



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:28 PM UTC

PDB ID : 5C44 / pdb_00005c44
Title : Crystal structure of a transcribing RNA Polymerase II complex reveals a complete transcription bubble
Authors : Barnes, C.O.; Calero, M.; Malik, I.; Spahr, H.; Zhang, Q.; Pullara, F.; Kaplan, C.D.; Calero, G.
Deposited on : 2015-06-17
Resolution : 3.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

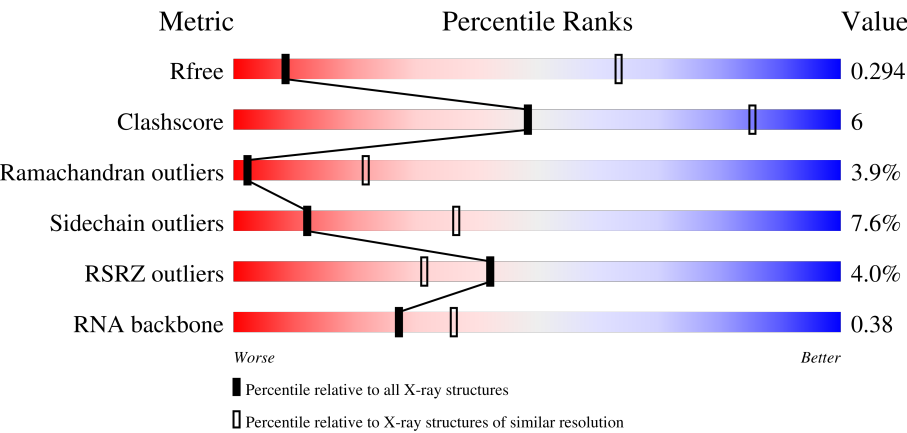
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 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	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)
RNA backbone	3983	1016 (4.80-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	1733	2% 64% 16% • 17%
2	B	1224	3% 70% 22% • 5%
3	C	318	2% 66% 14% • 17%
4	D	221	2% 64% 15% • 19%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	179	
8	H	146	
9	I	120	
10	J	70	
11	K	120	
12	L	70	
13	R	9	
14	S	53	
15	U	53	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 32540 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	1434	Total	C	N	O	S	0	0	0
			11249	7083	1967	2137	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1158	Total	C	N	O	S	0	0	0
			9175	5795	1603	1721	56			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2086	1312	347	414	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
			1417	875	254	286	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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 RPABC2.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1339	861	222	248	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	172	LEU	-	expression tag	UNP P34087
G	173	GLU	-	expression tag	UNP P34087
G	174	HIS	-	expression tag	UNP P34087
G	175	HIS	-	expression tag	UNP P34087
G	176	HIS	-	expression tag	UNP P34087
G	177	HIS	-	expression tag	UNP P34087
G	178	HIS	-	expression tag	UNP P34087
G	179	HIS	-	expression tag	UNP P34087

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	135	Total	C	N	O	S	0	0	0
			1080	679	182	214	5			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	114	Total	C	N	O	S	0	0	0
			921	568	165	178	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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	0
			924	593	157	172	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			346	214	67	61	4			

- Molecule 13 is a RNA chain called Synthetic RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	9	Total	C	N	O	P	0	0	0
			197	88	40	60	9			

- Molecule 14 is a DNA chain called Synthetic DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	S	13	Total	C	N	O	P	0	0	0
			268	128	46	81	13			

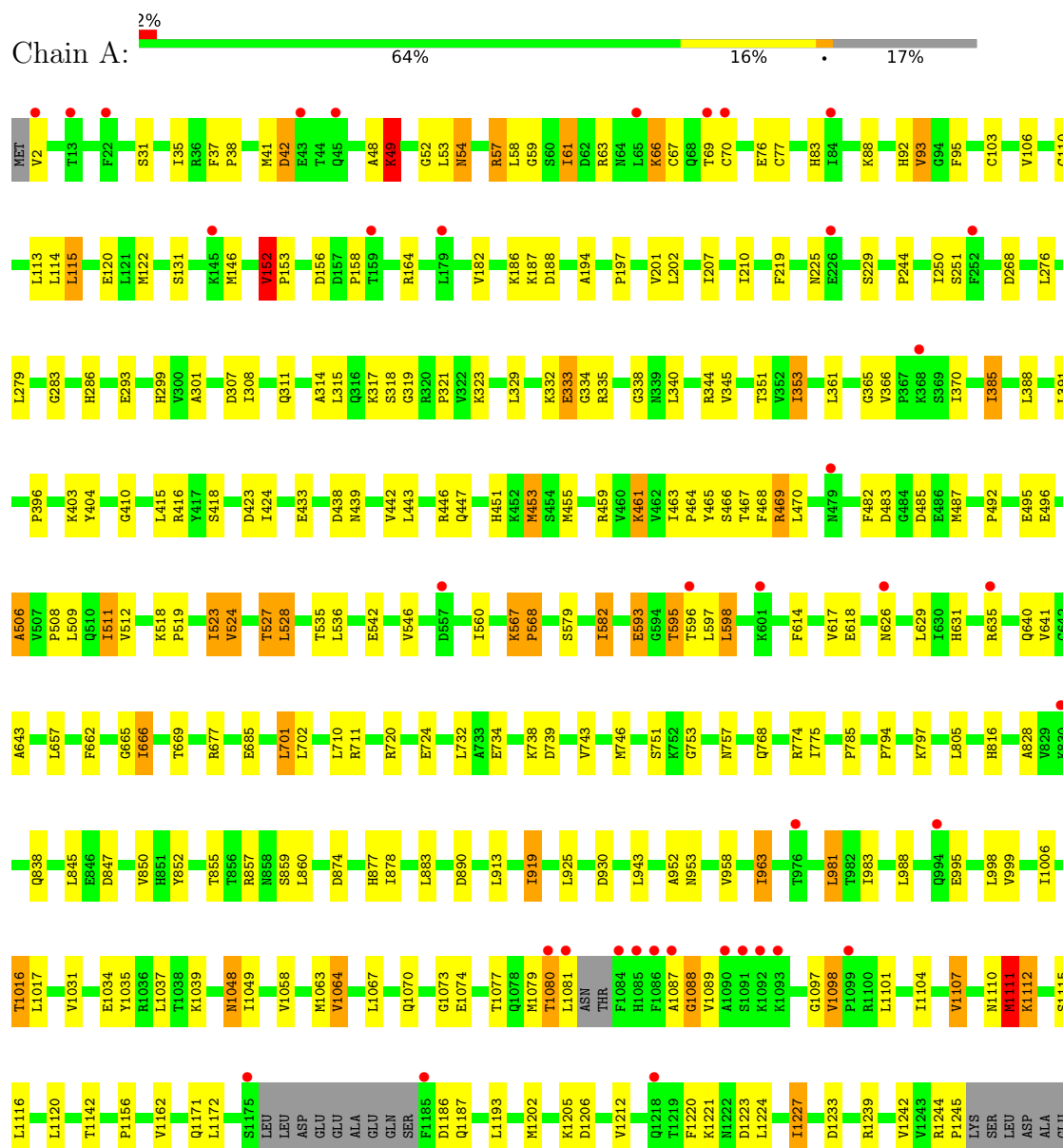
- Molecule 15 is a DNA chain called Synthetic DNA.

