



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:53 PM UTC

PDB ID : 4A3K / pdb_00004a3k
Title : RNA Polymerase II initial transcribing complex with a 7nt DNA-RNA hybrid
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on : 2011-09-30
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

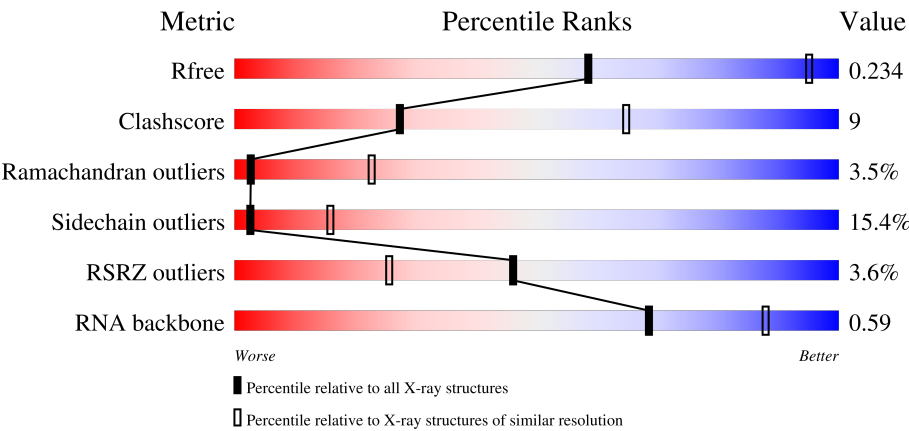
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1732	2% 54% 22% 5% 18%
2	B	1224	4% 58% 27% 5% 9%
3	C	318	54% 23% 6% 16%
4	D	221	7% 50% 24% 6% 19%

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

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31940 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	1422	Total	C	N	O	S	0	0	0
			11174	7037	1954	2121	62			

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

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

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

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

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

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

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT 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 SUB-UNIT RPABC 2.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	10	Total	C	N	O	P	0	0	0
			207	99	39	59	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	7	Total	C	N	O	P	0	0	0
			152	68	31	46	7			

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

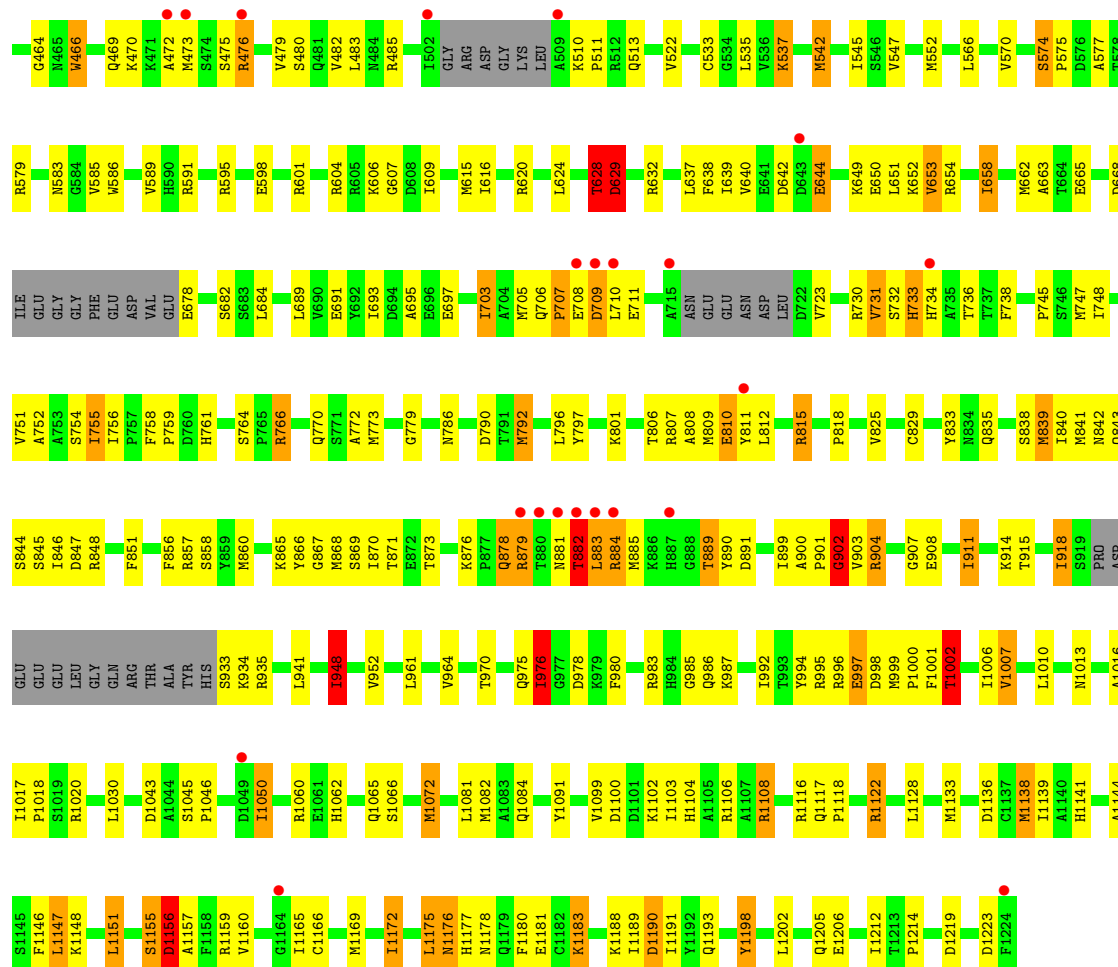
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	19	Total	Br	C	N	O	P	0	0
			385	1	185	60	120	19		

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

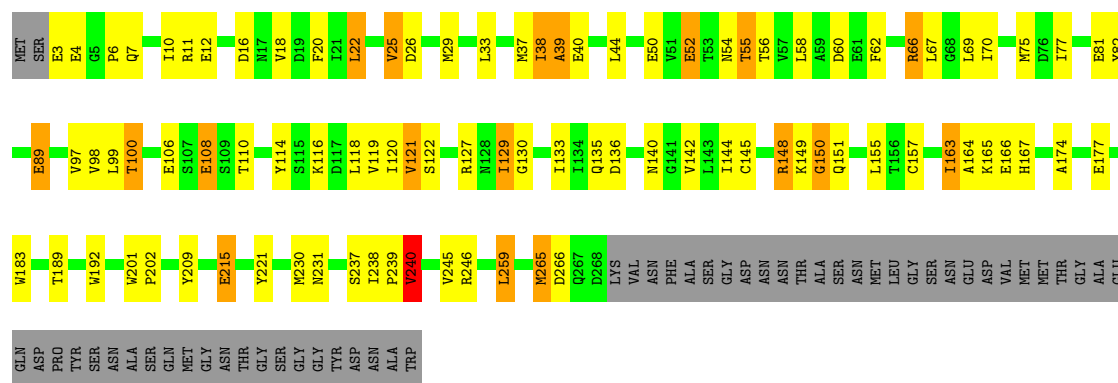
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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



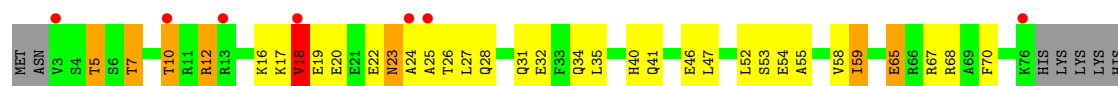
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

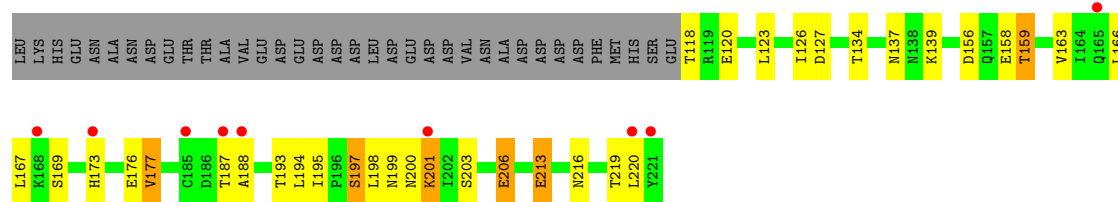
Chain C: 54% 23% 6% 16%



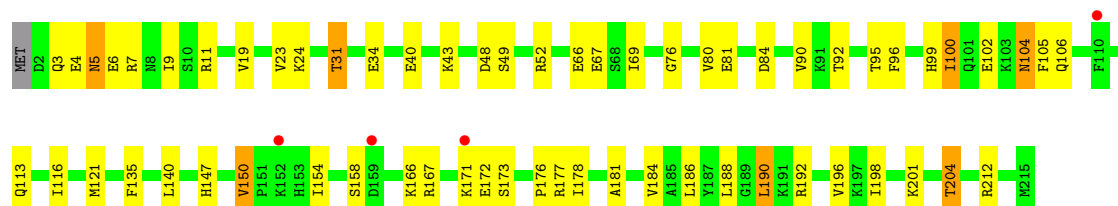
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D: 7% 50% 24% 6% 19%

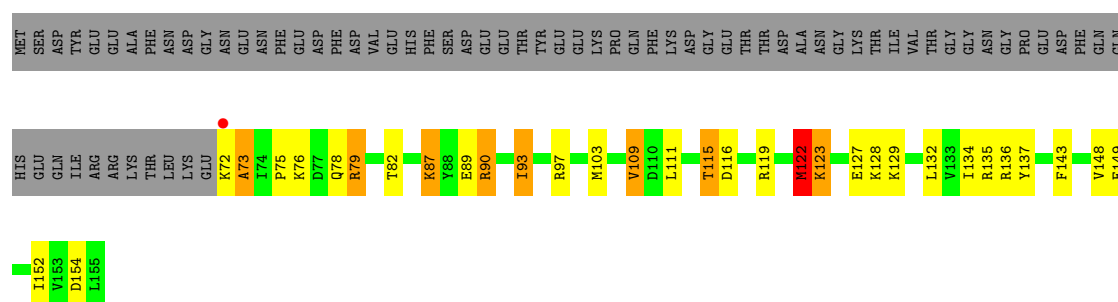
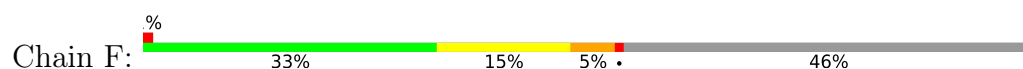




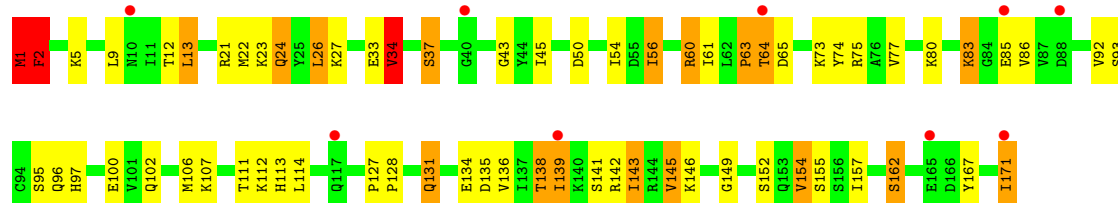
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



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

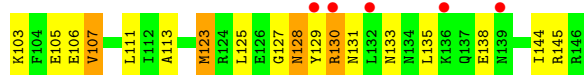


• Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

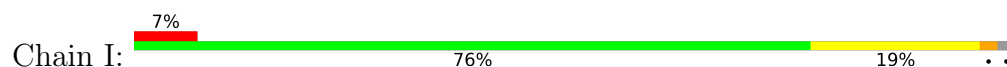


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

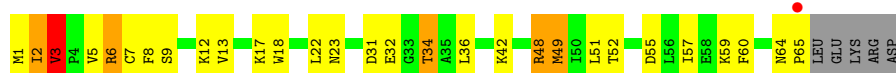




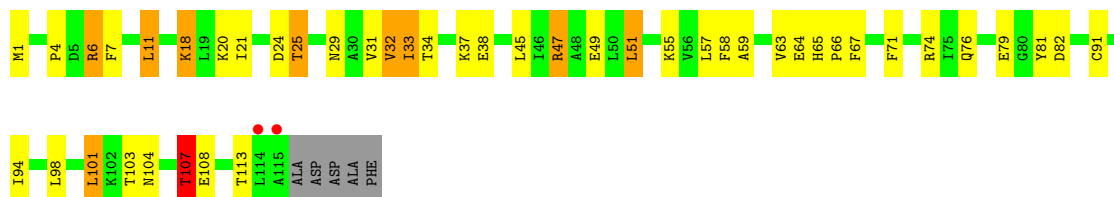
- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



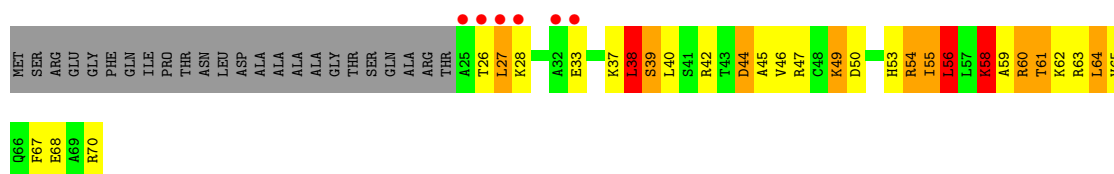
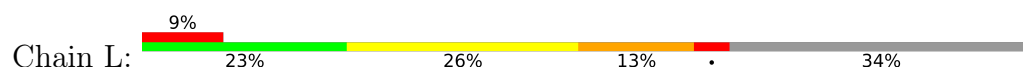
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



