VAL:HA	1:A:519:PRO:HA	1.99	0.44
1:A:524:VAL:HG12	1:A:525:GLN:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ILE:HG23	2:B:337:ARG:HB3	2.00	0.44
4:D:8:PHE:CE1	4:D:37:GLN:HB2	2.53	0.44
1:A:605:MET:HG2	1:A:621:THR:HG21	2.00	0.44
5:E:78:LEU:HD21	5:E:109:ILE:HD12	2.00	0.44
4:D:24:ALA:HB1	4:D:25:ALA:H	1.60	0.43
4:D:135:GLY:C	4:D:137:ASN:H	2.26	0.43
7:G:10:ASN:HA	7:G:70:PHE:O	2.18	0.43
1:A:690:VAL:HG11	1:A:794:PRO:HD3	2.00	0.43
1:A:767:GLN:HA	1:A:799:PHE:HA	1.99	0.43
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.18	0.43
2:B:205:ILE:HD13	2:B:461:LEU:HB3	2.00	0.43
3:C:173:ALA:HB2	3:C:243:VAL:HG11	1.99	0.43
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.99	0.43
9:I:19:ASP:HB2	9:I:26:LEU:HD11	2.00	0.43
1:A:396:PRO:HB3	1:A:403:LYS:HA	1.99	0.43
1:A:1445:ILE:HD11	7:G:68:ALA:CB	2.48	0.43
2:B:806:THR:HG22	2:B:808:ALA:H	1.82	0.43
3:C:166:GLU:HG2	11:K:10:PHE:HZ	1.83	0.43
4:D:23:ASN:HA	4:D:28:GLN:O	2.18	0.43
6:F:75:PRO:HG2	6:F:78:GLN:HB2	2.00	0.43
1:A:260:ASP:OD1	1:A:328:ARG:NH2	2.45	0.43
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.19	0.43
1:A:265:LYS:CG	1:A:303:TYR:HB2	2.48	0.43
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.49	0.43
4:D:52:LEU:O	4:D:53:SER:HB2	2.19	0.43
10:J:1:MET:N	10:J:56:LEU:H	2.16	0.43
1:A:824:LEU:HD21	2:B:769:TYR:HE1	1.83	0.43
2:B:309:GLN:HG3	9:I:52:ILE:HD11	2.01	0.43
8:H:42:ILE:O	8:H:44:VAL:HG23	2.18	0.43
1:A:265:LYS:NZ	1:A:299:HIS:HD2	2.17	0.43
2:B:199:MET:HE2	2:B:492:LEU:HD23	2.00	0.43
11:K:61:TYR:HA	11:K:72:LYS:O	2.19	0.43
4:D:168:LYS:HD2	4:D:168:LYS:HA	1.88	0.43
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.53	0.43
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.01	0.43
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.82	0.43
8:H:23:VAL:HA	8:H:42:ILE:O	2.19	0.43
1:A:369:SER:HB3	11:K:2:ASN:ND2	2.32	0.43
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	2.00	0.43
3:C:166:GLU:HG2	11:K:10:PHE:CZ	2.53	0.43
1:A:202:LEU:HB3	1:A:207:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.01	0.42
1:A:919:ILE:HG12	1:A:983:ILE:HD13	2.00	0.42
1:A:1170:ILE:H	1:A:1170:ILE:HG13	1.62	0.42
2:B:597:MET:HA	2:B:600:LEU:HD12	2.00	0.42
5:E:151:PRO:HD2	5:E:153:HIS:HE1	1.83	0.42
11:K:81:TYR:OH	11:K:86:ALA:HA	2.19	0.42
4:D:53:SER:HB3	4:D:154:PHE:O	2.19	0.42
8:H:80:ARG:HG2	11:K:57:LEU:HD22	2.00	0.42
12:L:40:LEU:HD11	12:L:49:LYS:NZ	2.34	0.42
1:A:845:LEU:HA	1:A:848:ILE:HD12	2.01	0.42
1:A:1225:PHE:H	1:A:1242:VAL:H	1.67	0.42
7:G:43:GLY:HA2	7:G:157:ILE:HD11	2.00	0.42
7:G:91:VAL:HG23	7:G:143:ILE:HD13	2.00	0.42
1:A:356:ASP:OD2	11:K:65:HIS:HE1	2.02	0.42
1:A:573:SER:O	1:A:576:GLN:HB3	2.19	0.42
1:A:1311:VAL:HG21	1:A:1329:THR:HG23	2.02	0.42
2:B:123:THR:HG23	2:B:205:ILE:HA	2.01	0.42
2:B:169:ARG:HB2	2:B:454:THR:HG23	2.01	0.42
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	2.00	0.42
1:A:443:LEU:CD1	1:A:455:MET:HE2	2.49	0.42
1:A:535:THR:HG21	1:A:617:VAL:H	1.84	0.42
1:A:1220:PHE:HE2	1:A:1271:ILE:HD11	1.84	0.42
2:B:684:LEU:HB3	2:B:690:VAL:HG22	2.00	0.42
2:B:751:VAL:HG13	2:B:812:LEU:HD22	2.01	0.42
2:B:852:ARG:HH22	12:L:70:ARG:C	2.28	0.42
2:B:976:ILE:HD11	2:B:992:ILE:HA	2.01	0.42
4:D:167:LEU:HB3	4:D:177:VAL:HG12	2.01	0.42
10:J:25:LEU:O	10:J:29:GLU:HA	2.19	0.42
1:A:116:ASP:HB3	1:A:118:HIS:H	1.84	0.42
1:A:265:LYS:HZ1	1:A:299:HIS:CD2	2.37	0.42
2:B:1181:GLU:HG3	2:B:1188:LYS:HG2	2.02	0.42
1:A:5:GLN:HG3	2:B:1175:LEU:HD12	2.02	0.42
1:A:197:PRO:HG2	1:A:199:LEU:HD11	2.01	0.42
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.20	0.42
2:B:758:PHE:CE2	2:B:1027:ILE:HG22	2.54	0.42
3:C:15:LYS:HZ1	3:C:135:GLN:HG2	1.83	0.42
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.54	0.42
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.54	0.42
1:A:50:ILE:C	1:A:52:GLY:H	2.28	0.42
1:A:128:ILE:HB	1:A:134:ARG:HG3	2.01	0.42
1:A:265:LYS:NZ	1:A:299:HIS:CD2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:NZ	13:M:94:THR:OG1	2.52	0.42
1:A:1076:ALA:HA	1:A:1079:MET:HE2	2.01	0.42
1:A:1140:HIS:CE1	1:A:1272:THR:HG23	2.54	0.42
2:B:1124:ARG:HG3	13:M:58:ASP:OD2	2.20	0.42
1:A:800:VAL:HA	1:A:812:GLU:HG2	2.02	0.42
2:B:345:LYS:HG2	2:B:349:ILE:HD11	2.02	0.42
2:B:786:ASN:HA	2:B:967:ARG:NH2	2.35	0.42
2:B:1181:GLU:HA	2:B:1187:ASN:O	2.20	0.42
5:E:39:LEU:HG	5:E:43:LYS:HE2	2.02	0.42
12:L:61:THR:HB	12:L:63:ARG:CG	2.37	0.42
1:A:986:ILE:O	1:A:990:VAL:HG23	2.20	0.42
2:B:69:LEU:HD22	2:B:425:THR:HG23	2.01	0.42
2:B:486:TYR:HA	2:B:1096:ARG:NH2	2.29	0.42
