



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:04 PM UTC

PDB ID : 4A3I / pdb_00004a3i
Title : RNA Polymerase II binary complex with DNA
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on : 2011-09-30
Resolution : 3.80 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:

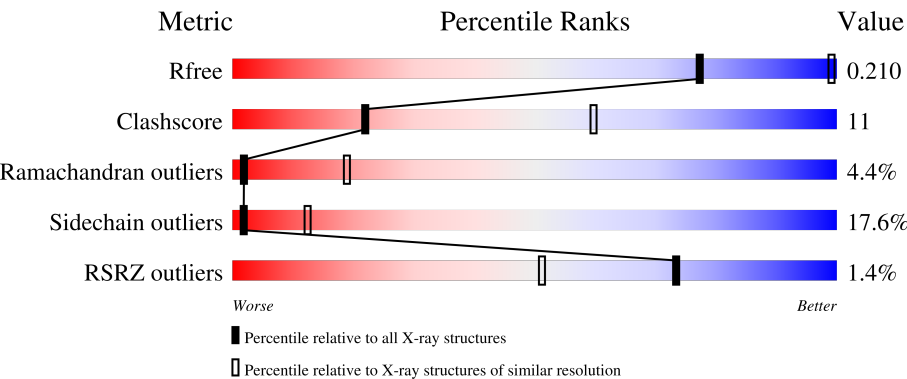
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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% 48%26%6%18%
2	B	1224	2% 57%27%7%9%
3	C	318	46%30%8%16%
4	D	221	2% 44%27%9%19%
5	E	215	58%34%7%

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Mol	Chain	Length	Quality of chain
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	15	
14	T	27	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 31768 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 SUBUNIT RPABC 1.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	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(*GP*GP*CP*AP*CP*AP*AP*CP*TP*GP*CP*GP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	11	Total	C	N	O	P	0	0	0
			222	106	44	62	10			

- Molecule 14 is a DNA chain called TEMPLATE DNA 27-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	17	Total	Br	C	N	O	P	0	0
			350	1	166	61	105	17		

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

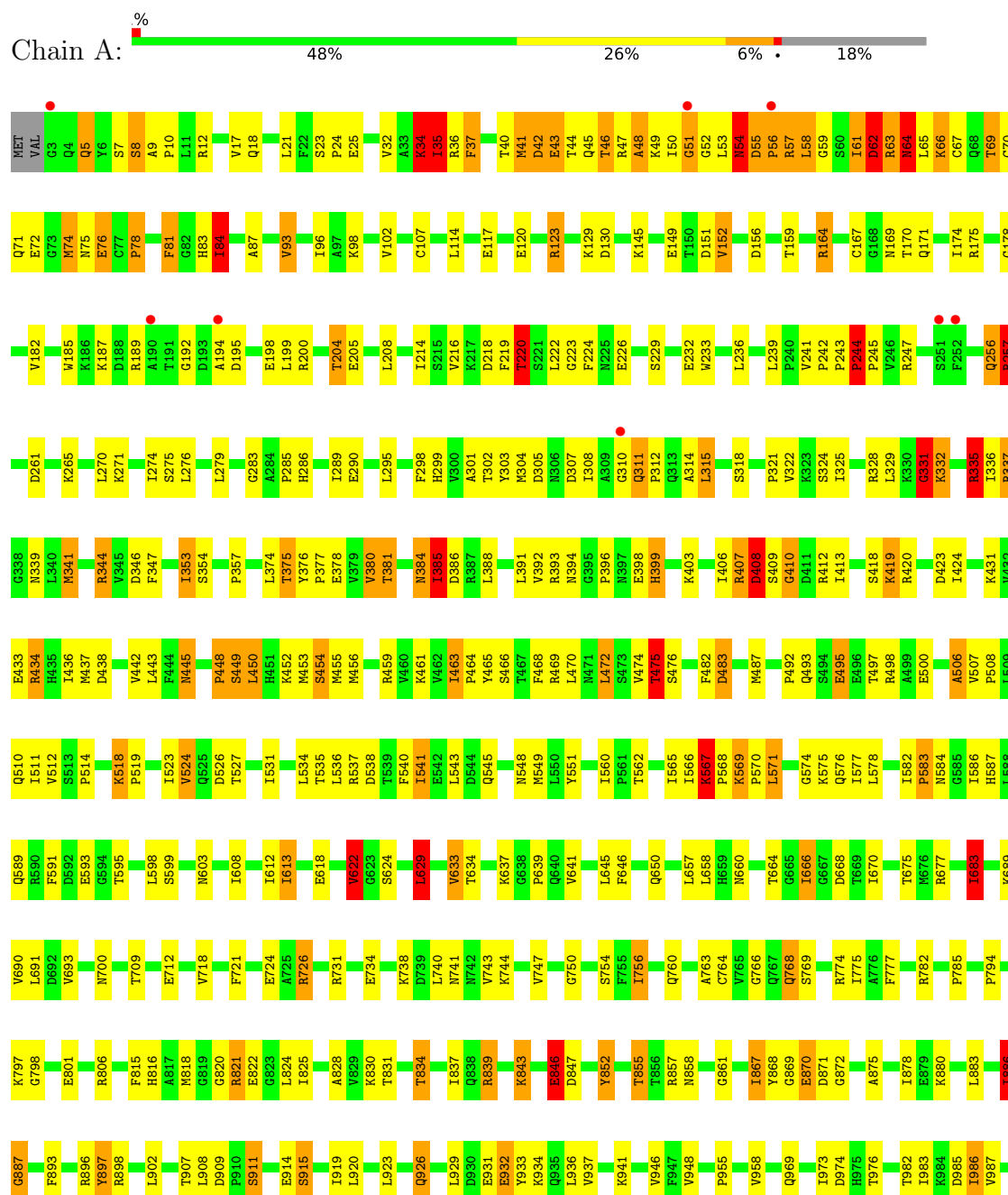
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

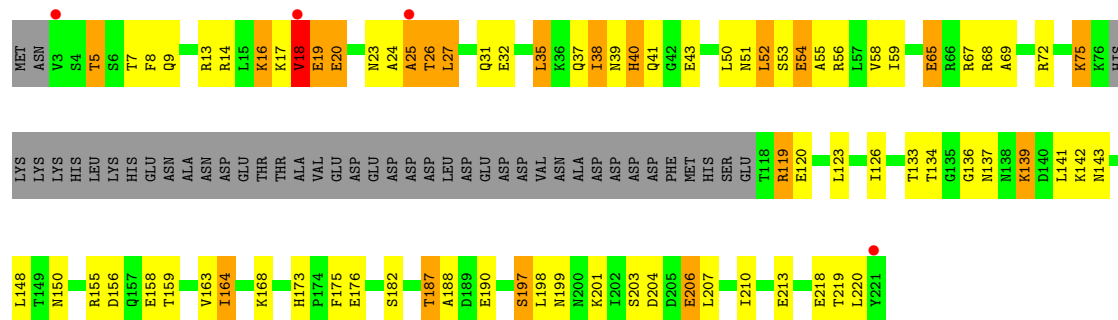
3 Residue-property plots

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.

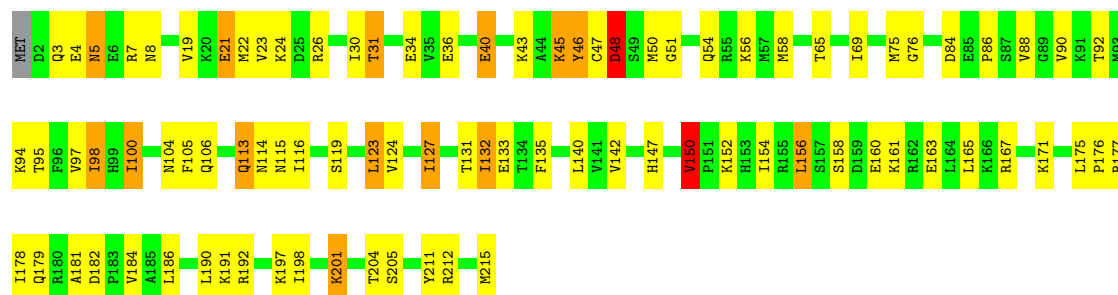
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



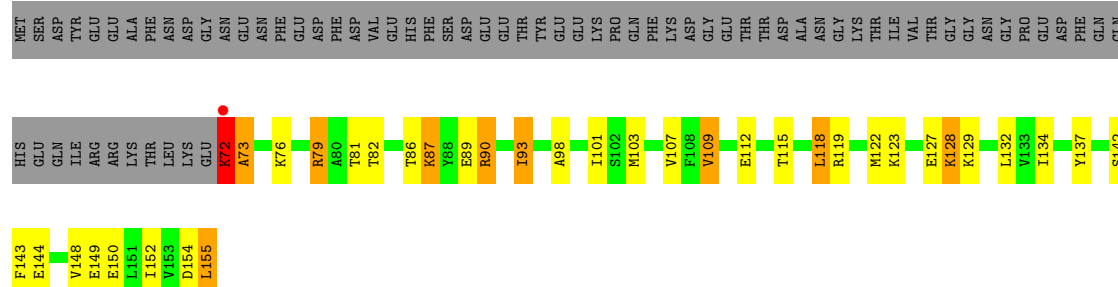
Chain D:



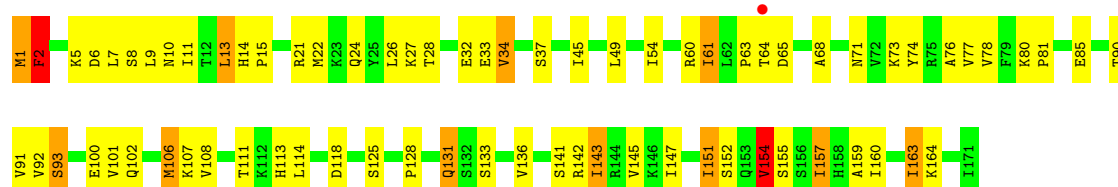
Chain E: 58% 34% 7%



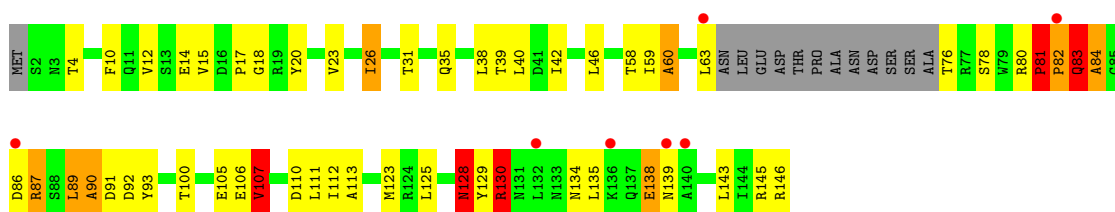
Chain F:



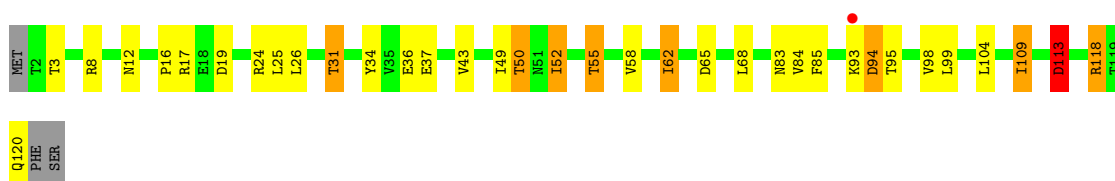
Chain G: %



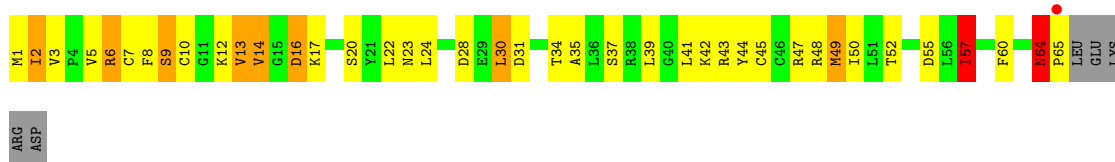
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



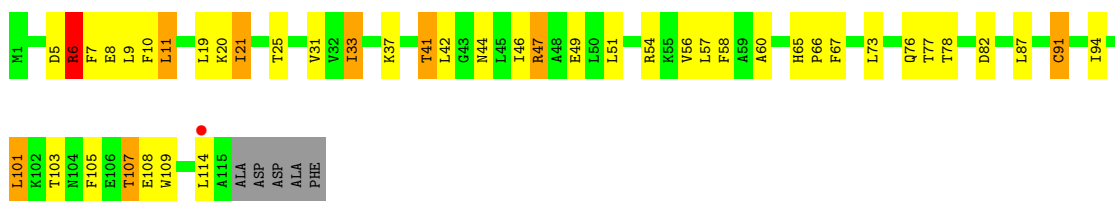
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



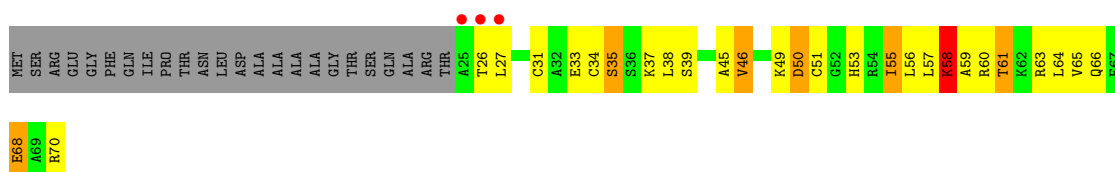
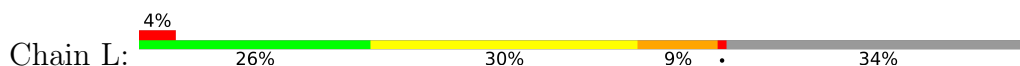
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



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



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



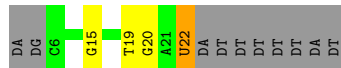
- Molecule 13: 5'-D(*GP*GP*CP*AP*CP*AP*AP*CP*TP*GP*CP*GP*GP*CP*T)-3'

Chain N:  40% 33% 27%



- Molecule 14: TEMPLATE DNA 27-MER

Chain T:  48% 11% 37%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.14Å 393.18Å 282.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 3.80 49.80 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.80-3.80) 99.9 (49.80-3.80)	Depositor EDS
R_{merge}	0.89	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 3.77Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.159 , 0.191 0.183 , 0.210	Depositor DCC
R_{free} test set	2395 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	111.3	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 138.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.026 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.034 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31768	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, BRU