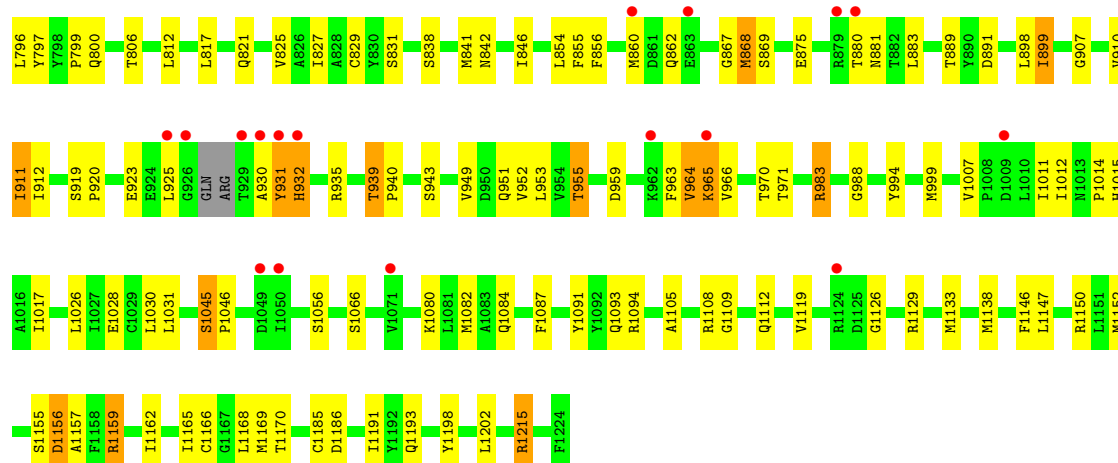
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	27	Total	C	N	O	P	0	0	0
			549	261	102	159	27			

3 Residue-property plots

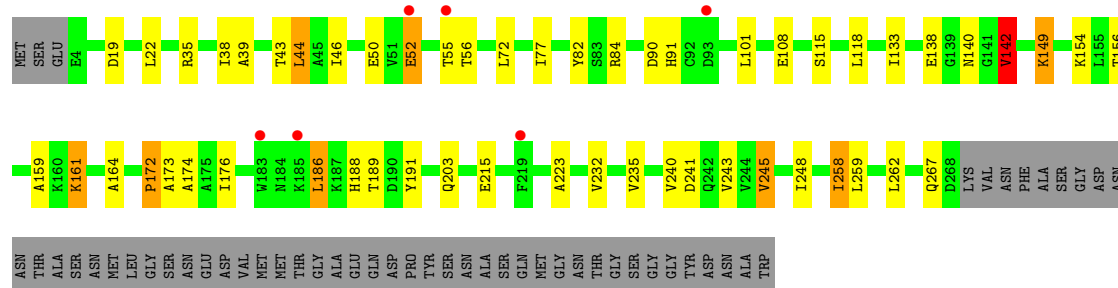
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

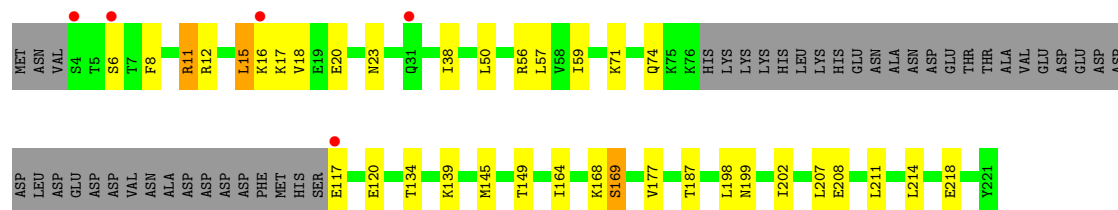




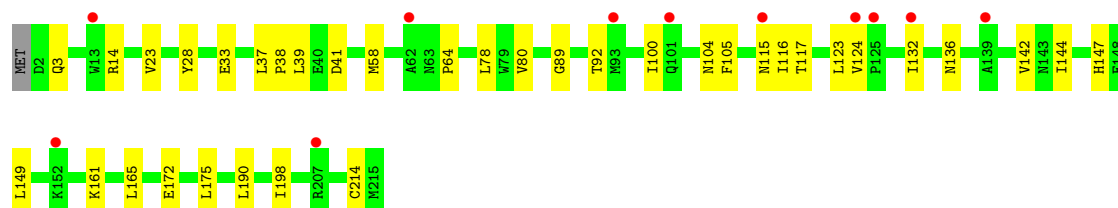
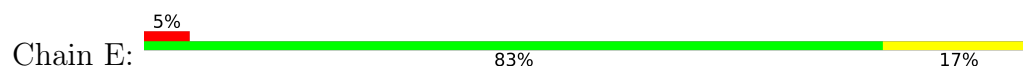
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



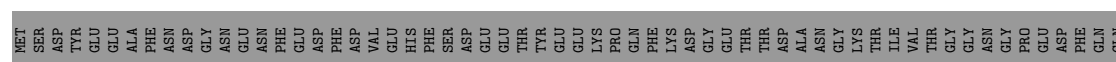
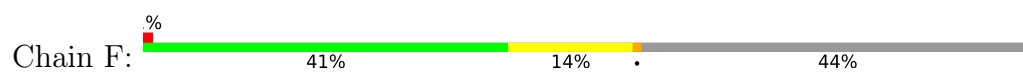
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