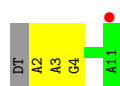
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



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



- Molecule 13: 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP)-3'

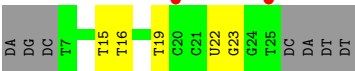


- Molecule 14: 5'-R(*AP*CP*CP*AP*GP*GP*AP)-3'





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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.91Å 391.36Å 283.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.95 – 3.50 48.95 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.95-3.50) 99.9 (48.95-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.158 , 0.185 0.220 , 0.234	Depositor DCC
R_{free} test set	3353 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	97.8	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 114.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.019 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.028 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	31940	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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, BRU, 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	0.90	12/11374 (0.1%)	1.56	148/15383 (1.0%)
2	B	0.87	5/9029 (0.1%)	1.47	94/12171 (0.8%)
3	C	0.84	0/2133	1.46	22/2891 (0.8%)
4	D	0.90	2/1444 (0.1%)	1.60	20/1935 (1.0%)
5	E	0.80	0/1788	1.44	13/2406 (0.5%)
6	F	1.00	1/691 (0.1%)	1.40	6/933 (0.6%)
7	G	0.86	2/1368 (0.1%)	1.45	11/1844 (0.6%)
8	H	0.84	0/1086	1.43	12/1470 (0.8%)
9	I	0.79	0/989	1.38	7/1331 (0.5%)
10	J	0.92	1/541 (0.2%)	1.46	2/727 (0.3%)
11	K	0.80	0/938	1.43	8/1267 (0.6%)
12	L	1.01	0/365	1.69	12/485 (2.5%)
13	N	0.50	0/232	0.65	0/356
14	P	0.67	0/170	0.71	0/263
15	T	0.57	0/405	0.70	0/620
All	All	0.87	23/32553 (0.1%)	1.48	355/44082 (0.8%)

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

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

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	867	ILE	CG1-CD1	8.86	1.86	1.51
1	A	57	ARG	CA-C	7.06	1.62	1.52
1	A	54	ASN	CA-C	6.84	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1454	MET	CA-C	6.77	1.59	1.52
4	D	18	VAL	CA-C	6.58	1.61	1.52
1	A	52	GLY	C-N	6.56	1.43	1.33
2	B	881	ASN	C-N	6.56	1.42	1.33
1	A	437	MET	SD-CE	6.35	1.95	1.79
7	G	1	MET	C-N	6.30	1.42	1.33
6	F	122	MET	SD-CE	5.99	1.94	1.79
10	J	49	MET	SD-CE	-5.89	1.64	1.79
1	A	332	LYS	CA-C	-5.78	1.45	1.52
1	A	56	PRO	C-N	5.66	1.41	1.33
2	B	1017	ILE	CA-C	5.51	1.57	1.52
1	A	1398	MET	SD-CE	5.50	1.93	1.79
2	B	948	ILE	CG1-CD1	5.46	1.73	1.51
2	B	167	ILE	CA-CB	5.45	1.59	1.53
1	A	53	LEU	N-CA	5.43	1.53	1.46
2	B	882	THR	N-CA	5.36	1.52	1.46
1	A	56	PRO	CA-C	5.21	1.59	1.52
1	A	57	ARG	C-N	5.13	1.40	1.33
7	G	56	ILE	CA-C	5.08	1.59	1.52
4	D	24	ALA	CA-C	5.04	1.59	1.52