2:B:1057:LYS:HD2	2:B:1058:LEU:HD23	2.02	0.42
5:E:147:HIS:CD2	5:E:149:LEU:H	2.38	0.42
9:I:5:ARG:HG3	9:I:14:LEU:HD12	2.02	0.42
1:A:46:THR:HG22	1:A:47:ARG:N	2.34	0.41
2:B:601:ARG:CA	2:B:615:MET:HE1	2.46	0.41
2:B:1202:LEU:HD22	2:B:1202:LEU:HA	1.94	0.41
3:C:65:HIS:CE1	3:C:69:LEU:HD11	2.55	0.41
6:F:116:ASP:HB3	6:F:119:ARG:HB2	2.02	0.41
1:A:320:ARG:HH21	13:M:78:ARG:NH2	2.18	0.41
1:A:599:SER:HA	1:A:600:PRO:HD2	1.96	0.41
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.55	0.41
1:A:1442:ASP:HB2	6:F:137:TYR:CE2	2.46	0.41
2:B:269:ILE:HD12	2:B:317:CYS:SG	2.61	0.41
1:A:1005:GLU:HG3	1:A:1009:ASN:ND2	2.33	0.41
2:B:175:ARG:HB2	2:B:200:GLY:HA3	2.01	0.41
2:B:515:HIS:H	2:B:518:HIS:HD2	1.63	0.41
2:B:843:GLN:HA	2:B:846:ILE:HD12	2.02	0.41
5:E:46:TYR:HD1	5:E:57:MET:HB3	1.85	0.41
5:E:88:VAL:HB	5:E:116:ILE:HA	2.02	0.41
2:B:102:VAL:HG21	2:B:122:LEU:HD13	2.02	0.41
2:B:555:ILE:HA	2:B:558:LEU:HD12	2.01	0.41
3:C:58:LEU:HD12	3:C:145:CYS:HB2	2.01	0.41
3:C:73:GLN:HE21	3:C:75:MET:N	2.09	0.41
3:C:143:LEU:HD21	3:C:146:LYS:HE3	2.02	0.41
3:C:164:ALA:HA	3:C:167:HIS:O	2.21	0.41
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.54	0.41
1:A:72:GLU:HB3	1:A:76:GLU:HB3	2.01	0.41
1:A:337:ARG:NH1	2:B:1132:GLU:OE1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:LEU:HD13	1:A:597:LEU:HA	1.90	0.41
1:A:774:ARG:HB2	1:A:797:LYS:HB3	2.03	0.41
2:B:428:ILE:O	2:B:432:MET:HG3	2.20	0.41
2:B:848:ARG:HD2	10:J:8:PHE:O	2.21	0.41
2:B:859:TYR:OH	2:B:942:ARG:HG2	2.21	0.41
2:B:1048:THR:HB	2:B:1050:ILE:HD12	2.03	0.41
3:C:259:LEU:HD13	11:K:91:CYS:HB2	2.01	0.41
9:I:77:LYS:HB2	9:I:108:HIS:CD2	2.56	0.41
13:M:160:GLU:HG3	13:M:213:ILE:HD13	2.03	0.41
1:A:752:LYS:HG3	2:B:1015:HIS:HB3	2.02	0.41
1:A:844:ALA:HA	1:A:1389:PHE:CD2	2.56	0.41
10:J:48:ARG:O	10:J:52:THR:HB	2.21	0.41
1:A:253:ASN:C	1:A:255:SER:H	2.28	0.41
1:A:626:ASN:O	1:A:631:HIS:CD2	2.74	0.41
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.56	0.41
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	2.02	0.41
3:C:169:LYS:HE3	3:C:170:TRP:CH2	2.56	0.41
7:G:127:PRO:HD2	7:G:138:THR:HG21	2.03	0.41
8:H:130:ARG:H	8:H:130:ARG:CD	2.14	0.41
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.36	0.41
1:A:465:TYR:CE1	11:K:4:PRO:HD3	2.56	0.41
2:B:106:ASP:O	2:B:108:VAL:N	2.54	0.41
2:B:311:LEU:HB3	9:I:4:PHE:CZ	2.56	0.41
2:B:658:ILE:HA	2:B:661:LEU:HD12	2.02	0.41
2:B:841:MET:HB3	2:B:993:THR:HG22	2.03	0.41
3:C:252:GLN:HG2	11:K:95:ILE:HG23	2.03	0.41
4:D:23:ASN:HB3	7:G:82:PHE:HD1	1.86	0.41
4:D:68:ARG:HB2	4:D:72:ARG:HH21	1.86	0.41
5:E:86:PRO:HA	5:E:113:GLN:HB2	2.03	0.41
7:G:15:PRO:HD3	7:G:67:SER:HA	2.03	0.41
10:J:1:MET:H1	10:J:56:LEU:H	1.69	0.41
12:L:27:LEU:HA	12:L:39:SER:HB2	2.01	0.41
2:B:199:MET:SD	2:B:199:MET:N	2.84	0.41
4:D:180:LEU:HD23	4:D:180:LEU:HA	1.93	0.40
8:H:105:GLU:HB3	8:H:113:ALA:HB3	2.03	0.40
10:J:7:CYS:HA	10:J:49:MET:HG2	2.02	0.40
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.49	0.40
2:B:47:GLN:HE21	2:B:408:LEU:HD23	1.85	0.40
4:D:52:LEU:HB3	4:D:148:LEU:CD2	2.49	0.40
1:A:709:THR:HG22	1:A:711:ARG:H	1.84	0.40
2:B:466:TRP:HB2	2:B:479:VAL:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:644:GLU:CD	2:B:654:ARG:HH12	2.29	0.40
2:B:1159:ARG:HG3	2:B:1195:HIS:CE1	2.56	0.40
3:C:20:PHE:HE2	3:C:22:LEU:HD13	1.87	0.40
1:A:928:LEU:HD22	1:A:987:VAL:HG11	2.02	0.40
3:C:176:ILE:HG12	3:C:232:VAL:HG13	2.04	0.40
5:E:147:HIS:HB3	5:E:150:VAL:HG23	2.03	0.40
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	2.03	0.40
2:B:74:LEU:HA	2:B:85:SER:HA	2.04	0.40
2:B:256:VAL:HG12	2:B:385:LEU:HD22	2.02	0.40
2:B:283:VAL:HG22	2:B:297:ILE:HG21	2.04	0.40
2:B:1085:ILE:N	2:B:1085:ILE:HD12	2.37	0.40
3:C:93:ASP:O	3:C:127:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1404/1733 (81%)	1248 (89%)	107 (8%)	49 (4%)	3	16
2	B	1134/1224 (93%)	1007 (89%)	94 (8%)	33 (3%)	3	19
3	C	264/318 (83%)	239 (90%)	22 (8%)	3 (1%)	11	38
4	D	174/221 (79%)	152 (87%)	16 (9%)	6 (3%)	3	17
5	E	212/215 (99%)	196 (92%)	14 (7%)	2 (1%)	14	42
6	F	85/155 (55%)	79 (93%)	4 (5%)	2 (2%)	4	22
7	G	169/171 (99%)	151 (89%)	14 (8%)	4 (2%)	4	22
8	H	130/146 (89%)	110 (85%)	14 (11%)	6 (5%)	2	12
9	I	117/122 (96%)	96 (82%)	19 (16%)	2 (2%)	7	28
10	J	63/70 (90%)	54 (86%)	6 (10%)	3 (5%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	112/120 (93%)	107 (96%)	4 (4%)	1 (1%)	14	42
12	L	42/70 (60%)	28 (67%)	12 (29%)	2 (5%)	2	11
13	M	191/345 (55%)	176 (92%)	12 (6%)	3 (2%)	7	29
All	All	4097/4910 (83%)	3643 (89%)	338 (8%)	116 (3%)	4	19