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	0.91	6/11374 (0.1%)	1.60	161/15383 (1.0%)
2	B	0.89	1/9029 (0.0%)	1.51	100/12171 (0.8%)
3	C	0.83	0/2133	1.52	22/2891 (0.8%)
4	D	0.87	1/1444 (0.1%)	1.63	27/1935 (1.4%)
5	E	0.83	0/1788	1.50	24/2406 (1.0%)
6	F	0.95	0/691	1.46	8/933 (0.9%)
7	G	0.89	1/1368 (0.1%)	1.45	11/1844 (0.6%)
8	H	0.86	0/1086	1.52	21/1470 (1.4%)
9	I	0.78	0/989	1.37	7/1331 (0.5%)
10	J	0.95	1/541 (0.2%)	1.65	10/727 (1.4%)
11	K	0.79	0/938	1.46	6/1267 (0.5%)
12	L	0.98	0/365	1.55	5/485 (1.0%)
13	N	0.48	0/249	0.54	0/382
14	T	0.49	0/369	0.57	0/568
All	All	0.88	10/32364 (0.0%)	1.53	402/43793 (0.9%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	867	ILE	CG1-CD1	7.74	1.81	1.51
1	A	507	VAL	CA-CB	7.37	1.57	1.54
7	G	1	MET	C-N	6.78	1.43	1.33
4	D	18	VAL	CA-C	6.48	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	ARG	CA-C	5.79	1.60	1.52
1	A	56	PRO	CA-C	5.56	1.60	1.52
2	B	881	ASN	C-N	5.54	1.41	1.33
1	A	1398	MET	SD-CE	5.43	1.93	1.79
10	J	64	ASN	CA-C	5.10	1.59	1.52
1	A	56	PRO	C-N	5.07	1.40	1.33