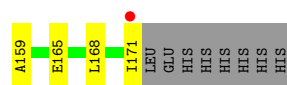
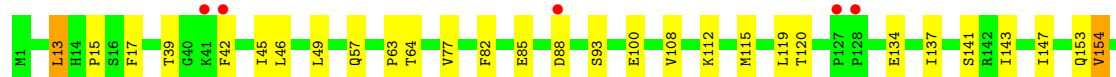
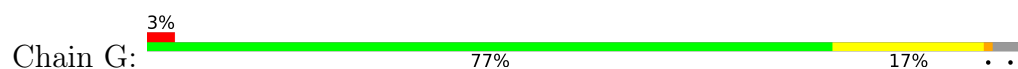
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



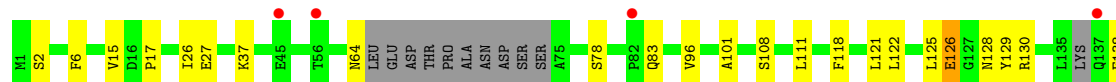
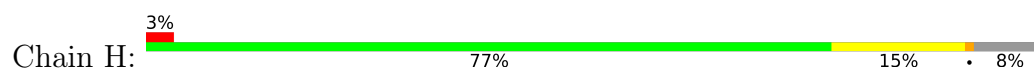
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



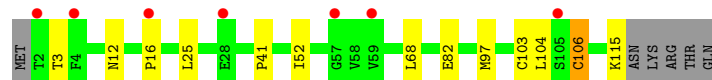
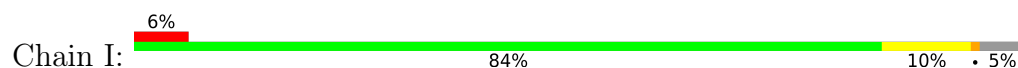
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



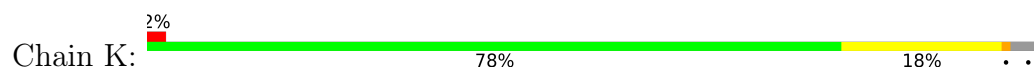
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

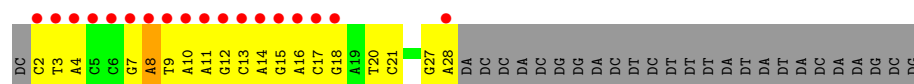


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.22Å 391.84Å 282.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.00 – 3.95 79.00 – 3.95	Depositor EDS
% Data completeness (in resolution range)	94.3 (79.00-3.95) 94.5 (79.00-3.95)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 4.01Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.215 , 0.236 0.272 , 0.294	Depositor DCC
R_{free} test set	3013 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å ²)	114.2	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 232.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.178 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.186 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	32540	wwPDB-VP
Average B, all atoms (Å ²)	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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

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	0.79	1/11452 (0.0%)	1.36	35/15492 (0.2%)
2	B	0.76	3/9347 (0.0%)	1.27	22/12601 (0.2%)
3	C	0.77	0/2124	1.26	2/2879 (0.1%)
4	D	0.71	0/1427	1.35	3/1911 (0.2%)
5	E	0.72	0/1788	1.25	4/2406 (0.2%)
6	F	0.74	0/717	1.28	0/967
7	G	0.76	0/1367	1.20	1/1844 (0.1%)
8	H	0.73	0/1097	1.10	2/1484 (0.1%)
9	I	0.72	0/939	1.21	0/1266
10	J	0.70	0/541	1.28	0/727
11	K	0.70	0/942	1.31	0/1272
12	L	0.75	0/348	1.21	0/461
13	R	0.56	0/221	0.73	1/343 (0.3%)
14	S	1.42	2/299 (0.7%)	0.85	0/460
15	U	1.05	0/615	0.63	0/945
All	All	0.77	6/33224 (0.0%)	1.28	70/45058 (0.2%)

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
14	S	0	1
15	U	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	260	GLY	C-N	7.77	1.47	1.33
2	B	265	SER	C-N	7.64	1.44	1.33
2	B	932	HIS	CG-ND1	5.63	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	S	27	DT	O5'-C5'	5.54	1.59	1.42
1	A	1107	VAL	CA-C	5.37	1.59	1.52
14	S	27	DT	P-O5'	5.29	1.71	1.60

