



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:07 AM UTC

PDB ID : 3S2D / pdb_00003s2d
Title : RNA Polymerase II Initiation Complex with a 5-nt RNA containing a 5Br-U
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
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

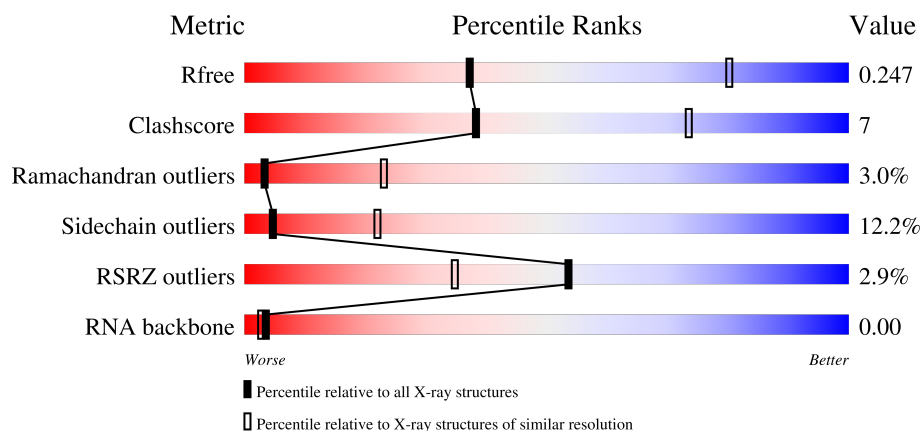
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

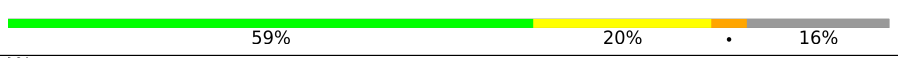
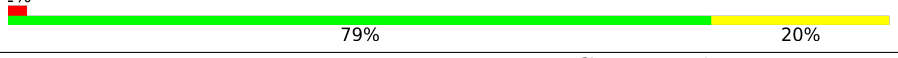
The reported resolution of this entry is 3.20 Å.

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	B	1224	
3	C	318	
4	E	215	

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Mol	Chain	Length	Quality of chain
5	F	155	53% 45%
6	H	146	5% 65% 20% 5% 9%
7	I	122	3% 80% 16%
8	J	70	% 57% 26% 10% 7%
9	K	120	% 59% 33% 5%
10	L	70	9% 39% 17% 9% 34%
11	R	5	40% 60%
12	T	29	3% 28% 17% 55%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 28672 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*GP*(5BU)P*G)-3').

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
11	R	5	Total	Br	C	N	O	P		0	0	0
			109	1	49	22	33	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*AP*CP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	13	Total	C	N	O	P	0	0	0
			262	125	46	78	13			

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

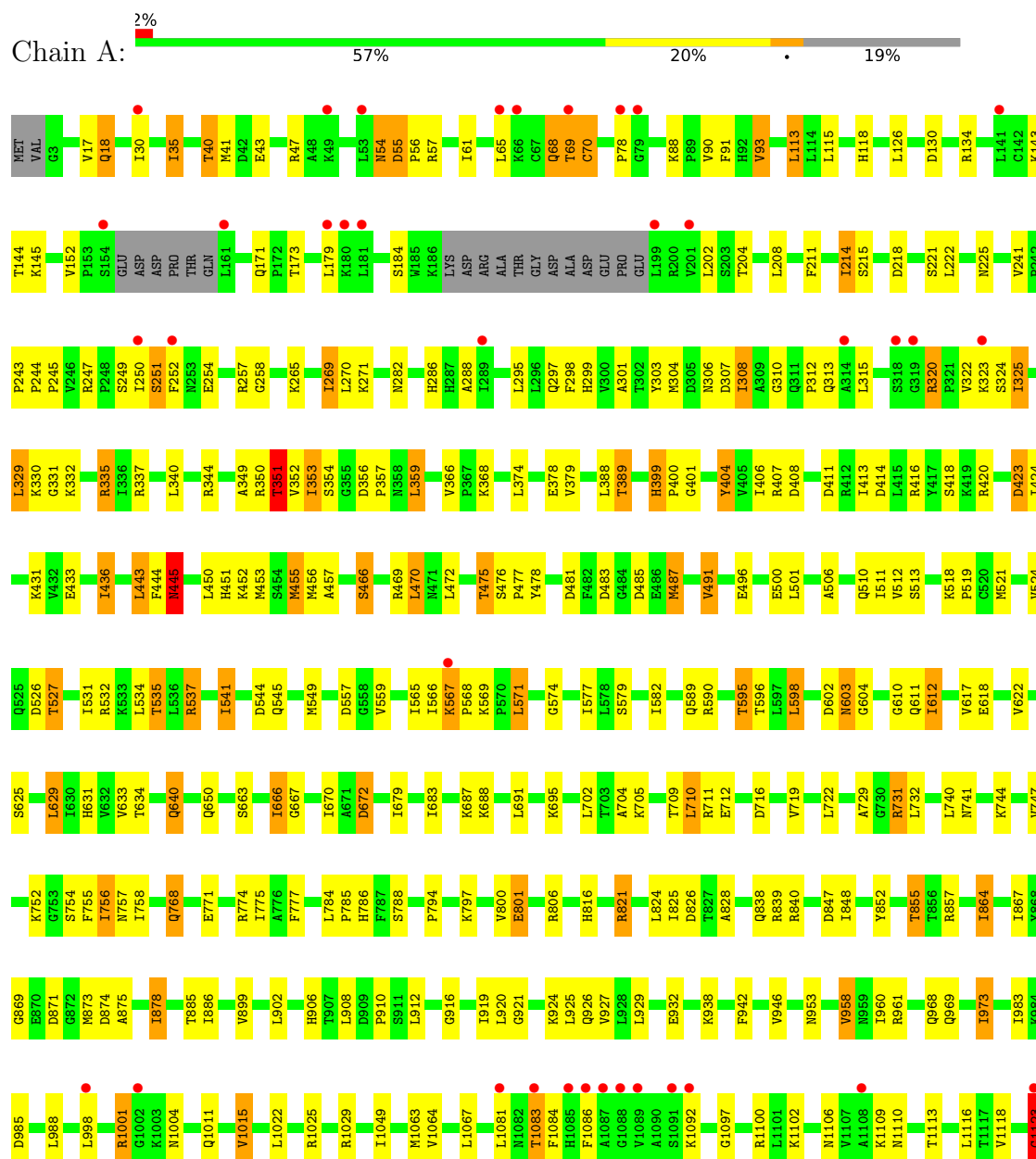
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

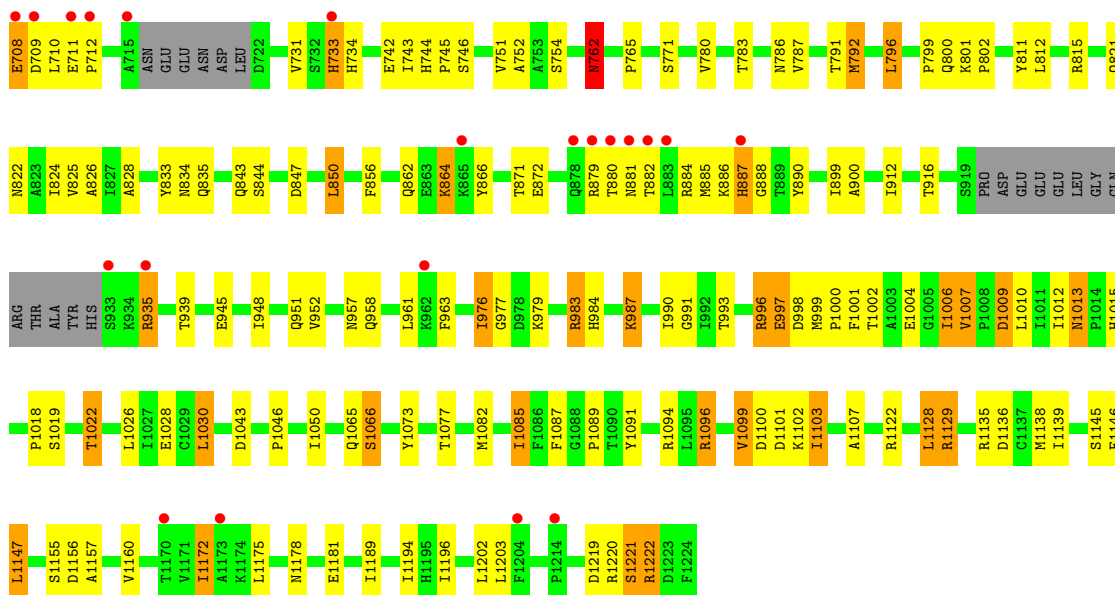
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