All (355) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	39	ALA	N-CA-C	12.99	124.97	111.07
1	A	34	LYS	CA-C-N	11.32	142.07	121.70
1	A	34	LYS	C-N-CA	11.32	142.07	121.70
1	A	72	GLU	N-CA-C	10.31	122.11	111.07
4	D	26	THR	N-CA-C	-10.07	99.81	113.30
4	D	31	GLN	N-CA-C	-9.99	100.35	111.14
7	G	34	VAL	N-CA-C	9.86	119.69	110.42
5	E	150	VAL	N-CA-C	9.70	116.39	107.56
1	A	452	LYS	N-CA-C	-9.53	100.88	111.07
10	J	5	VAL	N-CA-C	-9.26	97.49	109.80
8	H	81	PRO	N-CA-C	8.86	121.51	110.70
1	A	1419	ASP	CA-C-N	8.50	132.03	120.38
1	A	1419	ASP	C-N-CA	8.50	132.03	120.38
2	B	976	ILE	N-CA-C	8.28	119.06	110.62
3	C	135	GLN	CA-C-N	8.02	132.52	121.05
3	C	135	GLN	C-N-CA	8.02	132.52	121.05
4	D	25	ALA	CA-C-N	7.95	134.81	122.49
4	D	25	ALA	C-N-CA	7.95	134.81	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1112	LYS	N-CA-C	7.91	119.68	111.14
1	A	194	ALA	CA-C-N	7.88	135.88	121.70
1	A	194	ALA	C-N-CA	7.88	135.88	121.70
2	B	1017	ILE	N-CA-C	7.77	121.67	112.35
12	L	58	LYS	N-CA-C	7.73	121.97	112.54
8	H	92	ASP	N-CA-C	-7.63	101.65	113.02
1	A	56	PRO	CA-C-N	7.55	135.96	121.54
1	A	56	PRO	C-N-CA	7.55	135.96	121.54
2	B	628	THR	CA-C-N	7.52	135.90	121.54
2	B	628	THR	C-N-CA	7.52	135.90	121.54
1	A	35	ILE	N-CA-CB	7.46	124.19	111.50
12	L	60	ARG	N-CA-C	7.42	119.89	110.24
2	B	902	GLY	CA-C-N	7.40	130.47	120.63
2	B	902	GLY	C-N-CA	7.40	130.47	120.63
1	A	42	ASP	CA-CB-CG	7.39	119.99	112.60
2	B	296	GLU	N-CA-C	-7.32	102.28	112.45
2	B	338	GLY	CA-C-N	7.31	134.87	121.70
2	B	338	GLY	C-N-CA	7.31	134.87	121.70
3	C	40	GLU	N-CA-C	7.28	122.27	112.88
1	A	399	HIS	N-CA-CB	7.25	123.28	110.37
1	A	672	ASP	CA-CB-CG	7.19	119.79	112.60
1	A	54	ASN	CA-CB-CG	7.11	119.71	112.60
2	B	1122	ARG	CA-C-N	7.06	130.61	120.79
2	B	1122	ARG	C-N-CA	7.06	130.61	120.79
8	H	129	TYR	N-CA-C	7.03	119.02	111.36
1	A	224	PHE	N-CA-C	6.96	119.54	110.43
2	B	41	LYS	N-CA-C	6.92	119.42	111.11
3	C	183	TRP	N-CA-C	-6.90	97.48	108.73
1	A	1445	ILE	N-CA-CB	6.89	118.23	110.72
2	B	1016	ALA	CA-C-N	6.88	125.83	120.33
2	B	1016	ALA	C-N-CA	6.88	125.83	120.33
1	A	70	CYS	N-CA-C	-6.84	100.36	110.48
8	H	128	ASN	CA-C-N	6.83	129.99	120.29
8	H	128	ASN	C-N-CA	6.83	129.99	120.29
1	A	229	SER	N-CA-C	6.71	118.39	107.32
2	B	707	PRO	CA-C-N	6.71	129.60	120.54
2	B	707	PRO	C-N-CA	6.71	129.60	120.54
1	A	886	ILE	N-CA-C	6.69	118.25	110.62
1	A	1404	GLU	N-CA-C	6.69	121.14	112.92
1	A	219	PHE	CA-CB-CG	6.65	120.45	113.80
11	K	24	ASP	CA-C-N	6.59	129.11	120.28
11	K	24	ASP	C-N-CA	6.59	129.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	55	ILE	N-CA-C	6.58	117.37	110.72
2	B	1219	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	998	LEU	N-CA-C	6.56	120.35	109.46
2	B	1013	ASN	N-CA-C	6.55	119.13	109.50
1	A	218	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	825	ILE	N-CA-C	-6.49	104.83	110.74
1	A	1127	ASP	CA-CB-CG	6.49	119.09	112.60
7	G	141	SER	N-CA-C	6.49	119.64	110.23
2	B	663	ALA	N-CA-C	-6.48	104.14	111.14
1	A	485	ASP	CA-CB-CG	6.47	119.07	112.60
3	C	38	ILE	CA-C-N	6.47	128.85	120.44
3	C	38	ILE	C-N-CA	6.47	128.85	120.44
5	E	171	LYS	N-CA-C	-6.47	100.04	110.32
2	B	1169	MET	CA-C-N	6.43	129.19	120.38
2	B	1169	MET	C-N-CA	6.43	129.19	120.38
2	B	188	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	411	ASP	CA-C-N	6.40	129.84	120.82
1	A	411	ASP	C-N-CA	6.40	129.84	120.82
3	C	26	ASP	CA-CB-CG	6.40	119.00	112.60
2	B	818	PRO	N-CA-C	6.39	120.17	111.22
1	A	53	LEU	N-CA-CB	6.34	121.31	110.65
1	A	1436	ILE	N-CA-CB	-6.32	102.69	111.41
1	A	84	ILE	N-CA-CB	6.32	119.85	111.64
2	B	294	ASP	CA-CB-CG	6.30	118.90	112.60
7	G	50	ASP	CA-CB-CG	6.30	118.90	112.60
10	J	3	VAL	CB-CA-C	-6.28	104.73	110.88
1	A	331	GLY	CA-C-N	6.27	133.52	121.54
1	A	331	GLY	C-N-CA	6.27	133.52	121.54
1	A	537	ARG	CA-C-N	6.25	129.51	120.38
1	A	537	ARG	C-N-CA	6.25	129.51	120.38
1	A	123	ARG	CA-C-N	6.23	128.92	120.44
1	A	123	ARG	C-N-CA	6.23	128.92	120.44
1	A	436	ILE	CB-CA-C	6.21	119.65	111.33
1	A	636	GLU	N-CA-C	6.21	118.05	111.28
11	K	64	GLU	N-CA-C	6.20	118.84	111.71
2	B	733	HIS	CA-C-N	6.20	129.43	120.38
2	B	733	HIS	C-N-CA	6.20	129.43	120.38
1	A	346	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	825	ILE	N-CA-CB	6.15	118.02	110.64
4	D	53	SER	CA-C-N	6.14	128.43	120.44
4	D	53	SER	C-N-CA	6.14	128.43	120.44
8	H	12	VAL	N-CA-C	6.14	116.34	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	GLU	CA-C-N	6.13	128.41	120.44
1	A	495	GLU	C-N-CA	6.13	128.41	120.44
3	C	110	THR	CB-CA-C	6.13	119.70	109.89
1	A	54	ASN	CA-C-N	6.13	136.75	121.80
1	A	54	ASN	C-N-CA	6.13	136.75	121.80
1	A	1403	GLU	N-CA-C	6.13	123.85	110.80
2	B	472	ALA	CA-C-N	6.11	133.22	121.54
2	B	472	ALA	C-N-CA	6.11	133.22	121.54
1	A	78	PRO	CA-C-N	-6.10	112.34	121.01
1	A	78	PRO	C-N-CA	-6.10	112.34	121.01
1	A	341	MET	CA-C-N	6.10	127.25	121.46
1	A	341	MET	C-N-CA	6.10	127.25	121.46
1	A	64	ASN	N-CA-C	-6.09	101.92	110.50
1	A	224	PHE	CA-CB-CG	-6.09	107.71	113.80
12	L	64	LEU	N-CA-C	6.08	119.28	110.28
2	B	736	THR	N-CA-C	-6.07	106.20	113.97
5	E	95	THR	CA-C-N	6.07	128.33	120.44
5	E	95	THR	C-N-CA	6.07	128.33	120.44
9	I	93	LYS	CA-C-N	6.06	128.72	120.54
9	I	93	LYS	C-N-CA	6.06	128.72	120.54
1	A	535	THR	N-CA-C	6.06	119.41	112.57
1	A	532	ARG	CA-C-N	6.05	128.67	120.38
1	A	532	ARG	C-N-CA	6.05	128.67	120.38
4	D	25	ALA	N-CA-C	-6.04	103.15	110.88
12	L	49	LYS	CA-C-N	6.04	133.07	121.54
12	L	49	LYS	C-N-CA	6.04	133.07	121.54
1	A	524	VAL	N-CA-CB	-6.03	105.69	112.45
1	A	1403	GLU	CA-C-N	-6.02	113.02	122.65
1	A	1403	GLU	C-N-CA	-6.02	113.02	122.65
8	H	36	CYS	N-CA-C	6.01	118.09	108.41
2	B	102	VAL	N-CA-C	6.01	117.34	107.24
1	A	73	GLY	CA-C-N	6.00	132.99	121.54
1	A	73	GLY	C-N-CA	6.00	132.99	121.54
1	A	592	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	1237	ILE	N-CA-C	6.00	117.11	108.48
1	A	1161	THR	CB-CA-C	5.99	119.55	109.48
1	A	897	TYR	N-CA-C	5.97	120.75	112.45
2	B	903	VAL	N-CA-C	5.96	117.41	109.37
1	A	70	CYS	CA-C-N	-5.94	112.34	122.56
1	A	70	CYS	C-N-CA	-5.94	112.34	122.56
1	A	481	ASP	CA-CB-CG	5.92	118.53	112.60
1	A	408	ASP	CA-C-N	5.92	130.16	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	ASP	C-N-CA	5.92	130.16	120.63
2	B	890	TYR	N-CA-C	-5.92	106.22	113.50
4	D	26	THR	CA-C-N	5.91	130.97	122.40
4	D	26	THR	C-N-CA	5.91	130.97	122.40
3	C	136	ASP	CA-CB-CG	5.89	118.49	112.60
11	K	107	THR	CB-CA-C	5.88	120.23	110.81
1	A	900	ASP	CA-CB-CG	5.88	118.48	112.60
2	B	186	GLU	CA-C-N	5.88	128.44	120.38
2	B	186	GLU	C-N-CA	5.88	128.44	120.38
8	H	83	GLN	CA-C-N	5.88	130.00	120.60
8	H	83	GLN	C-N-CA	5.88	130.00	120.60
1	A	1371	LEU	CA-C-N	5.87	128.18	120.60
1	A	1371	LEU	C-N-CA	5.87	128.18	120.60
2	B	1156	ASP	CA-C-N	5.87	132.76	121.54
2	B	1156	ASP	C-N-CA	5.87	132.76	121.54
1	A	794	PRO	CA-C-N	5.87	128.15	120.28
1	A	794	PRO	C-N-CA	5.87	128.15	120.28
2	B	881	ASN	CA-C-N	5.87	128.40	120.65
2	B	881	ASN	C-N-CA	5.87	128.40	120.65
1	A	1005	GLU	CB-CG-CD	5.83	122.51	112.60
2	B	998	ASP	CA-CB-CG	5.81	118.41	112.60
3	C	265	MET	CA-C-N	5.80	128.64	120.28
3	C	265	MET	C-N-CA	5.80	128.64	120.28
1	A	524	VAL	N-CA-C	5.80	115.90	108.82
2	B	825	VAL	N-CA-C	5.80	116.23	108.11
1	A	472	LEU	N-CA-C	5.77	119.14	111.75
1	A	602	ASP	N-CA-C	-5.76	103.45	111.52
1	A	646	PHE	CA-C-N	5.76	126.50	119.99
1	A	646	PHE	C-N-CA	5.76	126.50	119.99
1	A	308	ILE	CA-C-N	5.76	128.80	120.79
1	A	308	ILE	C-N-CA	5.76	128.80	120.79
6	F	154	ASP	CA-CB-CG	5.76	118.36	112.60
4	D	188	ALA	N-CA-C	-5.74	105.37	112.38