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	58	LEU
1	A	72	GLU
1	A	74	MET
1	A	254	GLU
1	A	317	LYS
1	A	330	LYS
1	A	424	ILE
1	A	466	SER
1	A	626	ASN
1	A	629	LEU
1	A	885	THR
1	A	1064	VAL
1	A	1122	PRO
1	A	1405	THR
2	B	107	GLY
2	B	251	ILE
2	B	369	GLY
2	B	531	GLN
2	B	708	GLU
2	B	733	HIS
2	B	1066	SER
4	D	18	VAL
7	G	154	VAL
7	G	155	SER
8	H	82	PRO
8	H	139	ASN
10	J	2	ILE
13	M	197	HIS
1	A	66	LYS
1	A	68	GLN
1	A	252	PHE
1	A	333	GLU

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Mol	Chain	Res	Type
1	A	775	ILE
1	A	884	ASP
2	B	108	VAL
2	B	471	LYS
2	B	643	ASP
2	B	723	VAL
2	B	1046	PRO
2	B	1156	ASP
2	B	1157	ALA
2	B	1221	SER
3	C	215	GLU
4	D	5	THR
4	D	199	ASN
5	E	3	GLN
6	F	78	GLN
7	G	139	ILE
8	H	18	GLY
9	I	57	GLY
12	L	45	ALA
12	L	50	ASP
1	A	62	ASP
1	A	69	THR
1	A	71	GLN
1	A	167	CYS
1	A	286	HIS
1	A	517	ASN
1	A	543	LEU
1	A	593	GLU
1	A	1206	ASP
1	A	1242	VAL
1	A	1255	GLU
1	A	1377	THR
1	A	1403	GLU
2	B	229	ALA
2	B	266	ALA
2	B	440	HIS
2	B	466	TRP
2	B	629	ASP
2	B	792	MET
2	B	992	ILE
3	C	90	ASP
4	D	4	SER