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	260	GLY	O-C-N	-10.39	109.19	122.70
2	B	79	THR	CA-C-N	8.20	136.46	121.70
2	B	79	THR	C-N-CA	8.20	136.46	121.70
2	B	136	THR	CA-C-N	7.63	135.43	121.70
2	B	136	THR	C-N-CA	7.63	135.43	121.70
1	A	1098	VAL	N-CA-CB	7.58	115.28	110.50
1	A	1097	GLY	CA-C-N	7.57	125.01	120.24
1	A	1097	GLY	C-N-CA	7.57	125.01	120.24
1	A	1111	MET	N-CA-C	7.54	119.28	111.14
2	B	260	GLY	CA-C-N	7.51	135.71	122.42
2	B	260	GLY	C-N-CA	7.51	135.71	122.42
1	A	506	ALA	CA-C-N	6.82	126.98	120.43
1	A	506	ALA	C-N-CA	6.82	126.98	120.43
1	A	1107	VAL	CA-C-N	6.75	133.86	121.70
1	A	1107	VAL	C-N-CA	6.75	133.86	121.70
2	B	145	ARG	CA-C-N	6.57	133.53	121.70
2	B	145	ARG	C-N-CA	6.57	133.53	121.70
1	A	1079	MET	CA-C-N	6.54	133.47	121.70
1	A	1079	MET	C-N-CA	6.54	133.47	121.70
2	B	867	GLY	CA-C-N	6.32	133.07	121.70
2	B	867	GLY	C-N-CA	6.32	133.07	121.70
2	B	469	GLN	CA-C-N	6.29	129.33	120.28
2	B	469	GLN	C-N-CA	6.29	129.33	120.28
1	A	930	ASP	N-CA-C	-6.07	104.02	112.45
3	C	172	PRO	CA-C-N	6.06	128.68	120.38
3	C	172	PRO	C-N-CA	6.06	128.68	120.38
5	E	147	HIS	CA-C-N	6.02	128.62	120.38
5	E	147	HIS	C-N-CA	6.02	128.62	120.38
2	B	150	GLU	CA-C-N	5.95	132.42	121.70
2	B	150	GLU	C-N-CA	5.95	132.42	121.70
1	A	641	VAL	N-CA-C	-5.91	104.55	111.00
1	A	48	ALA	CA-C-N	5.79	132.60	121.54
1	A	48	ALA	C-N-CA	5.79	132.60	121.54
1	A	1063	MET	CA-C-N	5.74	132.30	121.97
1	A	1063	MET	C-N-CA	5.74	132.30	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	999	VAL	N-CA-C	-5.69	105.56	110.74
1	A	54	ASN	CA-C-N	5.66	128.53	123.10
1	A	54	ASN	C-N-CA	5.66	128.53	123.10
1	A	1088	GLY	CA-C-N	5.64	131.85	121.70
1	A	1088	GLY	C-N-CA	5.64	131.85	121.70
1	A	307	ASP	CA-C-N	5.64	131.84	121.70
1	A	307	ASP	C-N-CA	5.64	131.84	121.70
2	B	694	ASP	CA-CB-CG	5.62	118.22	112.60
4	D	117	GLU	CB-CG-CD	5.60	122.12	112.60
2	B	332	ASP	CA-CB-CG	5.52	118.12	112.60
2	B	939	THR	CB-CA-C	5.48	115.60	110.17
1	A	219	PHE	CA-CB-CG	5.45	119.25	113.80
8	H	128	ASN	CA-C-N	5.41	131.87	121.54
8	H	128	ASN	C-N-CA	5.41	131.87	121.54
2	B	1152	MET	CA-C-N	5.35	127.71	120.38
2	B	1152	MET	C-N-CA	5.35	127.71	120.38
1	A	1331	SER	CA-C-N	5.31	127.93	120.28
1	A	1331	SER	C-N-CA	5.31	127.93	120.28
2	B	265	SER	O-C-N	-5.29	114.37	121.78
1	A	49	LYS	CA-C-N	5.25	127.64	120.35
1	A	49	LYS	C-N-CA	5.25	127.64	120.35
7	G	88	ASP	CA-CB-CG	5.23	117.83	112.60
2	B	221	ASN	CA-CB-CG	5.18	117.78	112.60
1	A	244	PRO	N-CA-C	5.17	117.01	110.70
1	A	739	ASP	CA-C-N	5.13	127.67	120.28
1	A	739	ASP	C-N-CA	5.13	127.67	120.28
4	D	169	SER	CA-C-N	5.13	127.87	120.38
4	D	169	SER	C-N-CA	5.13	127.87	120.38
13	R	2	U	P-O3'-C3'	-5.08	112.58	120.20
1	A	42	ASP	CA-C-N	5.06	128.41	120.82
1	A	42	ASP	C-N-CA	5.06	128.41	120.82
1	A	629	LEU	CA-C-N	5.01	127.07	120.60
1	A	629	LEU	C-N-CA	5.01	127.07	120.60
5	E	136	ASN	CA-C-N	5.00	126.94	120.44
5	E	136	ASN	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	S	32	DA	Sidechain
15	U	8	DA	Sidechain

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	11249	0	11277	121	0
2	B	9175	0	9138	128	0
3	C	2086	0	2049	24	0
4	D	1417	0	1428	10	0
5	E	1752	0	1776	11	0
6	F	705	0	731	13	0
7	G	1339	0	1357	13	0
8	H	1080	0	1049	9	0
9	I	921	0	877	10	0
10	J	532	0	546	5	0
11	K	924	0	934	11	0
12	L	346	0	367	3	0
13	R	197	0	97	4	0
14	S	268	0	149	25	0
15	U	549	0	303	33	0
All	All	32540	0	32078	354	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 6.