5	E	5	ASN	N-CA-C	-5.74	104.63	111.69
1	A	334	GLY	CA-C-N	5.74	132.50	121.54
1	A	334	GLY	C-N-CA	5.74	132.50	121.54
1	A	629	LEU	N-CA-C	-5.74	105.03	111.28
6	F	87	LYS	CA-C-N	5.74	127.90	120.44
6	F	87	LYS	C-N-CA	5.74	127.90	120.44
1	A	1435	PRO	CA-C-N	5.72	130.63	123.14
1	A	1435	PRO	C-N-CA	5.72	130.63	123.14
1	A	1360	GLY	CA-C-N	5.69	128.93	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1360	GLY	C-N-CA	5.69	128.93	120.90
1	A	35	ILE	CA-C-N	5.69	132.49	122.42
1	A	35	ILE	C-N-CA	5.69	132.49	122.42
2	B	851	PHE	N-CA-C	5.69	120.04	113.38
1	A	1416	ALA	CA-C-N	5.68	128.77	120.71
1	A	1416	ALA	C-N-CA	5.68	128.77	120.71
1	A	322	VAL	N-CA-C	5.67	116.37	108.89
1	A	1097	GLY	CA-C-N	5.66	125.87	120.43
1	A	1097	GLY	C-N-CA	5.66	125.87	120.43
3	C	89	GLU	N-CA-C	-5.66	101.47	109.96
2	B	343	ILE	CA-C-N	5.64	132.31	121.54
2	B	343	ILE	C-N-CA	5.64	132.31	121.54
1	A	411	ASP	N-CA-C	5.63	117.87	109.25
2	B	1099	VAL	N-CA-C	5.62	116.26	110.36
1	A	948	VAL	N-CA-C	5.62	116.35	110.62
1	A	398	GLU	CA-C-O	-5.60	114.64	121.36
7	G	64	THR	N-CA-C	5.60	117.39	111.28
1	A	1001	ARG	N-CA-C	5.59	120.23	113.41
5	E	172	GLU	CA-C-N	5.59	128.09	120.54
5	E	172	GLU	C-N-CA	5.59	128.09	120.54
4	D	46	GLU	CA-C-N	5.59	129.64	121.31
4	D	46	GLU	C-N-CA	5.59	129.64	121.31
1	A	5	GLN	N-CA-C	5.58	117.72	110.53
12	L	62	LYS	N-CA-C	-5.57	106.65	113.50
1	A	78	PRO	N-CA-C	-5.54	102.87	111.13
1	A	399	HIS	CA-CB-CG	-5.54	108.26	113.80
2	B	918	ILE	N-CA-C	5.54	116.64	108.45
1	A	1117	THR	CB-CA-C	5.54	120.53	111.23
2	B	883	LEU	CA-C-N	5.53	130.24	122.05
2	B	883	LEU	C-N-CA	5.53	130.24	122.05
1	A	408	ASP	CA-CB-CG	5.53	118.13	112.60
3	C	82	TYR	N-CA-C	-5.52	100.99	109.76
1	A	452	LYS	CA-C-N	5.51	131.23	120.99
1	A	452	LYS	C-N-CA	5.51	131.23	120.99
2	B	978	ASP	CA-CB-CG	5.50	118.10	112.60
8	H	128	ASN	CA-CB-CG	5.50	118.10	112.60
5	E	96	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	885	THR	CA-C-N	5.50	128.28	120.53
1	A	885	THR	C-N-CA	5.50	128.28	120.53
1	A	193	ASP	CA-C-N	5.49	131.59	121.70
1	A	193	ASP	C-N-CA	5.49	131.59	121.70
2	B	294	ASP	N-CA-C	-5.49	102.75	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	82	ASP	CA-CB-CG	5.49	118.09	112.60
2	B	339	THR	CB-CA-C	5.49	121.17	109.10
4	D	18	VAL	CA-C-N	5.48	131.57	121.70
4	D	18	VAL	C-N-CA	5.48	131.57	121.70
1	A	1147	THR	N-CA-C	5.47	118.17	109.96
2	B	266	ALA	N-CA-C	5.47	117.31	110.91
8	H	16	ASP	N-CA-C	5.47	119.13	108.85
1	A	932	GLU	CB-CG-CD	5.46	121.88	112.60
2	B	535	LEU	N-CA-C	-5.45	106.99	113.97
2	B	366	GLN	N-CA-C	-5.45	106.00	113.30
1	A	1376	THR	N-CA-C	5.44	118.04	111.40
2	B	1155	SER	CA-C-N	5.44	131.93	121.54
2	B	1155	SER	C-N-CA	5.44	131.93	121.54
2	B	858	SER	N-CA-C	5.44	117.50	108.20
4	D	200	ASN	CA-C-N	5.43	127.56	120.28
4	D	200	ASN	C-N-CA	5.43	127.56	120.28
1	A	1295	THR	CB-CA-C	5.43	120.43	110.11
1	A	99	ILE	N-CA-C	-5.43	105.03	110.30
2	B	359	GLU	N-CA-C	5.43	119.07	112.23
1	A	511	ILE	N-CA-C	5.41	115.86	110.23
2	B	1177	HIS	N-CA-C	-5.40	105.36	113.89
1	A	445	ASN	CA-CB-CG	5.40	118.00	112.60
2	B	629	ASP	CA-CB-CG	5.39	117.99	112.60
12	L	64	LEU	CA-C-N	5.39	129.32	122.37
12	L	64	LEU	C-N-CA	5.39	129.32	122.37
4	D	120	GLU	N-CA-C	-5.38	105.50	111.36
3	C	108	GLU	N-CA-C	-5.37	105.47	112.23
7	G	1	MET	CA-C-N	5.37	131.79	121.54
7	G	1	MET	C-N-CA	5.37	131.79	121.54
11	K	32	VAL	N-CA-C	5.37	115.81	107.28
1	A	1072	ILE	N-CA-C	-5.37	107.19	111.81
12	L	55	ILE	N-CA-CB	5.36	118.62	110.58
5	E	66	GLU	CA-C-N	5.36	127.77	120.54
5	E	66	GLU	C-N-CA	5.36	127.77	120.54
12	L	56	LEU	N-CA-C	5.35	122.20	110.80
1	A	71	GLN	CA-C-N	5.35	127.39	120.44
1	A	71	GLN	C-N-CA	5.35	127.39	120.44
7	G	2	PHE	CA-CB-CG	5.35	119.15	113.80
3	C	266	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	1420	ASP	CA-CB-CG	5.34	117.94	112.60
2	B	1180	PHE	CA-CB-CG	-5.33	108.47	113.80
2	B	684	LEU	CA-C-N	5.33	127.42	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	684	LEU	C-N-CA	5.33	127.42	120.28
1	A	898	ARG	N-CA-C	5.33	118.04	110.10
7	G	131	GLN	N-CA-C	5.32	117.09	108.41
1	A	311	GLN	N-CA-C	5.32	121.56	109.81
1	A	511	ILE	N-CA-CB	5.31	116.20	110.62
1	A	762	SER	N-CA-C	5.29	118.20	111.69
8	H	131	ASN	CA-CB-CG	5.29	117.89	112.60
5	E	48	ASP	CA-CB-CG	5.29	117.89	112.60
11	K	25	THR	CA-C-N	5.28	127.30	120.44
11	K	25	THR	C-N-CA	5.28	127.30	120.44
1	A	890	ASP	CA-C-N	5.26	127.79	120.63
1	A	890	ASP	C-N-CA	5.26	127.79	120.63
1	A	1138	ILE	N-CA-C	5.25	116.15	111.90
2	B	609	ILE	N-CA-C	-5.25	100.89	108.71
1	A	35	ILE	CB-CA-C	5.24	122.09	111.60
2	B	40	GLU	CA-C-N	5.24	127.61	120.54
2	B	40	GLU	C-N-CA	5.24	127.61	120.54
2	B	650	GLU	CA-C-N	5.23	128.76	121.02
2	B	650	GLU	C-N-CA	5.23	128.76	121.02
2	B	607	GLY	CA-C-N	5.23	127.24	120.44
2	B	607	GLY	C-N-CA	5.23	127.24	120.44
12	L	55	ILE	CA-C-O	-5.23	115.31	120.85
2	B	1190	ASP	CA-CB-CG	5.23	117.83	112.60
4	D	31	GLN	CA-C-N	5.23	127.28	120.28
4	D	31	GLN	C-N-CA	5.23	127.28	120.28
1	A	24	PRO	CA-C-N	5.22	127.53	120.38
1	A	24	PRO	C-N-CA	5.22	127.53	120.38
2	B	1198	TYR	CA-C-N	5.21	127.79	120.28
2	B	1198	TYR	C-N-CA	5.21	127.79	120.28
2	B	1001	PHE	N-CA-C	5.21	118.06	109.72
3	C	240	VAL	N-CA-C	5.20	120.15	109.34
6	F	122	MET	CA-C-N	5.20	127.19	120.44
6	F	122	MET	C-N-CA	5.20	127.19	120.44
9	I	94	ASP	CA-C-N	5.18	131.44	121.54
9	I	94	ASP	C-N-CA	5.18	131.44	121.54
3	C	245	VAL	N-CA-C	5.18	115.33	110.30
2	B	1102	LYS	CA-C-N	5.18	128.25	120.69
2	B	1102	LYS	C-N-CA	5.18	128.25	120.69
2	B	222	ILE	CA-C-N	5.17	129.04	121.80
2	B	222	ILE	C-N-CA	5.17	129.04	121.80
2	B	228	LYS	CA-C-N	5.17	131.41	121.54
2	B	228	LYS	C-N-CA	5.17	131.41	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	SER	N-CA-C	5.17	117.67	109.50
2	B	339	THR	CA-C-N	5.15	131.37	121.54
2	B	339	THR	C-N-CA	5.15	131.37	121.54
2	B	829	CYS	N-CA-C	-5.14	100.79	108.96
3	C	120	ILE	N-CA-CB	5.12	116.69	110.95
1	A	223	GLY	CA-C-N	5.11	129.51	120.87
1	A	223	GLY	C-N-CA	5.11	129.51	120.87
9	I	68	LEU	N-CA-C	5.10	116.08	109.65
1	A	1270	ASN	N-CA-C	5.10	117.62	111.40
1	A	602	ASP	CA-CB-CG	5.08	117.68	112.60
7	G	135	ASP	N-CA-C	5.08	118.03	109.95
9	I	52	ILE	N-CA-CB	5.08	117.69	111.60
7	G	33	GLU	CA-C-N	5.07	126.90	120.72
7	G	33	GLU	C-N-CA	5.07	126.90	120.72
3	C	145	CYS	N-CA-C	5.06	115.99	108.60
1	A	130	ASP	CA-C-N	5.06	127.37	120.54
1	A	130	ASP	C-N-CA	5.06	127.37	120.54
9	I	28	GLU	CB-CG-CD	5.06	121.20	112.60
2	B	752	ALA	N-CA-C	5.05	116.48	111.07
2	B	320	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	173	THR	CB-CA-C	5.05	119.88	111.30
2	B	703	ILE	N-CA-C	5.05	116.23	108.71
2	B	810	GLU	CA-C-N	5.05	127.98	120.31
2	B	810	GLU	C-N-CA	5.05	127.98	120.31
4	D	70	PHE	CA-CB-CG	5.05	118.85	113.80
6	F	116	ASP	CA-CB-CG	5.04	117.64	112.60
2	B	1018	PRO	CA-C-N	5.04	127.45	120.29
2	B	1018	PRO	C-N-CA	5.04	127.45	120.29
1	A	1231	ASP	CA-C-N	5.04	127.48	120.63
1	A	1231	ASP	C-N-CA	5.04	127.48	120.63
2	B	1002	THR	CA-C-N	5.04	127.28	120.38
2	B	1002	THR	C-N-CA	5.04	127.28	120.38
1	A	827	THR	CA-C-N	5.03	127.02	120.28
1	A	827	THR	C-N-CA	5.03	127.02	120.28
3	C	62	PHE	CA-C-N	5.03	127.00	120.56
3	C	62	PHE	C-N-CA	5.03	127.00	120.56
5	E	24	LYS	CA-C-N	5.02	127.01	120.28
5	E	24	LYS	C-N-CA	5.02	127.01	120.28
1	A	1447	GLU	CB-CG-CD	5.02	121.14	112.60
2	B	881	ASN	CA-CB-CG	5.02	117.62	112.60
2	B	1018	PRO	N-CA-C	5.02	120.65	113.47
2	B	732	SER	N-CA-C	5.01	115.92	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	763	ALA	N-CA-C	5.01	118.99	112.13