All (402) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	THR	N-CA-C	-12.45	98.53	112.72
3	C	39	ALA	N-CA-C	10.44	122.42	111.14
5	E	5	ASN	N-CA-C	-9.99	101.22	113.41
7	G	34	VAL	N-CA-C	9.42	119.39	110.53
1	A	56	PRO	CA-C-N	9.34	139.38	121.54
1	A	56	PRO	C-N-CA	9.34	139.38	121.54
8	H	92	ASP	N-CA-C	-9.30	99.66	112.30
1	A	452	LYS	N-CA-C	-9.25	101.20	111.28
1	A	224	PHE	N-CA-C	9.22	122.89	110.35
12	L	58	LYS	N-CA-C	9.00	123.81	113.01
1	A	341	MET	CA-C-N	8.93	129.26	121.58
1	A	341	MET	C-N-CA	8.93	129.26	121.58
1	A	223	GLY	CA-C-N	8.57	133.69	120.75
1	A	223	GLY	C-N-CA	8.57	133.69	120.75
1	A	34	LYS	CA-C-N	8.48	136.96	121.70
1	A	34	LYS	C-N-CA	8.48	136.96	121.70
1	A	42	ASP	CA-CB-CG	8.47	121.07	112.60
2	B	1009	ASP	N-CA-C	-8.45	103.11	113.50
8	H	128	ASN	CA-C-N	8.30	131.75	120.54
8	H	128	ASN	C-N-CA	8.30	131.75	120.54
2	B	339	THR	CA-C-N	8.22	137.25	121.54
2	B	339	THR	C-N-CA	8.22	137.25	121.54
1	A	346	ASP	CA-CB-CG	8.14	120.74	112.60
1	A	998	LEU	N-CA-C	8.11	122.92	109.46
1	A	194	ALA	CA-C-N	8.05	136.19	121.70
1	A	194	ALA	C-N-CA	8.05	136.19	121.70
8	H	81	PRO	N-CA-C	8.03	120.49	110.70
2	B	736	THR	N-CA-C	-8.02	103.96	114.31
1	A	399	HIS	N-CA-CB	7.90	124.42	110.37
1	A	629	LEU	N-CA-C	-7.89	102.67	111.82
10	J	5	VAL	N-CA-C	-7.88	99.45	109.30
2	B	628	THR	N-CA-C	-7.66	104.06	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	38	ILE	CA-C-N	7.64	130.83	120.44
3	C	38	ILE	C-N-CA	7.64	130.83	120.44
8	H	110	ASP	N-CA-C	-7.62	103.98	113.28
1	A	54	ASN	CA-CB-CG	7.49	120.08	112.60
2	B	1155	SER	CA-C-N	7.43	130.56	120.38
2	B	1155	SER	C-N-CA	7.43	130.56	120.38
2	B	1121	GLY	CA-C-N	7.42	131.95	120.82
2	B	1121	GLY	C-N-CA	7.42	131.95	120.82
2	B	818	PRO	N-CA-C	7.37	121.54	111.22
8	H	129	TYR	N-CA-C	7.37	119.95	111.11
9	I	93	LYS	CA-C-N	7.37	130.48	120.54
9	I	93	LYS	C-N-CA	7.37	130.48	120.54
2	B	1156	ASP	N-CA-C	7.36	120.23	111.33
2	B	294	ASP	CA-CB-CG	7.34	119.94	112.60
1	A	35	ILE	N-CA-CB	7.33	123.97	111.50
3	C	40	GLU	CA-C-N	-7.13	117.45	122.59
3	C	40	GLU	C-N-CA	-7.13	117.45	122.59
8	H	138	GLU	N-CA-C	-7.08	103.65	111.36
1	A	483	ASP	CA-CB-CG	7.06	119.66	112.60
3	C	136	ASP	CA-CB-CG	7.01	119.61	112.60
4	D	23	ASN	CA-CB-CG	7.00	119.60	112.60
2	B	296	GLU	N-CA-C	-6.99	103.71	111.82
2	B	340	ALA	CA-C-N	6.96	134.83	121.54
2	B	340	ALA	C-N-CA	6.96	134.83	121.54
1	A	1112	LYS	N-CA-C	6.90	119.82	111.40
1	A	47	ARG	CA-C-N	6.85	134.62	121.54
1	A	47	ARG	C-N-CA	6.85	134.62	121.54
1	A	1189	SER	N-CA-C	6.83	117.97	109.57
8	H	128	ASN	CA-CB-CG	6.80	119.40	112.60
3	C	162	GLY	N-CA-C	6.78	120.68	112.48
4	D	18	VAL	CA-C-N	6.78	133.91	121.70
4	D	18	VAL	C-N-CA	6.78	133.91	121.70
2	B	366	GLN	N-CA-C	-6.75	104.94	113.72
11	K	6	ARG	N-CA-C	6.73	118.70	111.36
1	A	5	GLN	N-CA-C	6.72	120.47	110.52
1	A	64	ASN	N-CA-C	-6.71	100.58	110.52
4	D	158	GLU	CA-C-N	6.67	129.10	120.44
4	D	158	GLU	C-N-CA	6.67	129.10	120.44
4	D	26	THR	CA-C-N	6.62	131.53	122.07
4	D	26	THR	C-N-CA	6.62	131.53	122.07
1	A	1376	THR	CB-CA-C	6.62	121.78	110.86
1	A	399	HIS	CA-CB-CG	-6.58	107.22	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	44	ASN	CA-C-N	6.58	129.00	120.44
11	K	44	ASN	C-N-CA	6.58	129.00	120.44
2	B	1188	LYS	CA-C-N	6.57	129.41	122.97
2	B	1188	LYS	C-N-CA	6.57	129.41	122.97
1	A	445	ASN	CA-CB-CG	6.56	119.16	112.60
2	B	1122	ARG	CA-C-N	6.54	129.36	120.54
2	B	1122	ARG	C-N-CA	6.54	129.36	120.54
2	B	943	SER	CA-C-N	6.53	129.04	120.28
2	B	943	SER	C-N-CA	6.53	129.04	120.28
1	A	511	ILE	N-CA-C	6.49	117.17	110.36
2	B	681	TRP	N-CA-C	-6.44	104.18	111.14
2	B	628	THR	CA-C-N	6.44	133.83	121.54
2	B	628	THR	C-N-CA	6.44	133.83	121.54
8	H	110	ASP	CA-CB-CG	6.44	119.04	112.60
2	B	1222	ARG	N-CA-C	6.43	118.83	111.11
1	A	1333	ILE	N-CA-C	-6.43	104.24	110.42
4	D	25	ALA	CA-C-N	6.43	133.09	122.73
4	D	25	ALA	C-N-CA	6.43	133.09	122.73
5	E	123	LEU	CA-C-N	6.43	125.47	120.33
5	E	123	LEU	C-N-CA	6.43	125.47	120.33
2	B	322	PHE	CA-CB-CG	6.41	120.21	113.80
1	A	34	LYS	N-CA-C	-6.40	96.73	107.80
8	H	87	ARG	N-CA-C	6.38	119.28	110.35
2	B	964	VAL	N-CA-C	6.38	117.89	108.45
3	C	225	ALA	N-CA-C	6.37	118.95	109.59
2	B	102	VAL	N-CA-C	6.35	117.03	107.75
2	B	1041	GLU	CA-C-N	6.34	126.78	120.31
2	B	1041	GLU	C-N-CA	6.34	126.78	120.31
2	B	732	SER	N-CA-C	6.31	117.45	108.74
2	B	41	LYS	N-CA-C	6.30	119.44	111.69
2	B	340	ALA	N-CA-C	-6.29	97.41	110.80
2	B	881	ASN	CA-C-N	6.29	128.61	120.44
2	B	881	ASN	C-N-CA	6.29	128.61	120.44
11	K	41	THR	N-CA-C	-6.17	103.70	111.11
12	L	55	ILE	N-CA-CB	6.16	121.39	111.23
1	A	81	PHE	N-CA-C	6.14	118.70	110.35
3	C	213	PRO	N-CA-C	6.11	121.59	113.40
10	J	64	ASN	N-CA-C	6.09	123.27	109.81
5	E	161	LYS	CA-C-N	6.05	128.71	120.54
5	E	161	LYS	C-N-CA	6.05	128.71	120.54
2	B	945	GLU	N-CA-C	6.04	118.84	109.60
1	A	510	GLN	CA-C-N	6.03	128.38	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	GLN	C-N-CA	6.03	128.38	120.60
4	D	54	GLU	N-CA-C	-6.02	104.78	111.71
1	A	244	PRO	N-CA-C	6.02	118.04	110.70
7	G	1	MET	CA-C-N	6.02	133.04	121.54
7	G	1	MET	C-N-CA	6.02	133.04	121.54
4	D	7	THR	CA-C-N	6.02	128.94	120.28
4	D	7	THR	C-N-CA	6.02	128.94	120.28
2	B	343	ILE	CA-C-N	5.99	132.97	121.54
2	B	343	ILE	C-N-CA	5.99	132.97	121.54
7	G	2	PHE	CA-CB-CG	5.99	119.79	113.80
11	K	107	THR	CB-CA-C	5.96	120.24	110.88
3	C	212	PRO	N-CA-C	5.95	117.96	110.70
2	B	1201	LYS	CA-C-N	5.93	128.48	120.65
2	B	1201	LYS	C-N-CA	5.93	128.48	120.65
2	B	708	GLU	CA-C-N	5.91	128.20	120.28
2	B	708	GLU	C-N-CA	5.91	128.20	120.28
3	C	40	GLU	N-CA-C	5.91	120.19	112.92
1	A	893	PHE	CA-C-N	5.91	128.51	120.54
1	A	893	PHE	C-N-CA	5.91	128.51	120.54
5	E	54	GLN	CA-C-N	5.90	128.99	120.38
5	E	54	GLN	C-N-CA	5.90	128.99	120.38
2	B	1011	ILE	N-CA-CB	5.89	119.36	112.35
1	A	551	TYR	CA-C-N	5.89	128.76	120.28
1	A	551	TYR	C-N-CA	5.89	128.76	120.28
9	I	31	THR	N-CA-C	-5.88	105.94	113.23
1	A	1422	ARG	N-CA-C	-5.88	106.24	113.41
1	A	718	VAL	CA-C-N	5.87	128.51	120.46
1	A	718	VAL	C-N-CA	5.87	128.51	120.46
4	D	173	HIS	CB-CA-C	5.87	117.89	109.26
1	A	1056	SER	N-CA-C	5.87	118.46	111.71
2	B	69	LEU	CA-C-N	5.86	132.25	121.70
2	B	69	LEU	C-N-CA	5.86	132.25	121.70
1	A	1233	ASP	CA-C-N	5.86	130.07	120.63
1	A	1233	ASP	C-N-CA	5.86	130.07	120.63
1	A	689	LYS	CA-C-N	5.86	128.06	120.56
1	A	689	LYS	C-N-CA	5.86	128.06	120.56
1	A	683	ILE	N-CA-C	-5.85	104.81	110.42
4	D	188	ALA	N-CA-C	-5.85	105.03	111.82
7	G	33	GLU	CA-C-N	5.83	128.02	120.56
7	G	33	GLU	C-N-CA	5.83	128.02	120.56
2	B	320	ASP	CA-CB-CG	5.83	118.42	112.60
1	A	275	SER	CA-C-N	5.82	128.07	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	SER	C-N-CA	5.82	128.07	120.28
1	A	524	VAL	N-CA-C	5.81	117.28	108.80
4	D	75	LYS	N-CA-C	-5.81	105.28	112.72
5	E	171	LYS	N-CA-C	-5.80	99.94	109.40
1	A	794	PRO	CA-C-N	5.80	128.37	120.54
1	A	794	PRO	C-N-CA	5.80	128.37	120.54
1	A	8	SER	CA-C-N	5.80	129.12	120.83
1	A	8	SER	C-N-CA	5.80	129.12	120.83
1	A	683	ILE	N-CA-CB	5.79	117.33	110.55
1	A	55	ASP	N-CA-CB	5.79	120.68	110.37
1	A	677	ARG	CA-C-N	5.79	128.03	120.28
1	A	677	ARG	C-N-CA	5.79	128.03	120.28
2	B	1121	GLY	N-CA-C	5.77	126.85	113.18
1	A	1419	ASP	CA-C-N	5.76	128.00	120.28
1	A	1419	ASP	C-N-CA	5.76	128.00	120.28
3	C	62	PHE	CA-C-N	5.75	127.81	120.56
3	C	62	PHE	C-N-CA	5.75	127.81	120.56
3	C	55	THR	N-CA-C	-5.74	106.41	113.41
10	J	49	MET	CA-C-N	5.74	128.95	120.74
10	J	49	MET	C-N-CA	5.74	128.95	120.74
5	E	21	GLU	CA-C-N	5.73	127.96	120.28
5	E	21	GLU	C-N-CA	5.73	127.96	120.28
4	D	143	ASN	CA-CB-CG	5.72	118.33	112.60
8	H	130	ARG	CA-C-N	5.71	127.87	120.44
8	H	130	ARG	C-N-CA	5.71	127.87	120.44
2	B	454	THR	CA-C-N	5.70	127.92	120.28
2	B	454	THR	C-N-CA	5.70	127.92	120.28
4	D	31	GLN	N-CA-C	-5.70	104.97	111.07
2	B	363	HIS	N-CA-C	-5.69	101.62	110.10
1	A	764	CYS	CA-C-N	5.69	127.73	120.56
1	A	764	CYS	C-N-CA	5.69	127.73	120.56
1	A	468	PHE	CA-CB-CG	5.69	119.49	113.80
1	A	78	PRO	N-CA-C	-5.68	102.88	111.41
1	A	331	GLY	N-CA-C	5.67	126.61	113.18
1	A	870	GLU	CB-CG-CD	5.67	122.24	112.60
2	B	1171	VAL	N-CA-C	5.67	117.02	109.37
1	A	219	PHE	CA-CB-CG	5.65	119.45	113.80
2	B	642	ASP	N-CA-C	-5.62	105.25	111.71
1	A	214	ILE	N-CA-CB	5.61	117.05	110.82
1	A	123	ARG	CA-C-N	5.60	127.78	120.28
1	A	123	ARG	C-N-CA	5.60	127.78	120.28
1	A	285	PRO	CA-C-N	5.60	132.23	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	PRO	C-N-CA	5.60	132.23	121.54
6	F	154	ASP	CA-CB-CG	5.57	118.17	112.60
10	J	50	ILE	CA-C-N	5.57	127.68	120.44
10	J	50	ILE	C-N-CA	5.57	127.68	120.44
1	A	887	GLY	N-CA-C	5.57	119.47	112.79
2	B	709	ASP	CA-CB-CG	5.57	118.17	112.60
2	B	1221	SER	CA-C-N	5.57	128.05	120.54
2	B	1221	SER	C-N-CA	5.57	128.05	120.54
5	E	160	GLU	CA-C-N	5.56	127.67	120.44
5	E	160	GLU	C-N-CA	5.56	127.67	120.44
2	B	998	ASP	CA-C-N	5.56	128.38	120.49
2	B	998	ASP	C-N-CA	5.56	128.38	120.49
1	A	130	ASP	CA-C-N	5.56	129.16	120.82
1	A	130	ASP	C-N-CA	5.56	129.16	120.82
4	D	37	GLN	N-CA-C	5.56	117.24	108.96
2	B	1177	HIS	N-CA-C	-5.55	106.09	112.92
1	A	7	SER	CA-C-N	5.55	128.27	120.28
1	A	7	SER	C-N-CA	5.55	128.27	120.28
1	A	466	SER	N-CA-C	5.54	122.61	110.80
1	A	937	VAL	CA-C-N	5.54	127.97	120.65
1	A	937	VAL	C-N-CA	5.54	127.97	120.65
4	D	136	GLY	CA-C-N	5.54	128.26	120.28
4	D	136	GLY	C-N-CA	5.54	128.26	120.28
2	B	609	ILE	N-CA-C	-5.54	100.61	108.58
1	A	495	GLU	CA-C-N	5.53	130.04	120.58
1	A	495	GLU	C-N-CA	5.53	130.04	120.58
1	A	424	ILE	CA-C-N	-5.52	115.08	122.42
1	A	424	ILE	C-N-CA	-5.52	115.08	122.42
9	I	52	ILE	N-CA-CB	5.52	118.22	111.60
1	A	1424	VAL	CB-CA-C	-5.51	104.92	111.97
1	A	750	GLY	CA-C-N	5.51	127.66	120.28
1	A	750	GLY	C-N-CA	5.51	127.66	120.28
5	E	5	ASN	CA-C-N	5.50	128.20	120.28
5	E	5	ASN	C-N-CA	5.50	128.20	120.28
1	A	633	VAL	N-CA-CB	5.49	116.61	110.62
1	A	932	GLU	CB-CG-CD	5.49	121.93	112.60
3	C	62	PHE	N-CA-C	-5.48	105.22	111.14
5	E	150	VAL	N-CA-C	5.48	112.98	107.55
2	B	693	ILE	N-CA-C	5.48	115.75	107.75
1	A	820	GLY	CA-C-N	5.47	127.62	120.28
1	A	820	GLY	C-N-CA	5.47	127.62	120.28
2	B	825	VAL	N-CA-C	5.47	116.19	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	603	ASN	CA-CB-CG	5.47	118.07	112.60
2	B	213	ILE	N-CA-C	5.47	116.06	108.84
1	A	1336	MET	CA-C-N	5.45	127.58	120.28
1	A	1336	MET	C-N-CA	5.45	127.58	120.28
11	K	82	ASP	CA-CB-CG	5.44	118.04	112.60
2	B	918	ILE	N-CA-C	5.44	115.95	108.12
8	H	31	THR	CA-C-N	5.44	127.51	120.44
8	H	31	THR	C-N-CA	5.44	127.51	120.44
1	A	331	GLY	CA-C-N	5.42	131.89	121.54
1	A	331	GLY	C-N-CA	5.42	131.89	121.54
2	B	109	THR	CB-CA-C	5.42	118.33	110.79
1	A	724	GLU	CA-C-N	5.42	127.80	120.65
1	A	724	GLU	C-N-CA	5.42	127.80	120.65
8	H	139	ASN	CA-CB-CG	5.41	118.01	112.60
2	B	1130	PHE	N-CA-C	-5.41	102.09	109.71
9	I	113	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	17	VAL	N-CA-CB	5.40	118.70	111.90
2	B	338	GLY	CA-C-N	5.40	131.42	121.70
2	B	338	GLY	C-N-CA	5.40	131.42	121.70
8	H	83	GLN	CA-C-N	5.40	131.85	121.54
8	H	83	GLN	C-N-CA	5.40	131.85	121.54
1	A	915	SER	CA-C-N	5.39	126.07	120.03
1	A	915	SER	C-N-CA	5.39	126.07	120.03
7	G	131	GLN	N-CA-C	5.39	117.20	108.41
6	F	87	LYS	CA-C-N	5.38	129.78	120.58
6	F	87	LYS	C-N-CA	5.38	129.78	120.58
9	I	94	ASP	CA-C-N	5.38	131.81	121.54
9	I	94	ASP	C-N-CA	5.38	131.81	121.54
4	D	31	GLN	CA-C-N	5.38	127.74	120.38
4	D	31	GLN	C-N-CA	5.38	127.74	120.38
5	E	48	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	897	TYR	N-CA-C	5.35	119.94	113.41
2	B	530	GLY	N-CA-C	5.35	120.70	110.86
1	A	463	ILE	N-CA-C	5.35	113.78	107.84
1	A	575	LYS	CA-C-N	5.35	127.76	120.54
1	A	575	LYS	C-N-CA	5.35	127.76	120.54
3	C	84	ARG	N-CA-C	5.34	117.79	111.33
4	D	18	VAL	CB-CA-C	5.34	120.04	111.29
1	A	1393	ASN	CA-CB-CG	5.33	117.93	112.60
8	H	10	PHE	CA-CB-CG	5.32	119.12	113.80
2	B	1215	ARG	N-CA-C	5.32	116.81	109.15
10	J	55	ASP	CA-CB-CG	5.31	117.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	THR	CA-C-N	5.31	129.96	121.62
1	A	475	THR	C-N-CA	5.31	129.96	121.62
1	A	70	CYS	CA-C-N	-5.31	115.21	121.90
1	A	70	CYS	C-N-CA	-5.31	115.21	121.90
1	A	384	ASN	N-CA-C	5.30	117.87	111.40
1	A	506	ALA	CA-C-N	5.30	125.52	120.43
1	A	506	ALA	C-N-CA	5.30	125.52	120.43
2	B	450	ALA	CA-C-N	5.30	128.16	120.79
2	B	450	ALA	C-N-CA	5.30	128.16	120.79
1	A	84	ILE	N-CA-CB	5.29	118.72	111.41
1	A	914	GLU	CA-C-N	5.29	129.06	120.60
1	A	914	GLU	C-N-CA	5.29	129.06	120.60
1	A	398	GLU	CA-C-O	-5.29	115.70	121.89
1	A	886	ILE	N-CA-C	5.29	120.34	109.34
6	F	119	ARG	CA-C-N	5.29	127.70	120.46
6	F	119	ARG	C-N-CA	5.29	127.70	120.46
1	A	931	GLU	N-CA-C	-5.28	105.42	111.07
1	A	1406	VAL	CA-C-N	5.28	127.62	120.38
1	A	1406	VAL	C-N-CA	5.28	127.62	120.38
5	E	65	THR	N-CA-C	-5.28	103.56	110.53
12	L	49	LYS	CA-C-N	5.28	131.62	121.54
12	L	49	LYS	C-N-CA	5.28	131.62	121.54
1	A	1325	THR	N-CA-C	-5.27	105.99	112.90
2	B	684	LEU	CA-C-N	5.27	127.34	120.28
2	B	684	LEU	C-N-CA	5.27	127.34	120.28
1	A	381	THR	CB-CA-C	5.27	117.03	108.87
3	C	135	GLN	CA-C-N	5.26	129.77	121.56
3	C	135	GLN	C-N-CA	5.26	129.77	121.56
1	A	408	ASP	N-CA-C	-5.25	105.64	111.36
2	B	1022	THR	CB-CA-C	5.25	119.83	112.07
8	H	110	ASP	CA-C-N	5.24	128.53	120.82
8	H	110	ASP	C-N-CA	5.24	128.53	120.82
1	A	1231	ASP	CA-C-N	5.24	127.56	120.44
1	A	1231	ASP	C-N-CA	5.24	127.56	120.44
1	A	535	THR	N-CA-C	5.23	119.53	113.20
1	A	646	PHE	CA-C-N	5.23	125.75	119.94
1	A	646	PHE	C-N-CA	5.23	125.75	119.94
2	B	319	GLU	CA-C-N	5.23	128.02	120.38
2	B	319	GLU	C-N-CA	5.23	128.02	120.38
2	B	56	ASP	CA-CB-CG	5.23	117.83	112.60
5	E	95	THR	CA-C-N	5.21	127.53	120.44
5	E	95	THR	C-N-CA	5.21	127.53	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	GLU	CA-C-N	5.21	127.51	120.38
2	B	116	GLU	C-N-CA	5.21	127.51	120.38
1	A	218	ASP	CA-CB-CG	5.21	117.81	112.60
2	B	282	ILE	CA-C-N	5.20	127.31	120.60
2	B	282	ILE	C-N-CA	5.20	127.31	120.60
7	G	61	ILE	N-CA-CB	5.20	116.77	110.95
1	A	650	GLN	N-CA-C	5.19	117.68	111.71
2	B	958	GLN	CA-C-N	5.18	127.65	120.29
2	B	958	GLN	C-N-CA	5.18	127.65	120.29
1	A	1351	GLU	CA-C-N	5.18	127.08	120.56
1	A	1351	GLU	C-N-CA	5.18	127.08	120.56
1	A	1226	VAL	N-CA-C	5.17	115.35	108.11
1	A	622	VAL	N-CA-CB	-5.16	105.42	112.28
2	B	722	ASP	CA-C-N	5.15	127.41	120.50
2	B	722	ASP	C-N-CA	5.15	127.41	120.50
1	A	726	ARG	CA-C-N	5.15	127.64	120.63
1	A	726	ARG	C-N-CA	5.15	127.64	120.63
7	G	106	MET	N-CA-C	5.15	118.14	109.95
3	C	172	PRO	CA-C-N	5.15	130.88	122.07
3	C	172	PRO	C-N-CA	5.15	130.88	122.07
10	J	57	ILE	CA-C-N	5.15	127.18	120.28
10	J	57	ILE	C-N-CA	5.15	127.18	120.28
1	A	35	ILE	CB-CA-C	5.14	121.89	111.60
2	B	790	ASP	CA-CB-CG	5.14	117.74	112.60
2	B	807	ARG	CA-C-N	5.14	127.68	120.28
2	B	807	ARG	C-N-CA	5.14	127.68	120.28
12	L	35	SER	N-CA-C	5.14	119.13	112.86
1	A	1445	ILE	N-CA-CB	5.13	116.32	110.72
5	E	119	SER	CA-C-N	5.13	127.67	120.28
5	E	119	SER	C-N-CA	5.13	127.67	120.28
6	F	72	LYS	CA-C-N	5.13	131.33	121.54
6	F	72	LYS	C-N-CA	5.13	131.33	121.54
2	B	336	ARG	N-CA-C	-5.11	105.62	111.14
1	A	24	PRO	CA-C-N	5.11	127.44	120.54
1	A	24	PRO	C-N-CA	5.11	127.44	120.54
5	E	158	SER	CA-C-N	5.11	127.55	120.29
5	E	158	SER	C-N-CA	5.11	127.55	120.29
3	C	215	GLU	CA-C-N	5.11	125.65	119.98
3	C	215	GLU	C-N-CA	5.11	125.65	119.98
4	D	35	LEU	CA-C-N	5.11	129.48	122.84
4	D	35	LEU	C-N-CA	5.11	129.48	122.84
2	B	276	ILE	N-CA-C	5.10	115.20	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	890	TYR	N-CA-C	-5.10	106.56	112.89
1	A	220	THR	CB-CA-C	5.10	119.52	110.85
8	H	59	ILE	CB-CA-C	5.10	119.65	111.29
1	A	66	LYS	CA-C-N	5.10	128.31	120.82
1	A	66	LYS	C-N-CA	5.10	128.31	120.82
1	A	204	THR	CA-C-N	5.09	127.10	120.28
1	A	204	THR	C-N-CA	5.09	127.10	120.28
2	B	292	ILE	N-CA-C	5.08	119.86	108.88
2	B	354	ASP	CA-CB-CG	5.08	117.67	112.60
2	B	190	TYR	CA-C-N	5.07	127.49	120.29
2	B	190	TYR	C-N-CA	5.07	127.49	120.29
1	A	9	ALA	N-CA-C	5.07	115.80	109.57
1	A	1269	GLU	N-CA-C	5.07	117.78	111.24
1	A	769	SER	N-CA-C	5.07	117.08	109.23
7	G	32	GLU	CA-C-N	5.07	127.03	120.44
7	G	32	GLU	C-N-CA	5.07	127.03	120.44
1	A	763	ALA	N-CA-C	5.05	118.86	111.34
5	E	163	GLU	CB-CG-CD	5.05	121.18	112.60
1	A	583	PRO	N-CA-C	5.05	120.11	111.68
1	A	69	THR	CB-CA-C	5.04	118.91	111.65
10	J	16	ASP	CA-CB-CG	5.04	117.64	112.60
2	B	707	PRO	CA-C-N	5.04	128.37	120.82
2	B	707	PRO	C-N-CA	5.04	128.37	120.82
4	D	51	ASN	CA-CB-CG	5.04	117.64	112.60
2	B	945	GLU	CA-C-N	5.03	131.15	121.54
2	B	945	GLU	C-N-CA	5.03	131.15	121.54
1	A	271	LYS	CA-C-N	5.03	127.52	120.28
1	A	271	LYS	C-N-CA	5.03	127.52	120.28
6	F	150	GLU	N-CA-C	5.01	118.49	112.38
1	A	911	SER	CA-C-N	5.00	127.24	120.44
1	A	911	SER	C-N-CA	5.00	127.24	120.44
1	A	311	GLN	N-CA-C	5.00	120.86	109.81
1	A	991	LYS	CA-C-N	5.00	127.68	120.38
1	A	991	LYS	C-N-CA	5.00	127.68	120.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