All (354) 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)
14:S:38:DA:N6	15:U:2:DC:N4	2.15	0.93
14:S:38:DA:N6	15:U:2:DC:C4	2.43	0.86
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.07	0.85
1:A:67:CYS:HG	1:A:77:CYS:HG	1.12	0.85
14:S:38:DA:H62	15:U:2:DC:N4	1.74	0.83
14:S:30:DT:H3	15:U:11:DA:H61	1.26	0.81
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.62	0.80
15:U:14:DA:H4'	15:U:15:DG:OP1	1.85	0.77
1:A:225:ASN:HB3	1:A:229:SER:H	1.50	0.77
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.68	0.75
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.69	0.75
2:B:79:THR:HA	2:B:81:SER:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:33:DT:H3	15:U:8:DA:H2	1.30	0.73
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.72	0.70
2:B:880:THR:HA	2:B:931:TYR:CD2	2.27	0.69
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.75	0.69
1:A:443:LEU:HD11	1:A:455:MET:HE2	1.76	0.68
2:B:136:THR:HA	2:B:137:TYR:HB3	1.77	0.67
15:U:11:DA:H2''	15:U:12:DG:O5'	1.96	0.66
1:A:365:GLY:HA3	1:A:469:ARG:HB3	1.76	0.66
14:S:30:DT:H3	15:U:11:DA:N6	1.94	0.66
1:A:1280:GLU:HB3	1:A:1309:ASP:HB3	1.76	0.66
14:S:27:DT:H3	15:U:15:DG:N2	1.94	0.66
1:A:1142:THR:HA	1:A:1273:LEU:HD13	1.79	0.65
14:S:27:DT:H1'	14:S:28:DG:C1'	2.28	0.64
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.80	0.64
2:B:644:GLU:HG3	2:B:647:GLY:H	1.64	0.63
1:A:496:GLU:HB2	6:F:99:LEU:HD12	1.82	0.62
4:D:23:ASN:HB3	7:G:82:PHE:HD1	1.66	0.61
14:S:33:DT:N3	15:U:8:DA:C2	2.57	0.61
14:S:34:DC:H2'	14:S:35:DG:C8	2.35	0.61
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.83	0.61
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.82	0.61
2:B:145:ARG:HA	2:B:146:GLU:CB	2.31	0.60
2:B:269:ILE:HG23	2:B:282:ILE:HG12	1.82	0.60
3:C:172:PRO:HA	3:C:235:VAL:HG22	1.84	0.60
14:S:31:DT:H2''	14:S:32:DA:H5''	1.84	0.59
2:B:1082:MET:HA	3:C:189:THR:HA	1.84	0.59
1:A:874:ASP:HB3	1:A:877:HIS:HD2	1.67	0.59
14:S:32:DA:N6	15:U:8:DA:C6	2.70	0.59
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.84	0.58
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.84	0.58
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.39	0.58
2:B:600:LEU:HA	2:B:603:LEU:HD12	1.85	0.58
2:B:654:ARG:H	2:B:657:HIS:HD2	1.50	0.58
1:A:49:LYS:HG3	1:A:61:ILE:HG13	1.85	0.58
14:S:27:DT:H1'	14:S:28:DG:O4'	2.03	0.58
7:G:137:ILE:HG12	7:G:143:ILE:HD11	1.86	0.57
3:C:186:LEU:HG	3:C:223:ALA:HB1	1.86	0.57
1:A:847:ASP:HB2	1:A:859:SER:H	1.69	0.57
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.87	0.56
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.86	0.56
7:G:49:LEU:HD11	7:G:77:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:VAL:HG22	1:A:468:PHE:HE1	1.70	0.56
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.88	0.56
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.88	0.56
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.87	0.56
2:B:899:ILE:HG12	2:B:949:VAL:HG21	1.87	0.56
1:A:451:HIS:CD2	1:A:453:MET:HB2	2.41	0.55
10:J:14:VAL:HA	10:J:17:LYS:HD3	1.88	0.55
1:A:438:ASP:HB3	1:A:461:LYS:HE3	1.88	0.55
1:A:315:LEU:HA	1:A:321:PRO:HA	1.89	0.55
1:A:451:HIS:HA	1:A:1070:GLN:HB3	1.89	0.55
3:C:77:ILE:HG13	3:C:161:LYS:HE3	1.88	0.55
14:S:29:DC:H42	15:U:12:DG:H1	1.54	0.55
14:S:32:DA:N6	15:U:8:DA:N6	2.55	0.55
1:A:396:PRO:HB3	1:A:403:LYS:HG3	1.90	0.54
1:A:524:VAL:HA	1:A:528:LEU:HB2	1.89	0.54
7:G:46:LEU:HB2	7:G:77:VAL:HG23	1.90	0.54
8:H:37:LYS:H	8:H:126:GLU:HB2	1.71	0.54
12:L:30:ILE:HG12	12:L:59:ALA:HB2	1.90	0.54
2:B:267:ARG:HD3	2:B:313:MET:HG2	1.90	0.53
1:A:370:ILE:HG12	2:B:1105:ALA:HB2	1.89	0.53
2:B:919:SER:HB2	2:B:920:PRO:HA	1.91	0.53
1:A:207:ILE:HA	1:A:210:ILE:HD12	1.90	0.53
2:B:638:PHE:HB2	2:B:741:CYS:HB3	1.91	0.53
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.91	0.53
1:A:838:GLN:HG3	1:A:1073:GLY:HA3	1.91	0.53
2:B:145:ARG:HA	2:B:146:GLU:HB2	1.90	0.53
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.74	0.53
3:C:258:ILE:HG13	11:K:19:LEU:HD11	1.90	0.53
1:A:669:THR:HG23	1:A:805:LEU:HD13	1.91	0.52
1:A:506:ALA:HB3	1:A:509:LEU:HD12	1.91	0.52
2:B:778:MET:SD	2:B:794:ASN:HB3	2.50	0.52
14:S:32:DA:H61	15:U:9:DT:H3	1.56	0.52
2:B:883:LEU:HG	2:B:931:TYR:HB2	1.92	0.52
15:U:15:DG:C2'	15:U:16:DA:H5'	2.40	0.52
1:A:333:GLU:HA	1:A:338:GLY:HA3	1.91	0.52
1:A:467:THR:HG23	1:A:469:ARG:HH12	1.75	0.52
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.92	0.52
5:E:28:TYR:HA	5:E:64:PRO:HA	1.92	0.52