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11174	0	11233	216	1
2	B	8859	0	8901	182	0
3	C	2095	0	2051	50	0
4	D	1434	0	1460	24	0
5	E	1752	0	1776	27	0
6	F	679	0	701	20	0
7	G	1340	0	1357	44	1
8	H	1068	0	1040	19	0
9	I	971	0	927	6	1
10	J	532	0	542	15	0
11	K	920	0	929	30	0
12	L	363	0	386	17	0
13	N	207	0	114	4	0
14	P	152	0	77	0	0
15	T	385	0	216	5	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31940	0	31710	579	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 9.

All (579) 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	1.86	1.53
1:A:53:LEU:HD23	1:A:54:ASN:H	0.97	1.11
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.34	1.08
7:G:1:MET:HE2	7:G:2:PHE:H	1.14	1.04
1:A:53:LEU:CD2	1:A:54:ASN:H	1.78	0.97
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.99	0.96
1:A:53:LEU:HD23	1:A:54:ASN:N	1.81	0.94
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.49	0.92
7:G:1:MET:CE	7:G:2:PHE:H	1.82	0.92
7:G:1:MET:HE1	7:G:80:LYS:H	1.33	0.92
1:A:855:THR:HG21	1:A:857:ARG:HE	1.36	0.88
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.55	0.86
1:A:41:MET:HB3	1:A:49:LYS:HA	1.59	0.83
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.58	0.82
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.15	0.82
1:A:63:ARG:HA	1:A:74:MET:HG3	1.62	0.82
2:B:815:ARG:HG3	2:B:815:ARG:HH11	1.43	0.81
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.62	0.81
1:A:61:ILE:HG22	1:A:62:ASP:H	1.43	0.80
1:A:869:GLY:O	5:E:204:THR:HG21	1.83	0.79
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.47	0.79
7:G:34:VAL:O	7:G:37:SER:HB3	1.82	0.79
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.12	0.78
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.67	0.77
7:G:111:THR:HG22	7:G:113:HIS:H	1.48	0.77
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.67	0.76
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.68	0.75
1:A:254:GLU:HB3	2:B:935:ARG:HH21	1.52	0.74
12:L:28:LYS:HB2	12:L:39:SER:HA	1.70	0.74
10:J:48:ARG:O	10:J:52:THR:HG22	1.88	0.73
1:A:383:TYR:HB3	6:F:115:THR:HG22	1.70	0.73
7:G:1:MET:HE2	7:G:2:PHE:N	1.97	0.73
2:B:705:MET:H	2:B:710:LEU:HD12	1.53	0.73
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.71	0.72
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.70	0.72
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.72	0.71
2:B:882:THR:HG1	2:B:935:ARG:N	1.88	0.71
2:B:1172:ILE:HD11	2:B:1183:LYS:HE2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.71	0.71
3:C:66:ARG:NH2	10:J:3:VAL:O	2.23	0.70
2:B:662:MET:HA	2:B:665:GLU:HB2	1.72	0.70
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.74	0.69
12:L:27:LEU:HD13	12:L:37:LYS:HG2	1.73	0.69
2:B:638:PHE:HB3	2:B:651:LEU:HD21	1.75	0.69
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.27	0.69
1:A:64:ASN:O	1:A:65:LEU:HB3	1.93	0.68
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.73	0.68
3:C:56:THR:HG22	3:C:58:LEU:H	1.57	0.68
3:C:163:ILE:HD12	3:C:165:LYS:HB2	1.74	0.67
1:A:219:PHE:HA	1:A:222:LEU:HD12	1.77	0.67
1:A:497:THR:HG22	2:B:1146:PHE:HA	1.76	0.67
8:H:82:PRO:C	8:H:84:ALA:H	2.02	0.67
2:B:446:LEU:HD12	2:B:448:ILE:HD11	1.77	0.67
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.60	0.66
2:B:466:TRP:HB2	2:B:479:VAL:HG21	1.77	0.66
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.77	0.65
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.78	0.65
2:B:296:GLU:O	2:B:300:HIS:HD2	1.80	0.65
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.78	0.65
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.30	0.65
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.31	0.65
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.79	0.65
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.79	0.64
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.79	0.64
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.77	0.64
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.79	0.64
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.12	0.64
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.79	0.64
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.79	0.64
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.62	0.64
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.78	0.64
2:B:865:LYS:HE2	2:B:869:SER:HA	1.80	0.64
6:F:90:ARG:HH11	6:F:90:ARG:HG3	1.61	0.63
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.38	0.63
2:B:882:THR:HB	2:B:934:LYS:O	1.99	0.63
2:B:642:ASP:HA	2:B:649:LYS:HA	1.81	0.63
7:G:26:LEU:HD13	7:G:56:ILE:HD11	1.80	0.63
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.81	0.62
1:A:41:MET:CB	1:A:49:LYS:HA	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.81	0.62
13:N:2:DA:H4'	13:N:3:DA:OP1	1.98	0.62
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	1.99	0.62
4:D:18:VAL:HG22	4:D:20:GLU:H	1.64	0.62
1:A:472:LEU:O	1:A:475:THR:HB	2.00	0.61
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.82	0.61
2:B:35:SER:HA	2:B:811:TYR:HE1	1.65	0.61
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.82	0.61
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.33	0.61
1:A:855:THR:CG2	1:A:857:ARG:HE	2.11	0.61
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.83	0.61
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.35	0.61
1:A:341:MET:HE2	1:A:843:LYS:HZ1	1.65	0.61
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.83	0.61
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.82	0.61
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.82	0.61
1:A:847:ASP:HB3	1:A:1398:MET:HE1	1.82	0.61
3:C:98:VAL:H	3:C:122:SER:CB	2.13	0.61
7:G:143:ILE:HG22	7:G:145:VAL:HG22	1.82	0.61
7:G:111:THR:HB	7:G:114:LEU:HD23	1.83	0.61
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.30	0.61
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.81	0.60
2:B:901:PRO:HD3	12:L:58:LYS:HB3	1.83	0.60
12:L:47:ARG:HH21	12:L:54:ARG:HE	1.48	0.60
2:B:996:ARG:NH2	3:C:174:ALA:O	2.32	0.60
6:F:89:GLU:O	6:F:93:ILE:HD12	2.01	0.60
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.82	0.60
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.84	0.60
3:C:55:THR:HB	3:C:151:GLN:HA	1.84	0.59
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.83	0.59
12:L:60:ARG:HH22	12:L:65:VAL:HG22	1.66	0.59
2:B:815:ARG:HH11	2:B:815:ARG:CG	2.14	0.59
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.84	0.59
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.85	0.59
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.84	0.58
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.85	0.58
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.68	0.58
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.86	0.58
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.39	0.58
2:B:902:GLY:O	12:L:65:VAL:HG11	2.03	0.58
7:G:1:MET:CE	7:G:80:LYS:H	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.03	0.57
7:G:114:LEU:HD12	7:G:162:SER:HB2	1.85	0.57
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.86	0.57
1:A:62:ASP:HB2	1:A:65:LEU:HD22	1.86	0.57
2:B:1002:THR:HG22	2:B:1072:MET:HE2	1.86	0.57
2:B:344:LYS:HB3	2:B:347:LYS:HB2	1.84	0.57
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.70	0.57
1:A:1402:PHE:CE2	1:A:1403:GLU:HG2	2.40	0.57
2:B:542:MET:HE2	2:B:747:MET:HG3	1.87	0.57
2:B:878:GLN:HA	2:B:885:MET:HE1	1.86	0.57
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.87	0.56
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.87	0.56
1:A:253:ASN:HA	2:B:884:ARG:HH22	1.70	0.56
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.86	0.56
1:A:392:VAL:HG11	1:A:424:ILE:HG21	1.88	0.56
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.86	0.56
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.87	0.56
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.88	0.56
4:D:167:LEU:HB3	4:D:177:VAL:HG22	1.88	0.56
1:A:646:PHE:O	1:A:650:GLN:HG2	2.05	0.55
1:A:1433:MET:CE	7:G:63:PRO:HB3	2.36	0.55
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.88	0.55
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.89	0.55
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.72	0.55
2:B:311:LEU:HB3	9:I:4:PHE:HE1	1.70	0.55
4:D:59:ILE:HD11	7:G:77:VAL:HG11	1.89	0.55
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.89	0.55
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.69	0.55
2:B:1172:ILE:HD11	2:B:1183:LYS:CE	2.37	0.55
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.07	0.55
2:B:839:MET:CE	2:B:980:PHE:HB2	2.36	0.55
1:A:392:VAL:CG1	1:A:424:ILE:HG21	2.37	0.55
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.89	0.54
1:A:448:PRO:O	1:A:449:SER:HB2	2.07	0.54
2:B:343:ILE:O	2:B:344:LYS:HB2	2.08	0.54
1:A:315:LEU:HA	1:A:321:PRO:HA	1.89	0.54
8:H:130:ARG:HA	8:H:133:ASN:HD22	1.72	0.54
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.90	0.54
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.08	0.54
13:N:2:DA:H61	15:T:16:DT:H3	1.55	0.54
7:G:127:PRO:HB2	7:G:139:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.88	0.53
7:G:138:THR:HG22	7:G:139:ILE:H	1.73	0.53
2:B:35:SER:HA	2:B:811:TYR:CE1	2.42	0.53
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.90	0.53
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.44	0.53
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.73	0.53
2:B:882:THR:C	2:B:884:ARG:H	2.16	0.53
7:G:1:MET:SD	7:G:2:PHE:N	2.82	0.53
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.90	0.53
1:A:579:SER:HA	1:A:582:ILE:HD12	1.91	0.53
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.90	0.53
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.08	0.53
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.41	0.53
3:C:98:VAL:H	3:C:122:SER:HB2	1.74	0.53
1:A:741:ASN:HB3	1:A:744:LYS:HB2	1.90	0.52
2:B:247:GLY:H	2:B:418:LYS:NZ	2.07	0.52
2:B:577:ALA:HB1	2:B:589:VAL:HB	1.91	0.52
1:A:49:LYS:NZ	1:A:60:SER:HA	2.24	0.52
4:D:55:ALA:O	4:D:59:ILE:HD12	2.08	0.52
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.73	0.52
1:A:915:SER:HB2	1:A:919:ILE:HD13	1.91	0.52
1:A:1386:ARG:HB3	1:A:1403:GLU:HG3	1.92	0.52
1:A:982:THR:HB	1:A:985:ASP:H	1.75	0.52
2:B:706:GLN:HB3	2:B:709:ASP:OD1	2.10	0.52
2:B:848:ARG:HD2	10:J:8:PHE:O	2.08	0.52
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.92	0.52
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.90	0.52
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.10	0.52
2:B:1165:ILE:HG21	4:D:17:LYS:HB3	1.91	0.52
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.92	0.52
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.90	0.52
2:B:428:ILE:HG22	2:B:432:MET:HE2	1.91	0.52
1:A:49:LYS:HZ3	1:A:60:SER:HA	1.74	0.51
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.93	0.51
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.10	0.51
3:C:100:THR:HB	3:C:121:VAL:HG21	1.91	0.51
1:A:140:THR:HA	1:A:143:LYS:HE2	1.93	0.51
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.91	0.51
5:E:40:GLU:HA	5:E:43:LYS:HD2	1.93	0.51
2:B:296:GLU:O	2:B:300:HIS:CD2	2.61	0.51
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:4:GLU:HB3	5:E:7:ARG:NE	2.26	0.51
3:C:149:LYS:HG3	3:C:150:GLY:H	1.75	0.51
1:A:1172:LEU:C	1:A:1174:PHE:H	2.18	0.51
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.92	0.51
2:B:882:THR:OG1	2:B:935:ARG:N	2.41	0.51
1:A:709:THR:HB	1:A:712:GLU:H	1.75	0.51
1:A:1148:ILE:HA	9:I:49:ILE:HD12	1.93	0.51
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.93	0.51
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.93	0.51
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.76	0.51
5:E:5:ASN:HD21	5:E:52:ARG:HE	1.57	0.51
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.93	0.51
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.92	0.50
4:D:193:THR:HG21	7:G:167:TYR:HD2	1.76	0.50
2:B:313:MET:HG2	2:B:386:LEU:HD22	1.94	0.50
1:A:697:ALA:HB2	1:A:702:LEU:HD13	1.94	0.50
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.93	0.50
2:B:1100:ASP:OD2	11:K:1:MET:HB3	2.12	0.50
1:A:1148:ILE:HD12	1:A:1196:GLU:HG2	1.93	0.50
1:A:52:GLY:N	1:A:56:PRO:HB3	2.26	0.50
6:F:76:LYS:HA	6:F:79:ARG:CD	2.34	0.50
1:A:857:ARG:HD3	1:A:861:GLY:O	2.11	0.50
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.94	0.50
1:A:679:ILE:HG13	1:A:732:LEU:HD12	1.94	0.50
1:A:1400:CYS:HA	1:A:1408:ILE:HD12	1.94	0.49
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.93	0.49
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.47	0.49
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.94	0.49
2:B:242:SER:OG	2:B:362:PRO:HD2	2.12	0.49
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.93	0.49
3:C:33:LEU:HG	3:C:37:MET:HE2	1.94	0.49
3:C:149:LYS:C	3:C:151:GLN:H	2.20	0.49
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.94	0.49
3:C:4:GLU:H	3:C:7:GLN:HE22	1.59	0.49
1:A:216:VAL:O	1:A:220:THR:HB	2.13	0.49
1:A:448:PRO:O	1:A:449:SER:CB	2.60	0.49
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.94	0.49
10:J:9:SER:OG	10:J:48:ARG:NH2	2.45	0.49
1:A:452:LYS:HG2	2:B:1141:HIS:CE1	2.47	0.49
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.95	0.49
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ILE:HA	2:B:338:GLY:O	2.13	0.49
2:B:425:THR:HA	2:B:428:ILE:HD12	1.95	0.49
1:A:449:SER:HA	1:A:454:SER:CB	2.42	0.49
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.95	0.49
8:H:107:VAL:HG23	8:H:111:LEU:HB3	1.95	0.49
10:J:32:GLU:CD	10:J:32:GLU:H	2.20	0.49
1:A:49:LYS:HG2	1:A:61:ILE:HD12	1.95	0.49
1:A:511:ILE:HA	1:A:521:MET:HE3	1.95	0.49
3:C:6:PRO:HB2	11:K:101:LEU:HD23	1.95	0.48
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.94	0.48
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.95	0.48
11:K:32:VAL:HG22	11:K:74:ARG:HG3	1.94	0.48
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.94	0.48
2:B:745:PRO:O	2:B:748:ILE:HG12	2.13	0.48
2:B:842:ASN:HB3	2:B:845:SER:HB2	1.95	0.48
2:B:918:ILE:HG12	2:B:935:ARG:HH22	1.78	0.48
8:H:105:GLU:HB3	8:H:113:ALA:HB3	1.94	0.48
8:H:125:LEU:HG	8:H:130:ARG:NH2	2.28	0.48
7:G:1:MET:HE3	7:G:80:LYS:O	2.13	0.48
8:H:82:PRO:O	8:H:84:ALA:N	2.45	0.48
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.78	0.48
1:A:353:ILE:HD12	1:A:482:PHE:CD1	2.48	0.48
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.96	0.48
2:B:33:VAL:HG21	2:B:638:PHE:CZ	2.48	0.48
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.44	0.48
4:D:23:ASN:HA	4:D:28:GLN:O	2.14	0.48
4:D:34:GLN:O	4:D:47:LEU:HD12	2.14	0.48
5:E:76:GLY:H	5:E:106:GLN:CD	2.22	0.48
3:C:11:ARG:HD3	3:C:209:TYR:CE2	2.49	0.48
7:G:93:SER:OG	7:G:100:GLU:HB2	2.13	0.48
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.95	0.47
7:G:142:ARG:HB3	7:G:171:ILE:HD12	1.95	0.47
1:A:567:LYS:HA	1:A:568:PRO:C	2.38	0.47