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Mol	Chain	Res	Type
6	F	104	ASN
8	H	17	PRO
8	H	86	ASP
9	I	105	SER
13	M	167	SER
1	A	31	SER
1	A	948	VAL
1	A	1365	TYR
2	B	230	ALA
2	B	245	GLU
2	B	711	GLU
2	B	1155	SER
2	B	1223	ASP
4	D	14	ARG
4	D	198	LEU
7	G	112	LYS
10	J	6	ARG
13	M	200	THR
1	A	42	ASP
1	A	44	THR
1	A	399	HIS
1	A	465	TYR
1	A	597	LEU
1	A	599	SER
1	A	958	VAL
1	A	1280	GLU
2	B	247	GLY
2	B	441	ASP
2	B	809	MET
2	B	1181	GLU
2	B	1222	ARG
5	E	36	GLU
11	K	26	LYS
1	A	196	GLU
2	B	250	PHE
8	H	130	ARG
1	A	52	GLY
3	C	105	GLY
1	A	35	ILE
10	J	64	ASN
1	A	51	GLY

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	1236/1520 (81%)	1041 (84%)	195 (16%)	2	10
2	B	980/1061 (92%)	824 (84%)	156 (16%)	2	10
3	C	234/274 (85%)	196 (84%)	38 (16%)	2	10
4	D	160/200 (80%)	124 (78%)	36 (22%)	1	3
5	E	196/197 (100%)	173 (88%)	23 (12%)	5	20
6	F	77/137 (56%)	64 (83%)	13 (17%)	2	9
7	G	152/152 (100%)	134 (88%)	18 (12%)	5	20
8	H	118/128 (92%)	99 (84%)	19 (16%)	2	10
9	I	113/116 (97%)	100 (88%)	13 (12%)	5	20
10	J	60/65 (92%)	48 (80%)	12 (20%)	1	4
11	K	99/102 (97%)	86 (87%)	13 (13%)	4	16
12	L	39/57 (68%)	31 (80%)	8 (20%)	1	4
13	M	142/299 (48%)	109 (77%)	33 (23%)	1	2
All	All	3606/4308 (84%)	3029 (84%)	577 (16%)	2	10

All (577) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	15	LYS
1	A	36	ARG
1	A	41	MET
1	A	42	ASP
1	A	43	GLU
1	A	45	GLN
1	A	47	ARG
1	A	53	LEU
1	A	57	ARG
1	A	61	ILE
1	A	62	ASP

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Mol	Chain	Res	Type
1	A	64	ASN
1	A	65	LEU
1	A	66	LYS
1	A	68	GLN
1	A	74	MET
1	A	85	ASP
1	A	93	VAL
1	A	98	LYS
1	A	109	HIS
1	A	113	LEU
1	A	131	SER
1	A	141	LEU
1	A	145	LYS
1	A	146	MET
1	A	149	GLU
1	A	151	ASP
1	A	152	VAL
1	A	159	THR
1	A	160	GLN
1	A	167	CYS
1	A	196	GLU
1	A	198	GLU
1	A	200	ARG
1	A	204	THR
1	A	208	LEU
1	A	210	ILE
1	A	220	THR
1	A	227	VAL
1	A	237	THR
1	A	239	LEU
1	A	249	SER
1	A	250	ILE
1	A	257	ARG
1	A	265	LYS
1	A	277	GLU
1	A	279	LEU
1	A	280	GLU
1	A	302	THR
1	A	307	ASP
1	A	311	GLN
1	A	335	ARG
1	A	337	ARG

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Mol	Chain	Res	Type
1	A	344	ARG
1	A	369	SER
1	A	375	THR
1	A	385	ILE
1	A	397	ASN
1	A	403	LYS
1	A	407	ARG
1	A	408	ASP
1	A	419	LYS
1	A	420	ARG
1	A	425	GLN
1	A	434	ARG
1	A	443	LEU
1	A	444	PHE
1	A	445	ASN
1	A	451	HIS
1	A	461	LYS
1	A	463	ILE
1	A	470	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	493	GLN
1	A	504	LEU
1	A	516	SER
1	A	527	THR
1	A	566	ILE
1	A	567	LYS
1	A	571	LEU
1	A	577	ILE
1	A	597	LEU
1	A	609	ASP
1	A	618	GLU
1	A	621	THR
1	A	622	VAL
1	A	626	ASN
1	A	629	LEU
1	A	632	VAL
1	A	634	THR
1	A	636	GLU
1	A	644	LYS
1	A	652	VAL