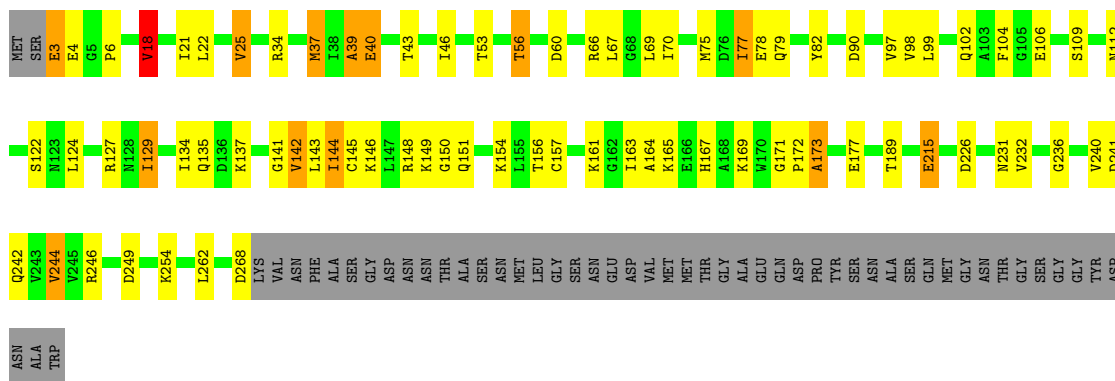
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





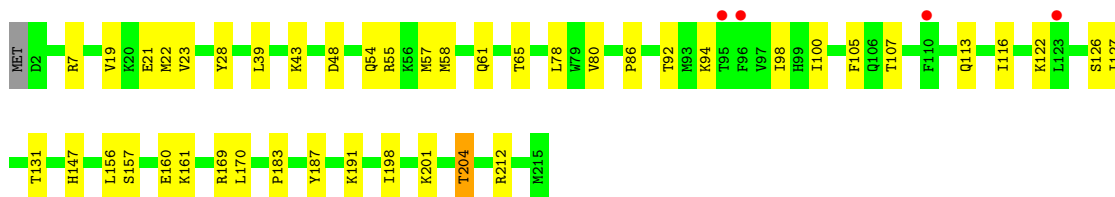
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 59% 20% 16%



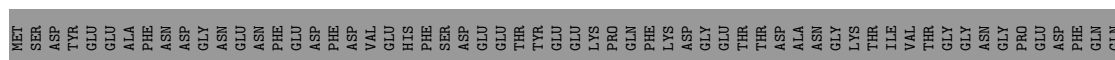
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

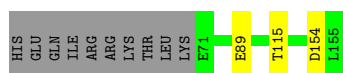
Chain E: 2% 79% 20%



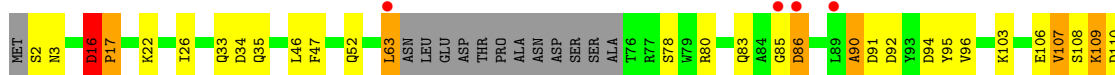
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 53% 45% 2%

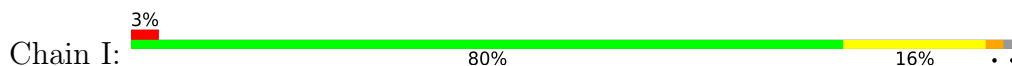




- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



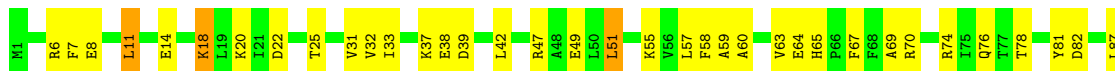
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



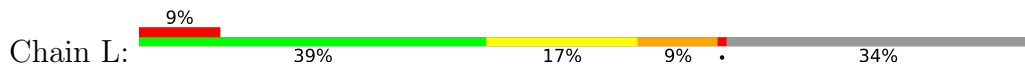
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



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

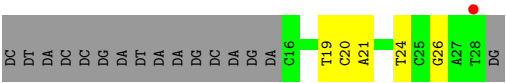


- Molecule 11: RNA (5'-R(*AP*GP*GP*(5BU)P*G)-3')





● Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*C
P*GP*AP*TP*CP*AP*CP*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	158.29Å 220.77Å 192.24Å 90.00° 97.69° 90.00°	Depositor
Resolution (Å)	47.76 – 3.20 47.76 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.76-3.20) 99.0 (47.76-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 3.19Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.183 , 0.231 0.202 , 0.247	Depositor DCC
R_{free} test set	5360 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 92.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28672	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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, 5BU, 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	0.80	2/11241 (0.0%)	1.44	61/15199 (0.4%)
2	B	0.81	1/9033 (0.0%)	1.42	61/12181 (0.5%)
3	C	0.76	0/2133	1.43	17/2891 (0.6%)
4	E	0.77	0/1788	1.40	9/2406 (0.4%)
5	F	0.77	0/700	1.33	0/945
6	H	0.74	0/1086	1.29	14/1470 (1.0%)
7	I	0.75	0/989	1.31	5/1331 (0.4%)
8	J	0.83	0/541	1.55	6/727 (0.8%)
9	K	0.71	0/937	1.34	6/1265 (0.5%)
10	L	0.86	0/365	1.43	9/485 (1.9%)
11	R	0.58	0/99	1.32	1/154 (0.6%)
12	T	0.43	0/292	1.14	1/447 (0.2%)
All	All	0.79	3/29204 (0.0%)	1.41	190/39501 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	487	MET	SD-CE	-5.96	1.64	1.79
2	B	563	MET	SD-CE	-5.91	1.64	1.79
1	A	249	SER	CA-C	5.67	1.55	1.52