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	11174	0	11233	265	0
2	B	8859	0	8901	180	0
3	C	2095	0	2051	64	0
4	D	1434	0	1460	38	0
5	E	1752	0	1776	41	0
6	F	679	0	701	23	0
7	G	1340	0	1357	47	0
8	H	1068	0	1040	26	0
9	I	971	0	927	17	0
10	J	532	0	542	24	0
11	K	920	0	929	28	0
12	L	363	0	386	9	0
13	N	222	0	124	4	0
14	T	350	0	191	3	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	1	0	0	0	0
All	All	31768	0	31618	676	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (676) 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	1.81	1.53
1:A:37:PHE:HD1	1:A:52:GLY:HA3	1.26	1.01
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.49	0.94
1:A:35:ILE:HG22	1:A:84:ILE:HG22	1.51	0.92
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.52	0.90
7:G:1:MET:HE1	7:G:80:LYS:O	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.10	0.87
1:A:855:THR:HG21	1:A:857:ARG:HE	1.40	0.87
10:J:48:ARG:O	10:J:52:THR:HG22	1.75	0.86
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.57	0.85
2:B:766:ARG:HE	2:B:1020:ARG:HG2	1.44	0.82
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.60	0.82
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.60	0.81
4:D:24:ALA:HB3	4:D:26:THR:HG23	1.63	0.81
12:L:61:THR:HG21	12:L:63:ARG:HE	1.46	0.80
8:H:4:THR:HA	8:H:60:ALA:HB2	1.64	0.80
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.63	0.80
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.66	0.79
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.63	0.78
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.66	0.78
1:A:37:PHE:HD1	1:A:52:GLY:CA	1.97	0.77
8:H:82:PRO:C	8:H:84:ALA:H	1.92	0.77
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.66	0.77
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.67	0.77
5:E:90:VAL:HG23	5:E:123:LEU:HD11	1.65	0.76
7:G:1:MET:CG	7:G:2:PHE:H	1.99	0.76
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.68	0.76
2:B:498:THR:HG22	2:B:537:LYS:HB2	1.69	0.75
4:D:155:ARG:HB3	4:D:219:THR:HG21	1.69	0.75
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.68	0.74
1:A:54:ASN:HD22	1:A:247:ARG:HH12	1.33	0.74
2:B:276:ILE:HD11	2:B:355:ILE:HD13	1.69	0.74
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.70	0.74
1:A:55:ASP:N	1:A:56:PRO:HD3	2.02	0.73
3:C:148:ARG:H	3:C:151:GLN:HG3	1.52	0.72
1:A:472:LEU:O	1:A:475:THR:HB	1.90	0.72
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.72	0.71
4:D:24:ALA:CB	4:D:26:THR:HG23	2.20	0.71
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.55	0.71
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.73	0.70
1:A:41:MET:HB2	1:A:49:LYS:HA	1.73	0.70
7:G:1:MET:HG3	7:G:2:PHE:H	1.57	0.70
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.57	0.70
3:C:46:ILE:HD13	3:C:67:LEU:O	1.92	0.69
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.56	0.69
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.58	0.69
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:34:VAL:O	7:G:37:SER:HB3	1.93	0.69
1:A:41:MET:CB	1:A:49:LYS:HA	2.24	0.68
4:D:54:GLU:O	4:D:58:VAL:HG23	1.94	0.68
1:A:35:ILE:HG22	1:A:84:ILE:CG2	2.24	0.67
8:H:63:LEU:HB3	8:H:90:ALA:HB2	1.74	0.67
1:A:37:PHE:CD1	1:A:52:GLY:HA3	2.18	0.67
1:A:61:ILE:HG22	1:A:62:ASP:H	1.60	0.67
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.77	0.67
11:K:42:LEU:HG	11:K:46:ILE:HD11	1.75	0.67
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.76	0.66
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.77	0.66
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.28	0.66
1:A:1288:ASP:HA	1:A:1302:PRO:HB3	1.78	0.66
6:F:87:LYS:HA	6:F:155:LEU:HD21	1.77	0.66
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.77	0.66
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.77	0.65
1:A:830:LYS:O	1:A:834:THR:HB	1.97	0.65
1:A:53:LEU:HD23	1:A:54:ASN:N	2.12	0.65
1:A:347:PHE:HE2	1:A:375:THR:HG22	1.63	0.64
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.27	0.64
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.79	0.64
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.78	0.64
2:B:172:ILE:CD1	2:B:178:ASN:HB3	2.27	0.64
3:C:100:THR:HG23	3:C:119:VAL:HG13	1.80	0.64
6:F:72:LYS:HE3	6:F:142:SER:HB3	1.80	0.64
1:A:741:ASN:HB3	1:A:744:LYS:HB2	1.79	0.64
1:A:53:LEU:HD23	1:A:54:ASN:H	1.63	0.64
4:D:220:LEU:H	4:D:220:LEU:HD12	1.64	0.63
1:A:56:PRO:CD	1:A:58:LEU:HG	2.27	0.63
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.80	0.63
1:A:1393:ASN:ND2	1:A:1393:ASN:H	1.97	0.63
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.32	0.62
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.81	0.62
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.81	0.62
1:A:315:LEU:HA	1:A:321:PRO:HA	1.81	0.62
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.81	0.62
2:B:933:SER:O	2:B:935:ARG:N	2.34	0.61
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.81	0.61
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.81	0.61
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.82	0.61
4:D:24:ALA:HB3	4:D:26:THR:CG2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLN:HB2	2:B:337:ARG:HG2	1.83	0.60
3:C:259:LEU:CD2	11:K:91:CYS:HB3	2.30	0.60
4:D:8:PHE:HB2	4:D:38:ILE:HB	1.82	0.60
13:N:3:DC:H2'	13:N:4:DA:C8	2.37	0.60
2:B:975:GLN:O	2:B:990:ILE:HD13	2.01	0.60
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.83	0.60
1:A:1445:ILE:HD11	7:G:68:ALA:CB	2.31	0.60
10:J:64:ASN:HB2	10:J:65:PRO:HD3	1.84	0.60
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.84	0.60
1:A:376:TYR:CE1	1:A:498:ARG:HD2	2.37	0.60
3:C:262:LEU:HD11	11:K:87:LEU:HD23	1.83	0.60
2:B:113:TYR:CD2	2:B:192:LEU:HD21	2.37	0.59
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.84	0.59
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.37	0.59
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.02	0.59
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.31	0.59
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.84	0.59
3:C:11:ARG:HH12	3:C:205:LYS:HD3	1.66	0.59
1:A:1172:LEU:C	1:A:1174:PHE:H	2.11	0.59
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.84	0.59
1:A:315:LEU:H	1:A:315:LEU:HD12	1.68	0.59
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.83	0.59
6:F:89:GLU:O	6:F:93:ILE:HD12	2.03	0.59
1:A:1393:ASN:H	1:A:1393:ASN:HD22	1.48	0.59
1:A:42:ASP:O	1:A:44:THR:N	2.36	0.58
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.84	0.58
1:A:982:THR:HB	1:A:985:ASP:H	1.68	0.58
2:B:558:LEU:HB3	2:B:563:MET:HE3	1.84	0.58
13:N:3:DC:H2''	13:N:4:DA:O5'	2.04	0.58
1:A:152:VAL:HB	1:A:164:ARG:HG2	1.85	0.58
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.41	0.58
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.85	0.58
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.85	0.58
1:A:63:ARG:HA	1:A:74:MET:HG3	1.85	0.58
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.68	0.58
1:A:64:ASN:O	1:A:65:LEU:HB3	2.03	0.58
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.39	0.57
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.85	0.57
4:D:38:ILE:HG22	4:D:39:ASN:H	1.69	0.57
1:A:216:VAL:O	1:A:220:THR:HB	2.05	0.57
10:J:44:TYR:HA	10:J:47:ARG:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.40	0.57
2:B:711:GLU:HB2	2:B:712:PRO:HD3	1.87	0.57
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.87	0.57
4:D:65:GLU:HA	4:D:68:ARG:HG3	1.87	0.57
7:G:9:LEU:HD22	7:G:34:VAL:HG23	1.87	0.57
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.87	0.57
1:A:35:ILE:HG21	1:A:241:VAL:HG21	1.86	0.57
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.86	0.56
1:A:1116:LEU:HD21	1:A:1327:ILE:HD11	1.86	0.56
4:D:5:THR:HG21	7:G:74:TYR:OH	2.06	0.56
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.87	0.56
1:A:62:ASP:HB3	1:A:64:ASN:O	2.06	0.56
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.87	0.56
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.88	0.56
2:B:424:LEU:O	2:B:428:ILE:HG13	2.04	0.56
4:D:25:ALA:C	4:D:27:LEU:H	2.14	0.56
11:K:60:ALA:O	11:K:73:LEU:HD12	2.04	0.56
1:A:93:VAL:HG23	1:A:304:MET:HE3	1.88	0.56
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.88	0.55
2:B:1193:GLN:HE21	2:B:1195:HIS:HE1	1.52	0.55
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.87	0.55
1:A:43:GLU:CD	1:A:48:ALA:HB3	2.31	0.55
1:A:565:ILE:O	1:A:570:PRO:HA	2.06	0.55
3:C:183:TRP:O	3:C:185:LYS:N	2.39	0.55
12:L:27:LEU:HD13	12:L:37:LYS:HG2	1.89	0.55
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.89	0.55
2:B:996:ARG:HD2	10:J:9:SER:O	2.07	0.55
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.89	0.55
3:C:66:ARG:NH2	10:J:3:VAL:O	2.39	0.55
3:C:255:VAL:HG21	11:K:94:ILE:HG21	1.89	0.55
1:A:56:PRO:HD3	1:A:58:LEU:HG	1.87	0.55
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.20	0.55
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.88	0.55
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.88	0.55
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.71	0.55
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	1.88	0.55
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.21	0.55
7:G:93:SER:OG	7:G:100:GLU:HB3	2.07	0.55
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.89	0.55
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.88	0.55
2:B:1084:GLN:OE1	3:C:189:THR:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PHE:CD1	1:A:52:GLY:CA	2.82	0.54
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.88	0.54
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.89	0.54
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.08	0.54
8:H:105:GLU:HB3	8:H:113:ALA:HB3	1.89	0.54
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.90	0.54
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.89	0.54
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.46	0.54
3:C:6:PRO:HB2	11:K:101:LEU:HD23	1.90	0.54
1:A:448:PRO:O	1:A:449:SER:HB2	2.07	0.54
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.90	0.54
7:G:1:MET:SD	7:G:2:PHE:N	2.81	0.54
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.89	0.54
7:G:143:ILE:HG23	7:G:145:VAL:HG23	1.89	0.54
1:A:1376:THR:CG2	5:E:212:ARG:HH22	2.21	0.54
4:D:52:LEU:HB3	4:D:148:LEU:HD23	1.89	0.54
5:E:176:PRO:O	5:E:212:ARG:HA	2.07	0.54
2:B:490:SER:HB3	2:B:775:LYS:HA	1.90	0.53
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.43	0.53
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.38	0.53
2:B:882:THR:C	2:B:884:ARG:H	2.16	0.53
4:D:119:ARG:HH21	4:D:120:GLU:HB2	1.72	0.53
10:J:48:ARG:HE	10:J:49:MET:CE	2.20	0.53
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.73	0.53
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	1.90	0.53
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.90	0.53
4:D:150:ASN:HB3	7:G:142:ARG:NH2	2.24	0.53
1:A:145:LYS:NZ	1:A:149:GLU:HB2	2.23	0.53
1:A:1148:ILE:HA	9:I:49:ILE:HD12	1.91	0.53
3:C:46:ILE:HD12	3:C:46:ILE:H	1.73	0.53
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.90	0.53
7:G:1:MET:CG	7:G:2:PHE:N	2.70	0.53
7:G:106:MET:HG2	7:G:107:LYS:N	2.24	0.53
9:I:17:ARG:HG2	9:I:26:LEU:HB2	1.90	0.53
9:I:50:THR:HG22	9:I:52:ILE:H	1.74	0.53
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.91	0.53
2:B:1002:THR:HG22	2:B:1072:MET:HE2	1.91	0.53
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.57	0.53
2:B:247:GLY:H	2:B:418:LYS:HZ3	1.55	0.53
1:A:332:LYS:H	1:A:337:ARG:CB	2.22	0.53
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:PRO:HA	1:A:1167:GLU:HG3	1.91	0.53
1:A:1329:THR:HG22	1:A:1331:SER:H	1.74	0.53
3:C:149:LYS:C	3:C:151:GLN:H	2.17	0.53
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.90	0.52
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.91	0.52
2:B:996:ARG:NH2	3:C:174:ALA:O	2.43	0.52
5:E:19:VAL:O	5:E:23:VAL:HG23	2.08	0.52
2:B:102:VAL:HG11	2:B:122:LEU:HD13	1.90	0.52
2:B:373:ARG:HH21	2:B:567:GLU:HG2	1.74	0.52
3:C:43:THR:HG22	3:C:44:LEU:H	1.72	0.52
3:C:148:ARG:HG3	3:C:149:LYS:H	1.74	0.52
1:A:629:LEU:O	1:A:633:VAL:HG23	2.10	0.52
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.91	0.52
4:D:164:ILE:HG23	4:D:168:LYS:HD2	1.91	0.52
1:A:567:LYS:HA	1:A:568:PRO:C	2.35	0.52
6:F:132:LEU:HD22	7:G:61:ILE:HD11	1.92	0.52
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.90	0.52
1:A:512:VAL:HA	1:A:519:PRO:HA	1.91	0.52
2:B:577:ALA:HB1	2:B:589:VAL:HB	1.92	0.51
1:A:1389:PHE:CZ	1:A:1402:PHE:CE2	2.99	0.51
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.41	0.51
7:G:106:MET:HG3	7:G:157:ILE:O	2.10	0.51
1:A:50:ILE:C	1:A:52:GLY:H	2.19	0.51
2:B:880:THR:O	2:B:934:LYS:HG3	2.10	0.51
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.91	0.51
1:A:587:HIS:HB2	1:A:969:GLN:HE22	1.75	0.51
1:A:855:THR:CG2	1:A:857:ARG:HE	2.17	0.51
4:D:18:VAL:HG13	4:D:19:GLU:HA	1.91	0.51
7:G:1:MET:CE	7:G:80:LYS:O	2.54	0.51
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.25	0.51
2:B:303:TYR:HD1	2:B:571:PRO:HB3	1.76	0.51
2:B:314:LEU:O	2:B:318:VAL:HG23	2.10	0.51
1:A:756:ILE:HD13	1:A:760:GLN:HG3	1.92	0.51
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.92	0.51
2:B:35:SER:HA	2:B:811:TYR:CE1	2.46	0.51
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.76	0.51
7:G:101:VAL:HG21	7:G:143:ILE:HG21	1.93	0.51
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.46	0.51
2:B:345:LYS:HA	2:B:348:ARG:CD	2.38	0.51
3:C:66:ARG:NH2	10:J:2:ILE:HG23	2.26	0.51
1:A:869:GLY:O	5:E:204:THR:HG21	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:542:MET:HG2	2:B:747:MET:HE3	1.92	0.51
9:I:19:ASP:HB3	9:I:24:ARG:HG2	1.93	0.51
1:A:84:ILE:HG13	1:A:239:LEU:HB3	1.93	0.51
1:A:265:LYS:HG3	1:A:303:TYR:HB2	1.93	0.51
1:A:541:ILE:HG21	1:A:549:MET:HE2	1.92	0.51
2:B:341:LEU:HD13	2:B:343:ILE:HB	1.93	0.51
3:C:100:THR:CG2	3:C:119:VAL:HG13	2.41	0.51
12:L:68:GLU:HB2	12:L:70:ARG:HD2	1.93	0.51
1:A:25:GLU:CD	1:A:25:GLU:H	2.19	0.51
1:A:768:GLN:CG	1:A:816:HIS:HA	2.33	0.51
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.93	0.51
11:K:8:GLU:O	11:K:37:LYS:HD2	2.10	0.51
3:C:4:GLU:H	3:C:7:GLN:HE22	1.59	0.50
10:J:48:ARG:HE	10:J:49:MET:HE2	1.76	0.50
2:B:323:VAL:HG23	2:B:324:ILE:HD12	1.93	0.50
2:B:510:LYS:H	2:B:510:LYS:HD3	1.75	0.50
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.93	0.50
2:B:745:PRO:O	2:B:748:ILE:HG12	2.11	0.50
11:K:10:PHE:HD1	11:K:11:LEU:HD13	1.76	0.50
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	1.94	0.50
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.93	0.50
1:A:883:LEU:HD23	1:A:1021:LEU:HB2	1.93	0.50
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.93	0.50
2:B:882:THR:HB	2:B:934:LYS:C	2.36	0.50
4:D:207:LEU:HA	4:D:210:ILE:HD12	1.93	0.50
4:D:176:GLU:OE2	4:D:197:SER:HB2	2.12	0.50
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.42	0.49
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	1.92	0.49
1:A:83:HIS:HA	1:A:239:LEU:O	2.12	0.49
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.94	0.49
1:A:374:LEU:HB2	1:A:436:ILE:HG12	1.93	0.49
1:A:743:VAL:O	1:A:747:VAL:HG23	2.12	0.49
1:A:843:LYS:NZ	1:A:846:GLU:OE2	2.45	0.49
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.75	0.49
9:I:85:PHE:HD2	9:I:99:LEU:HD22	1.76	0.49
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.47	0.49
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.94	0.49
2:B:34:ILE:HG12	2:B:542:MET:CE	2.43	0.49
7:G:81:PRO:HD2	7:G:157:ILE:HD13	1.95	0.49
8:H:15:VAL:HG22	8:H:26:ILE:HG13	1.94	0.49
2:B:1033:LYS:HD3	2:B:1059:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:26:ILE:HB	8:H:40:LEU:O	2.13	0.49
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.94	0.49
1:A:388:LEU:O	1:A:392:VAL:HG23	2.13	0.49
1:A:880:LYS:HA	1:A:955:PRO:HA	1.94	0.49
8:H:100:THR:HG23	8:H:138:GLU:HA	1.95	0.49
1:A:453:MET:O	1:A:456:MET:HE2	2.13	0.49
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.13	0.49
8:H:82:PRO:O	8:H:84:ALA:N	2.42	0.49
8:H:130:ARG:HD3	8:H:134:ASN:HD22	1.76	0.49
9:I:34:TYR:OH	9:I:36:GLU:HB3	2.13	0.49
1:A:506:ALA:HB1	1:A:508:PRO:HD2	1.95	0.49
6:F:127:GLU:HB3	6:F:129:LYS:HE3	1.95	0.49
1:A:21:LEU:HD12	1:A:229:SER:HB2	1.95	0.48
1:A:335:ARG:HD3	2:B:1202:LEU:HD13	1.94	0.48
1:A:51:GLY:C	1:A:56:PRO:HB3	2.37	0.48
5:E:97:VAL:HG13	5:E:127:ILE:HG12	1.95	0.48
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.94	0.48
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.94	0.48
10:J:6:ARG:H	10:J:14:VAL:H	1.60	0.48
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.38	0.48
2:B:343:ILE:O	2:B:344:LYS:HB2	2.13	0.48
2:B:564:GLU:HB3	2:B:589:VAL:HG23	1.96	0.48
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.29	0.48
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.94	0.48
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.95	0.48
5:E:40:GLU:HA	5:E:43:LYS:HD2	1.94	0.48
1:A:986:ILE:O	1:A:990:VAL:HG23	2.13	0.48
1:A:1445:ILE:HD11	7:G:68:ALA:HB3	1.96	0.48
2:B:213:ILE:HD13	2:B:213:ILE:HA	1.76	0.48
2:B:789:MET:HE3	2:B:953:LEU:HB2	1.95	0.48
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.95	0.48
1:A:1329:THR:HG22	1:A:1331:SER:N	2.28	0.48
2:B:766:ARG:NE	2:B:1020:ARG:HG2	2.21	0.48
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.96	0.48