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.96	0.47
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.96	0.47
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.95	0.47
11:K:103:THR:O	11:K:107:THR:HB	2.14	0.47
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.44	0.47
1:A:185:TRP:HE3	1:A:185:TRP:H	1.61	0.47
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.95	0.47
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:LYS:O	11:K:6:ARG:NH1	2.40	0.47
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.96	0.47
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.79	0.47
1:A:1338:VAL:HG12	1:A:1339:LEU:HG	1.95	0.47
1:A:358:ASN:HB2	11:K:65:HIS:HD2	1.79	0.47
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.62	0.47
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.94	0.47
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.96	0.47
1:A:84:ILE:HD11	1:A:86:LEU:HD23	1.97	0.47
3:C:114:TYR:CD1	3:C:140:ASN:HB3	2.49	0.47
3:C:148:ARG:HG2	3:C:149:LYS:HG2	1.97	0.47
1:A:358:ASN:HB2	11:K:65:HIS:CD2	2.50	0.47
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.96	0.47
1:A:528:LEU:HD23	1:A:751:SER:HA	1.96	0.47
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.25	0.47
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.97	0.47
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.96	0.47
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.45	0.47
2:B:865:LYS:HB2	2:B:961:LEU:HD21	1.97	0.47
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.50	0.47
8:H:63:LEU:HB3	8:H:90:ALA:CB	2.45	0.47
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.79	0.47
1:A:61:ILE:HG22	1:A:62:ASP:N	2.23	0.47
1:A:88:LYS:HB2	1:A:276:LEU:HD21	1.97	0.47
1:A:886:ILE:HG12	1:A:943:LEU:HB3	1.97	0.47
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.48	0.47
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.97	0.47
2:B:755:ILE:HG22	2:B:809:MET:HE2	1.96	0.47
2:B:806:THR:HG22	2:B:808:ALA:H	1.79	0.47
3:C:166:GLU:HG2	12:L:70:ARG:HH22	1.80	0.47
7:G:92:VAL:HG21	7:G:102:GLN:HB2	1.97	0.47
6:F:128:LYS:HD3	6:F:149:GLU:O	2.15	0.46
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.97	0.46
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.97	0.46
1:A:62:ASP:HB3	1:A:64:ASN:O	2.15	0.46
1:A:1004:ASN:HD21	1:A:1007:ILE:HG12	1.80	0.46
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	1.96	0.46
10:J:64:ASN:HB2	10:J:65:PRO:HD3	1.96	0.46
2:B:435:THR:C	2:B:437:GLU:H	2.24	0.46
2:B:449:ASN:HD21	2:B:451:LYS:HB2	1.80	0.46
2:B:649:LYS:HE2	2:B:738:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:O	1:A:55:ASP:CG	2.59	0.46
1:A:497:THR:CG2	2:B:1146:PHE:HA	2.46	0.46
1:A:871:ASP:CG	1:A:1366:ARG:HH22	2.24	0.46
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.31	0.46
6:F:90:ARG:HH11	6:F:90:ARG:CG	2.29	0.46
1:A:941:LYS:HE3	1:A:941:LYS:O	2.15	0.46
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.55	0.46
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.97	0.46
1:A:1433:MET:HE1	7:G:63:PRO:HB3	1.98	0.46
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.97	0.46
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.98	0.46
1:A:672:ASP:HB3	1:A:736:ASN:OD1	2.16	0.46
3:C:259:LEU:HD22	11:K:91:CYS:HB3	1.97	0.46
8:H:89:LEU:C	8:H:91:ASP:H	2.24	0.46
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.63	0.46
3:C:98:VAL:H	3:C:122:SER:HB3	1.79	0.46
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.97	0.46
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.51	0.46
5:E:6:GLU:HA	5:E:9:ILE:HD12	1.98	0.46
5:E:198:ILE:HD13	5:E:212:ARG:HG3	1.97	0.46
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.97	0.46
1:A:587:HIS:HB2	1:A:969:GLN:HE22	1.80	0.46
2:B:341:LEU:HD12	2:B:343:ILE:H	1.81	0.46
2:B:756:ILE:O	2:B:759:PRO:HD3	2.16	0.46
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.98	0.46
12:L:38:LEU:HD22	12:L:56:LEU:HD21	1.97	0.45
1:A:53:LEU:O	1:A:54:ASN:C	2.59	0.45
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.46	0.45
6:F:132:LEU:O	6:F:148:VAL:HG22	2.15	0.45
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.97	0.45
1:A:38:PRO:HD3	1:A:270:LEU:HD12	1.98	0.45
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.98	0.45
7:G:106:MET:HG3	7:G:157:ILE:O	2.16	0.45
5:E:19:VAL:HG22	5:E:140:LEU:HD22	1.97	0.45
1:A:425:GLN:HA	1:A:425:GLN:NE2	2.31	0.45
1:A:527:THR:HG23	1:A:653:VAL:HB	1.97	0.45
2:B:365:THR:HG21	2:B:370:PHE:CD2	2.52	0.45
7:G:23:LYS:HA	7:G:56:ILE:HD12	1.99	0.45
2:B:363:HIS:O	2:B:364:ILE:HB	2.16	0.45
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.82	0.45
8:H:82:PRO:C	8:H:84:ALA:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HG22	1:A:84:ILE:HG22	1.99	0.45
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.46	0.45
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.99	0.45
2:B:583:ASN:HD21	2:B:628:THR:HB	1.81	0.45
1:A:385:ILE:O	1:A:389:THR:OG1	2.34	0.45
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.16	0.45
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.47	0.45
1:A:121:LEU:O	1:A:124:GLN:HB3	2.16	0.45
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.99	0.45
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.50	0.45
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.81	0.45
6:F:109:VAL:HG11	6:F:123:LYS:HG2	2.00	0.45
7:G:106:MET:HG2	7:G:107:LYS:N	2.32	0.45
10:J:7:CYS:HA	10:J:49:MET:HG2	1.99	0.45
2:B:310:MET:HE1	2:B:387:LEU:HD12	1.99	0.44
5:E:116:ILE:HB	5:E:121:MET:HE2	1.98	0.44
5:E:176:PRO:O	5:E:212:ARG:HA	2.16	0.44
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.98	0.44
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.46	0.44
2:B:693:ILE:HG23	2:B:697:GLU:HB3	1.99	0.44
1:A:626:ASN:O	1:A:631:HIS:ND1	2.48	0.44
2:B:295:GLY:HA2	2:B:298:LEU:HB2	2.00	0.44
2:B:792:MET:HA	2:B:856:PHE:O	2.18	0.44
2:B:900:ALA:HB3	12:L:61:THR:HG23	2.00	0.44
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.82	0.44
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.30	0.44
1:A:1402:PHE:CD2	1:A:1403:GLU:HG2	2.53	0.44
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.99	0.44
2:B:873:THR:O	2:B:914:LYS:HA	2.17	0.44
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.15	0.44
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.99	0.44
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	2.00	0.44
1:A:880:LYS:HA	1:A:955:PRO:HA	1.99	0.44
1:A:1313:LEU:HD23	1:A:1338:VAL:HB	2.00	0.44
2:B:510:LYS:N	2:B:511:PRO:HD3	2.32	0.44
2:B:705:MET:HE3	2:B:705:MET:HA	1.99	0.44
1:A:388:LEU:O	1:A:392:VAL:HG23	2.18	0.44
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.42	0.44
2:B:338:GLY:HA3	2:B:340:ALA:H	1.83	0.44
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.90	0.44
7:G:128:PRO:O	7:G:138:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.99	0.44
11:K:45:LEU:HG	11:K:94:ILE:HD13	2.00	0.44
1:A:1076:ALA:HA	1:A:1079:MET:HE2	2.00	0.44
2:B:574:SER:HB3	2:B:591:ARG:HE	1.81	0.44
5:E:100:ILE:HA	5:E:105:PHE:HD2	1.83	0.44
6:F:119:ARG:HA	6:F:122:MET:HG3	2.00	0.44
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.51	0.44
2:B:475:SER:O	2:B:476:ARG:HB3	2.18	0.44
6:F:134:ILE:HG22	6:F:136:ARG:HG3	2.00	0.44
7:G:21:ARG:NH1	7:G:24:GLN:OE1	2.51	0.44
1:A:1276:VAL:HB	1:A:1279:ILE:HD13	2.00	0.44
2:B:291:ILE:HD12	2:B:291:ILE:H	1.83	0.44
1:A:1158:PRO:HA	1:A:1241:ARG:NH1	2.33	0.43
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.17	0.43
1:A:816:HIS:HE2	2:B:764:SER:H	1.64	0.43
1:A:1444:MET:HB2	1:A:1444:MET:HE2	1.60	0.43
2:B:1116:ARG:HB2	2:B:1198:TYR:CD2	2.53	0.43
1:A:464:PRO:HB2	11:K:4:PRO:HD3	2.01	0.43
2:B:121:ASN:ND2	2:B:860:MET:HE2	2.34	0.43
3:C:60:ASP:HB3	12:L:67:PHE:CE2	2.54	0.43
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.82	0.43
2:B:283:VAL:HG13	2:B:297:ILE:HD13	1.99	0.43
3:C:54:ASN:OD1	3:C:56:THR:HB	2.19	0.43
4:D:176:GLU:OE2	4:D:197:SER:HB2	2.19	0.43
7:G:43:GLY:HA2	7:G:157:ILE:HD11	2.00	0.43
8:H:16:ASP:HA	8:H:17:PRO:HD3	1.90	0.43
1:A:767:GLN:HA	1:A:799:PHE:HA	2.01	0.43
2:B:1122:ARG:HB3	15:T:23:DG:OP1	2.19	0.43
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.83	0.43
3:C:75:MET:O	3:C:246:ARG:NH2	2.50	0.43
4:D:18:VAL:HG13	4:D:19:GLU:HA	2.00	0.43
5:E:19:VAL:O	5:E:23:VAL:HG23	2.19	0.43
2:B:128:LEU:HB2	2:B:167:ILE:O	2.18	0.43
2:B:766:ARG:NH2	2:B:1020:ARG:HD3	2.33	0.43
3:C:22:LEU:HD22	3:C:230:MET:HE1	2.00	0.43
5:E:19:VAL:HG11	5:E:80:VAL:HG11	2.01	0.43
7:G:106:MET:HB3	7:G:106:MET:HE2	1.83	0.43
1:A:1076:ALA:HA	1:A:1079:MET:HG3	2.01	0.43
2:B:754:SER:HB2	2:B:812:LEU:HD11	2.01	0.43
1:A:658:LEU:HD23	1:A:659:HIS:NE2	2.33	0.43
1:A:1436:ILE:O	1:A:1437:GLY:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.18	0.43
11:K:51:LEU:HD12	11:K:51:LEU:HA	1.87	0.43
2:B:847:ASP:HB3	3:C:167:HIS:CE1	2.53	0.43
1:A:901:LEU:HD22	1:A:919:ILE:HG23	2.00	0.43
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.18	0.43
5:E:102:GLU:C	5:E:104:ASN:H	2.25	0.43
2:B:1138:MET:HB3	2:B:1147:LEU:HG	2.01	0.42
6:F:90:ARG:HG3	6:F:90:ARG:NH1	2.31	0.42
9:I:50:THR:HG22	9:I:52:ILE:H	1.83	0.42
13:N:2:DA:N6	15:T:16:DT:H3	2.16	0.42
1:A:194:ALA:HA	1:A:195:ASP:C	2.44	0.42
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.52	0.42
3:C:58:LEU:HD21	10:J:57:ILE:HD12	2.01	0.42
4:D:65:GLU:HA	4:D:68:ARG:HG3	2.00	0.42
8:H:63:LEU:HB3	8:H:90:ALA:HB2	2.01	0.42
1:A:868:TYR:CE2	1:A:1058:VAL:HG11	2.54	0.42
2:B:801:LYS:O	10:J:52:THR:OG1	2.35	0.42
2:B:911:ILE:HD11	2:B:941:LEU:HD13	2.01	0.42
11:K:7:PHE:CD1	11:K:7:PHE:C	2.97	0.42
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.55	0.42
1:A:605:MET:HE2	1:A:607:ILE:HG13	2.00	0.42
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.54	0.42
1:A:1155:ASP:HB3	1:A:1241:ARG:NH2	2.32	0.42
2:B:328:GLU:CD	2:B:328:GLU:H	2.28	0.42
3:C:52:GLU:HG2	12:L:64:LEU:HD11	2.01	0.42
4:D:213:GLU:HA	4:D:216:ASN:HD22	1.84	0.42
1:A:1128:GLN:HG3	1:A:1304:TRP:CE2	2.54	0.42
8:H:93:TYR:HA	8:H:145:ARG:HB3	2.01	0.42
1:A:216:VAL:HG13	1:A:226:GLU:HB3	2.00	0.42
2:B:766:ARG:HH21	2:B:1020:ARG:HH11	1.68	0.42
2:B:464:GLY:HA2	2:B:480:SER:HB3	2.02	0.42
2:B:848:ARG:HA	3:C:69:LEU:HD21	2.01	0.42
4:D:5:THR:HG21	7:G:74:TYR:OH	2.20	0.42
13:N:4:DG:N2	15:T:15:DT:O2	2.53	0.42
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.55	0.42
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.02	0.42
2:B:168:GLY:H	2:B:450:ALA:HB1	1.85	0.42
2:B:216:GLU:OE1	2:B:537:LYS:HD2	2.20	0.42
2:B:601:ARG:HA	2:B:615:MET:HE1	2.01	0.42
4:D:10:THR:O	4:D:12:ARG:NH2	2.53	0.42
4:D:195:ILE:HG22	4:D:198:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:65:HIS:HE1	11:K:67:PHE:CG	2.37	0.42
1:A:200:ARG:HH22	1:A:206:GLU:CD	2.28	0.41
1:A:868:TYR:HD2	1:A:1058:VAL:HG11	1.83	0.41
2:B:70:ILE:HD12	2:B:70:ILE:H	1.85	0.41
2:B:542:MET:HG3	2:B:747:MET:HB3	2.02	0.41
3:C:4:GLU:HB2	11:K:104:ASN:HD21	1.84	0.41
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.79	0.41
11:K:51:LEU:CD1	11:K:59:ALA:HB3	2.45	0.41
1:A:1323:ASP:CG	1:A:1326:ARG:HG3	2.46	0.41
2:B:637:LEU:HD12	2:B:693:ILE:HD13	2.01	0.41
2:B:876:LYS:NZ	2:B:891:ASP:HA	2.35	0.41
4:D:173:HIS:CE1	4:D:201:LYS:HE3	2.56	0.41
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.85	0.41
2:B:211:VAL:HG23	2:B:483:LEU:HB2	2.01	0.41
2:B:1050:ILE:H	2:B:1050:ILE:HG13	1.73	0.41
3:C:75:MET:HE1	3:C:239:PRO:HG3	2.01	0.41
1:A:122:MET:HG3	1:A:126:LEU:HD12	2.02	0.41
1:A:786:HIS:CD2	2:B:703:ILE:HB	2.54	0.41
1:A:1433:MET:HE3	7:G:63:PRO:CB	2.51	0.41
4:D:7:THR:HG21	7:G:5:LYS:HZ1	1.85	0.41
4:D:54:GLU:O	4:D:58:VAL:HG23	2.21	0.41
11:K:18:LYS:HE3	11:K:38:GLU:HG2	2.03	0.41
1:A:270:LEU:HD22	1:A:270:LEU:HA	1.89	0.41
1:A:629:LEU:HD13	1:A:645:LEU:HD21	2.03	0.41
2:B:102:VAL:HG13	2:B:112:LEU:HD22	2.03	0.41
2:B:1104:HIS:HB2	2:B:1122:ARG:HG3	2.03	0.41
5:E:188:LEU:HB2	5:E:190:LEU:HD23	2.02	0.41
12:L:47:ARG:HG3	12:L:54:ARG:HG3	2.02	0.41
1:A:1387:HIS:O	1:A:1391:ARG:HG2	2.21	0.41
2:B:205:ILE:HD13	2:B:461:LEU:HB3	2.02	0.41
2:B:315:LYS:N	2:B:316:PRO:HD2	2.35	0.41
4:D:18:VAL:HG22	4:D:19:GLU:HA	2.03	0.41
5:E:181:ALA:HA	5:E:186:LEU:HD21	2.02	0.41
1:A:436:ILE:HD13	1:A:436:ILE:HA	1.60	0.41
2:B:770:GLN:HG2	2:B:983:ARG:C	2.46	0.41
4:D:159:THR:O	4:D:163:VAL:HG23	2.20	0.41
12:L:40:LEU:HB2	12:L:44:ASP:HB3	2.01	0.41
1:A:35:ILE:HA	1:A:52:GLY:O	2.20	0.41
1:A:605:MET:CE	1:A:612:ILE:HG23	2.51	0.41
1:A:856:THR:HB	1:A:865:GLN:HB2	2.02	0.41
1:A:923:LEU:HD12	1:A:923:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:HD21	1:A:1327:ILE:HD11	2.03	0.41
2:B:169:ARG:HB2	2:B:454:THR:HG23	2.02	0.41
2:B:889:THR:HG22	2:B:891:ASP:OD1	2.20	0.41
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	2.03	0.41
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.79	0.41
3:C:29:MET:HE2	11:K:98:LEU:HG	2.03	0.41
15:T:19:DT:O2	15:T:19:DT:H2'	2.21	0.41
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.03	0.41
2:B:273:LEU:HD23	2:B:273:LEU:HA	1.92	0.41
2:B:640:VAL:HA	2:B:651:LEU:HA	2.02	0.41
2:B:644:GLU:HG2	2:B:654:ARG:HH22	1.86	0.41
3:C:201:TRP:HA	3:C:202:PRO:HD3	1.95	0.41
6:F:90:ARG:CG	6:F:90:ARG:NH1	2.84	0.41
10:J:31:ASP:OD1	10:J:34:THR:OG1	2.37	0.41
10:J:48:ARG:CZ	10:J:49:MET:HE1	2.51	0.41
1:A:413:ILE:HD13	1:A:424:ILE:HD11	2.02	0.41
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	2.03	0.41
7:G:73:LYS:HD2	7:G:73:LYS:HA	1.93	0.41
11:K:65:HIS:CE1	11:K:67:PHE:CG	3.08	0.41
1:A:354:SER:O	1:A:469:ARG:HA	2.21	0.40
1:A:629:LEU:O	1:A:633:VAL:HG23	2.20	0.40
1:A:1318:THR:HB	5:E:11:ARG:HH12	1.86	0.40
2:B:840:ILE:HG21	2:B:994:TYR:HD2	1.85	0.40
8:H:63:LEU:CB	8:H:90:ALA:CB	2.99	0.40
8:H:127:GLY:N	8:H:130:ARG:HH21	2.19	0.40
2:B:101:MET:HG2	2:B:111:ALA:HA	2.02	0.40
12:L:60:ARG:NH2	12:L:65:VAL:HG22	2.33	0.40
1:A:41:MET:HA	1:A:50:ILE:HB	2.02	0.40
1:A:399:HIS:O	1:A:401:GLY:N	2.54	0.40
1:A:709:THR:HG23	9:I:94:ASP:HA	2.03	0.40
1:A:946:VAL:HG22	5:E:201:LYS:HD2	2.04	0.40
2:B:39:ARG:NE	2:B:665:GLU:HG2	2.37	0.40
2:B:121:ASN:HA	2:B:207:GLY:HA3	2.03	0.40
2:B:280:ILE:H	2:B:280:ILE:HG13	1.78	0.40
2:B:373:ARG:HA	2:B:566:LEU:HD23	2.03	0.40
2:B:915:THR:HG21	2:B:934:LYS:HB2	2.02	0.40
2:B:1082:MET:HA	3:C:189:THR:HA	2.04	0.40
3:C:18:VAL:HG23	3:C:240:VAL:HB	2.04	0.40
7:G:13:LEU:HD23	7:G:13:LEU:HA	1.92	0.40
1:A:93:VAL:HG13	1:A:301:ALA:HB1	2.03	0.40
1:A:974:ASP:C	1:A:976:THR:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.85	0.40
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.22	0.40
7:G:9:LEU:HD22	7:G:34:VAL:HG23	2.04	0.40
1:A:151:ASP:HA	1:A:163:SER:HA	2.02	0.40
1:A:353:ILE:HD13	1:A:487:MET:CE	2.51	0.40
1:A:567:LYS:HA	1:A:569:LYS:N	2.36	0.40
2:B:992:ILE:HD11	11:K:66:PRO:HB2	2.03	0.40
7:G:83:LYS:HD2	7:G:149:GLY:HA2	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:THR:N	9:I:33:SER:O[8_555]	2.18	0.02
7:G:95:SER:OG	7:G:97:HIS:CD2[3_654]	2.18	0.02