7:G:93:SER:HB2	7:G:100:GLU:HB2	1.92	0.52
2:B:581:PHE:HB2	2:B:625:LYS:HG2	1.92	0.51
1:A:774:ARG:HG3	1:A:797:LYS:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:LEU:HD23	2:B:545:ILE:HG21	1.93	0.51
2:B:373:ARG:HG2	2:B:566:LEU:HB3	1.92	0.51
7:G:112:LYS:HA	7:G:115:MET:HE3	1.91	0.51
14:S:38:DA:H61	15:U:3:DT:H3	1.59	0.51
15:U:27:DG:H2''	15:U:28:DA:O5'	2.11	0.51
6:F:74:ILE:HB	6:F:144:GLU:HG2	1.92	0.51
2:B:20:ASP:HB3	2:B:23:ALA:HB2	1.91	0.51
14:S:37:DT:O4	15:U:4:DA:N1	2.44	0.51
1:A:560:ILE:HD12	8:H:78:SER:HB2	1.92	0.51
1:A:2:VAL:HG12	2:B:1159:ARG:HG3	1.92	0.51
2:B:1112:GLN:HG3	13:R:2:U:OP1	2.11	0.51
8:H:2:SER:HB2	8:H:64:ASN:HB2	1.92	0.51
1:A:774:ARG:HH21	1:A:794:PRO:HA	1.76	0.51
2:B:806:THR:HG23	2:B:1045:SER:HA	1.93	0.51
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.93	0.50
2:B:1084:GLN:HE22	3:C:191:TYR:HA	1.75	0.50
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.93	0.50
1:A:567:LYS:H	8:H:96:VAL:HB	1.76	0.50
1:A:662:PHE:HB3	2:B:829:CYS:SG	2.51	0.50
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.93	0.50
2:B:420:LEU:HD21	2:B:456:GLY:HA3	1.92	0.50
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.92	0.50
2:B:642:ASP:HA	2:B:649:LYS:HG2	1.92	0.50
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.94	0.50
1:A:31:SER:HB2	1:A:83:HIS:HB3	1.92	0.50
1:A:182:VAL:HG12	1:A:201:VAL:HA	1.94	0.50
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.93	0.50
3:C:46:ILE:HA	3:C:159:ALA:HA	1.92	0.50
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.93	0.50
1:A:1331:SER:HB3	1:A:1333:ILE:HG22	1.93	0.50
2:B:604:ARG:HD2	2:B:611:PRO:HA	1.93	0.50
2:B:74:LEU:HD12	2:B:85:SER:HB2	1.93	0.49
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.94	0.49
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.94	0.49
2:B:994:TYR:HB2	2:B:999:MET:HE3	1.93	0.49
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.93	0.49
1:A:596:THR:C	1:A:598:LEU:H	2.20	0.49
9:I:82:GLU:HG2	9:I:104:LEU:HD23	1.93	0.49
1:A:508:PRO:HB3	1:A:643:ALA:HB2	1.94	0.49
1:A:92:HIS:HB3	1:A:95:PHE:HD2	1.78	0.49
2:B:125:SER:HB2	2:B:169:ARG:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:7:PHE:HB2	11:K:11:LEU:HD12	1.95	0.49
2:B:999:MET:HG3	2:B:1011:ILE:HD11	1.95	0.49
2:B:1129:ARG:HG2	15:U:21:DC:H5''	1.95	0.49
2:B:55:VAL:HA	2:B:59:LEU:HD12	1.94	0.48
14:S:27:DT:H1'	14:S:28:DG:H1'	1.95	0.48
4:D:56:ARG:HD2	4:D:149:THR:HA	1.96	0.48
1:A:1080:THR:HG22	1:A:1081:LEU:HD12	1.94	0.48
2:B:238:ALA:HB2	2:B:385:LEU:HD13	1.95	0.48
1:A:1453:TYR:HB3	6:F:129:LYS:HE2	1.95	0.48
2:B:796:LEU:HD23	2:B:799:PRO:HA	1.95	0.48
2:B:880:THR:HA	2:B:931:TYR:HD2	1.72	0.48
3:C:142:VAL:H	10:J:16:ASP:HB3	1.77	0.48
14:S:35:DG:H2''	14:S:36:DG:C8	2.49	0.48
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.94	0.48
1:A:88:LYS:HD3	1:A:293:GLU:HG3	1.96	0.48
1:A:453:MET:C	1:A:455:MET:H	2.22	0.48
1:A:1227:ILE:HB	1:A:1239:ARG:HB2	1.95	0.48
14:S:35:DG:C2	15:U:7:DG:N2	2.82	0.48
2:B:31:TRP:HA	2:B:34:ILE:HD12	1.95	0.47
4:D:208:GLU:HA	4:D:211:LEU:HD12	1.96	0.47
15:U:3:DT:H2''	15:U:4:DA:C8	2.49	0.47
15:U:10:DA:H2''	15:U:11:DA:H8	1.79	0.47
14:S:33:DT:N3	15:U:8:DA:H2	2.04	0.47
1:A:1313:LEU:HD23	1:A:1338:VAL:HG11	1.96	0.47
2:B:661:LEU:HD21	2:B:684:LEU:HD11	1.96	0.47
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.96	0.47
1:A:579:SER:HA	1:A:582:ILE:HD12	1.97	0.47
1:A:702:LEU:HB3	1:A:710:LEU:HD11	1.97	0.47
1:A:1220:PHE:HB3	1:A:1223:ASP:HB2	1.96	0.47
2:B:127:GLY:HA2	2:B:169:ARG:HG2	1.97	0.47
2:B:420:LEU:HD22	2:B:453:ILE:HA	1.97	0.47
2:B:640:VAL:HA	2:B:651:LEU:HA	1.96	0.47
2:B:1133:MET:HG3	15:U:20:DT:H4'	1.97	0.47
2:B:505:ASP:H	2:B:506:GLY:HA2	1.80	0.47
2:B:855:PHE:HB3	2:B:970:THR:HB	1.96	0.47
1:A:852:TYR:HB3	6:F:81:THR:HG22	1.96	0.47
1:A:1345:ARG:HB3	1:A:1376:THR:HG21	1.95	0.47
3:C:108:GLU:HG3	3:C:149:LYS:HE2	1.96	0.47
10:J:7:CYS:SG	10:J:10:CYS:SG	3.12	0.47
1:A:711:ARG:HG2	9:I:97:MET:HE2	1.97	0.47
2:B:910:VAL:HA	2:B:940:PRO:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:LEU:HA	1:A:1104:ILE:HD12	1.96	0.46
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.97	0.46
15:U:14:DA:H1'	15:U:15:DG:O4'	2.16	0.46
1:A:701:LEU:HA	9:I:115:LYS:HE3	1.98	0.46
2:B:1080:LYS:HB2	3:C:188:HIS:HB3	1.95	0.46
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	1.96	0.46
2:B:705:MET:HE3	2:B:742:GLU:HG2	1.96	0.46
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.50	0.46