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.96	0.48
4:D:159:THR:O	4:D:163:VAL:HG23	2.14	0.48
1:A:98:LYS:O	1:A:102:VAL:HG23	2.13	0.48
1:A:709:THR:HB	1:A:712:GLU:H	1.78	0.48
1:A:1436:ILE:O	1:A:1437:GLY:C	2.57	0.48
3:C:146:LYS:C	3:C:147:LEU:HD12	2.39	0.48
8:H:83:GLN:HA	11:K:54:ARG:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.95	0.47
10:J:8:PHE:H	10:J:49:MET:HE3	1.78	0.47
1:A:298:PHE:HZ	1:A:314:ALA:HB2	1.79	0.47
4:D:13:ARG:HH12	4:D:20:GLU:HG3	1.78	0.47
5:E:156:LEU:HD11	5:E:197:LYS:HB2	1.95	0.47
8:H:89:LEU:C	8:H:91:ASP:H	2.21	0.47
14:T:19:DT:H2'	14:T:20:DG:C8	2.50	0.47
6:F:101:ILE:HG12	6:F:107:VAL:HG22	1.96	0.47
1:A:418:SER:C	1:A:420:ARG:H	2.22	0.47
1:A:1170:ILE:O	1:A:1174:PHE:HB2	2.14	0.47
2:B:658:ILE:HG23	2:B:662:MET:HE2	1.96	0.47
8:H:89:LEU:HB2	8:H:91:ASP:OD1	2.15	0.47
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.96	0.47
1:A:55:ASP:H	1:A:56:PRO:HD3	1.77	0.47
1:A:495:GLU:HG3	6:F:98:ALA:HB1	1.97	0.47
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.97	0.47
2:B:101:MET:HA	2:B:112:LEU:H	1.79	0.47
3:C:37:MET:HE3	3:C:176:ILE:HD13	1.96	0.47
3:C:242:GLN:O	3:C:246:ARG:HB2	2.14	0.47
1:A:50:ILE:HG22	1:A:52:GLY:H	1.80	0.47
2:B:839:MET:HE3	2:B:1012:ILE:HG22	1.96	0.47
1:A:1379:GLY:HA2	5:E:177:ARG:O	2.15	0.47
6:F:128:LYS:HD3	6:F:149:GLU:O	2.14	0.47
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.97	0.47
4:D:175:PHE:CZ	7:G:85:GLU:HG3	2.42	0.47
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.79	0.47
5:E:197:LYS:HG3	5:E:211:TYR:CE2	2.50	0.47
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.50	0.47
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.95	0.47
2:B:35:SER:HA	2:B:811:TYR:HE1	1.80	0.46
1:A:35:ILE:CG2	1:A:84:ILE:HG22	2.37	0.46
2:B:1160:VAL:HG23	2:B:1194:ILE:HG13	1.98	0.46
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.80	0.46
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.96	0.46
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.80	0.46
1:A:469:ARG:NH2	2:B:991:GLY:O	2.48	0.46
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.97	0.46
1:A:591:PHE:HD2	1:A:595:THR:HB	1.80	0.46
1:A:1116:LEU:CD2	1:A:1327:ILE:HD11	2.46	0.46
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.81	0.46
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.97	0.46
2:B:753:ALA:HA	2:B:756:ILE:HD12	1.98	0.46
6:F:132:LEU:O	6:F:148:VAL:HG22	2.15	0.46
1:A:448:PRO:HB2	1:A:450:LEU:HD21	1.97	0.46
1:A:1035:TYR:N	1:A:1035:TYR:CD1	2.82	0.46
1:A:63:ARG:HE	1:A:74:MET:HE2	1.80	0.46
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.98	0.46
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.97	0.46
10:J:45:CYS:O	10:J:48:ARG:HG3	2.15	0.46
1:A:518:LYS:HE2	1:A:624:SER:O	2.16	0.46
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.96	0.46
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.51	0.46
10:J:9:SER:OG	10:J:48:ARG:NH2	2.48	0.46
3:C:66:ARG:HH21	10:J:2:ILE:HG23	1.81	0.46
6:F:76:LYS:HA	6:F:79:ARG:CD	2.46	0.46
7:G:111:THR:HG22	7:G:113:HIS:H	1.80	0.46
1:A:1308:THR:HG22	1:A:1309:ASP:N	2.31	0.46
2:B:620:ARG:HD2	9:I:62:ILE:HD11	1.98	0.46
1:A:187:LYS:HD2	1:A:198:GLU:HB2	1.99	0.45
1:A:837:ILE:HG21	1:A:1101:LEU:HD21	1.98	0.45
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.51	0.45
4:D:187:THR:HB	4:D:190:GLU:H	1.81	0.45
5:E:47:CYS:HB3	5:E:51:GLY:HA2	1.97	0.45
2:B:1163:CYS:HB3	2:B:1166:CYS:O	2.16	0.45
6:F:90:ARG:HD2	6:F:155:LEU:HD22	1.98	0.45
1:A:406:ILE:HG12	1:A:412:ARG:HG3	1.98	0.45
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.46	0.45
2:B:350:GLN:O	2:B:351:TYR:C	2.58	0.45
3:C:58:LEU:HD11	10:J:2:ILE:HG21	1.97	0.45
8:H:80:ARG:HB3	8:H:87:ARG:HH22	1.82	0.45
1:A:909:ASP:C	1:A:911:SER:H	2.24	0.45
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.99	0.45
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.98	0.45
2:B:906:SER:O	2:B:941:LEU:HD23	2.17	0.45
2:B:501:PRO:O	2:B:502:ILE:HB	2.17	0.45
2:B:879:ARG:HG3	2:B:883:LEU:HG	1.99	0.45
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.98	0.45
3:C:33:LEU:HG	3:C:37:MET:HE2	1.98	0.45
1:A:34:LYS:HA	1:A:83:HIS:O	2.16	0.45
1:A:1308:THR:HG22	1:A:1309:ASP:H	1.82	0.45
2:B:25:ILE:HG12	2:B:29:ASP:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:16:PRO:HB3	9:I:25:LEU:HD11	1.98	0.45
1:A:857:ARG:HD3	1:A:861:GLY:O	2.17	0.45
3:C:125:MET:HE3	3:C:125:MET:HA	1.97	0.45
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.99	0.45
6:F:118:LEU:O	6:F:122:MET:HG3	2.17	0.45
1:A:40:THR:HB	1:A:257:ARG:CZ	2.47	0.45
1:A:302:THR:HA	1:A:305:ASP:O	2.17	0.45
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.31	0.45
5:E:24:LYS:HB2	5:E:30:ILE:HB	1.99	0.45
7:G:10:ASN:ND2	7:G:71:ASN:HD22	2.15	0.45
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.98	0.45
10:J:37:SER:OG	10:J:47:ARG:NH2	2.50	0.45
1:A:731:ARG:HA	1:A:734:GLU:HG2	1.99	0.45
2:B:220:GLY:HA2	2:B:241:ARG:HB3	1.99	0.45
4:D:14:ARG:C	4:D:16:LYS:H	2.24	0.45
2:B:486:TYR:HB3	2:B:1096:ARG:NH1	2.31	0.44
2:B:707:PRO:O	2:B:711:GLU:HG2	2.17	0.44
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	1.99	0.44
2:B:1173:ALA:HB1	2:B:1175:LEU:HD23	1.99	0.44
7:G:49:LEU:HG	7:G:76:ALA:HA	1.98	0.44
13:N:6:DA:H2"	13:N:7:DA:C8	2.52	0.44
12:L:68:GLU:CD	12:L:68:GLU:H	2.24	0.44
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.82	0.44
1:A:396:PRO:HB3	1:A:403:LYS:HA	1.99	0.44
1:A:537:ARG:HB2	8:H:20:TYR:CE1	2.52	0.44
1:A:982:THR:H	1:A:985:ASP:HB2	1.82	0.44
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.99	0.44
3:C:50:GLU:HB3	12:L:64:LEU:HD12	1.99	0.44
7:G:92:VAL:CG2	7:G:102:GLN:HB2	2.48	0.44
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.82	0.44
10:J:9:SER:OG	10:J:45:CYS:HB2	2.17	0.44
10:J:24:LEU:O	10:J:30:LEU:HB2	2.17	0.44
1:A:34:LYS:HD2	1:A:36:ARG:HE	1.83	0.44
1:A:1376:THR:HG23	5:E:212:ARG:NH2	2.32	0.44
1:A:1444:MET:HE2	1:A:1444:MET:HB2	1.83	0.44
2:B:472:ALA:HB1	2:B:475:SER:HB2	1.99	0.44
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.99	0.44
2:B:865:LYS:HD2	2:B:961:LEU:HD21	2.00	0.44
8:H:4:THR:HA	8:H:60:ALA:CB	2.40	0.44
1:A:872:GLY:O	1:A:1057:VAL:HG13	2.17	0.44
2:B:770:GLN:CD	2:B:983:ARG:HA	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:GLN:H	2:B:46:GLN:HG3	1.60	0.44
7:G:21:ARG:NH1	7:G:24:GLN:OE1	2.50	0.44
14:T:22:BRU:H6	14:T:22:BRU:H5'	1.99	0.44
1:A:608:ILE:HD12	1:A:613:ILE:HD13	2.00	0.44
3:C:184:ASN:HD21	3:C:189:THR:H	1.65	0.44
5:E:26:ARG:HH22	5:E:133:GLU:CD	2.26	0.44
1:A:449:SER:HA	1:A:454:SER:CB	2.47	0.44
1:A:806:ARG:HH21	2:B:729:ILE:HG13	1.83	0.44
1:A:818:MET:HA	2:B:514:LEU:HB3	2.00	0.44
2:B:815:ARG:HG3	2:B:815:ARG:HH11	1.82	0.44
2:B:973:ILE:HD12	2:B:973:ILE:H	1.83	0.44
5:E:181:ALA:HA	5:E:186:LEU:HD21	2.00	0.44
9:I:55:THR:HG21	9:I:109:ILE:HG21	1.98	0.44
1:A:897:TYR:HB3	1:A:936:LEU:HD13	1.98	0.44
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.99	0.44
2:B:881:ASN:OD1	2:B:933:SER:N	2.51	0.44
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.99	0.44
3:C:149:LYS:HG3	3:C:150:GLY:H	1.83	0.44
4:D:59:ILE:HG21	4:D:141:LEU:HD11	2.00	0.44
6:F:109:VAL:HG22	6:F:127:GLU:OE1	2.18	0.44
7:G:125:SER:OG	7:G:128:PRO:HA	2.17	0.44
2:B:1181:GLU:HG3	2:B:1188:LYS:HG2	1.99	0.43
5:E:124:VAL:HG13	5:E:132:ILE:HG22	2.00	0.43
1:A:76:GLU:O	1:A:78:PRO:HD3	2.18	0.43
1:A:325:ILE:O	1:A:328:ARG:HB2	2.17	0.43
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.33	0.43
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	2.00	0.43
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	2.00	0.43
2:B:599:THR:O	2:B:603:LEU:HB2	2.17	0.43
2:B:792:MET:H	2:B:857:ARG:HA	1.83	0.43
8:H:107:VAL:HG23	8:H:111:LEU:HB3	2.00	0.43
1:A:464:PRO:HD2	11:K:67:PHE:HD2	1.83	0.43
2:B:542:MET:HE2	2:B:747:MET:HE2	2.00	0.43
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.45	0.43
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	1.99	0.43
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.84	0.43
2:B:446:LEU:HD12	2:B:448:ILE:HD11	2.01	0.43
1:A:51:GLY:HA2	1:A:56:PRO:HA	2.00	0.43
1:A:58:LEU:HB3	1:A:59:GLY:H	1.54	0.43
1:A:265:LYS:HZ2	1:A:299:HIS:CE1	2.36	0.43
2:B:400:HIS:CD2	2:B:517:THR:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:HG21	2:B:935:ARG:HA	1.99	0.43
1:A:66:LYS:HB3	1:A:71:GLN:O	2.18	0.43
1:A:591:PHE:CD2	1:A:595:THR:HB	2.53	0.43
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.53	0.43
2:B:295:GLY:HA2	2:B:298:LEU:HB2	2.01	0.43
7:G:6:ASP:HB3	7:G:73:LYS:NZ	2.33	0.43
1:A:120:GLU:HA	1:A:123:ARG:HG2	2.01	0.43
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.52	0.43
1:A:562:THR:O	1:A:576:GLN:NE2	2.51	0.43
2:B:309:GLN:HB2	9:I:52:ILE:HD11	1.99	0.43
2:B:498:THR:CG2	2:B:537:LYS:HB2	2.46	0.43
7:G:91:VAL:HG22	7:G:101:VAL:HG22	2.01	0.43
1:A:43:GLU:HB2	1:A:46:THR:HB	2.01	0.43
1:A:568:PRO:HG2	8:H:46:LEU:HB3	2.00	0.43
1:A:578:LEU:HD23	1:A:612:ILE:HD11	2.01	0.43
1:A:1014:ALA:HA	5:E:205:SER:HB2	2.01	0.43
2:B:292:ILE:HD11	2:B:327:ARG:HB2	2.01	0.43
5:E:23:VAL:HG12	5:E:30:ILE:HD11	2.00	0.43
8:H:82:PRO:C	8:H:84:ALA:N	2.68	0.43
1:A:35:ILE:HA	1:A:52:GLY:O	2.18	0.43
5:E:86:PRO:HA	5:E:113:GLN:HB2	2.01	0.43
7:G:154:VAL:HB	7:G:155:SER:H	1.67	0.43
1:A:55:ASP:N	1:A:56:PRO:CD	2.77	0.43
2:B:291:ILE:HD12	2:B:291:ILE:N	2.34	0.43
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.99	0.43
7:G:151:ILE:HD11	7:G:160:ILE:CD1	2.49	0.43
8:H:80:ARG:HG2	11:K:57:LEU:HD22	2.00	0.43
1:A:408:ASP:C	1:A:410:GLY:H	2.27	0.42
1:A:482:PHE:HB2	2:B:838:SER:HB3	2.01	0.42
2:B:615:MET:HG2	2:B:626:ILE:HG23	2.00	0.42
2:B:901:PRO:HD2	12:L:60:ARG:HA	2.00	0.42
7:G:45:ILE:HA	7:G:78:VAL:HG12	2.00	0.42
1:A:353:ILE:HD12	1:A:482:PHE:CD1	2.54	0.42
2:B:1006:ILE:H	2:B:1006:ILE:HG13	1.66	0.42
3:C:35:ARG:HD3	11:K:41:THR:HA	2.01	0.42
1:A:244:PRO:HB2	1:A:245:PRO:HD3	2.01	0.42
1:A:569:LYS:HG2	1:A:571:LEU:HD13	2.01	0.42
2:B:294:ASP:HB2	9:I:12:ASN:HA	2.01	0.42
4:D:139:LYS:HA	4:D:142:LYS:HD2	2.02	0.42
1:A:32:VAL:HB	1:A:69:THR:HG21	2.00	0.42
1:A:381:THR:HG22	1:A:384:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:VAL:HG22	5:E:201:LYS:HB3	2.01	0.42
1:A:1386:ARG:NH2	14:T:15:DG:H1'	2.34	0.42
5:E:179:GLN:HA	5:E:215:MET:HB2	2.00	0.42
7:G:14:HIS:CD2	7:G:15:PRO:HD2	2.53	0.42
9:I:98:VAL:HG11	9:I:113:ASP:HB2	2.02	0.42
10:J:48:ARG:O	10:J:52:THR:CG2	2.56	0.42
11:K:11:LEU:HD12	11:K:11:LEU:HA	1.93	0.42
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.55	0.42
1:A:41:MET:HB3	1:A:49:LYS:HA	1.99	0.42
1:A:582:ILE:HA	1:A:583:PRO:HD3	1.93	0.42
2:B:882:THR:OG1	2:B:935:ARG:HA	2.20	0.42
1:A:34:LYS:HG3	1:A:36:ARG:HH21	1.85	0.42
1:A:331:GLY:HA2	1:A:337:ARG:HB2	2.02	0.42
1:A:445:ASN:HB2	1:A:455:MET:HG2	2.02	0.42
1:A:760:GLN:OE1	2:B:1021:MET:HE1	2.20	0.42
1:A:1100:ARG:HE	1:A:1351:GLU:HG3	1.85	0.42
2:B:1165:ILE:HG21	4:D:17:LYS:HB3	2.02	0.42
3:C:124:LEU:HD22	3:C:129:ILE:HG22	2.02	0.42
4:D:50:LEU:HD13	4:D:55:ALA:HA	2.01	0.42
1:A:683:ILE:HG21	1:A:801:GLU:HG3	2.02	0.42
2:B:313:MET:HE1	2:B:390:LEU:HG	2.02	0.42
2:B:336:ARG:HG3	2:B:348:ARG:NH2	2.35	0.42
6:F:89:GLU:C	6:F:93:ILE:HD12	2.43	0.42
7:G:34:VAL:HG13	7:G:45:ILE:HG21	2.01	0.42
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.35	0.42
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.54	0.42
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.55	0.42
3:C:22:LEU:HD22	3:C:230:MET:HE1	2.01	0.42
3:C:82:TYR:HB2	3:C:85:ASP:OD2	2.20	0.42
3:C:114:TYR:HB2	3:C:116:LYS:HG2	2.02	0.42
11:K:65:HIS:ND1	11:K:66:PRO:HD2	2.34	0.42
1:A:455:MET:HE1	2:B:1130:PHE:CE1	2.55	0.42
1:A:1158:PRO:HA	1:A:1241:ARG:CZ	2.50	0.42
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	2.01	0.42
2:B:212:LEU:HA	2:B:212:LEU:HD22	1.77	0.42
2:B:352:ALA:HA	2:B:355:ILE:HD12	2.02	0.42
2:B:708:GLU:H	2:B:708:GLU:HG3	1.50	0.42
9:I:118:ARG:HD3	9:I:120:GLN:HG3	2.00	0.42
10:J:7:CYS:HA	10:J:49:MET:HG2	2.01	0.42
1:A:1159:ARG:HG2	1:A:1174:PHE:CE2	2.55	0.42
2:B:1154:ALA:O	2:B:1155:SER:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:7:DA:H2'	13:N:8:DC:O4'	2.19	0.41
1:A:81:PHE:HE1	2:B:1205:GLN:HG2	1.85	0.41
1:A:353:ILE:HD12	1:A:482:PHE:HD1	1.84	0.41
2:B:284:ILE:HG12	2:B:324:ILE:HD13	2.02	0.41
2:B:758:PHE:CE2	2:B:1027:ILE:HG22	2.55	0.41
2:B:957:ASN:HB3	2:B:961:LEU:H	1.85	0.41
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.85	0.41
3:C:40:GLU:OE2	3:C:254:LYS:HE3	2.20	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.55	0.41
1:A:534:LEU:O	1:A:574:GLY:HA3	2.20	0.41
1:A:709:THR:HG23	9:I:94:ASP:HA	2.01	0.41
2:B:274:PRO:HG2	2:B:359:GLU:HB3	2.02	0.41
7:G:8:SER:HB3	7:G:73:LYS:HA	2.02	0.41
12:L:31:CYS:O	12:L:35:SER:HA	2.20	0.41
2:B:666:TYR:C	2:B:668:ASP:H	2.29	0.41
4:D:69:ALA:HA	4:D:72:ARG:HB2	2.01	0.41
5:E:5:ASN:HA	5:E:8:ASN:ND2	2.35	0.41
5:E:46:TYR:CD2	5:E:58:MET:HG3	2.56	0.41
8:H:58:THR:HB	8:H:143:LEU:HB2	2.02	0.41
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.21	0.41
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.55	0.41
1:A:1341:ILE:HG13	1:A:1379:GLY:O	2.19	0.41
2:B:823:ALA:O	2:B:1089:PRO:HA	2.21	0.41
2:B:1185:CYS:HA	4:D:17:LYS:HD3	2.03	0.41
5:E:76:GLY:HA3	5:E:106:GLN:HB2	2.02	0.41
1:A:448:PRO:O	1:A:449:SER:CB	2.68	0.41
1:A:1116:LEU:HD12	1:A:1311:VAL:HA	2.03	0.41
1:A:1422:ARG:HH12	2:B:1224:PHE:C	2.28	0.41
2:B:770:GLN:HG2	2:B:983:ARG:C	2.46	0.41
2:B:1037:LEU:HD21	2:B:1064:TYR:CE2	2.56	0.41
3:C:175:ALA:HB2	10:J:10:CYS:HB2	2.03	0.41
5:E:56:LYS:HG3	5:E:84:ASP:HB2	2.03	0.41
8:H:80:ARG:HA	8:H:81:PRO:HD3	1.91	0.41
1:A:75:ASN:O	1:A:76:GLU:HB2	2.20	0.41
1:A:974:ASP:C	1:A:976:THR:H	2.29	0.41
2:B:551:PRO:HG3	2:B:628:THR:HG21	2.02	0.41
3:C:82:TYR:O	3:C:83:SER:C	2.63	0.41
1:A:23:SER:HB2	1:A:25:GLU:OE1	2.20	0.41
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.21	0.41
1:A:847:ASP:OD2	1:A:858:ASN:HB2	2.21	0.41
1:A:852:TYR:O	6:F:81:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ILE:HG23	1:A:887:GLY:N	2.36	0.41
1:A:1019:CYS:HA	1:A:1022:LEU:HB3	2.02	0.41
1:A:1297:GLU:H	1:A:1297:GLU:HG3	1.55	0.41
1:A:1317:MET:HE2	5:E:142:VAL:HG11	2.02	0.41
2:B:188:ASP:O	2:B:192:LEU:HB2	2.21	0.41
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.86	0.41
2:B:848:ARG:HA	3:C:69:LEU:HD21	2.03	0.41
3:C:43:THR:HG22	3:C:44:LEU:N	2.36	0.41
5:E:48:ASP:C	5:E:50:MET:H	2.29	0.41
7:G:13:LEU:HD23	7:G:13:LEU:HA	1.86	0.41
3:C:258:ILE:HG23	11:K:19:LEU:HD21	2.01	0.41
4:D:5:THR:HG21	7:G:74:TYR:HH	1.86	0.41
1:A:114:LEU:HD21	1:A:171:GLN:HG3	2.03	0.40
2:B:363:HIS:O	2:B:364:ILE:HB	2.20	0.40
2:B:580:VAL:HG13	2:B:624:LEU:HD23	2.03	0.40
2:B:847:ASP:C	2:B:849:GLY:H	2.27	0.40
10:J:35:ALA:O	10:J:39:LEU:HD12	2.22	0.40
11:K:10:PHE:HA	11:K:37:LYS:HB3	2.03	0.40
1:A:376:TYR:HA	1:A:377:PRO:HD3	1.96	0.40
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.55	0.40
1:A:855:THR:HG21	1:A:857:ARG:NE	2.21	0.40
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.54	0.40
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.22	0.40
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.86	0.40
1:A:1377:THR:HG22	5:E:176:PRO:HB3	2.03	0.40
2:B:332:ASP:HB2	2:B:349:ILE:HG12	2.03	0.40
2:B:542:MET:HG2	2:B:747:MET:CE	2.50	0.40
2:B:706:GLN:H	2:B:710:LEU:HD12	1.85	0.40
2:B:852:ARG:HH22	12:L:70:ARG:C	2.30	0.40
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.86	0.40
3:C:245:VAL:HA	3:C:248:ILE:HD12	2.03	0.40
5:E:152:LYS:HZ1	5:E:201:LYS:HE3	1.85	0.40
7:G:145:VAL:HG22	7:G:163:ILE:CG2	2.51	0.40
7:G:147:ILE:HG23	7:G:159:ALA:HB1	2.02	0.40
1:A:347:PHE:H	2:B:1107:ALA:HA	1.86	0.40
5:E:178:ILE:HB	5:E:212:ARG:HD3	2.03	0.40
6:F:128:LYS:HG2	6:F:149:GLU:HA	2.02	0.40
1:A:450:LEU:H	1:A:450:LEU:HG	1.76	0.40
1:A:907:THR:HG22	1:A:908:LEU:N	2.36	0.40
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.57	0.40
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1202:LEU:HD23	2:B:1202:LEU:HA	1.90	0.40
3:C:172:PRO:O	3:C:235:VAL:HG23	2.22	0.40
7:G:101:VAL:HG11	7:G:143:ILE:HG22	2.03	0.40
11:K:56:VAL:HG22	11:K:77:THR:HG22	2.03	0.40
1:A:18:GLN:HB2	1:A:1418:LEU:HD12	2.04	0.40
1:A:519:PRO:O	1:A:624:SER:HB2	2.21	0.40
1:A:540:PHE:HB3	1:A:571:LEU:HG	2.03	0.40
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	2.04	0.40
1:A:1095:THR:HG21	1:A:1112:LYS:HB3	2.03	0.40
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	2.03	0.40
1:A:1430:LEU:CB	1:A:1432:GLN:HG3	2.51	0.40
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	2.04	0.40
4:D:52:LEU:H	4:D:52:LEU:HG	1.60	0.40
7:G:106:MET:HE2	7:G:106:MET:HB3	1.99	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	1414/1732 (82%)	1207 (85%)	137 (10%)	70 (5%)	1	17
2	B	1095/1224 (90%)	929 (85%)	122 (11%)	44 (4%)	2	20
3	C	264/318 (83%)	231 (88%)	25 (10%)	8 (3%)	3	25
4	D	174/221 (79%)	152 (87%)	13 (8%)	9 (5%)	1	17
5	E	212/215 (99%)	186 (88%)	19 (9%)	7 (3%)	3	24
6	F	82/155 (53%)	75 (92%)	6 (7%)	1 (1%)	10	40
7	G	169/171 (99%)	149 (88%)	17 (10%)	3 (2%)	6	33
8	H	129/146 (88%)	102 (79%)	16 (12%)	11 (8%)	0	9
9	I	117/122 (96%)	91 (78%)	23 (20%)	3 (3%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	63/70 (90%)	52 (82%)	6 (10%)	5 (8%)	1	10
11	K	113/120 (94%)	107 (95%)	6 (5%)	0	100	100
12	L	44/70 (63%)	26 (59%)	10 (23%)	8 (18%)	0	2
All	All	3876/4564 (85%)	3307 (85%)	400 (10%)	169 (4%)	2	19