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	647	GLY	CA-C-N	10.56	140.72	121.70
2	B	647	GLY	C-N-CA	10.56	140.72	121.70
3	C	172	PRO	CA-C-N	9.02	138.77	121.54
3	C	172	PRO	C-N-CA	9.02	138.77	121.54
1	A	1097	GLY	CA-C-N	8.63	125.68	120.24
1	A	1097	GLY	C-N-CA	8.63	125.68	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	39	ALA	N-CA-C	8.58	123.88	113.41
6	H	92	ASP	N-CA-C	-8.14	102.66	112.59
2	B	37	PHE	N-CA-C	-8.06	99.89	110.53
1	A	506	ALA	CA-C-N	8.01	128.12	120.43
1	A	506	ALA	C-N-CA	8.01	128.12	120.43
2	B	628	THR	CA-C-N	7.97	136.77	121.54
2	B	628	THR	C-N-CA	7.97	136.77	121.54
2	B	733	HIS	N-CA-C	-7.56	102.97	111.14
8	J	18	TRP	N-CA-C	7.33	118.95	110.97
1	A	864	ILE	N-CA-C	-7.32	104.71	111.67
2	B	140	ILE	CA-C-N	7.26	134.76	121.70
2	B	140	ILE	C-N-CA	7.26	134.76	121.70
1	A	1123	GLY	CA-C-N	7.16	134.58	121.70
1	A	1123	GLY	C-N-CA	7.16	134.58	121.70
1	A	603	ASN	CA-CB-CG	7.13	119.73	112.60
2	B	39	ARG	N-CA-C	-7.13	103.43	111.14
1	A	445	ASN	CA-CB-CG	7.13	119.73	112.60
8	J	5	VAL	N-CA-C	-7.05	99.63	109.21
6	H	91	ASP	N-CA-C	7.01	121.10	108.69
2	B	581	PHE	CA-CB-CG	6.90	120.70	113.80
3	C	172	PRO	N-CA-C	-6.76	106.09	114.20
10	L	58	LYS	N-CA-C	6.74	121.67	113.38
2	B	276	ILE	CA-C-N	6.74	130.93	120.82
2	B	276	ILE	C-N-CA	6.74	130.93	120.82
1	A	1063	MET	CA-C-N	6.67	133.97	121.97
1	A	1063	MET	C-N-CA	6.67	133.97	121.97
1	A	411	ASP	N-CA-C	6.67	120.04	110.24
1	A	351	THR	CA-C-N	6.59	129.34	120.50
1	A	351	THR	C-N-CA	6.59	129.34	120.50
2	B	882	THR	N-CA-C	6.58	118.14	110.97
1	A	537	ARG	CA-C-N	6.53	129.03	120.28
1	A	537	ARG	C-N-CA	6.53	129.03	120.28
2	B	1009	ASP	N-CA-C	-6.48	105.20	113.23
2	B	1066	SER	N-CA-C	6.35	119.88	111.75
2	B	629	ASP	CA-CB-CG	6.34	118.94	112.60
2	B	345	LYS	CA-C-N	6.29	133.01	121.70
2	B	345	LYS	C-N-CA	6.29	133.01	121.70
1	A	466	SER	N-CA-C	6.26	120.76	113.18
1	A	152	VAL	N-CA-C	6.24	114.76	107.84
1	A	244	PRO	N-CA-C	6.18	118.24	110.70
2	B	394	ASP	CA-CB-CG	6.17	118.77	112.60
2	B	1222	ARG	CA-C-N	6.00	130.25	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1222	ARG	C-N-CA	6.00	130.25	121.31
11	R	8	G	C4'-C3'-C2'	-6.00	96.60	102.60
1	A	69	THR	CA-C-N	5.97	128.28	120.28
1	A	69	THR	C-N-CA	5.97	128.28	120.28
3	C	56	THR	CA-C-N	5.97	128.64	120.46
3	C	56	THR	C-N-CA	5.97	128.64	120.46
1	A	251	SER	CA-C-N	5.97	128.76	120.29
1	A	251	SER	C-N-CA	5.97	128.76	120.29
2	B	294	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	777	PHE	CA-CB-CG	5.91	119.71	113.80
1	A	800	VAL	CA-C-N	5.91	128.79	120.28
1	A	800	VAL	C-N-CA	5.91	128.79	120.28
1	A	1256	GLU	N-CA-C	5.86	117.75	111.36
2	B	834	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	1004	ASN	CA-C-N	5.83	129.56	120.82
1	A	1004	ASN	C-N-CA	5.83	129.56	120.82
10	L	55	ILE	N-CA-C	5.82	116.59	110.72
9	K	18	LYS	N-CA-C	5.80	117.29	110.97
1	A	288	ALA	N-CA-C	-5.74	106.05	113.16
4	E	48	ASP	CA-CB-CG	5.73	118.33	112.60
6	H	2	SER	CA-C-N	5.72	132.00	121.70
6	H	2	SER	C-N-CA	5.72	132.00	121.70
2	B	648	HIS	N-CA-CB	5.70	120.18	110.50
8	J	64	ASN	N-CA-C	5.70	122.40	109.81
6	H	138	GLU	N-CA-C	-5.69	106.19	113.01
7	I	118	ARG	N-CA-C	5.67	118.72	109.24
1	A	794	PRO	CA-C-N	5.67	128.15	120.38
1	A	794	PRO	C-N-CA	5.67	128.15	120.38
2	B	648	HIS	CA-C-N	5.65	128.74	120.71
2	B	648	HIS	C-N-CA	5.65	128.74	120.71
10	L	56	LEU	N-CA-C	5.65	122.83	110.80
2	B	825	VAL	N-CA-C	5.64	116.01	108.11
1	A	389	THR	CB-CA-C	5.63	119.72	110.88
2	B	363	HIS	N-CA-C	-5.61	101.04	109.79
2	B	890	TYR	CA-C-N	5.60	129.65	120.63
2	B	890	TYR	C-N-CA	5.60	129.65	120.63
1	A	491	VAL	N-CA-C	5.54	114.05	107.73
1	A	983	ILE	N-CA-C	-5.52	105.12	110.42
1	A	485	ASP	CA-CB-CG	5.51	118.11	112.60
3	C	150	GLY	CA-C-N	5.49	128.91	121.05
3	C	150	GLY	C-N-CA	5.49	128.91	121.05
12	T	26	DG	P-O3'-C3'	5.49	128.43	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	50	THR	N-CA-C	5.48	118.16	109.50
2	B	1085	ILE	N-CA-C	5.46	116.17	108.36
6	H	129	TYR	CA-C-N	5.46	127.53	120.44
6	H	129	TYR	C-N-CA	5.46	127.53	120.44
1	A	307	ASP	CA-CB-CG	5.46	118.06	112.60
7	I	113	ASP	CA-CB-CG	5.44	118.04	112.60
8	J	55	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	602	ASP	CA-CB-CG	5.42	118.03	112.60
1	A	886	ILE	N-CA-C	5.42	116.49	111.45
2	B	476	ARG	CA-C-N	5.42	131.89	121.54
2	B	476	ARG	C-N-CA	5.42	131.89	121.54
10	L	62	LYS	N-CA-C	-5.41	106.36	113.17
1	A	481	ASP	CA-CB-CG	5.40	118.00	112.60
3	C	40	GLU	N-CA-C	5.39	120.55	112.94
6	H	3	ASN	CA-C-N	5.39	129.13	121.42
6	H	3	ASN	C-N-CA	5.39	129.13	121.42
1	A	1424	VAL	CA-C-N	5.37	127.79	120.54
1	A	1424	VAL	C-N-CA	5.37	127.79	120.54
8	J	13	VAL	N-CA-CB	5.36	116.65	110.49
2	B	638	PHE	CA-CB-CG	5.35	119.15	113.80
2	B	945	GLU	N-CA-C	5.34	117.42	110.53
9	K	39	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	1419	ASP	CA-C-N	5.32	127.41	120.28
1	A	1419	ASP	C-N-CA	5.32	127.41	120.28
3	C	135	GLN	CA-C-N	5.32	128.32	120.82
3	C	135	GLN	C-N-CA	5.32	128.32	120.82
2	B	997	GLU	N-CA-C	5.31	117.06	111.28
2	B	1022	THR	CB-CA-C	5.31	120.08	112.12
4	E	21	GLU	CA-C-N	5.29	127.32	120.44
4	E	21	GLU	C-N-CA	5.29	127.32	120.44
1	A	1354	ASN	N-CA-C	5.28	117.78	111.71
1	A	985	ASP	CA-CB-CG	5.28	117.88	112.60
3	C	82	TYR	N-CA-C	-5.26	101.39	109.76
9	K	82	ASP	CA-CB-CG	5.26	117.86	112.60
2	B	351	TYR	N-CA-C	-5.25	105.47	111.14
1	A	452	LYS	N-CA-C	-5.25	105.73	111.82
2	B	276	ILE	N-CA-C	5.24	115.40	107.80
2	B	490	SER	CA-C-N	5.24	127.56	120.65
2	B	490	SER	C-N-CA	5.24	127.56	120.65
4	E	113	GLN	N-CA-C	5.24	117.07	111.36
1	A	1198	ASP	CA-C-N	5.23	127.29	120.28
1	A	1198	ASP	C-N-CA	5.23	127.29	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	236	GLY	CA-C-N	5.22	127.53	120.38
3	C	236	GLY	C-N-CA	5.22	127.53	120.38
1	A	1437	GLY	CA-C-N	5.21	127.27	120.28
1	A	1437	GLY	C-N-CA	5.21	127.27	120.28
2	B	99	LYS	N-CA-C	-5.21	102.63	110.24
2	B	294	ASP	CA-C-N	5.21	125.76	119.98
2	B	294	ASP	C-N-CA	5.21	125.76	119.98
2	B	1122	ARG	CA-C-N	5.20	128.92	120.60
2	B	1122	ARG	C-N-CA	5.20	128.92	120.60
2	B	828	ALA	N-CA-C	5.19	116.41	108.52
4	E	161	LYS	CA-C-N	5.19	127.49	120.38
4	E	161	LYS	C-N-CA	5.19	127.49	120.38
1	A	906	HIS	N-CA-C	5.18	119.15	112.41
3	C	60	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	557	ASP	CA-CB-CG	5.15	117.75	112.60
2	B	425	THR	CA-C-N	5.14	127.16	120.28
2	B	425	THR	C-N-CA	5.14	127.16	120.28
6	H	16	ASP	N-CA-C	5.14	118.44	107.91
3	C	78	GLU	CB-CG-CD	5.13	121.32	112.60
1	A	513	SER	N-CA-C	5.13	116.53	110.07
2	B	392	ARG	N-CA-C	-5.12	107.41	113.97
1	A	612	ILE	N-CA-CB	5.12	116.68	110.95
1	A	366	VAL	N-CA-C	5.11	113.49	107.77
2	B	1101	ASP	CA-CB-CG	5.11	117.71	112.60
10	L	59	ALA	CA-C-N	5.11	128.33	120.82
10	L	59	ALA	C-N-CA	5.11	128.33	120.82
9	K	70	ARG	N-CA-C	5.11	116.88	110.24
8	J	2	ILE	N-CA-C	5.10	119.94	109.34
6	H	130	ARG	CA-C-N	5.09	131.26	121.54
6	H	130	ARG	C-N-CA	5.09	131.26	121.54
2	B	762	ASN	CA-CB-CG	5.08	117.68	112.60
2	B	230	ALA	N-CA-C	5.07	121.01	109.81
10	L	40	LEU	N-CA-C	5.06	117.08	109.23
2	B	681	TRP	N-CA-C	-5.06	105.95	111.82
7	I	52	ILE	CB-CA-C	5.05	116.86	111.35
2	B	1222	ARG	N-CA-C	-5.04	104.30	110.65
3	C	18	VAL	N-CA-CB	5.04	118.89	112.34
1	A	1001	ARG	N-CA-C	5.03	119.14	113.15
9	K	113	THR	CA-C-N	5.03	130.76	121.70
9	K	113	THR	C-N-CA	5.03	130.76	121.70
4	E	170	LEU	N-CA-C	5.03	117.53	110.14
2	B	1013	ASN	N-CA-C	5.03	116.21	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1030	LEU	CA-C-N	5.02	126.97	120.44
2	B	1030	LEU	C-N-CA	5.02	126.97	120.44
2	B	1022	THR	CA-C-N	5.02	127.55	120.42
2	B	1022	THR	C-N-CA	5.02	127.55	120.42
7	I	10	CYS	N-CA-C	5.02	116.83	111.36
10	L	40	LEU	CA-C-N	5.02	127.90	120.82
10	L	40	LEU	C-N-CA	5.02	127.90	120.82
2	B	711	GLU	N-CA-C	5.01	120.88	109.81
1	A	874	ASP	CA-C-N	5.01	127.69	120.38
1	A	874	ASP	C-N-CA	5.01	127.69	120.38
4	E	57	MET	CA-C-N	5.01	126.95	120.44
4	E	57	MET	C-N-CA	5.01	126.95	120.44
1	A	526	ASP	CA-CB-CG	5.00	117.60	112.60
6	H	91	ASP	CA-C-N	5.00	130.62	122.67
6	H	91	ASP	C-N-CA	5.00	130.62	122.67
1	A	1228	TRP	N-CA-C	5.00	116.67	109.07