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Mol	Chain	Res	Type
1	A	666	ILE
1	A	670	ILE
1	A	680	THR
1	A	682	THR
1	A	685	GLU
1	A	688	LYS
1	A	691	LEU
1	A	722	LEU
1	A	732	LEU
1	A	739	ASP
1	A	756	ILE
1	A	768	GLN
1	A	769	SER
1	A	782	ARG
1	A	795	GLU
1	A	801	GLU
1	A	805	LEU
1	A	821	ARG
1	A	830	LYS
1	A	834	THR
1	A	846	GLU
1	A	855	THR
1	A	864	ILE
1	A	880	LYS
1	A	882	SER
1	A	884	ASP
1	A	886	ILE
1	A	896	ARG
1	A	898	ARG
1	A	905	ASP
1	A	915	SER
1	A	918	GLU
1	A	919	ILE
1	A	920	LEU
1	A	924	LYS
1	A	926	GLN
1	A	929	LEU
1	A	931	GLU
1	A	937	VAL
1	A	964	ILE
1	A	973	ILE
1	A	976	THR

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Mol	Chain	Res	Type
1	A	991	LYS
1	A	992	ASP
1	A	998	LEU
1	A	1001	ARG
1	A	1006	ILE
1	A	1029	ARG
1	A	1030	ARG
1	A	1038	THR
1	A	1047	SER
1	A	1052	GLN
1	A	1058	VAL
1	A	1064	VAL
1	A	1081	LEU
1	A	1093	LYS
1	A	1098	VAL
1	A	1110	ASN
1	A	1113	THR
1	A	1116	LEU
1	A	1120	LEU
1	A	1142	THR
1	A	1147	THR
1	A	1163	ILE
1	A	1170	ILE
1	A	1171	GLN
1	A	1193	LEU
1	A	1195	LEU
1	A	1196	GLU
1	A	1215	ARG
1	A	1218	GLN
1	A	1222	ASN
1	A	1227	ILE
1	A	1230	GLU
1	A	1237	ILE
1	A	1259	MET
1	A	1260	LEU
1	A	1267	MET
1	A	1273	LEU
1	A	1274	ARG
1	A	1280	GLU
1	A	1284	MET
1	A	1297	GLU
1	A	1299	VAL

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Mol	Chain	Res	Type
1	A	1308	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1356	ILE
1	A	1366	ARG
1	A	1370	LEU
1	A	1391	ARG
1	A	1405	THR
1	A	1406	VAL
1	A	1422	ARG
1	A	1424	VAL
1	A	1426	GLU
1	A	1433	MET
1	A	1444	MET
1	A	1445	ILE
2	B	25	ILE
2	B	26	THR
2	B	45	SER
2	B	46	GLN
2	B	63	ILE
2	B	69	LEU
2	B	72	GLU
2	B	73	GLN
2	B	101	MET
2	B	102	VAL
2	B	104	GLU
2	B	112	LEU
2	B	128	LEU
2	B	164	LYS
2	B	175	ARG
2	B	178	ASN
2	B	183	GLU
2	B	211	VAL
2	B	216	GLU
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	223	VAL
2	B	227	LYS
2	B	228	LYS
2	B	232	SER
2	B	237	VAL

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Mol	Chain	Res	Type
2	B	240	ILE
2	B	244	LEU
2	B	245	GLU
2	B	249	ARG
2	B	254	LEU
2	B	273	LEU
2	B	284	ILE
2	B	298	LEU
2	B	309	GLN
2	B	313	MET
2	B	323	VAL
2	B	331	LEU
2	B	358	LYS
2	B	367	LEU
2	B	371	GLU
2	B	384	ARG
2	B	387	LEU
2	B	391	ASP
2	B	393	LYS
2	B	394	ASP
2	B	408	LEU
2	B	416	LEU
2	B	419	THR
2	B	425	THR
2	B	440	HIS
2	B	442	PHE
2	B	471	LYS
2	B	476	ARG
2	B	479	VAL
2	B	480	SER
2	B	482	VAL
2	B	485	ARG
2	B	490	SER
2	B	495	LEU
2	B	496	ARG
2	B	498	THR
2	B	502	ILE
2	B	516	ASN
2	B	531	GLN
2	B	541	LEU
2	B	544	CYS
2	B	547	VAL

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Mol	Chain	Res	Type
2	B	549	THR
2	B	574	SER
2	B	589	VAL
2	B	596	LEU
2	B	598	GLU
2	B	603	LEU
2	B	604	ARG
2	B	609	ILE
2	B	610	ASN
2	B	616	ILE
2	B	620	ARG
2	B	621	GLU
2	B	623	GLU
2	B	625	LYS
2	B	628	THR
2	B	637	LEU
2	B	651	LEU
2	B	658	ILE
2	B	685	LEU
2	B	689	LEU
2	B	694	ASP
2	B	706	GLN
2	B	710	LEU
2	B	730	ARG
2	B	733	HIS
2	B	736	THR
2	B	764	SER
2	B	766	ARG
2	B	786	ASN
2	B	795	ILE
2	B	805	THR
2	B	812	LEU
2	B	813	LYS
2	B	831	SER
2	B	835	GLN
2	B	838	SER
2	B	868	MET
2	B	879	ARG
2	B	883	LEU
2	B	905	VAL
2	B	906	SER
2	B	934	LYS