All (169) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	48	ALA
1	A	54	ASN
1	A	57	ARG
1	A	58	LEU
1	A	72	GLU
1	A	76	GLU
1	A	195	ASP
1	A	286	HIS
1	A	311	GLN
1	A	312	PRO
1	A	318	SER
1	A	335	ARG
1	A	385	ILE
1	A	449	SER
1	A	775	ILE
1	A	1016	THR
1	A	1124	HIS
2	B	67	SER
2	B	229	ALA
2	B	344	LYS
2	B	364	ILE
2	B	476	ARG
2	B	629	ASP
2	B	707	PRO
2	B	1155	SER
2	B	1175	LEU
3	C	161	LYS
3	C	184	ASN
4	D	18	VAL
5	E	36	GLU
5	E	104	ASN
7	G	2	PHE

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Mol	Chain	Res	Type
9	I	95	THR
12	L	50	ASP
12	L	53	HIS
1	A	178	GLY
1	A	257	ARG
1	A	331	GLY
1	A	410	GLY
1	A	586	ILE
1	A	777	PHE
1	A	886	ILE
1	A	986	ILE
1	A	987	VAL
1	A	1123	GLY
1	A	1167	GLU
1	A	1175	SER
1	A	1437	GLY
2	B	108	VAL
2	B	184	ALA
2	B	322	PHE
2	B	338	GLY
2	B	341	LEU
2	B	343	ILE
2	B	368	GLU
2	B	369	GLY
2	B	531	GLN
2	B	533	CYS
2	B	655	LYS
2	B	711	GLU
2	B	731	VAL
2	B	751	VAL
2	B	792	MET
2	B	879	ARG
2	B	881	ASN
2	B	1046	PRO
2	B	1223	ASP
4	D	16	LYS
4	D	20	GLU
4	D	53	SER
5	E	45	LYS
6	F	73	ALA
8	H	81	PRO
8	H	82	PRO