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	181	0
2	B	8861	0	8884	152	0
3	C	2095	0	2051	39	0
4	E	1752	0	1776	17	0
5	F	688	0	707	1	0
6	H	1068	0	1040	11	0
7	I	971	0	927	8	0
8	J	532	0	542	18	0
9	K	919	0	929	19	0
10	L	363	0	386	5	0
11	R	109	0	54	1	0
12	T	262	0	147	3	0
13	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	28672	0	28576	397	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (397) 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:1123:GLY:HA3	1:A:1124:HIS:HB2	1.59	0.83
1:A:869:GLY:O	4:E:204:THR:HG21	1.79	0.82
8:J:48:ARG:O	8:J:52:THR:HB	1.80	0.82
2:B:1013:ASN:HD21	2:B:1015:HIS:HD2	1.28	0.81
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.45	0.81
3:C:98:VAL:H	3:C:122:SER:HB2	1.44	0.81
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.46	0.80
1:A:535:THR:HG21	1:A:617:VAL:H	1.46	0.79
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.66	0.78
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.66	0.75
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.69	0.73
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.68	0.73
2:B:345:LYS:HA	2:B:347:LYS:H	1.52	0.73
1:A:855:THR:HG21	1:A:857:ARG:HE	1.55	0.72
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.71	0.71
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.73	0.71
3:C:142:VAL:H	8:J:16:ASP:HB3	1.57	0.69
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.28	0.68
1:A:469:ARG:NH2	2:B:991:GLY:O	2.26	0.68
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.09	0.68
1:A:756:ILE:HD13	1:A:756:ILE:H	1.59	0.67
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.75	0.67
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.29	0.67
1:A:998:LEU:HD12	1:A:1001:ARG:HG3	1.77	0.66
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.76	0.66
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.76	0.66
1:A:399:HIS:O	1:A:401:GLY:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.28	0.66
2:B:864:LYS:H	2:B:872:GLU:HB2	1.60	0.66
2:B:654:ARG:H	2:B:657:HIS:HD2	1.44	0.65
1:A:754:SER:H	1:A:757:ASN:HD22	1.45	0.65
4:E:19:VAL:O	4:E:23:VAL:HG23	1.98	0.64
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.80	0.63
3:C:167:HIS:HD2	3:C:169:LYS:H	1.45	0.63
1:A:511:ILE:HA	1:A:521:MET:HE3	1.80	0.63
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.81	0.62
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.62
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.82	0.62
1:A:567:LYS:HD3	6:H:95:TYR:CE1	2.35	0.62
2:B:996:ARG:HH22	3:C:173:ALA:HB1	1.65	0.61
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.81	0.61
3:C:6:PRO:HB3	3:C:25:VAL:HG22	1.82	0.61
2:B:43:LEU:HD11	2:B:811:TYR:O	2.00	0.61
2:B:1002:THR:HG22	2:B:1004:GLU:H	1.65	0.61
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.83	0.61
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.82	0.61
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.82	0.61
3:C:171:GLY:C	3:C:173:ALA:H	2.07	0.61
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.47	0.60
1:A:640:GLN:CD	1:A:640:GLN:H	2.09	0.60
1:A:596:THR:C	1:A:598:LEU:H	2.10	0.60
2:B:1013:ASN:ND2	2:B:1015:HIS:HD2	2.00	0.60
1:A:741:ASN:HD22	1:A:744:LYS:H	1.50	0.60
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.68	0.59
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.84	0.59
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.85	0.58
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.85	0.58
2:B:801:LYS:O	8:J:52:THR:HG23	2.04	0.58
2:B:1013:ASN:HD21	2:B:1015:HIS:CD2	2.16	0.58
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.86	0.58
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.86	0.57
1:A:265:LYS:HD3	1:A:322:VAL:HG11	1.86	0.57
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.33	0.57
2:B:38:PHE:H	2:B:41:LYS:HB2	1.69	0.57
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.87	0.57
2:B:976:ILE:O	2:B:990:ILE:HB	2.05	0.57
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.86	0.57
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:125:LEU:HG	6:H:130:ARG:NH1	2.20	0.56
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.69	0.56
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.69	0.56
2:B:744:HIS:HD2	2:B:746:SER:H	1.54	0.56
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.88	0.56
1:A:472:LEU:O	1:A:475:THR:HB	2.05	0.56
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.88	0.56
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.86	0.56
2:B:887:HIS:HA	2:B:888:GLY:C	2.31	0.56
2:B:843:GLN:HB2	2:B:993:THR:HB	1.88	0.56
1:A:251:SER:HB3	1:A:258:GLY:HA3	1.88	0.56
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.88	0.56
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.89	0.55
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.88	0.55
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.22	0.55
9:K:65:HIS:HD2	9:K:67:PHE:H	1.55	0.55
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.89	0.55
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.89	0.55
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.89	0.54
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.42	0.54
2:B:128:LEU:HB2	2:B:167:ILE:HG22	1.88	0.54
1:A:456:MET:HE3	1:A:510:GLN:HB2	1.88	0.54
2:B:313:MET:HE2	2:B:390:LEU:HG	1.88	0.54
2:B:706:GLN:O	2:B:710:LEU:HB2	2.07	0.54
1:A:472:LEU:HD21	2:B:835:GLN:HB2	1.89	0.54
11:R:6:A:H61	12:T:24:DT:H3	1.54	0.54
6:H:125:LEU:HG	6:H:130:ARG:HH12	1.73	0.54
3:C:262:LEU:HD11	9:K:87:LEU:HD23	1.89	0.54
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.38	0.54
1:A:527:THR:HG21	1:A:650:GLN:HA	1.90	0.53
1:A:855:THR:CG2	1:A:857:ARG:HE	2.21	0.53
2:B:884:ARG:HG3	2:B:935:ARG:HE	1.73	0.53
6:H:63:LEU:HB2	6:H:90:ALA:H	1.74	0.53
1:A:579:SER:HA	1:A:582:ILE:HD12	1.90	0.53
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.91	0.53
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.90	0.53
2:B:241:ARG:HA	2:B:253:THR:HG22	1.89	0.53
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.89	0.53
2:B:984:HIS:HB3	2:B:1022:THR:OG1	2.09	0.53
2:B:1129:ARG:HB3	12:T:21:DA:H5"	1.91	0.53
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:HG2	7:I:97:MET:HE2	1.91	0.53
1:A:535:THR:HG21	1:A:617:VAL:N	2.18	0.52
2:B:195:CYS:SG	2:B:783:THR:HB	2.49	0.52
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.91	0.52
4:E:22:MET:HE2	4:E:187:TYR:HA	1.91	0.52
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.74	0.52
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.92	0.52
1:A:946:VAL:HG13	4:E:201:LYS:HB3	1.92	0.52
1:A:404:TYR:HA	1:A:413:ILE:O	2.09	0.52
2:B:1013:ASN:ND2	2:B:1015:HIS:CD2	2.77	0.52
3:C:56:THR:HG21	3:C:145:CYS:SG	2.50	0.52
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.92	0.52
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.92	0.51
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.92	0.51
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.92	0.51
3:C:134:ILE:HG12	3:C:141:GLY:H	1.75	0.51
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.93	0.51
1:A:709:THR:HG22	1:A:711:ARG:H	1.76	0.51
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.93	0.51
6:H:80:ARG:HG2	9:K:57:LEU:HD22	1.92	0.51
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.76	0.51
1:A:134:ARG:HD2	1:A:221:SER:O	2.11	0.51
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.37	0.51
2:B:515:HIS:H	2:B:518:HIS:CD2	2.29	0.51
2:B:570:VAL:HB	2:B:573:GLN:HG2	1.93	0.50
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.93	0.50
1:A:113:LEU:HD12	1:A:218:ASP:HB3	1.94	0.50
1:A:571:LEU:HD23	6:H:46:LEU:HD11	1.94	0.50
1:A:1422:ARG:HG3	2:B:1220:ARG:HH12	1.75	0.50
2:B:563:MET:HE3	2:B:580:VAL:HB	1.93	0.50
1:A:663:SER:HB2	2:B:1085:ILE:HG13	1.94	0.50
1:A:729:ALA:HA	1:A:732:LEU:HD12	1.93	0.50
1:A:406:ILE:HD11	1:A:433:GLU:HG3	1.94	0.50
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.94	0.50
2:B:579:ARG:HG3	2:B:623:GLU:HG2	1.93	0.50
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.94	0.50
1:A:1123:GLY:CA	1:A:1124:HIS:HB2	2.38	0.49
9:K:38:GLU:O	9:K:69:ALA:O	2.30	0.49
12:T:19:DT:H2'	12:T:20:DC:C6	2.48	0.49
1:A:667:GLY:HA2	1:A:670:ILE:HG12	1.95	0.49
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.46	0.49
3:C:165:LYS:O	9:K:6:ARG:NH1	2.46	0.49
1:A:839:ARG:NH2	1:A:1402:PHE:O	2.44	0.49
3:C:167:HIS:CD2	3:C:169:LYS:H	2.30	0.49
1:A:211:PHE:HA	1:A:214:ILE:HD11	1.95	0.49
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.78	0.49
3:C:171:GLY:C	3:C:173:ALA:N	2.70	0.49
1:A:899:VAL:HB	1:A:929:LEU:HD22	1.95	0.48
3:C:66:ARG:NH2	8:J:3:VAL:O	2.35	0.48
1:A:70:CYS:HB2	2:B:1172:ILE:HG23	1.95	0.48
1:A:531:ILE:O	1:A:535:THR:HB	2.13	0.48
2:B:69:LEU:HD12	2:B:90:ILE:HB	1.95	0.48
2:B:792:MET:HA	2:B:856:PHE:O	2.14	0.48
2:B:976:ILE:HG23	2:B:977:GLY:H	1.79	0.48
1:A:567:LYS:HB3	6:H:96:VAL:H	1.79	0.48
1:A:1086:PHE:HB3	1:A:1092:LYS:HB3	1.96	0.48
1:A:55:ASP:O	1:A:57:ARG:N	2.46	0.48
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.96	0.48
7:I:26:LEU:HD23	7:I:37:GLU:HA	1.95	0.48
1:A:683:ILE:HG21	1:A:801:GLU:HG2	1.96	0.47
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.14	0.47
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.94	0.47
2:B:245:GLU:HG3	2:B:249:ARG:HH22	1.79	0.47
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.96	0.47
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.96	0.47
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.79	0.47
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.96	0.47
9:K:108:GLU:HA	9:K:111:LEU:HD12	1.96	0.47
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.97	0.47
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.67	0.47
4:E:39:LEU:HG	4:E:43:LYS:HE3	1.96	0.47
1:A:115:LEU:HD21	1:A:145:LYS:HE3	1.96	0.47
1:A:445:ASN:HB2	1:A:455:MET:HG3	1.96	0.47
1:A:565:ILE:HG22	1:A:569:LYS:O	2.15	0.47
2:B:542:MET:HE1	2:B:743:ILE:HG13	1.97	0.47
4:E:107:THR:HG22	4:E:131:THR:HB	1.97	0.47
4:E:157:SER:HB3	4:E:160:GLU:HG3	1.97	0.47
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.96	0.47
1:A:1130:GLN:O	1:A:1134:ILE:HG12	2.15	0.47
3:C:3:GLU:HB3	9:K:104:ASN:HD21	1.80	0.47
1:A:357:PRO:HD2	2:B:833:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:LYS:HA	2:B:347:LYS:N	2.27	0.47
2:B:428:ILE:HD11	2:B:448:ILE:HG23	1.97	0.47
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.97	0.47
9:K:65:HIS:CD2	9:K:67:PHE:H	2.33	0.46
1:A:535:THR:CG2	1:A:617:VAL:H	2.21	0.46
1:A:545:GLN:HG2	1:A:549:MET:HE2	1.98	0.46