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Mol	Chain	Res	Type
2	B	935	ARG
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	946	ASN
2	B	956	THR
2	B	958	GLN
2	B	959	ASP
2	B	967	ARG
2	B	975	GLN
2	B	976	ILE
2	B	983	ARG
2	B	986	GLN
2	B	987	LYS
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1007	VAL
2	B	1010	LEU
2	B	1028	GLU
2	B	1034	VAL
2	B	1057	LYS
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1108	ARG
2	B	1111	MET
2	B	1112	GLN
2	B	1113	VAL
2	B	1123	SER
2	B	1128	LEU
2	B	1135	ARG
2	B	1145	SER
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1160	VAL
2	B	1162	ILE
2	B	1169	MET
2	B	1183	LYS
2	B	1189	ILE
2	B	1202	LEU

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Mol	Chain	Res	Type
2	B	1211	ASN
2	B	1216	LEU
2	B	1224	PHE
3	C	3	GLU
3	C	7	GLN
3	C	9	LYS
3	C	22	LEU
3	C	25	VAL
3	C	40	GLU
3	C	43	THR
3	C	50	GLU
3	C	56	THR
3	C	74	SER
3	C	79	GLN
3	C	106	GLU
3	C	107	SER
3	C	108	GLU
3	C	111	THR
3	C	113	VAL
3	C	121	VAL
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	145	CYS
3	C	149	LYS
3	C	156	THR
3	C	163	ILE
3	C	166	GLU
3	C	186	LEU
3	C	187	LYS
3	C	189	THR
3	C	203	GLN
3	C	208	GLU
3	C	215	GLU
3	C	237	SER
3	C	238	ILE
3	C	240	VAL
3	C	260	LEU
3	C	263	THR
3	C	265	MET
3	C	268	ASP
4	D	11	ARG

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Mol	Chain	Res	Type
4	D	12	ARG
4	D	13	ARG
4	D	15	LEU
4	D	16	LYS
4	D	17	LYS
4	D	19	GLU
4	D	20	GLU
4	D	22	GLU
4	D	29	LEU
4	D	31	GLN
4	D	34	GLN
4	D	35	LEU
4	D	40	HIS
4	D	45	GLU
4	D	46	GLU
4	D	47	LEU
4	D	48	ILE
4	D	50	LEU
4	D	51	ASN
4	D	52	LEU
4	D	65	GLU
4	D	118	THR
4	D	120	GLU
4	D	123	LEU
4	D	142	LYS
4	D	156	ASP
4	D	164	ILE
4	D	165	GLN
4	D	166	LEU
4	D	168	LYS
4	D	169	SER
4	D	177	VAL
4	D	201	LYS
4	D	203	SER
4	D	210	ILE
5	E	6	GLU
5	E	25	ASP
5	E	31	THR
5	E	37	LEU
5	E	40	GLU
5	E	48	ASP
5	E	61	GLN

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Mol	Chain	Res	Type
5	E	71	LYS
5	E	94	LYS
5	E	95	THR
5	E	100	ILE
5	E	101	GLN
5	E	102	GLU
5	E	107	THR
5	E	131	THR
5	E	150	VAL
5	E	152	LYS
5	E	159	ASP
5	E	162	ARG
5	E	165	LEU
5	E	171	LYS
5	E	173	SER
5	E	196	VAL
6	F	69	LEU
6	F	70	LYS
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	86	THR
6	F	90	ARG
6	F	93	ILE
6	F	111	LEU
6	F	112	GLU
6	F	133	VAL
6	F	152	ILE
6	F	153	VAL
7	G	1	MET
7	G	8	SER
7	G	13	LEU
7	G	22	MET
7	G	29	LYS
7	G	34	VAL
7	G	62	LEU
7	G	64	THR
7	G	106	MET
7	G	111	THR
7	G	112	LYS
7	G	131	GLN
7	G	134	GLU

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Mol	Chain	Res	Type
7	G	138	THR
7	G	139	ILE
7	G	141	SER
7	G	143	ILE
7	G	165	GLU
8	H	3	ASN
8	H	11	GLN
8	H	26	ILE
8	H	32	THR
8	H	35	GLN
8	H	54	SER
8	H	89	LEU
8	H	103	LYS
8	H	106	GLU
8	H	107	VAL
8	H	108	SER
8	H	110	ASP
8	H	111	LEU
8	H	112	ILE
8	H	129	TYR
8	H	130	ARG
8	H	131	ASN
8	H	135	LEU
8	H	136	LYS
9	I	17	ARG
9	I	21	GLU
9	I	36	GLU
9	I	49	ILE
9	I	50	THR
9	I	70	ARG
9	I	72	ASP
9	I	83	ASN
9	I	84	VAL
9	I	93	LYS
9	I	95	THR
9	I	104	LEU
9	I	114	GLN
10	J	2	ILE
10	J	6	ARG
10	J	13	VAL
10	J	14	VAL
10	J	20	SER

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Mol	Chain	Res	Type
10	J	22	LEU
10	J	23	ASN
10	J	27	GLU
10	J	38	ARG
10	J	42	LYS
10	J	48	ARG
10	J	57	ILE
11	K	14	GLU
11	K	20	LYS
11	K	25	THR
11	K	31	VAL
11	K	34	THR
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	101	LEU
11	K	102	LYS
11	K	108	GLU
11	K	110	ASN
11	K	114	LEU
12	L	27	LEU
12	L	38	LEU
12	L	50	ASP
12	L	54	ARG
12	L	58	LYS
12	L	65	VAL
12	L	68	GLU
12	L	70	ARG
13	M	22	LEU
13	M	26	GLU
13	M	27	CYS
13	M	35	VAL
13	M	39	SER
13	M	47	LEU
13	M	51	VAL
13	M	52	LEU
13	M	56	LEU
13	M	59	THR
13	M	60	ARG
13	M	74	ASP
13	M	79	VAL
13	M	83	SER