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	1414/1732 (82%)	1252 (88%)	112 (8%)	50 (4%)	3	23
2	B	1095/1224 (90%)	969 (88%)	82 (8%)	44 (4%)	2	19
3	C	264/318 (83%)	236 (89%)	24 (9%)	4 (2%)	8	37
4	D	174/221 (79%)	154 (88%)	14 (8%)	6 (3%)	3	23
5	E	212/215 (99%)	186 (88%)	24 (11%)	2 (1%)	14	47
6	F	82/155 (53%)	77 (94%)	4 (5%)	1 (1%)	10	41
7	G	169/171 (99%)	160 (95%)	6 (4%)	3 (2%)	6	34
8	H	129/146 (88%)	101 (78%)	19 (15%)	9 (7%)	1	10
9	I	117/122 (96%)	96 (82%)	18 (15%)	3 (3%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	63/70 (90%)	55 (87%)	4 (6%)	4 (6%)	1	12
11	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
12	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0	1
All	All	3876/4564 (85%)	3421 (88%)	321 (8%)	134 (4%)	3	23

All (134) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	57	ARG
1	A	58	LEU
1	A	74	MET
1	A	193	ASP
1	A	257	ARG
1	A	286	HIS
1	A	318	SER
1	A	332	LYS
1	A	335	ARG
1	A	399	HIS
1	A	448	PRO
1	A	449	SER
1	A	1175	SER
1	A	1403	GLU
1	A	1405	THR
2	B	229	ALA
2	B	307	ASP
2	B	344	LYS
2	B	473	MET
2	B	629	ASP
2	B	707	PRO
2	B	731	VAL
2	B	751	VAL
2	B	879	ARG
2	B	1066	SER
2	B	1157	ALA
2	B	1176	ASN
3	C	215	GLU
3	C	240	VAL
4	D	18	VAL
9	I	9	ASP
10	J	6	ARG

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Mol	Chain	Res	Type
12	L	53	HIS
12	L	56	LEU
1	A	54	ASN
1	A	76	GLU
1	A	178	GLY
1	A	187	LYS
1	A	189	ARG
1	A	195	ASP
1	A	311	GLN
1	A	312	PRO
1	A	1124	HIS
1	A	1206	ASP
1	A	1281	ARG
2	B	340	ALA
2	B	341	LEU
2	B	466	TRP
2	B	867	GLY
2	B	1046	PRO
2	B	1156	ASP
2	B	1181	GLU
2	B	1190	ASP
4	D	169	SER
8	H	17	PRO
8	H	81	PRO
8	H	83	GLN
9	I	95	THR
10	J	2	ILE
10	J	55	ASP
12	L	39	SER
12	L	50	ASP
1	A	43	GLU
1	A	167	CYS
1	A	251	SER
1	A	336	ILE
1	A	593	GLU
1	A	1173	HIS
1	A	1255	GLU
2	B	343	ILE
2	B	575	PRO
2	B	883	LEU
2	B	1223	ASP
4	D	16	LYS

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Mol	Chain	Res	Type
4	D	52	LEU
4	D	199	ASN
5	E	3	GLN
7	G	154	VAL
8	H	52	GLN
8	H	60	ALA
8	H	82	PRO
10	J	17	LYS
12	L	45	ALA
1	A	35	ILE
1	A	62	ASP
1	A	283	GLY
1	A	331	GLY
1	A	423	ASP
1	A	567	LYS
1	A	569	LYS
1	A	775	ILE
1	A	1122	PRO
2	B	262	GLU
2	B	338	GLY
2	B	449	ASN
2	B	533	CYS
2	B	711	GLU
3	C	150	GLY
4	D	220	LEU
7	G	63	PRO
8	H	18	GLY
8	H	90	ALA
9	I	105	SER
12	L	38	LEU
12	L	59	ALA
1	A	52	GLY
1	A	156	ASP
1	A	958	VAL
1	A	1437	GLY
2	B	368	GLU
2	B	772	ALA
2	B	792	MET
2	B	1155	SER
6	F	73	ALA
7	G	139	ILE
8	H	32	THR

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Mol	Chain	Res	Type
12	L	26	THR
2	B	1108	ARG
3	C	38	ILE
2	B	108	VAL
5	E	90	VAL
1	A	196	GLU
2	B	168	GLY
2	B	251	ILE
2	B	436	VAL
2	B	902	GLY
2	B	907	GLY
2	B	369	GLY
1	A	1123	GLY
2	B	1214	PRO
1	A	55	ASP
2	B	231	PRO
2	B	364	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1240/1519 (82%)	1046 (84%)	194 (16%)	2	15
2	B	966/1061 (91%)	824 (85%)	142 (15%)	3	17
3	C	234/274 (85%)	205 (88%)	29 (12%)	4	22
4	D	160/200 (80%)	128 (80%)	32 (20%)	1	7
5	E	196/197 (100%)	174 (89%)	22 (11%)	6	25
6	F	74/137 (54%)	59 (80%)	15 (20%)	1	7
7	G	152/152 (100%)	124 (82%)	28 (18%)	1	9
8	H	117/128 (91%)	97 (83%)	20 (17%)	2	12
9	I	113/116 (97%)	101 (89%)	12 (11%)	6	27
10	J	60/65 (92%)	49 (82%)	11 (18%)	2	10
11	K	99/102 (97%)	83 (84%)	16 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	40/57 (70%)	28 (70%)	12 (30%)	0	2
All	All	3451/4008 (86%)	2918 (85%)	533 (15%)	2	16

All (533) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	12	ARG
1	A	13	THR
1	A	28	ARG
1	A	34	LYS
1	A	41	MET
1	A	44	THR
1	A	47	ARG
1	A	50	ILE
1	A	62	ASP
1	A	64	ASN
1	A	65	LEU
1	A	84	ILE
1	A	88	LYS
1	A	93	VAL
1	A	96	ILE
1	A	117	GLU
1	A	126	LEU
1	A	129	LYS
1	A	132	LYS
1	A	141	LEU
1	A	144	THR
1	A	145	LYS
1	A	152	VAL
1	A	157	ASP
1	A	164	ARG
1	A	174	ILE
1	A	185	TRP
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	215	SER
1	A	220	THR
1	A	226	GLU
1	A	227	VAL
1	A	252	PHE

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Mol	Chain	Res	Type
1	A	257	ARG
1	A	261	ASP
1	A	270	LEU
1	A	307	ASP
1	A	315	LEU
1	A	322	VAL
1	A	324	SER
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	389	THR
1	A	393	ARG
1	A	408	ASP
1	A	412	ARG
1	A	424	ILE
1	A	425	GLN
1	A	427	GLN
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	450	LEU
1	A	451	HIS
1	A	461	LYS
1	A	462	VAL
1	A	463	ILE
1	A	466	SER
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	496	GLU
1	A	497	THR
1	A	500	GLU
1	A	518	LYS
1	A	527	THR

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Mol	Chain	Res	Type
1	A	536	LEU
1	A	538	ASP
1	A	541	ILE
1	A	544	ASP
1	A	549	MET
1	A	555	ASP
1	A	566	ILE
1	A	571	LEU
1	A	577	ILE
1	A	593	GLU
1	A	597	LEU
1	A	598	LEU
1	A	603	ASN
1	A	613	ILE
1	A	618	GLU
1	A	629	LEU
1	A	630	ILE
1	A	634	THR
1	A	644	LYS
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	675	THR
1	A	685	GLU
1	A	702	LEU
1	A	738	LYS
1	A	740	LEU
1	A	756	ILE
1	A	768	GLN
1	A	788	SER
1	A	795	GLU
1	A	806	ARG
1	A	821	ARG
1	A	824	LEU
1	A	826	ASP
1	A	831	THR
1	A	834	THR
1	A	839	ARG
1	A	855	THR
1	A	867	ILE
1	A	885	THR
1	A	886	ILE

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Mol	Chain	Res	Type
1	A	904	THR
1	A	906	HIS
1	A	915	SER
1	A	919	ILE
1	A	920	LEU
1	A	929	LEU
1	A	941	LYS
1	A	943	LEU
1	A	948	VAL
1	A	960	ILE
1	A	973	ILE
1	A	998	LEU
1	A	999	VAL
1	A	1001	ARG
1	A	1015	VAL
1	A	1024	SER
1	A	1064	VAL
1	A	1067	LEU
1	A	1116	LEU
1	A	1118	VAL
1	A	1124	HIS
1	A	1128	GLN
1	A	1135	ARG
1	A	1145	SER
1	A	1147	THR
1	A	1161	THR
1	A	1170	ILE
1	A	1171	GLN
1	A	1173	HIS
1	A	1176	LEU
1	A	1192	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1222	ASN
1	A	1223	ASP
1	A	1226	VAL
1	A	1230	GLU
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1256	GLU

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Mol	Chain	Res	Type
1	A	1257	ASP
1	A	1260	LEU
1	A	1264	GLU
1	A	1265	ASN
1	A	1266	THR
1	A	1277	GLU
1	A	1293	SER
1	A	1295	THR
1	A	1297	GLU
1	A	1309	ASP
1	A	1319	VAL
1	A	1322	ILE
1	A	1325	THR
1	A	1327	ILE
1	A	1333	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1370	LEU
1	A	1376	THR
1	A	1383	SER
1	A	1391	ARG
1	A	1400	CYS
1	A	1405	THR
1	A	1406	VAL
1	A	1424	VAL
1	A	1426	GLU
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
1	A	1454	MET
2	B	21	GLU
2	B	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	102	VAL
2	B	109	THR
2	B	118	ARG
2	B	128	LEU
2	B	134	LYS
2	B	167	ILE

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Mol	Chain	Res	Type
2	B	178	ASN
2	B	185	THR
2	B	187	SER
2	B	205	ILE
2	B	217	ARG
2	B	251	ILE
2	B	252	SER
2	B	261	ARG
2	B	272	THR
2	B	278	GLN
2	B	280	ILE
2	B	284	ILE
2	B	289	LEU
2	B	294	ASP
2	B	298	LEU
2	B	313	MET
2	B	323	VAL
2	B	324	ILE
2	B	328	GLU
2	B	336	ARG
2	B	337	ARG
2	B	339	THR
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	346	GLU
2	B	347	LYS
2	B	348	ARG
2	B	357	GLN
2	B	361	LEU
2	B	365	THR
2	B	368	GLU
2	B	387	LEU
2	B	393	LYS
2	B	394	ASP
2	B	398	ARG
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	436	VAL
2	B	446	LEU
2	B	452	THR

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Mol	Chain	Res	Type
2	B	453	ILE
2	B	469	GLN
2	B	470	LYS
2	B	476	ARG
2	B	482	VAL
2	B	485	ARG
2	B	513	GLN
2	B	522	VAL
2	B	537	LYS
2	B	542	MET
2	B	547	VAL
2	B	552	MET
2	B	570	VAL
2	B	574	SER
2	B	595	ARG
2	B	598	GLU
2	B	604	ARG
2	B	606	LYS
2	B	616	ILE
2	B	620	ARG
2	B	624	LEU
2	B	628	THR
2	B	644	GLU
2	B	653	VAL
2	B	658	ILE
2	B	668	ASP
2	B	678	GLU
2	B	682	SER
2	B	708	GLU
2	B	709	ASP
2	B	723	VAL
2	B	730	ARG
2	B	731	VAL
2	B	734	HIS
2	B	755	ILE
2	B	766	ARG
2	B	786	ASN
2	B	790	ASP
2	B	797	TYR
2	B	815	ARG
2	B	835	GLN
2	B	838	SER

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Mol	Chain	Res	Type
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	868	MET
2	B	871	THR
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	884	ARG
2	B	889	THR
2	B	904	ARG
2	B	908	GLU
2	B	911	ILE
2	B	933	SER
2	B	948	ILE
2	B	964	VAL
2	B	970	THR
2	B	975	GLN
2	B	976	ILE
2	B	986	GLN
2	B	997	GLU
2	B	1002	THR
2	B	1006	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1050	ILE
2	B	1060	ARG
2	B	1062	HIS
2	B	1065	GLN
2	B	1072	MET
2	B	1106	ARG
2	B	1128	LEU
2	B	1133	MET
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1151	LEU
2	B	1156	ASP
2	B	1160	VAL
2	B	1172	ILE
2	B	1175	LEU
2	B	1178	ASN

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Mol	Chain	Res	Type
2	B	1183	LYS
2	B	1188	LYS
2	B	1189	ILE
2	B	1191	ILE
2	B	1202	LEU
2	B	1212	ILE
3	C	3	GLU
3	C	12	GLU
3	C	16	ASP
3	C	22	LEU
3	C	25	VAL
3	C	50	GLU
3	C	52	GLU
3	C	55	THR
3	C	66	ARG
3	C	81	GLU
3	C	89	GLU
3	C	100	THR
3	C	106	GLU
3	C	108	GLU
3	C	119	VAL
3	C	121	VAL
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	142	VAL
3	C	148	ARG
3	C	155	LEU
3	C	163	ILE
3	C	215	GLU
3	C	237	SER
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	265	MET
4	D	5	THR
4	D	7	THR
4	D	10	THR
4	D	12	ARG
4	D	18	VAL
4	D	22	GLU
4	D	23	ASN

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Mol	Chain	Res	Type
4	D	27	LEU
4	D	32	GLU
4	D	35	LEU
4	D	41	GLN
4	D	59	ILE
4	D	65	GLU
4	D	67	ARG
4	D	118	THR
4	D	123	LEU
4	D	126	ILE
4	D	127	ASP
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	156	ASP
4	D	158	GLU
4	D	159	THR
4	D	166	LEU
4	D	177	VAL
4	D	187	THR
4	D	197	SER
4	D	201	LYS
4	D	206	GLU
4	D	213	GLU
4	D	219	THR
5	E	31	THR
5	E	49	SER
5	E	67	GLU
5	E	69	ILE
5	E	81	GLU
5	E	84	ASP
5	E	92	THR
5	E	99	HIS
5	E	100	ILE
5	E	104	ASN
5	E	113	GLN
5	E	154	ILE
5	E	158	SER
5	E	166	LYS
5	E	173	SER
5	E	177	ARG
5	E	178	ILE