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.51	0.46
3:C:69:LEU:O	8:J:6:ARG:HD2	2.15	0.46
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.97	0.46
9:K:55:LYS:HD2	9:K:81:TYR:HD1	1.81	0.46
1:A:752:LYS:HB3	2:B:1018:PRO:HG2	1.98	0.46
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.97	0.46
2:B:516:ASN:H	2:B:516:ASN:HD22	1.64	0.46
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.50	0.46
1:A:512:VAL:HA	1:A:519:PRO:HA	1.97	0.46
1:A:848:ILE:HD12	1:A:864:ILE:HG13	1.98	0.46
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.98	0.46
4:E:198:ILE:HD13	4:E:212:ARG:HG3	1.96	0.46
2:B:613:VAL:HG22	2:B:628:THR:HA	1.98	0.46
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.98	0.45
2:B:654:ARG:H	2:B:657:HIS:CD2	2.31	0.45
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.80	0.45
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.98	0.45
10:L:49:LYS:O	10:L:50:ASP:HB2	2.16	0.45
1:A:173:THR:HB	1:A:184:SER:HB3	1.97	0.45
1:A:306:ASN:HD21	1:A:313:GLN:HB2	1.80	0.45
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.96	0.45
1:A:456:MET:HG2	1:A:510:GLN:HG3	1.98	0.45
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.52	0.45
9:K:8:GLU:O	9:K:37:LYS:HD2	2.16	0.45
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.52	0.45
2:B:1100:ASP:HA	2:B:1103:ILE:HD11	1.98	0.45
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.98	0.45
2:B:36:ALA:HB2	2:B:661:LEU:HD22	1.98	0.45
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.99	0.45
1:A:1116:LEU:HB3	1:A:1308:THR:HB	1.98	0.45
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.98	0.45
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.99	0.45
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.17	0.45
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.99	0.45
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1266:THR:HA	1:A:1270:ASN:HD22	1.81	0.45
2:B:140:ILE:H	2:B:141:ASP:C	2.25	0.45
3:C:148:ARG:HB3	3:C:151:GLN:HG3	1.99	0.45
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.99	0.45
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.99	0.45
2:B:578:THR:OG1	2:B:593:PRO:HG3	2.17	0.45
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.52	0.45
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.32	0.44
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.98	0.44
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.99	0.44
1:A:756:ILE:H	1:A:756:ILE:CD1	2.27	0.44
7:I:69:PRO:HD2	7:I:85:PHE:O	2.18	0.44
1:A:443:LEU:HD11	1:A:455:MET:HG2	1.99	0.44
1:A:666:ILE:HG12	2:B:1026:LEU:HB2	1.99	0.44
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.32	0.44
1:A:350:ARG:HD2	2:B:1128:LEU:HD21	2.00	0.44
1:A:942:PHE:O	1:A:946:VAL:HG23	2.18	0.44
2:B:1082:MET:HA	3:C:189:THR:HA	2.00	0.44
1:A:747:VAL:HG21	1:A:758:ILE:HD11	1.99	0.44
1:A:821:ARG:O	1:A:825:ILE:HG12	2.17	0.44
1:A:774:ARG:HG3	1:A:797:LYS:HE3	2.00	0.44
3:C:104:PHE:HD2	3:C:106:GLU:HG3	1.82	0.44
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.17	0.44
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	2.00	0.44
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.98	0.44
3:C:37:MET:HE2	3:C:244:VAL:HA	1.99	0.44
10:L:61:THR:HB	10:L:63:ARG:H	1.82	0.44
1:A:353:ILE:HG12	1:A:487:MET:HG3	2.00	0.44
2:B:38:PHE:HA	2:B:42:GLY:H	1.83	0.44
2:B:405:ARG:HB3	2:B:631:GLY:HA3	1.98	0.44
6:H:33:GLN:HG3	6:H:129:TYR:OH	2.18	0.44
1:A:315:LEU:HA	1:A:320:ARG:HB3	2.00	0.44
1:A:1138:ILE:HG13	1:A:1282:VAL:HG21	2.00	0.44
2:B:63:ILE:O	2:B:67:SER:HB3	2.18	0.44
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.47	0.44
8:J:5:VAL:HG12	8:J:6:ARG:HG3	2.00	0.44
1:A:329:LEU:HA	1:A:335:ARG:H	1.83	0.43
1:A:924:LYS:O	1:A:927:VAL:HG12	2.18	0.43
2:B:356:LEU:HA	2:B:360:PHE:HB3	2.00	0.43
3:C:164:ALA:HA	3:C:167:HIS:O	2.18	0.43
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:LYS:H	2:B:277:LYS:HG3	1.53	0.43
1:A:567:LYS:CB	1:A:568:PRO:CD	2.96	0.43
1:A:1100:ARG:HH21	1:A:1330:ASN:HB2	1.82	0.43
8:J:44:TYR:HA	8:J:47:ARG:HB2	2.00	0.43
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.99	0.43
2:B:563:MET:HE1	2:B:587:HIS:HB2	2.00	0.43
2:B:708:GLU:O	2:B:710:LEU:N	2.52	0.43
1:A:873:MET:HB3	1:A:878:ILE:HD11	2.00	0.43
2:B:800:GLN:HB2	2:B:821:GLN:HA	2.01	0.43
3:C:143:LEU:HD21	3:C:146:LYS:HE3	2.00	0.43
7:I:97:MET:HE3	7:I:97:MET:HB2	1.79	0.43
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.99	0.43
1:A:958:VAL:HG11	1:A:1049:ILE:HG23	2.01	0.43
2:B:695:ALA:HA	2:B:698:GLU:HB2	2.01	0.43
2:B:824:ILE:HD13	2:B:1089:PRO:HB3	2.00	0.43
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.01	0.43
2:B:912:ILE:HB	2:B:939:THR:HB	2.00	0.43
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.33	0.43
2:B:640:VAL:CG1	2:B:649:LYS:HB3	2.49	0.43
2:B:706:GLN:HB2	2:B:710:LEU:HD23	2.01	0.43
3:C:18:VAL:HG23	3:C:232:VAL:HB	2.01	0.43
1:A:1129:GLU:HA	1:A:1132:LYS:HE3	2.00	0.42
1:A:1285:MET:HG3	1:A:1307:GLU:OE1	2.19	0.42
2:B:957:ASN:CG	2:B:958:GLN:H	2.27	0.42
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.01	0.42
2:B:653:VAL:HG22	2:B:689:LEU:HB3	2.01	0.42
3:C:70:ILE:CD1	3:C:144:ILE:HD12	2.49	0.42
2:B:29:ASP:HB3	2:B:658:ILE:HG12	2.01	0.42
4:E:61:GLN:HE21	4:E:105:PHE:HE2	1.67	0.42
9:K:7:PHE:HB2	9:K:11:LEU:HD22	2.01	0.42
1:A:1308:THR:HG22	1:A:1310:GLY:O	2.19	0.42
1:A:1393:ASN:ND2	1:A:1393:ASN:H	2.16	0.42
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.34	0.42
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.55	0.42
3:C:40:GLU:HG2	3:C:163:ILE:HD12	2.00	0.42
1:A:351:THR:HG21	1:A:466:SER:O	2.20	0.42
2:B:800:GLN:HG3	2:B:821:GLN:HG2	2.02	0.42
1:A:304:MET:HA	1:A:325:ILE:HD12	2.01	0.42
1:A:567:LYS:C	1:A:569:LYS:H	2.28	0.42
1:A:595:THR:HG21	1:A:604:GLY:HA3	2.02	0.42
1:A:1161:THR:OG1	1:A:1170:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:MET:HE3	2:B:386:LEU:HD22	2.01	0.42
2:B:379:GLY:HA2	2:B:382:ILE:HD12	2.01	0.42
2:B:577:ALA:HB1	2:B:589:VAL:HB	2.02	0.42
2:B:1002:THR:HB	2:B:1006:ILE:H	1.84	0.42
8:J:36:LEU:HD11	8:J:51:LEU:HB2	2.02	0.42
2:B:123:THR:HA	2:B:204:ILE:O	2.20	0.42
2:B:952:VAL:HB	10:L:58:LYS:CB	2.50	0.42
1:A:741:ASN:HB3	1:A:744:LYS:HB3	2.02	0.42
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	2.01	0.42
4:E:55:ARG:HA	4:E:58:MET:HE2	2.02	0.42
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	2.02	0.42
1:A:579:SER:HB3	1:A:611:GLN:HA	2.01	0.42
2:B:256:VAL:HG12	2:B:385:LEU:HD22	2.01	0.42
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.45	0.42
2:B:979:LYS:HE3	2:B:987:LYS:HB2	2.02	0.42
9:K:32:VAL:HG22	9:K:74:ARG:HG3	2.02	0.42
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.01	0.41
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.19	0.41
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.55	0.41
2:B:999:MET:HB3	2:B:1007:VAL:HG22	2.01	0.41
2:B:286:PHE:HB3	2:B:297:ILE:HG12	2.02	0.41
2:B:744:HIS:CD2	2:B:746:SER:OG	2.72	0.41
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.01	0.41
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.91	0.41
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.44	0.41
2:B:551:PRO:HB2	2:B:555:ILE:HD11	2.03	0.41
2:B:620:ARG:HD2	7:I:68:LEU:HD11	2.02	0.41
4:E:94:LYS:O	4:E:98:ILE:HG12	2.20	0.41
1:A:1152:ILE:HB	7:I:44:TYR:HB3	2.02	0.41
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.34	0.41
1:A:457:ALA:HB2	1:A:501:LEU:HB3	2.03	0.41
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.50	0.41
1:A:1342:GLU:HG3	4:E:198:ILE:HG21	2.03	0.41
2:B:363:HIS:O	2:B:364:ILE:HB	2.19	0.41
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.53	0.41
1:A:420:ARG:HE	1:A:423:ASP:CG	2.29	0.41
1:A:629:LEU:O	1:A:633:VAL:HG23	2.20	0.41
1:A:731:ARG:HD3	1:A:755:PHE:CZ	2.56	0.41
1:A:968:GLN:HA	1:A:973:ILE:HD13	2.02	0.41
1:A:1100:ARG:NH2	1:A:1330:ASN:HB2	2.35	0.41
2:B:291:ILE:HD12	2:B:291:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1135:ARG:HG3	2:B:1147:LEU:HD21	2.02	0.41
1:A:456:MET:HB2	1:A:478:TYR:OH	2.21	0.41
1:A:589:GLN:HB3	1:A:961:ARG:HH22	1.86	0.41
1:A:1191:TRP:HZ3	7:I:43:VAL:HG21	1.85	0.41
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.61	0.41
2:B:651:LEU:HD11	2:B:707:PRO:HB3	2.03	0.41
3:C:22:LEU:HD11	9:K:101:LEU:HD21	2.01	0.41
1:A:91:PHE:H	1:A:297:GLN:HE22	1.69	0.41
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.54	0.41
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	2.02	0.41
2:B:476:ARG:O	2:B:478:GLY:N	2.54	0.41
1:A:351:THR:HG22	1:A:352:VAL:H	1.84	0.41
1:A:534:LEU:O	1:A:574:GLY:HA3	2.21	0.41
1:A:567:LYS:HG3	1:A:568:PRO:HD2	2.03	0.41
1:A:666:ILE:HG12	2:B:1026:LEU:CB	2.51	0.41
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.21	0.41
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.53	0.41
2:B:1219:ASP:C	2:B:1221:SER:H	2.28	0.41
4:E:19:VAL:HG11	4:E:80:VAL:HG11	2.02	0.41
1:A:709:THR:HB	1:A:712:GLU:HB2	2.02	0.41
2:B:102:VAL:HG23	2:B:112:LEU:HD22	2.02	0.41
2:B:515:HIS:CD2	2:B:517:THR:H	2.39	0.41
1:A:559:VAL:HG13	6:H:78:SER:HA	2.02	0.40
1:A:828:ALA:HB2	2:B:530:GLY:HA2	2.02	0.40
1:A:1259:MET:HA	1:A:1262:LYS:HE2	2.03	0.40
1:A:68:GLN:C	1:A:70:CYS:H	2.29	0.40
1:A:374:LEU:HA	2:B:1107:ALA:HB2	2.03	0.40
1:A:1327:ILE:O	4:E:147:HIS:HE1	2.04	0.40
1:A:1338:VAL:HG12	1:A:1339:LEU:HG	2.03	0.40
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.86	0.40
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.44	0.40
2:B:708:GLU:H	2:B:708:GLU:HG2	1.63	0.40
1:A:18:GLN:HE21	1:A:1418:LEU:HB2	1.87	0.40
1:A:541:ILE:HD11	1:A:577:ILE:HG12	2.03	0.40
8:J:3:VAL:HG21	8:J:18:TRP:HB2	2.04	0.40
8:J:14:VAL:HA	8:J:17:LYS:HD3	2.02	0.40
1:A:179:LEU:HD11	1:A:298:PHE:HD1	1.87	0.40
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.21	0.40
1:A:785:PRO:HD2	1:A:786:HIS:CD2	2.57	0.40
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	2.04	0.40
2:B:211:VAL:HG21	2:B:483:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:7:PHE:O	9:K:11:LEU:HB2	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%)	1234 (88%)	124 (9%)	37 (3%)	4	25
2	B	1096/1224 (90%)	962 (88%)	96 (9%)	38 (4%)	3	20
3	C	264/318 (83%)	239 (90%)	21 (8%)	4 (2%)	8	37
4	E	212/215 (99%)	203 (96%)	7 (3%)	2 (1%)	14	47
5	F	83/155 (54%)	75 (90%)	7 (8%)	1 (1%)	10	42
6	H	129/146 (88%)	103 (80%)	16 (12%)	10 (8%)	1	5
7	I	117/122 (96%)	105 (90%)	11 (9%)	1 (1%)	14	47
8	J	63/70 (90%)	58 (92%)	2 (3%)	3 (5%)	2	14
9	K	112/120 (93%)	107 (96%)	4 (4%)	1 (1%)	14	47
10	L	44/70 (63%)	30 (68%)	7 (16%)	7 (16%)	0	0
All	All	3515/4173 (84%)	3116 (89%)	295 (8%)	104 (3%)	3	23