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Mol	Chain	Res	Type
13	M	86	LEU
13	M	88	ASP
13	M	90	ASN
13	M	93	SER
13	M	101	THR
13	M	107	THR
13	M	124	ASN
13	M	126	VAL
13	M	134	THR
13	M	136	LEU
13	M	142	LEU
13	M	145	ILE
13	M	158	HIS
13	M	168	MET
13	M	171	ILE
13	M	172	MET
13	M	182	ARG
13	M	198	VAL
13	M	209	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN
1	A	18	GLN
1	A	45	GLN
1	A	64	ASN
1	A	71	GLN
1	A	83	HIS
1	A	171	GLN
1	A	256	GLN
1	A	282	ASN
1	A	299	HIS
1	A	339	ASN
1	A	358	ASN
1	A	394	ASN
1	A	425	GLN
1	A	435	HIS
1	A	445	ASN
1	A	451	HIS
1	A	471	ASN

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Mol	Chain	Res	Type
1	A	503	GLN
1	A	517	ASN
1	A	525	GLN
1	A	631	HIS
1	A	660	ASN
1	A	698	GLN
1	A	741	ASN
1	A	757	ASN
1	A	760	GLN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	862	ASN
1	A	903	ASN
1	A	935	GLN
1	A	965	GLN
1	A	968	GLN
1	A	969	GLN
1	A	975	HIS
1	A	1033	GLN
1	A	1040	GLN
1	A	1106	ASN
1	A	1128	GLN
1	A	1140	HIS
1	A	1232	ASN
1	A	1270	ASN
1	A	1427	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	47	GLN
2	B	53	GLN
2	B	103	ASN
2	B	121	ASN
2	B	215	GLN
2	B	350	GLN
2	B	440	HIS
2	B	443	ASN
2	B	449	ASN
2	B	465	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN

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Mol	Chain	Res	Type
2	B	518	HIS
2	B	590	HIS
2	B	610	ASN
2	B	648	HIS
2	B	744	HIS
2	B	822	ASN
2	B	862	GLN
2	B	951	GLN
2	B	958	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1161	HIS
2	B	1178	ASN
2	B	1193	GLN
2	B	1195	HIS
3	C	7	GLN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	135	GLN
3	C	267	GLN
4	D	34	GLN
4	D	51	ASN
4	D	132	GLN
4	D	137	ASN
4	D	179	GLN
4	D	200	ASN
5	E	8	ASN
5	E	54	GLN
5	E	106	GLN
5	E	113	GLN
5	E	147	HIS
7	G	10	ASN
7	G	14	HIS
7	G	57	GLN
7	G	71	ASN
7	G	131	GLN
8	H	21	ASN
8	H	52	GLN
8	H	64	ASN
8	H	131	ASN
9	I	12	ASN