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Mol	Chain	Res	Type
8	H	83	GLN
10	J	2	ILE
10	J	6	ARG
12	L	59	ALA
1	A	74	MET
1	A	167	CYS
1	A	189	ARG
1	A	310	GLY
1	A	332	LYS
1	A	569	LYS
1	A	846	GLU
1	A	852	TYR
1	A	870	GLU
1	A	1122	PRO
1	A	1173	HIS
1	A	1361	SER
1	A	1388	GLY
2	B	58	THR
2	B	68	THR
2	B	275	TYR
2	B	880	THR
2	B	883	LEU
2	B	1066	SER
4	D	199	ASN
4	D	218	GLU
5	E	3	GLN
5	E	48	ASP
5	E	75	MET
7	G	154	VAL
8	H	17	PRO
8	H	84	ALA
9	I	3	THR
10	J	17	LYS
12	L	26	THR
12	L	56	LEU
1	A	62	ASP
1	A	256	GLN
1	A	419	LYS
1	A	448	PRO
1	A	465	TYR
1	A	567	LYS
1	A	599	SER

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Mol	Chain	Res	Type
1	A	639	PRO
1	A	700	ASN
1	A	1280	GLU
1	A	1416	ALA
2	B	340	ALA
2	B	526	GLU
2	B	643	ASP
2	B	667	GLN
2	B	1157	ALA
2	B	1176	ASN
4	D	119	ARG
4	D	198	LEU
5	E	113	GLN
8	H	60	ALA
9	I	113	ASP
10	J	64	ASN
1	A	169	ASN
1	A	399	HIS
1	A	409	SER
1	A	958	VAL
1	A	1378	GLN
2	B	510	LYS
2	B	1169	MET
3	C	90	ASP
4	D	40	HIS
7	G	63	PRO
8	H	107	VAL
8	H	128	ASN
8	H	130	ARG
10	J	13	VAL
12	L	39	SER
12	L	45	ALA
12	L	46	VAL
1	A	51	GLY
1	A	1454	MET
2	B	644	GLU
3	C	214	ASN
8	H	18	GLY
8	H	90	ALA
1	A	35	ILE
2	B	251	ILE
3	C	38	ILE

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Mol	Chain	Res	Type
1	A	244	PRO
3	C	150	GLY
3	C	212	PRO
1	A	192	GLY
1	A	283	GLY
1	A	380	VAL
1	A	1242	VAL
1	A	61	ILE
1	A	336	ILE
3	C	240	VAL

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%)	1013 (82%)	227 (18%)	2	11
2	B	966/1061 (91%)	795 (82%)	171 (18%)	2	12
3	C	234/274 (85%)	191 (82%)	43 (18%)	1	11
4	D	160/200 (80%)	131 (82%)	29 (18%)	2	12
5	E	196/197 (100%)	171 (87%)	25 (13%)	4	21
6	F	74/137 (54%)	60 (81%)	14 (19%)	1	10
7	G	152/152 (100%)	129 (85%)	23 (15%)	3	16
8	H	117/128 (91%)	99 (85%)	18 (15%)	2	15
9	I	113/116 (97%)	102 (90%)	11 (10%)	8	29
10	J	60/65 (92%)	44 (73%)	16 (27%)	0	3
11	K	99/102 (97%)	83 (84%)	16 (16%)	2	14
12	L	40/57 (70%)	27 (68%)	13 (32%)	0	1
All	All	3451/4008 (86%)	2845 (82%)	606 (18%)	2	12

All (606) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	12	ARG
1	A	34	LYS
1	A	37	PHE
1	A	41	MET
1	A	45	GLN
1	A	46	THR
1	A	62	ASP
1	A	63	ARG
1	A	64	ASN
1	A	67	CYS
1	A	84	ILE
1	A	93	VAL
1	A	96	ILE
1	A	107	CYS
1	A	117	GLU
1	A	129	LYS
1	A	151	ASP
1	A	152	VAL
1	A	156	ASP
1	A	159	THR
1	A	164	ARG
1	A	170	THR
1	A	174	ILE
1	A	175	ARG
1	A	182	VAL
1	A	199	LEU
1	A	204	THR
1	A	205	GLU
1	A	208	LEU
1	A	220	THR
1	A	222	LEU
1	A	226	GLU
1	A	232	GLU
1	A	236	LEU
1	A	256	GLN
1	A	257	ARG
1	A	261	ASP
1	A	270	LEU
1	A	274	ILE
1	A	279	LEU
1	A	289	ILE
1	A	290	GLU

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Mol	Chain	Res	Type
1	A	295	LEU
1	A	307	ASP
1	A	308	ILE
1	A	315	LEU
1	A	322	VAL
1	A	324	SER
1	A	329	LEU
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	354	SER
1	A	375	THR
1	A	385	ILE
1	A	386	ASP
1	A	391	LEU
1	A	393	ARG
1	A	394	ASN
1	A	407	ARG
1	A	408	ASP
1	A	419	LYS
1	A	423	ASP
1	A	431	LYS
1	A	434	ARG
1	A	437	MET
1	A	438	ASP
1	A	442	VAL
1	A	443	LEU
1	A	450	LEU
1	A	454	SER
1	A	459	ARG
1	A	461	LYS
1	A	463	ILE
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	483	ASP
1	A	493	GLN
1	A	500	GLU
1	A	518	LYS

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Mol	Chain	Res	Type
1	A	523	ILE
1	A	524	VAL
1	A	527	THR
1	A	536	LEU
1	A	538	ASP
1	A	541	ILE
1	A	543	LEU
1	A	545	GLN
1	A	560	ILE
1	A	566	ILE
1	A	567	LYS
1	A	571	LEU
1	A	577	ILE
1	A	584	ASN
1	A	589	GLN
1	A	593	GLU
1	A	598	LEU
1	A	613	ILE
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	634	THR
1	A	645	LEU
1	A	657	LEU
1	A	658	LEU
1	A	660	ASN
1	A	664	THR
1	A	666	ILE
1	A	670	ILE
1	A	675	THR
1	A	683	ILE
1	A	690	VAL
1	A	691	LEU
1	A	738	LYS
1	A	740	LEU
1	A	754	SER
1	A	756	ILE
1	A	768	GLN
1	A	782	ARG
1	A	821	ARG
1	A	822	GLU
1	A	831	THR

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Mol	Chain	Res	Type
1	A	834	THR
1	A	839	ARG
1	A	843	LYS
1	A	846	GLU
1	A	855	THR
1	A	878	ILE
1	A	886	ILE
1	A	896	ARG
1	A	915	SER
1	A	919	ILE
1	A	920	LEU
1	A	923	LEU
1	A	926	GLN
1	A	929	LEU
1	A	932	GLU
1	A	934	LYS
1	A	941	LYS
1	A	948	VAL
1	A	973	ILE
1	A	983	ILE
1	A	998	LEU
1	A	1001	ARG
1	A	1009	ASN
1	A	1015	VAL
1	A	1019	CYS
1	A	1024	SER
1	A	1029	ARG
1	A	1033	GLN
1	A	1038	THR
1	A	1040	GLN
1	A	1047	SER
1	A	1052	GLN
1	A	1062	GLU
1	A	1064	VAL
1	A	1067	LEU
1	A	1080	THR
1	A	1098	VAL
1	A	1100	ARG
1	A	1116	LEU
1	A	1118	VAL
1	A	1121	GLU
1	A	1124	HIS

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Mol	Chain	Res	Type
1	A	1133	LEU
1	A	1134	ILE
1	A	1135	ARG
1	A	1142	THR
1	A	1146	VAL
1	A	1147	THR
1	A	1170	ILE
1	A	1173	HIS
1	A	1174	PHE
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1223	ASP
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1243	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1265	ASN
1	A	1270	ASN
1	A	1288	ASP
1	A	1295	THR
1	A	1297	GLU
1	A	1301	GLU
1	A	1303	GLU
1	A	1315	GLU
1	A	1316	VAL
1	A	1317	MET
1	A	1325	THR
1	A	1327	ILE
1	A	1333	ILE
1	A	1334	ASP
1	A	1336	MET
1	A	1341	ILE
1	A	1356	ILE
1	A	1366	ARG
1	A	1376	THR
1	A	1378	GLN
1	A	1382	THR
1	A	1383	SER

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Mol	Chain	Res	Type
1	A	1386	ARG
1	A	1387	HIS
1	A	1391	ARG
1	A	1393	ASN
1	A	1405	THR
1	A	1418	LEU
1	A	1426	GLU
1	A	1428	VAL
1	A	1433	MET
1	A	1436	ILE
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
1	A	1453	TYR
2	B	25	ILE
2	B	26	THR
2	B	40	GLU
2	B	44	VAL
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	70	ILE
2	B	91	SER
2	B	101	MET
2	B	102	VAL
2	B	118	ARG
2	B	121	ASN
2	B	122	LEU
2	B	128	LEU
2	B	134	LYS
2	B	177	LYS
2	B	178	ASN
2	B	183	GLU
2	B	192	LEU
2	B	212	LEU
2	B	213	ILE
2	B	218	SER
2	B	222	ILE
2	B	223	VAL
2	B	240	ILE

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Mol	Chain	Res	Type
2	B	251	ILE
2	B	261	ARG
2	B	262	GLU
2	B	267	ARG
2	B	272	THR
2	B	278	GLN
2	B	284	ILE
2	B	299	GLU
2	B	317	CYS
2	B	324	ILE
2	B	325	GLN
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	348	ARG
2	B	350	GLN
2	B	365	THR
2	B	367	LEU
2	B	368	GLU
2	B	373	ARG
2	B	385	LEU
2	B	393	LYS
2	B	394	ASP
2	B	396	ASP
2	B	398	ARG
2	B	401	PHE
2	B	408	LEU
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	427	ASP
2	B	428	ILE
2	B	434	ARG
2	B	437	GLU
2	B	446	LEU
2	B	448	ILE
2	B	452	THR
2	B	453	ILE
2	B	461	LEU