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Mol	Chain	Res	Type
5	E	184	VAL
5	E	190	LEU
5	E	192	ARG
5	E	196	VAL
5	E	204	THR
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	87	LYS
6	F	90	ARG
6	F	93	ILE
6	F	103	MET
6	F	109	VAL
6	F	111	LEU
6	F	115	THR
6	F	122	MET
6	F	123	LYS
6	F	127	GLU
6	F	129	LYS
6	F	152	ILE
7	G	1	MET
7	G	2	PHE
7	G	12	THR
7	G	13	LEU
7	G	22	MET
7	G	24	GLN
7	G	26	LEU
7	G	34	VAL
7	G	37	SER
7	G	60	ARG
7	G	61	ILE
7	G	64	THR
7	G	65	ASP
7	G	75	ARG
7	G	83	LYS
7	G	85	GLU
7	G	96	GLN
7	G	112	LYS
7	G	134	GLU
7	G	138	THR
7	G	143	ILE
7	G	145	VAL

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Mol	Chain	Res	Type
7	G	146	LYS
7	G	152	SER
7	G	154	VAL
7	G	155	SER
7	G	162	SER
7	G	171	ILE
8	H	11	GLN
8	H	13	SER
8	H	14	GLU
8	H	26	ILE
8	H	31	THR
8	H	32	THR
8	H	39	THR
8	H	42	ILE
8	H	76	THR
8	H	89	LEU
8	H	91	ASP
8	H	103	LYS
8	H	106	GLU
8	H	107	VAL
8	H	123	MET
8	H	128	ASN
8	H	130	ARG
8	H	135	LEU
8	H	138	GLU
8	H	144	ILE
9	I	7	CYS
9	I	8	ARG
9	I	31	THR
9	I	35	VAL
9	I	42	LEU
9	I	43	VAL
9	I	50	THR
9	I	74	GLU
9	I	83	ASN
9	I	84	VAL
9	I	91	ARG
9	I	92	ARG
10	J	2	ILE
10	J	3	VAL
10	J	6	ARG
10	J	12	LYS

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Mol	Chain	Res	Type
10	J	13	VAL
10	J	22	LEU
10	J	23	ASN
10	J	34	THR
10	J	42	LYS
10	J	48	ARG
10	J	59	LYS
11	K	6	ARG
11	K	11	LEU
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	33	ILE
11	K	34	THR
11	K	37	LYS
11	K	47	ARG
11	K	51	LEU
11	K	79	GLU
11	K	101	LEU
11	K	107	THR
11	K	113	THR
12	L	27	LEU
12	L	33	GLU
12	L	38	LEU
12	L	42	ARG
12	L	44	ASP
12	L	46	VAL
12	L	49	LYS
12	L	54	ARG
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	71	GLN
1	A	109	HIS

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Mol	Chain	Res	Type
1	A	253	ASN
1	A	313	GLN
1	A	363	GLN
1	A	390	GLN
1	A	394	ASN
1	A	399	HIS
1	A	425	GLN
1	A	439	ASN
1	A	445	ASN
1	A	517	ASN
1	A	548	ASN
1	A	587	HIS
1	A	660	ASN
1	A	698	GLN
1	A	851	HIS
1	A	965	GLN
1	A	969	GLN
1	A	1033	GLN
1	A	1070	GLN
1	A	1106	ASN
1	A	1128	GLN
1	A	1203	ASN
1	A	1378	GLN
1	A	1393	ASN
2	B	46	GLN
2	B	103	ASN
2	B	255	GLN
2	B	300	HIS
2	B	357	GLN
2	B	433	GLN
2	B	449	ASN
2	B	465	ASN
2	B	538	ASN
2	B	572	HIS
2	B	587	HIS
2	B	686	ASN
2	B	786	ASN
2	B	842	ASN
2	B	975	GLN
2	B	1025	HIS
2	B	1040	ASN
2	B	1065	GLN

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Mol	Chain	Res	Type
2	B	1084	GLN
2	B	1117	GLN
2	B	1195	HIS
2	B	1205	GLN
3	C	7	GLN
3	C	135	GLN
3	C	214	ASN
4	D	9	GLN
4	D	37	GLN
4	D	41	GLN
4	D	132	GLN
4	D	137	ASN
4	D	143	ASN
4	D	216	ASN
5	E	3	GLN
5	E	5	ASN
5	E	101	GLN
5	E	113	GLN
5	E	114	ASN
5	E	115	ASN
6	F	78	GLN
7	G	53	ASN
7	G	71	ASN
7	G	102	GLN
7	G	158	HIS
8	H	131	ASN
8	H	133	ASN
8	H	139	ASN
9	I	46	HIS
9	I	83	ASN
9	I	87	GLN
9	I	89	GLN
11	K	104	ASN
11	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	6/7 (85%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	BRU	T	22	14,15	18,21,22	1.18	2 (11%)	25,30,33	2.18	8 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BRU	T	22	14,15	-	1/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C2-N3	-2.79	1.33	1.38
15	T	22	BRU	C4-N3	-2.61	1.34	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	O4'-C1'-N1	5.65	117.89	107.86
15	T	22	BRU	C5-C4-N3	4.52	118.54	113.34
15	T	22	BRU	C2'-C1'-N1	-3.60	104.82	113.81
15	T	22	BRU	O2-C2-N3	-3.13	115.71	121.49
15	T	22	BRU	BR-C5-C4	2.77	121.21	118.02
15	T	22	BRU	N3-C2-N1	2.69	118.39	114.89
15	T	22	BRU	O2-C2-N1	2.38	125.90	122.80
15	T	22	BRU	O4-C4-C5	-2.29	122.88	125.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	22	BRU	C2'-C1'-N1-C2

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	5.38

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	351:TYR	C	352:ALA	N	3.05

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	1422/1732 (82%)	0.38	34 (2%) 59 35	52, 99, 156, 225	0
2	B	1115/1224 (91%)	0.40	46 (4%) 41 22	59, 109, 169, 210	0
3	C	266/318 (83%)	0.28	0 100 100	71, 97, 136, 170	0
4	D	178/221 (80%)	0.81	16 (8%) 15 10	75, 111, 171, 186	0
5	E	214/215 (99%)	0.49	4 (1%) 66 41	75, 132, 177, 194	0
6	F	84/155 (54%)	0.19	1 (1%) 76 52	58, 79, 110, 126	0
7	G	171/171 (100%)	0.69	9 (5%) 32 18	67, 98, 134, 153	0
8	H	133/146 (91%)	0.80	11 (8%) 17 11	109, 140, 177, 200	0
9	I	119/122 (97%)	0.50	8 (6%) 24 15	105, 136, 174, 191	0
10	J	65/70 (92%)	0.35	1 (1%) 72 47	79, 94, 139, 159	0
11	K	115/120 (95%)	0.11	2 (1%) 69 43	69, 96, 132, 148	0
12	L	46/70 (65%)	1.18	6 (13%) 7 6	85, 165, 184, 194	0
13	N	10/11 (90%)	1.08	1 (10%) 12 8	173, 193, 239, 248	0
14	P	7/7 (100%)	0.42	1 (14%) 6 5	101, 108, 155, 173	0
15	T	18/26 (69%)	1.01	2 (11%) 10 7	125, 160, 250, 251	0
All	All	3963/4608 (86%)	0.44	142 (3%) 46 25	52, 105, 169, 251	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	7.8
2	B	883	LEU	5.8
2	B	509	ALA	5.7
1	A	1243	VAL	4.9
2	B	446	LEU	4.9
2	B	70	ILE	4.6
12	L	25	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	502	ILE	4.3
8	H	63	LEU	4.1
2	B	262	GLU	4.1
2	B	882	THR	4.0
2	B	1224	PHE	4.0
11	K	114	LEU	3.9
12	L	26	THR	3.8
4	D	3	VAL	3.8
4	D	24	ALA	3.8
1	A	194	ALA	3.8
7	G	88	ASP	3.8
1	A	1080	THR	3.7
2	B	715	ALA	3.6
2	B	134	LYS	3.6
4	D	173	HIS	3.6
2	B	709	ASP	3.5
2	B	230	ALA	3.4
2	B	251	ILE	3.4
8	H	84	ALA	3.4
10	J	65	PRO	3.4
1	A	1176	LEU	3.4
1	A	251	SER	3.2
9	I	2	THR	3.1
2	B	383	ASN	3.0
4	D	221	TYR	3.0
1	A	1257	ASP	2.9
1	A	190	ALA	2.9
1	A	1173	HIS	2.9
2	B	708	GLU	2.9
2	B	341	LEU	2.9
1	A	56	PRO	2.9
4	D	76	LYS	2.9
2	B	343	ILE	2.9
12	L	28	LYS	2.9
1	A	1254	ALA	2.8
2	B	340	ALA	2.8
2	B	881	ASN	2.8
2	B	266	ALA	2.8
1	A	252	PHE	2.8
6	F	72	LYS	2.8
1	A	57	ARG	2.8
4	D	18	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
9	I	120	GLN	2.8
1	A	1093	LYS	2.8
2	B	244	LEU	2.8
4	D	168	LYS	2.8
4	D	185	CYS	2.7
8	H	130	ARG	2.7
2	B	231	PRO	2.7
2	B	887	HIS	2.6
8	H	129	TYR	2.6
4	D	25	ALA	2.6
1	A	51	GLY	2.6
2	B	249	ARG	2.6
1	A	832	ALA	2.6
2	B	447	ALA	2.6
2	B	312	GLU	2.5
1	A	1187	GLN	2.5
1	A	830	LYS	2.5
2	B	643	ASP	2.5
4	D	13	ARG	2.5
4	D	187	THR	2.5
2	B	30	SER	2.5
1	A	1095	THR	2.5
2	B	880	THR	2.5
9	I	119	THR	2.5
2	B	164	LYS	2.4
8	H	90	ALA	2.4
1	A	292	ALA	2.4
4	D	165	GLN	2.4
1	A	49	LYS	2.4
2	B	879	ARG	2.4
9	I	118	ARG	2.4
1	A	79	GLY	2.4
7	G	40	GLY	2.4
13	N	11	DA	2.4
1	A	186	LYS	2.4
1	A	255	SER	2.4
4	D	10	THR	2.4
2	B	710	LEU	2.4
2	B	472	ALA	2.4
1	A	1391	ARG	2.4
2	B	884	ARG	2.4
2	B	342	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
7	G	64	THR	2.3
8	H	50	ALA	2.3
1	A	517	ASN	2.3
2	B	811	TYR	2.3
7	G	171	ILE	2.3
11	K	115	ALA	2.3
8	H	139	ASN	2.3
8	H	82	PRO	2.3
2	B	345	LYS	2.3
2	B	734	HIS	2.3
7	G	165	GLU	2.3
14	P	4	A	2.3
2	B	108	VAL	2.3
2	B	246	LYS	2.3
9	I	4	PHE	2.2
7	G	85	GLU	2.2
1	A	1455	PRO	2.2
2	B	243	ALA	2.2
4	D	188	ALA	2.2
1	A	176	LYS	2.2
9	I	93	LYS	2.2
2	B	1049	ASP	2.2
15	T	25	DT	2.2
1	A	567	LYS	2.2
5	E	171	LYS	2.2
8	H	136	LYS	2.2
7	G	117	GLN	2.2
2	B	1164	GLY	2.2
5	E	152	LYS	2.2
1	A	59	GLY	2.2
9	I	3	THR	2.2
7	G	10	ASN	2.2
1	A	36	ARG	2.2
2	B	437	GLU	2.2
5	E	110	PHE	2.2
9	I	117	LYS	2.2
8	H	132	LEU	2.2
12	L	32	ALA	2.1
2	B	473	MET	2.1
15	T	20	DC	2.1
7	G	139	ILE	2.1
2	B	476	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	256	GLN	2.1
5	E	159	ASP	2.0
4	D	220	LEU	2.0
1	A	61	ILE	2.0
1	A	1393	ASN	2.0
4	D	201	LYS	2.0
1	A	852	TYR	2.0
12	L	33	GLU	2.0
8	H	86	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	BRU	T	22	20/21	0.94	0.09	123,129,133,134	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	ZN	B	2225	1/1	0.96	0.07	82,82,82,82	0
16	ZN	A	2456	1/1	0.97	0.06	127,127,127,127	0
16	ZN	I	1122	1/1	0.97	0.04	175,175,175,175	0
16	ZN	C	1269	1/1	0.98	0.04	84,84,84,84	0
16	ZN	I	1121	1/1	0.98	0.04	125,125,125,125	0
16	ZN	A	2457	1/1	0.98	0.04	72,72,72,72	0
16	ZN	J	1066	1/1	0.98	0.05	82,82,82,82	0
16	ZN	L	1071	1/1	0.98	0.08	192,192,192,192	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	MG	A	2458	1/1	0.99	0.04	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.