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Mol	Chain	Res	Type
9	I	83	ASN
9	I	90	GLN
9	I	108	HIS
10	J	26	GLN
10	J	53	HIS
11	K	29	ASN
11	K	65	HIS
11	K	89	ASN
11	K	104	ASN
12	L	53	HIS
13	M	90	ASN
13	M	114	GLN
13	M	117	ASN
13	M	124	ASN
13	M	158	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 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	1414/1733 (81%)	-0.16	26 (1%) 67 53	30, 65, 118, 185	0
2	B	1150/1224 (93%)	-0.01	53 (4%) 37 27	29, 69, 132, 191	0
3	C	266/318 (83%)	-0.43	0 100 100	30, 53, 88, 140	0
4	D	178/221 (80%)	0.11	12 (6%) 24 19	43, 75, 120, 138	0
5	E	214/215 (99%)	0.19	7 (3%) 49 36	47, 101, 154, 173	0
6	F	87/155 (56%)	-0.38	1 (1%) 78 65	32, 56, 88, 98	0
7	G	171/171 (100%)	-0.31	2 (1%) 76 63	35, 56, 84, 104	0
8	H	134/146 (91%)	0.32	12 (8%) 15 14	55, 92, 134, 160	0
9	I	119/122 (97%)	0.43	12 (10%) 12 12	68, 98, 135, 166	0
10	J	65/70 (92%)	-0.39	1 (1%) 72 57	35, 50, 76, 92	0
11	K	114/120 (95%)	-0.48	2 (1%) 67 53	35, 56, 88, 100	0
12	L	44/70 (62%)	0.54	2 (4%) 38 28	52, 90, 122, 136	0
13	M	193/345 (55%)	0.65	15 (7%) 19 16	52, 101, 140, 154	0
All	All	4149/4910 (84%)	-0.05	145 (3%) 47 34	29, 68, 132, 191	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	250	PHE	6.8
2	B	141	ASP	6.7
1	A	61	ILE	5.9
2	B	715	ALA	5.2
2	B	709	ASP	5.1
1	A	69	THR	5.1
2	B	83	ASN	5.1
1	A	1081	LEU	5.0
8	H	132	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	4.7
1	A	1254	ALA	4.6
2	B	251	ILE	4.4
13	M	214	LEU	4.3
1	A	66	LYS	4.3
7	G	131	GLN	4.3
9	I	52	ILE	4.1
2	B	643	ASP	4.1
4	D	221	TYR	4.1
1	A	71	GLN	4.1
2	B	78	THR	3.9
13	M	196	ILE	3.9
2	B	151	LEU	3.9
8	H	90	ALA	3.8
1	A	56	PRO	3.6
4	D	18	VAL	3.6
2	B	734	HIS	3.5
1	A	62	ASP	3.5
2	B	442	PHE	3.5
2	B	146	GLU	3.4
2	B	646	LEU	3.4
2	B	246	LYS	3.3
8	H	139	ASN	3.2
1	A	49	LYS	3.2
2	B	74	LEU	3.1
9	I	118	ARG	3.1
2	B	732	SER	3.1
1	A	57	ARG	3.1
2	B	81	SER	3.1
9	I	119	THR	3.0
2	B	713	ALA	3.0
13	M	197	HIS	3.0
1	A	75	ASN	3.0
2	B	710	LEU	2.9
2	B	917	PRO	2.9
13	M	169	GLU	2.9
7	G	154	VAL	2.9
5	E	125	PRO	2.9
13	M	30	TYR	2.9
13	M	189	PHE	2.9
8	H	135	LEU	2.9
1	A	1093	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	248	SER	2.8
2	B	77	HIS	2.8
8	H	2	SER	2.8
2	B	265	SER	2.8
10	J	65	PRO	2.8
2	B	84	ILE	2.8
1	A	65	LEU	2.7
13	M	126	VAL	2.7
2	B	473	MET	2.7
1	A	59	GLY	2.7
2	B	249	ARG	2.7
9	I	53	GLY	2.7
2	B	509	ALA	2.7
9	I	60	GLN	2.6
4	D	24	ALA	2.6
5	E	50	MET	2.6
1	A	421	ALA	2.6
13	M	213	ILE	2.6
9	I	120	GLN	2.6
1	A	51	GLY	2.6
11	K	114	LEU	2.6
2	B	347	LYS	2.6
2	B	76	GLN	2.6
9	I	114	GLN	2.6
2	B	712	PRO	2.5
12	L	43	THR	2.5
1	A	253	ASN	2.5
8	H	76	THR	2.5
2	B	1224	PHE	2.5
4	D	8	PHE	2.5
8	H	18	GLY	2.5
9	I	56	ALA	2.5
2	B	441	ASP	2.5
2	B	884	ARG	2.5
9	I	117	LYS	2.5
1	A	158	PRO	2.5
2	B	733	HIS	2.5
13	M	118	VAL	2.5
1	A	254	GLU	2.4
2	B	82	ASP	2.4
2	B	247	GLY	2.4
2	B	959	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
11	K	113	THR	2.3
2	B	140	ILE	2.3
2	B	241	ARG	2.3
5	E	3	GLN	2.3
2	B	328	GLU	2.3
8	H	131	ASN	2.3
2	B	66	ASP	2.3
2	B	245	GLU	2.3
2	B	731	VAL	2.3
13	M	29	VAL	2.3
4	D	76	LYS	2.3
4	D	118	THR	2.3
5	E	90	VAL	2.3
1	A	159	THR	2.3
2	B	471	LYS	2.3
1	A	43	GLU	2.3
1	A	419	LYS	2.3
2	B	708	GLU	2.2
8	H	85	GLY	2.2
9	I	57	GLY	2.2
4	D	17	LYS	2.2
2	B	338	GLY	2.2
4	D	23	ASN	2.2
13	M	117	ASN	2.2
2	B	87	LYS	2.2
2	B	88	TYR	2.2
1	A	1175	SER	2.2
6	F	69	LEU	2.2
2	B	868	MET	2.2
13	M	141	GLU	2.2
1	A	155	GLU	2.1
4	D	10	THR	2.1
9	I	116	ASN	2.1
9	I	111	THR	2.1
4	D	136	GLY	2.1
2	B	560	GLU	2.1
5	E	129	PRO	2.1
2	B	134	LYS	2.1
13	M	90	ASN	2.1
2	B	1125	ASP	2.1
13	M	125	GLU	2.1
4	D	37	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	16	LYS	2.0
5	E	124	VAL	2.0
2	B	919	SER	2.0
1	A	40	THR	2.0
8	H	84	ALA	2.0
8	H	129	TYR	2.0
8	H	136	LYS	2.0
13	M	31	PRO	2.0
1	A	867	ILE	2.0
5	E	98	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	A	2458	1/1	0.80	0.13	75,75,75,75	0
15	MG	A	2459	1/1	0.81	0.15	80,80,80,80	0
14	ZN	I	1122	1/1	0.99	0.04	130,130,130,130	0
14	ZN	L	1071	1/1	0.99	0.03	98,98,98,98	0
14	ZN	M	1216	1/1	0.99	0.03	73,73,73,73	0
14	ZN	A	2456	1/1	0.99	0.03	91,91,91,91	0
14	ZN	A	2457	1/1	0.99	0.03	51,51,51,51	0
14	ZN	C	1269	1/1	1.00	0.02	64,64,64,64	0
14	ZN	I	1121	1/1	1.00	0.02	78,78,78,78	0
14	ZN	B	2225	1/1	1.00	0.02	46,46,46,46	0
14	ZN	J	1066	1/1	1.00	0.02	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.