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.50	0.46
3:C:82:TYR:HB3	3:C:84:ARG:HG2	1.97	0.46
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.97	0.46
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.97	0.46
1:A:855:THR:HG21	1:A:857:ARG:HE	1.81	0.46
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.98	0.46
2:B:79:THR:HA	2:B:81:SER:H	1.80	0.46
1:A:152:VAL:H	1:A:153:PRO:CD	2.28	0.46
1:A:746:MET:HE1	2:B:1014:PRO:HB2	1.98	0.46
2:B:215:GLN:HE22	2:B:499:ASN:HB3	1.80	0.46
2:B:246:LYS:HE3	2:B:249:ARG:HA	1.97	0.46
14:S:38:DA:N6	15:U:3:DT:H3	2.12	0.46
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.98	0.46
2:B:261:ARG:C	2:B:264:SER:N	2.74	0.46
2:B:526:GLU:HG3	2:B:771:SER:HB2	1.97	0.46
4:D:59:ILE:HD13	4:D:145:MET:HE1	1.98	0.46
1:A:396:PRO:HG2	1:A:416:ARG:HG3	1.98	0.45
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.98	0.45
1:A:874:ASP:HB3	1:A:877:HIS:CD2	2.50	0.45
1:A:883:LEU:H	1:A:952:ALA:HB1	1.80	0.45
4:D:71:LYS:HA	4:D:74:GLN:HG3	1.97	0.45
8:H:101:ALA:HB3	8:H:138:GLU:HA	1.98	0.45
1:A:753:GLY:HA2	1:A:757:ASN:HD22	1.80	0.45
2:B:309:GLN:HE22	9:I:52:ILE:HG12	1.81	0.45
3:C:115:SER:O	3:C:118:LEU:HG	2.17	0.45
5:E:89:GLY:HA2	5:E:117:THR:HG22	1.98	0.45
11:K:20:LYS:HB2	11:K:34:THR:HB	1.98	0.45
1:A:317:LYS:HA	1:A:318:SER:C	2.40	0.45
2:B:429:PHE:HA	2:B:432:MET:HB2	1.97	0.45
14:S:29:DC:N4	15:U:12:DG:H1	2.13	0.45
1:A:464:PRO:HB2	11:K:4:PRO:HD3	1.97	0.45
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.43	0.45
1:A:446:ARG:HG3	1:A:487:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1447:GLU:HA	1:A:1450:LEU:HD12	1.98	0.45
3:C:35:ARG:HH11	11:K:41:THR:HB	1.81	0.45
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.98	0.45
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.80	0.45
3:C:50:GLU:HB2	3:C:156:THR:HB	1.98	0.45
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.99	0.45
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.99	0.45
1:A:1313:LEU:HG	1:A:1317:MET:HB2	1.99	0.45
3:C:262:LEU:HD21	11:K:87:LEU:HD23	1.99	0.45
11:K:35:PHE:O	11:K:70:ARG:HA	2.17	0.45
5:E:38:PRO:HD2	5:E:41:ASP:HB2	1.99	0.45
1:A:403:LYS:HE2	1:A:416:ARG:HH21	1.82	0.44
2:B:136:THR:HA	2:B:137:TYR:CB	2.45	0.44
2:B:464:GLY:O	2:B:477:ALA:HA	2.17	0.44
4:D:59:ILE:HG12	7:G:77:VAL:HG21	1.99	0.44
2:B:364:ILE:HG12	2:B:585:VAL:CG1	2.45	0.44
5:E:161:LYS:HE2	5:E:165:LEU:HD11	1.99	0.44
15:U:11:DA:H2'	15:U:12:DG:C8	2.52	0.44
2:B:505:ASP:N	2:B:506:GLY:HA2	2.33	0.44
2:B:235:SER:HA	2:B:261:ARG:NH1	2.33	0.44
1:A:1171:GLN:HE21	1:A:1172:LEU:HG	1.83	0.44
8:H:15:VAL:HG22	8:H:26:ILE:HG12	2.00	0.44
1:A:351:THR:HG22	1:A:468:PHE:CD2	2.53	0.44
2:B:776:GLN:HE22	13:R:9:G:H5'	1.82	0.44
11:K:58:PHE:HE1	11:K:74:ARG:HB3	1.83	0.44
15:U:17:DC:H2''	15:U:18:DG:O5'	2.18	0.44
1:A:152:VAL:H	1:A:153:PRO:HD2	1.82	0.44
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.98	0.44
1:A:720:ARG:O	1:A:724:GLU:HB2	2.18	0.43
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.99	0.43
2:B:287:ARG:HG2	2:B:292:ILE:HA	2.00	0.43
2:B:294:ASP:HB2	9:I:12:ASN:HA	2.00	0.43
2:B:301:ILE:HD13	2:B:379:GLY:HA2	2.01	0.43
6:F:130:ILE:HG22	6:F:132:LEU:H	1.83	0.43
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.83	0.43
2:B:868:MET:HG3	2:B:869:SER:N	2.33	0.43
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.53	0.43
2:B:425:THR:HA	2:B:428:ILE:HD12	2.00	0.43
2:B:652:LYS:HB3	2:B:689:LEU:HD23	2.00	0.43
3:C:176:ILE:HG12	3:C:232:VAL:HG13	2.01	0.43
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ASN:HA	1:A:459:ARG:HG3	2.00	0.43
1:A:919:ILE:HG13	1:A:925:LEU:HD13	1.99	0.43
2:B:39:ARG:HH22	2:B:668:ASP:HA	1.83	0.43
2:B:392:ARG:HH21	9:I:52:ILE:HD13	1.84	0.43
2:B:526:GLU:HB3	2:B:538:ASN:HB2	2.00	0.43
2:B:754:SER:HB2	2:B:812:LEU:HD11	2.00	0.43
5:E:23:VAL:HG13	5:E:78:LEU:HD21	2.01	0.43
10:J:43:ARG:HB2	10:J:46:CYS:SG	2.58	0.43
6:F:84:TYR:HA	6:F:152:ILE:HG13	2.01	0.43
2:B:225:VAL:H	2:B:396:ASP:HB2	1.84	0.43
2:B:416:LEU:HD23	2:B:457:LEU:HD23	2.01	0.43
2:B:931:TYR:CD2	2:B:931:TYR:N	2.85	0.43
1:A:1087:ALA:HA	1:A:1088:GLY:HA3	1.67	0.43
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.54	0.42
2:B:842:ASN:O	2:B:846:ILE:HG12	2.19	0.42
2:B:800:GLN:HB2	2:B:821:GLN:HA	2.02	0.42
1:A:41:MET:HA	1:A:49:LYS:HD3	2.00	0.42
1:A:883:LEU:HD22	1:A:943:LEU:HD21	2.02	0.42
2:B:593:PRO:HG2	2:B:617:ARG:HH21	1.84	0.42
2:B:637:LEU:HD12	2:B:693:ILE:HD13	2.01	0.42
2:B:912:ILE:HB	2:B:939:THR:HB	2.01	0.42