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	54	ASN
1	A	55	ASP
1	A	250	ILE
1	A	399	HIS
1	A	418	SER

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Mol	Chain	Res	Type
1	A	424	ILE
1	A	567	LYS
1	A	1223	ASP
2	B	250	PHE
2	B	477	ALA
2	B	648	HIS
2	B	708	GLU
2	B	709	ASP
2	B	712	PRO
2	B	731	VAL
2	B	734	HIS
2	B	751	VAL
2	B	850	LEU
2	B	1046	PRO
2	B	1156	ASP
2	B	1181	GLU
3	C	173	ALA
8	J	2	ILE
8	J	6	ARG
10	L	50	ASP
10	L	56	LEU
1	A	118	HIS
1	A	286	HIS
1	A	312	PRO
1	A	324	SER
1	A	332	LYS
1	A	775	ILE
1	A	1123	GLY
1	A	1234	GLU
1	A	1437	GLY
2	B	367	LEU
2	B	465	ASN
2	B	469	GLN
2	B	526	GLU
2	B	629	ASP
2	B	887	HIS
2	B	976	ILE
2	B	1155	SER
3	C	142	VAL
4	E	126	SER
6	H	85	GLY
6	H	131	ASN

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Mol	Chain	Res	Type
10	L	64	LEU
1	A	56	PRO
1	A	68	GLN
1	A	308	ILE
1	A	423	ASP
1	A	1221	LYS
2	B	137	TYR
2	B	139	ALA
2	B	471	LYS
2	B	646	LEU
2	B	879	ARG
2	B	1221	SER
5	F	154	ASP
6	H	90	ALA
6	H	109	LYS
7	I	77	LYS
9	K	64	GLU
10	L	46	VAL
10	L	59	ALA
1	A	214	ILE
1	A	257	ARG
1	A	610	GLY
1	A	672	ASP
1	A	852	TYR
1	A	1083	THR
2	B	248	SER
2	B	478	GLY
2	B	1096	ARG
2	B	1157	ALA
2	B	1178	ASN
3	C	90	ASP
3	C	215	GLU
4	E	86	PRO
6	H	86	ASP
10	L	47	ARG
1	A	35	ILE
1	A	958	VAL
2	B	531	GLN
2	B	881	ASN
6	H	83	GLN
6	H	140	ALA
8	J	64	ASN