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Mol	Chain	Res	Type
2	B	470	LYS
2	B	476	ARG
2	B	479	VAL
2	B	485	ARG
2	B	498	THR
2	B	502	ILE
2	B	510	LYS
2	B	513	GLN
2	B	547	VAL
2	B	549	THR
2	B	555	ILE
2	B	563	MET
2	B	570	VAL
2	B	574	SER
2	B	578	THR
2	B	582	VAL
2	B	598	GLU
2	B	599	THR
2	B	603	LEU
2	B	604	ARG
2	B	615	MET
2	B	620	ARG
2	B	628	THR
2	B	644	GLU
2	B	651	LEU
2	B	653	VAL
2	B	658	ILE
2	B	685	LEU
2	B	689	LEU
2	B	696	GLU
2	B	708	GLU
2	B	709	ASP
2	B	722	ASP
2	B	730	ARG
2	B	734	HIS
2	B	737	THR
2	B	755	ILE
2	B	766	ARG
2	B	786	ASN
2	B	790	ASP
2	B	795	ILE
2	B	806	THR

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Mol	Chain	Res	Type
2	B	835	GLN
2	B	837	ASP
2	B	839	MET
2	B	844	SER
2	B	871	THR
2	B	878	GLN
2	B	882	THR
2	B	903	VAL
2	B	904	ARG
2	B	934	LYS
2	B	942	ARG
2	B	944	THR
2	B	945	GLU
2	B	946	ASN
2	B	953	LEU
2	B	954	VAL
2	B	956	THR
2	B	964	VAL
2	B	970	THR
2	B	972	LYS
2	B	973	ILE
2	B	975	GLN
2	B	976	ILE
2	B	986	GLN
2	B	987	LYS
2	B	992	ILE
2	B	997	GLU
2	B	1006	ILE
2	B	1007	VAL
2	B	1028	GLU
2	B	1031	LEU
2	B	1045	SER
2	B	1065	GLN
2	B	1072	MET
2	B	1084	GLN
2	B	1098	MET
2	B	1106	ARG
2	B	1112	GLN
2	B	1113	VAL
2	B	1117	GLN
2	B	1123	SER
2	B	1128	LEU

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Mol	Chain	Res	Type
2	B	1133	MET
2	B	1135	ARG
2	B	1137	CYS
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	1168	LEU
2	B	1175	LEU
2	B	1176	ASN
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1191	ILE
2	B	1202	LEU
2	B	1210	MET
2	B	1212	ILE
3	C	7	GLN
3	C	11	ARG
3	C	12	GLU
3	C	16	ASP
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	49	VAL
3	C	52	GLU
3	C	55	THR
3	C	57	VAL
3	C	70	ILE
3	C	78	GLU
3	C	80	LEU
3	C	89	GLU
3	C	102	GLN
3	C	106	GLU
3	C	119	VAL
3	C	121	VAL
3	C	125	MET
3	C	127	ARG
3	C	129	ILE

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Mol	Chain	Res	Type
3	C	133	ILE
3	C	148	ARG
3	C	154	LYS
3	C	179	GLU
3	C	189	THR
3	C	195	GLN
3	C	197	SER
3	C	211	ASP
3	C	215	GLU
3	C	226	ASP
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	245	VAL
3	C	260	LEU
3	C	262	LEU
3	C	263	THR
3	C	264	GLN
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	9	GLN
4	D	18	VAL
4	D	19	GLU
4	D	27	LEU
4	D	32	GLU
4	D	35	LEU
4	D	38	ILE
4	D	41	GLN
4	D	43	GLU
4	D	52	LEU
4	D	65	GLU
4	D	67	ARG
4	D	75	LYS
4	D	123	LEU
4	D	126	ILE
4	D	133	THR
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	156	ASP
4	D	164	ILE

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Mol	Chain	Res	Type
4	D	182	SER
4	D	187	THR
4	D	197	SER
4	D	201	LYS
4	D	204	ASP
4	D	206	GLU
4	D	213	GLU
5	E	21	GLU
5	E	31	THR
5	E	40	GLU
5	E	45	LYS
5	E	46	TYR
5	E	69	ILE
5	E	92	THR
5	E	98	ILE
5	E	100	ILE
5	E	114	ASN
5	E	115	ASN
5	E	127	ILE
5	E	131	THR
5	E	132	ILE
5	E	150	VAL
5	E	154	ILE
5	E	156	LEU
5	E	165	LEU
5	E	175	LEU
5	E	182	ASP
5	E	184	VAL
5	E	190	LEU
5	E	191	LYS
5	E	192	ARG
5	E	201	LYS
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	86	THR
6	F	90	ARG
6	F	93	ILE
6	F	103	MET
6	F	109	VAL
6	F	112	GLU
6	F	115	THR

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Mol	Chain	Res	Type
6	F	118	LEU
6	F	128	LYS
6	F	152	ILE
6	F	155	LEU
7	G	5	LYS
7	G	7	LEU
7	G	11	ILE
7	G	13	LEU
7	G	22	MET
7	G	26	LEU
7	G	28	THR
7	G	64	THR
7	G	65	ASP
7	G	90	THR
7	G	93	SER
7	G	108	VAL
7	G	114	LEU
7	G	118	ASP
7	G	133	SER
7	G	141	SER
7	G	143	ILE
7	G	151	ILE
7	G	152	SER
7	G	154	VAL
7	G	157	ILE
7	G	163	ILE
7	G	164	LYS
8	H	12	VAL
8	H	14	GLU
8	H	23	VAL
8	H	26	ILE
8	H	35	GLN
8	H	39	THR
8	H	42	ILE
8	H	76	THR
8	H	78	SER
8	H	86	ASP
8	H	89	LEU
8	H	106	GLU
8	H	107	VAL
8	H	112	ILE
8	H	128	ASN

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Mol	Chain	Res	Type
8	H	130	ARG
8	H	135	LEU
8	H	146	ARG
9	I	8	ARG
9	I	31	THR
9	I	43	VAL
9	I	50	THR
9	I	55	THR
9	I	62	ILE
9	I	83	ASN
9	I	84	VAL
9	I	104	LEU
9	I	109	ILE
9	I	118	ARG
10	J	9	SER
10	J	12	LYS
10	J	13	VAL
10	J	14	VAL
10	J	16	ASP
10	J	20	SER
10	J	22	LEU
10	J	23	ASN
10	J	28	ASP
10	J	30	LEU
10	J	31	ASP
10	J	34	THR
10	J	41	LEU
10	J	42	LYS
10	J	43	ARG
10	J	57	ILE
11	K	6	ARG
11	K	9	LEU
11	K	11	LEU
11	K	20	LYS
11	K	21	ILE
11	K	25	THR
11	K	31	VAL
11	K	33	ILE
11	K	47	ARG
11	K	51	LEU
11	K	78	THR
11	K	91	CYS

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Mol	Chain	Res	Type
11	K	101	LEU
11	K	103	THR
11	K	107	THR
11	K	114	LEU
12	L	33	GLU
12	L	34	CYS
12	L	38	LEU
12	L	46	VAL
12	L	50	ASP
12	L	51	CYS
12	L	55	ILE
12	L	57	LEU
12	L	58	LYS
12	L	61	THR
12	L	65	VAL
12	L	66	GLN
12	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	253	ASN
1	A	256	GLN
1	A	286	HIS
1	A	358	ASN
1	A	390	GLN
1	A	394	ASN
1	A	479	ASN
1	A	548	ASN
1	A	654	ASN
1	A	742	ASN
1	A	811	GLN
1	A	862	ASN
1	A	877	HIS
1	A	935	GLN
1	A	953	ASN
1	A	966	ASN
1	A	968	GLN
1	A	969	GLN
1	A	994	GLN
1	A	1040	GLN

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Mol	Chain	Res	Type
1	A	1070	GLN
1	A	1124	HIS
1	A	1140	HIS
1	A	1378	GLN
1	A	1393	ASN
1	A	1427	ASN
2	B	47	GLN
2	B	103	ASN
2	B	224	GLN
2	B	300	HIS
2	B	306	ASN
2	B	357	GLN
2	B	469	GLN
2	B	499	ASN
2	B	538	ASN
2	B	587	HIS
2	B	706	GLN
2	B	835	GLN
2	B	862	GLN
2	B	951	GLN
2	B	975	GLN
2	B	1025	HIS
2	B	1097	HIS
2	B	1112	GLN
2	B	1117	GLN
2	B	1195	HIS
3	C	7	GLN
3	C	24	ASN
3	C	79	GLN
3	C	151	GLN
3	C	264	GLN
4	D	23	ASN
4	D	143	ASN
5	E	3	GLN
5	E	8	ASN
5	E	54	GLN
5	E	99	HIS
5	E	104	ASN
5	E	174	GLN
7	G	10	ASN
7	G	57	GLN
7	G	126	ASN

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Mol	Chain	Res	Type
7	G	131	GLN
7	G	153	GLN
8	H	131	ASN
8	H	134	ASN
9	I	23	ASN
9	I	60	GLN
9	I	120	GLN
10	J	26	GLN
11	K	29	ASN
11	K	76	GLN
12	L	53	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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
14	BRU	T	22	14	18,21,22	1.60	4 (22%)	25,30,33	2.64	10 (40%)

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
14	BRU	T	22	14	-	2/7/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	22	BRU	C6-C5	3.72	1.41	1.34
14	T	22	BRU	BR-C5	3.31	1.96	1.88
14	T	22	BRU	C6-N1	2.79	1.42	1.38
14	T	22	BRU	C4-C5	2.57	1.50	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	22	BRU	BR-C5-C4	7.08	126.17	118.02
14	T	22	BRU	N3-C2-N1	4.54	120.80	114.89
14	T	22	BRU	O4'-C1'-N1	4.41	115.69	107.86
14	T	22	BRU	C6-C5-C4	-4.19	116.42	120.67
14	T	22	BRU	C5-C4-N3	4.05	118.00	113.34
14	T	22	BRU	C6-N1-C2	-3.43	117.89	121.30
14	T	22	BRU	C4-N3-C2	-3.28	123.04	127.34
14	T	22	BRU	C2'-C1'-N1	2.68	120.52	113.81
14	T	22	BRU	BR-C5-C6	-2.31	117.41	120.64
14	T	22	BRU	C1'-N1-C2	2.21	121.99	117.66

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	22	BRU	C3'-C4'-C5'-O5'
14	T	22	BRU	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	22	BRU	1	0

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	5.74
1	B	351:TYR	C	352:ALA	N	3.07

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%)	-0.27	15 (1%) 78 56	64, 116, 174, 247	0
2	B	1115/1224 (91%)	-0.10	22 (1%) 65 44	67, 130, 191, 222	0
3	C	266/318 (83%)	-0.38	0 100 100	90, 119, 163, 183	0
4	D	178/221 (80%)	-0.00	4 (2%) 62 44	102, 135, 182, 198	0
5	E	214/215 (99%)	-0.14	0 100 100	90, 151, 199, 208	0
6	F	84/155 (54%)	-0.63	1 (1%) 76 54	70, 95, 126, 149	0
7	G	171/171 (100%)	-0.26	1 (0%) 85 68	87, 116, 155, 179	0
8	H	133/146 (91%)	0.26	7 (5%) 32 24	122, 161, 195, 205	0
9	I	119/122 (97%)	-0.07	1 (0%) 82 62	123, 158, 192, 214	0
10	J	65/70 (92%)	-0.31	1 (1%) 72 50	97, 115, 153, 166	0
11	K	115/120 (95%)	-0.47	1 (0%) 81 60	83, 115, 163, 181	0
12	L	46/70 (65%)	0.46	3 (6%) 25 21	103, 159, 184, 191	0
13	N	11/15 (73%)	0.50	0 100 100	203, 219, 272, 273	0
14	T	16/27 (59%)	0.57	0 100 100	170, 216, 266, 270	0
All	All	3955/4606 (85%)	-0.19	56 (1%) 73 51	64, 125, 188, 273	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	446	LEU	5.0
8	H	63	LEU	4.4
12	L	27	LEU	4.3
1	A	251	SER	4.3
2	B	134	LYS	4.1
1	A	190	ALA	3.9
2	B	708	GLU	3.9
12	L	26	THR	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	251	ILE	3.7
2	B	883	LEU	3.7
2	B	1224	PHE	3.5
4	D	3	VAL	3.3
1	A	1176	LEU	3.1
1	A	1080	THR	3.0
1	A	1254	ALA	3.0
10	J	65	PRO	3.0
2	B	734	HIS	2.9
2	B	70	ILE	2.9
8	H	132	LEU	2.9
2	B	310	MET	2.9
8	H	139	ASN	2.9
2	B	305	VAL	2.9
6	F	72	LYS	2.9
1	A	1243	VAL	2.8
2	B	709	ASP	2.8
2	B	715	ALA	2.8
8	H	86	ASP	2.7
4	D	25	ALA	2.7
1	A	1321	GLY	2.6
7	G	64	THR	2.6
1	A	3	GLY	2.6
2	B	726	ALA	2.6
1	A	56	PRO	2.5
8	H	82	PRO	2.5
2	B	343	ILE	2.5
1	A	1455	PRO	2.4
9	I	93	LYS	2.4
4	D	221	TYR	2.4
2	B	502	ILE	2.3
8	H	140	ALA	2.3
1	A	1187	GLN	2.3
1	A	51	GLY	2.3
1	A	194	ALA	2.3
12	L	25	ALA	2.2
2	B	731	VAL	2.2
1	A	252	PHE	2.2
2	B	646	LEU	2.2
11	K	114	LEU	2.2
8	H	136	LYS	2.2
4	D	18	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	340	ALA	2.1
2	B	733	HIS	2.1
2	B	730	ARG	2.1
1	A	310	GLY	2.0
2	B	712	PRO	2.0
2	B	250	PHE	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
14	BRU	T	22	20/21	0.74	0.14	221,231,236,237	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	MG	A	2458	1/1	0.93	0.05	106,106,106,106	0
15	ZN	I	1122	1/1	0.99	0.03	197,197,197,197	0
15	ZN	B	2225	1/1	1.00	0.05	92,92,92,92	0
15	ZN	C	1269	1/1	1.00	0.03	88,88,88,88	0
15	ZN	I	1121	1/1	1.00	0.02	126,126,126,126	0
15	ZN	A	2456	1/1	1.00	0.01	146,146,146,146	0
15	ZN	J	1066	1/1	1.00	0.03	90,90,90,90	0
15	ZN	L	1071	1/1	1.00	0.02	164,164,164,164	0
15	ZN	A	2457	1/1	1.00	0.03	89,89,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.