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Mol	Chain	Res	Type
10	L	39	SER
1	A	310	GLY
1	A	404	TYR
2	B	563	MET
2	B	792	MET
2	B	1099	VAL
6	H	17	PRO
6	H	108	SER
1	A	78	PRO
1	A	331	GLY
1	A	400	PRO
1	A	1384	VAL
6	H	107	VAL
2	B	647	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	1225/1520 (81%)	1058 (86%)	167 (14%)	3	18
2	B	967/1061 (91%)	851 (88%)	116 (12%)	5	23
3	C	234/274 (85%)	207 (88%)	27 (12%)	5	24
4	E	196/197 (100%)	183 (93%)	13 (7%)	15	47
5	F	75/137 (55%)	74 (99%)	1 (1%)	61	78
6	H	117/128 (91%)	100 (86%)	17 (14%)	3	16
7	I	113/116 (97%)	103 (91%)	10 (9%)	9	35
8	J	60/65 (92%)	52 (87%)	8 (13%)	4	19
9	K	99/102 (97%)	85 (86%)	14 (14%)	3	17
10	L	40/57 (70%)	31 (78%)	9 (22%)	1	5
All	All	3126/3657 (86%)	2744 (88%)	382 (12%)	5	22

All (382) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	30	ILE
1	A	40	THR
1	A	41	MET
1	A	43	GLU
1	A	47	ARG
1	A	61	ILE
1	A	65	LEU
1	A	69	THR
1	A	70	CYS
1	A	88	LYS
1	A	90	VAL
1	A	93	VAL
1	A	113	LEU
1	A	126	LEU
1	A	130	ASP
1	A	143	LYS
1	A	144	THR
1	A	171	GLN
1	A	202	LEU
1	A	204	THR
1	A	208	LEU
1	A	222	LEU
1	A	225	ASN
1	A	252	PHE
1	A	254	GLU
1	A	269	ILE
1	A	270	LEU
1	A	271	LYS
1	A	282	ASN
1	A	295	LEU
1	A	303	TYR
1	A	308	ILE
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	329	LEU
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	351	THR
1	A	353	ILE

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Mol	Chain	Res	Type
1	A	354	SER
1	A	359	LEU
1	A	368	LYS
1	A	389	THR
1	A	407	ARG
1	A	408	ASP
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	455	MET
1	A	470	LEU
1	A	475	THR
1	A	476	SER
1	A	496	GLU
1	A	518	LYS
1	A	524	VAL
1	A	527	THR
1	A	532	ARG
1	A	535	THR
1	A	537	ARG
1	A	541	ILE
1	A	544	ASP
1	A	566	ILE
1	A	571	LEU
1	A	590	ARG
1	A	595	THR
1	A	598	LEU
1	A	603	ASN
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	625	SER
1	A	629	LEU
1	A	634	THR
1	A	640	GLN
1	A	666	ILE
1	A	672	ASP
1	A	687	LYS
1	A	688	LYS
1	A	691	LEU

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Mol	Chain	Res	Type
1	A	695	LYS
1	A	702	LEU
1	A	705	LYS
1	A	710	LEU
1	A	716	ASP
1	A	719	VAL
1	A	722	LEU
1	A	731	ARG
1	A	740	LEU
1	A	756	ILE
1	A	768	GLN
1	A	771	GLU
1	A	788	SER
1	A	801	GLU
1	A	806	ARG
1	A	821	ARG
1	A	826	ASP
1	A	838	GLN
1	A	847	ASP
1	A	855	THR
1	A	867	ILE
1	A	878	ILE
1	A	885	THR
1	A	908	LEU
1	A	912	LEU
1	A	919	ILE
1	A	920	LEU
1	A	925	LEU
1	A	932	GLU
1	A	938	LYS
1	A	953	ASN
1	A	960	ILE
1	A	969	GLN
1	A	973	ILE
1	A	988	LEU
1	A	1015	VAL
1	A	1022	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1064	VAL
1	A	1067	LEU
1	A	1081	LEU

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Mol	Chain	Res	Type
1	A	1083	THR
1	A	1084	PHE
1	A	1109	LYS
1	A	1110	ASN
1	A	1113	THR
1	A	1161	THR
1	A	1168	GLU
1	A	1169	ILE
1	A	1176	LEU
1	A	1187	GLN
1	A	1195	LEU
1	A	1221	LYS
1	A	1233	ASP
1	A	1237	ILE
1	A	1257	ASP
1	A	1261	LYS
1	A	1264	GLU
1	A	1267	MET
1	A	1269	GLU
1	A	1273	LEU
1	A	1277	GLU
1	A	1288	ASP
1	A	1297	GLU
1	A	1299	VAL
1	A	1303	GLU
1	A	1333	ILE
1	A	1334	ASP
1	A	1351	GLU
1	A	1354	ASN
1	A	1364	ASN
1	A	1366	ARG
1	A	1371	LEU
1	A	1382	THR
1	A	1384	VAL
1	A	1393	ASN
1	A	1394	THR
1	A	1398	MET
1	A	1403	GLU
1	A	1426	GLU
1	A	1438	THR
2	B	22	SER
2	B	25	ILE

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Mol	Chain	Res	Type
2	B	28	GLU
2	B	40	GLU
2	B	45	SER
2	B	46	GLN
2	B	63	ILE
2	B	65	GLU
2	B	66	ASP
2	B	68	THR
2	B	70	ILE
2	B	101	MET
2	B	135	ARG
2	B	167	ILE
2	B	175	ARG
2	B	194	GLU
2	B	208	SER
2	B	217	ARG
2	B	222	ILE
2	B	234	ILE
2	B	240	ILE
2	B	254	LEU
2	B	276	ILE
2	B	277	LYS
2	B	282	ILE
2	B	287	ARG
2	B	305	VAL
2	B	310	MET
2	B	311	LEU
2	B	324	ILE
2	B	355	ILE
2	B	365	THR
2	B	387	LEU
2	B	393	LYS
2	B	394	ASP
2	B	403	LYS
2	B	404	LYS
2	B	413	LEU
2	B	426	LYS
2	B	437	GLU
2	B	446	LEU
2	B	451	LYS
2	B	453	ILE
2	B	461	LEU

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Mol	Chain	Res	Type
2	B	468	GLU
2	B	479	VAL
2	B	485	ARG
2	B	487	THR
2	B	493	SER
2	B	531	GLN
2	B	547	VAL
2	B	555	ILE
2	B	567	GLU
2	B	574	SER
2	B	591	ARG
2	B	604	ARG
2	B	616	ILE
2	B	644	GLU
2	B	645	SER
2	B	653	VAL
2	B	655	LYS
2	B	658	ILE
2	B	696	GLU
2	B	733	HIS
2	B	762	ASN
2	B	780	VAL
2	B	786	ASN
2	B	787	VAL
2	B	791	THR
2	B	796	LEU
2	B	815	ARG
2	B	844	SER
2	B	850	LEU
2	B	862	GLN
2	B	864	LYS
2	B	866	TYR
2	B	880	THR
2	B	885	MET
2	B	886	LYS
2	B	899	ILE
2	B	935	ARG
2	B	948	ILE
2	B	951	GLN
2	B	963	PHE
2	B	983	ARG
2	B	987	LYS

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Mol	Chain	Res	Type
2	B	996	ARG
2	B	997	GLU
2	B	998	ASP
2	B	1006	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1012	ILE
2	B	1019	SER
2	B	1028	GLU
2	B	1030	LEU
2	B	1065	GLN
2	B	1066	SER
2	B	1077	THR
2	B	1094	ARG
2	B	1096	ARG
2	B	1099	VAL
2	B	1102	LYS
2	B	1103	ILE
2	B	1128	LEU
2	B	1129	ARG
2	B	1145	SER
2	B	1147	LEU
2	B	1160	VAL
2	B	1172	ILE
2	B	1175	LEU
2	B	1189	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1222	ARG
3	C	3	GLU
3	C	4	GLU
3	C	18	VAL
3	C	21	ILE
3	C	25	VAL
3	C	34	ARG
3	C	37	MET
3	C	43	THR
3	C	53	THR
3	C	75	MET
3	C	77	ILE
3	C	79	GLN

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Mol	Chain	Res	Type
3	C	109	SER
3	C	124	LEU
3	C	127	ARG
3	C	129	ILE
3	C	137	LYS
3	C	144	ILE
3	C	149	LYS
3	C	156	THR
3	C	215	GLU
3	C	226	ASP
3	C	240	VAL
3	C	244	VAL
3	C	249	ASP
3	C	254	LYS
3	C	268	ASP
4	E	7	ARG
4	E	54	GLN
4	E	65	THR
4	E	78	LEU
4	E	92	THR
4	E	100	ILE
4	E	116	ILE
4	E	122	LYS
4	E	127	ILE
4	E	156	LEU
4	E	169	ARG
4	E	191	LYS
4	E	204	THR
5	F	115	THR
6	H	16	ASP
6	H	22	LYS
6	H	26	ILE
6	H	34	ASP
6	H	35	GLN
6	H	52	GLN
6	H	63	LEU
6	H	86	ASP
6	H	94	ASP
6	H	103	LYS
6	H	106	GLU
6	H	107	VAL
6	H	109	LYS

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Mol	Chain	Res	Type
6	H	110	ASP
6	H	123	MET
6	H	130	ARG
6	H	145	ARG
7	I	21	GLU
7	I	35	VAL
7	I	52	ILE
7	I	70	ARG
7	I	77	LYS
7	I	84	VAL
7	I	87	GLN
7	I	97	MET
7	I	111	THR
7	I	119	THR
8	J	3	VAL
8	J	7	CYS
8	J	31	ASP
8	J	48	ARG
8	J	56	LEU
8	J	57	ILE
8	J	59	LYS
8	J	62	ARG
9	K	11	LEU
9	K	14	GLU
9	K	18	LYS
9	K	20	LYS
9	K	22	ASP
9	K	25	THR
9	K	31	VAL
9	K	33	ILE
9	K	42	LEU
9	K	49	GLU
9	K	51	LEU
9	K	63	VAL
9	K	78	THR
9	K	114	LEU
10	L	27	LEU
10	L	40	LEU
10	L	43	THR
10	L	55	ILE
10	L	58	LYS
10	L	61	THR

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Mol	Chain	Res	Type
10	L	65	VAL
10	L	66	GLN
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN
1	A	18	GLN
1	A	54	ASN
1	A	64	ASN
1	A	92	HIS
1	A	124	GLN
1	A	171	GLN
1	A	209	ASN
1	A	297	GLN
1	A	339	ASN
1	A	358	ASN
1	A	394	ASN
1	A	427	GLN
1	A	471	ASN
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	584	ASN
1	A	631	HIS
1	A	660	ASN
1	A	741	ASN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	851	HIS
1	A	862	ASN
1	A	906	HIS
1	A	926	GLN
1	A	1130	GLN
1	A	1140	HIS
1	A	1171	GLN
1	A	1258	HIS
1	A	1270	ASN
1	A	1364	ASN

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Mol	Chain	Res	Type
1	A	1393	ASN
2	B	47	GLN
2	B	103	ASN
2	B	215	GLN
2	B	255	GLN
2	B	363	HIS
2	B	415	GLN
2	B	484	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	657	HIS
2	B	734	HIS
2	B	744	HIS
2	B	762	ASN
2	B	767	ASN
2	B	786	ASN
2	B	794	ASN
2	B	957	ASN
2	B	984	HIS
2	B	1013	ASN
2	B	1015	HIS
2	B	1084	GLN
2	B	1176	ASN
2	B	1205	GLN
3	C	73	GLN
3	C	91	HIS
3	C	112	ASN
3	C	151	GLN
3	C	167	HIS
3	C	203	GLN
3	C	242	GLN
4	E	114	ASN
4	E	115	ASN
4	E	146	HIS
6	H	35	GLN
6	H	131	ASN
9	K	65	HIS
9	K	104	ASN
9	K	110	ASN
9	K	112	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	5/5 (100%)	4 (80%)	1 (20%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	7	G
11	R	8	G
11	R	9	5BU
11	R	10	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	R	6	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	5BU	R	9	11,12	19,22,23	1.10	2 (10%)	27,32,35	1.30	5 (18%)

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
11	5BU	R	9	11,12	-	2/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	9	5BU	C2-N1	2.64	1.42	1.38
11	R	9	5BU	C4-C5	2.44	1.49	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	9	5BU	O4-C4-C5	-2.46	122.66	125.80
11	R	9	5BU	O3'-C3'-C4'	-2.43	104.10	111.08
11	R	9	5BU	O4'-C4'-C3'	-2.29	100.62	105.15
11	R	9	5BU	C3'-C2'-C1'	-2.09	97.50	101.46
11	R	9	5BU	C2'-C3'-C4'	-2.04	98.66	102.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	R	9	5BU	C3'-C4'-C5'-O5'
11	R	9	5BU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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 [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%)	0.15	40 (2%)	55	35	42, 85, 175, 219	0
2	B	1114/1224 (91%)	0.11	37 (3%)	49	30	37, 78, 147, 189	0
3	C	266/318 (83%)	-0.11	0	100	100	49, 75, 114, 155	0
4	E	214/215 (99%)	0.27	4 (1%)	66	46	61, 115, 162, 175	0
5	F	85/155 (54%)	-0.10	0	100	100	66, 96, 133, 152	0
6	H	133/146 (91%)	0.45	8 (6%)	27	17	80, 119, 154, 166	0
7	I	119/122 (97%)	0.19	4 (3%)	48	30	55, 93, 129, 142	0
8	J	65/70 (92%)	-0.10	1 (1%)	72	52	49, 67, 102, 116	0
9	K	114/120 (95%)	-0.14	1 (0%)	81	64	51, 77, 104, 120	0
10	L	46/70 (65%)	0.85	6 (13%)	7	6	61, 116, 143, 158	0
11	R	4/5 (80%)	0.03	0	100	100	78, 91, 109, 113	0
12	T	13/29 (44%)	0.80	1 (7%)	19	13	84, 115, 174, 181	0
All	All	3578/4207 (85%)	0.13	102 (2%)	53	35	37, 84, 162, 219	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	5.9
1	A	1081	LEU	5.7
6	H	85	GLY	5.5
2	B	715	ALA	5.1
1	A	1087	ALA	5.0
2	B	335	GLY	4.9
1	A	65	LEU	4.8
2	B	882	THR	4.7
2	B	70	ILE	4.7
10	L	27	LEU	4.2
1	A	250	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	141	LEU	4.0
10	L	28	LYS	3.8
6	H	132	LEU	3.7
1	A	179	LEU	3.7
2	B	1173	ALA	3.7
2	B	709	ASP	3.6
6	H	86	ASP	3.6
6	H	63	LEU	3.6
2	B	446	LEU	3.5
2	B	1204	PHE	3.4
2	B	140	ILE	3.4
1	A	78	PRO	3.4
2	B	474	SER	3.3
1	A	1086	PHE	3.3
2	B	502	ILE	3.3
10	L	55	ILE	3.3
2	B	477	ALA	3.2
1	A	252	PHE	3.2
1	A	1083	THR	3.1
1	A	1123	GLY	3.1
1	A	154	SER	3.1
1	A	181	LEU	3.0
1	A	319	GLY	3.0
2	B	708	GLU	3.0
9	K	114	LEU	3.0
2	B	1214	PRO	2.9
4	E	96	PHE	2.9
2	B	881	ASN	2.9
6	H	89	LEU	2.9
1	A	1085	HIS	2.8
1	A	199	LEU	2.8
1	A	1088	GLY	2.8
10	L	26	THR	2.8
1	A	201	VAL	2.8
1	A	79	GLY	2.7
1	A	1176	LEU	2.7
1	A	1091	SER	2.7
1	A	69	THR	2.7
2	B	478	GLY	2.7
1	A	318	SER	2.7
1	A	1089	VAL	2.7
12	T	28	DT	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1002	GLY	2.6
1	A	66	LYS	2.6
1	A	567	LYS	2.6
2	B	711	GLU	2.6
2	B	865	LYS	2.6
2	B	137	TYR	2.6
1	A	314	ALA	2.6
4	E	123	LEU	2.5
2	B	887	HIS	2.5
6	H	139	ASN	2.5
7	I	4	PHE	2.5
1	A	53	LEU	2.4
2	B	733	HIS	2.4
2	B	246	LYS	2.4
4	E	110	PHE	2.4
2	B	1170	THR	2.4
1	A	180	LYS	2.4
6	H	131	ASN	2.3
2	B	879	ARG	2.3
2	B	878	GLN	2.3
2	B	468	GLU	2.3
1	A	1108	ALA	2.3
2	B	933	SER	2.3
2	B	472	ALA	2.3
2	B	962	LYS	2.3
1	A	1445	ILE	2.2
2	B	475	SER	2.2
2	B	880	THR	2.2
4	E	95	THR	2.2
1	A	289	ILE	2.2
1	A	1273	LEU	2.2
10	L	25	ALA	2.2
7	I	120	GLN	2.1
8	J	65	PRO	2.1
10	L	40	LEU	2.1
2	B	509	ALA	2.1
1	A	49	LYS	2.1
6	H	136	LYS	2.1
1	A	161	LEU	2.1
2	B	935	ARG	2.1
2	B	712	PRO	2.1
1	A	1092	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	30	ILE	2.1
7	I	82	GLU	2.1
1	A	998	LEU	2.0
7	I	104	LEU	2.0
1	A	323	LYS	2.0
2	B	108	VAL	2.0
2	B	345	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	5BU	R	9	21/22	0.91	0.09	77,80,90,102	1

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	ZN	A	1734	1/1	0.82	0.09	300,300,300,300	0
13	ZN	A	1735	1/1	0.95	0.07	135,135,135,135	0
13	ZN	B	1307	1/1	0.99	0.03	149,149,149,149	0
13	ZN	C	319	1/1	1.00	0.03	67,67,67,67	0
13	ZN	I	203	1/1	1.00	0.03	87,87,87,87	0
13	ZN	I	204	1/1	1.00	0.04	66,66,66,66	0
13	ZN	J	101	1/1	1.00	0.03	58,58,58,58	0
13	ZN	L	105	1/1	1.00	0.02	102,102,102,102	0
14	MG	A	2001	1/1	1.00	0.04	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.