5:E:190:LEU:HD12	5:E:214:CYS:HB2	2.01	0.42
6:F:86:THR:HG23	6:F:89:GLU:H	1.83	0.42
15:U:7:DG:H2"	15:U:8:DA:C8	2.54	0.42
1:A:106:VAL:HG22	1:A:113:LEU:HD23	2.02	0.42
1:A:1205:LYS:HB3	1:A:1274:ARG:NH2	2.34	0.42
4:D:6:SER:HA	7:G:42:PHE:HE2	1.85	0.42
5:E:100:ILE:HG23	5:E:105:PHE:HB2	2.00	0.42
11:K:49:GLU:HG3	11:K:94:ILE:HG12	2.02	0.42
1:A:115:LEU:HD23	1:A:122:MET:HB2	2.01	0.42
1:A:361:LEU:HD21	1:A:511:ILE:HD11	2.01	0.42
1:A:1031:VAL:HA	1:A:1035:TYR:CD2	2.55	0.42
2:B:356:LEU:HA	2:B:360:PHE:HB3	2.01	0.42
6:F:117:PRO:HA	6:F:120:ILE:HD12	2.02	0.42
1:A:482:PHE:HB2	2:B:838:SER:HB3	2.01	0.42
2:B:103:ASN:HD21	2:B:169:ARG:HH22	1.68	0.42
13:R:2:U:C4	13:R:3:C:N4	2.87	0.42
1:A:404:TYR:HB2	1:A:433:GLU:HG3	2.02	0.42
2:B:860:MET:HB3	2:B:965:LYS:HG2	2.01	0.42
9:I:16:PRO:HB2	9:I:25:LEU:HD11	2.01	0.42
1:A:1111:MET:O	1:A:1112:LYS:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:LEU:HA	2:B:495:LEU:HD12	2.01	0.41
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	2.01	0.41
1:A:523:ILE:HG23	1:A:527:THR:HB	2.02	0.41
2:B:276:ILE:HG22	2:B:278:GLN:H	1.85	0.41
2:B:234:ILE:HG12	2:B:257:LYS:HB3	2.02	0.41
1:A:1031:VAL:HA	1:A:1035:TYR:HD2	1.84	0.41
2:B:930:ALA:HB1	2:B:931:TYR:HA	2.01	0.41
7:G:165:GLU:HB2	7:G:168:LEU:HD12	2.03	0.41
2:B:1080:LYS:HE3	3:C:188:HIS:HB2	2.01	0.41
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.61	0.41
2:B:377:PHE:HE2	2:B:585:VAL:HA	1.86	0.41
2:B:542:MET:HB3	2:B:636:PRO:HD2	2.02	0.41
2:B:638:PHE:HE2	2:B:743:ILE:HA	1.86	0.41
5:E:23:VAL:HG12	5:E:28:TYR:HB2	2.02	0.41
1:A:665:GLY:HA2	2:B:1026:LEU:HD22	2.03	0.41
2:B:1168:LEU:C	2:B:1170:THR:H	2.29	0.41
3:C:259:LEU:HA	3:C:262:LEU:HD12	2.02	0.41
1:A:186:LYS:HD2	1:A:197:PRO:HB3	2.02	0.41
1:A:512:VAL:HA	1:A:519:PRO:HA	2.03	0.41
1:A:981:LEU:HD23	1:A:1039:LYS:HA	2.01	0.41
1:A:37:PHE:HA	1:A:38:PRO:HD3	1.98	0.41
1:A:93:VAL:HG13	1:A:301:ALA:HB1	2.03	0.41
1:A:746:MET:SD	2:B:1015:HIS:HA	2.61	0.41
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	2.02	0.41
2:B:1112:GLN:CG	13:R:2:U:OP1	2.69	0.41
4:D:11:ARG:HA	4:D:12:ARG:HA	1.77	0.41
4:D:168:LYS:HG3	4:D:177:VAL:HG11	2.02	0.41
8:H:6:PHE:HD1	8:H:130:ARG:HG3	1.86	0.41
11:K:91:CYS:HA	11:K:94:ILE:HD12	2.03	0.41
1:A:1187:GLN:HB2	1:A:1245:PRO:HG3	2.03	0.41
1:A:1292:PRO:HA	1:A:1298:TYR:HA	2.02	0.41
4:D:202:ILE:HG21	4:D:207:LEU:HD13	2.02	0.41
9:I:52:ILE:H	9:I:52:ILE:HG13	1.77	0.41
15:U:12:DG:H4'	15:U:13:DC:OP1	2.20	0.41
1:A:519:PRO:HD3	1:A:631:HIS:HD2	1.83	0.40
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	2.02	0.40
2:B:85:SER:HB3	2:B:139:ALA:HB3	2.03	0.40
2:B:144:GLY:HA2	2:B:145:ARG:HA	1.92	0.40
2:B:625:LYS:HD3	2:B:627:PHE:HE1	1.86	0.40
7:G:108:VAL:HG22	7:G:159:ALA:HB3	2.03	0.40
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:85:MET:HB2	6:F:151:LEU:HB3	2.02	0.40
6:F:97:ARG:HD3	6:F:130:ILE:HG23	2.02	0.40
14:S:37:DT:O4	15:U:4:DA:C2	2.74	0.40
1:A:785:PRO:HB2	2:B:703:ILE:HD12	2.03	0.40
2:B:778:MET:HB2	2:B:1094:ARG:HB3	2.02	0.40
2:B:792:MET:HG3	2:B:855:PHE:CE1	2.57	0.40
2:B:911:ILE:H	2:B:911:ILE:HG13	1.83	0.40
7:G:85:GLU:HB3	7:G:147:ILE:HD12	2.03	0.40
15:U:11:DA:H2'	15:U:12:DG:H8	1.86	0.40
1:A:442:VAL:HG22	1:A:492:PRO:HD2	2.04	0.40
2:B:120:ARG:HG2	2:B:955:THR:HG21	2.03	0.40
2:B:221:ASN:HB3	2:B:243:ALA:H	1.85	0.40
12:L:40:LEU:HB2	12:L:44:ASP:HB3	2.03	0.40
6:F:100:GLN:HG2	7:G:15:PRO:HB3	2.02	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	1426/1733 (82%)	1227 (86%)	135 (10%)	64 (4%)	2	20
2	B	1134/1224 (93%)	967 (85%)	121 (11%)	46 (4%)	2	21
3	C	263/318 (83%)	228 (87%)	26 (10%)	9 (3%)	3	24
4	D	174/221 (79%)	152 (87%)	12 (7%)	10 (6%)	1	17
5	E	212/215 (99%)	198 (93%)	10 (5%)	4 (2%)	6	33
6	F	85/155 (55%)	79 (93%)	3 (4%)	3 (4%)	3	23
7	G	169/179 (94%)	143 (85%)	21 (12%)	5 (3%)	3	26
8	H	129/146 (88%)	111 (86%)	14 (11%)	4 (3%)	3	25
9	I	112/120 (93%)	98 (88%)	13 (12%)	1 (1%)	14	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	63/70 (90%)	56 (89%)	3 (5%)	4 (6%)	1	15
11	K	113/120 (94%)	110 (97%)	3 (3%)	0	100	100
12	L	42/70 (60%)	31 (74%)	8 (19%)	3 (7%)	1	14
All	All	3922/4571 (86%)	3400 (87%)	369 (9%)	153 (4%)	2	22

All (153) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	66	LYS
1	A	319	GLY
1	A	385	ILE
1	A	567	LYS
1	A	751	SER
1	A	775	ILE
1	A	1016	THR
1	A	1064	VAL
2	B	80	GLU
2	B	137	TYR
2	B	334	ILE
2	B	648	HIS
2	B	712	PRO
3	C	91	HIS
6	F	73	ALA
7	G	141	SER
9	I	106	CYS
1	A	52	GLY
1	A	152	VAL
1	A	194	ALA
1	A	286	HIS
1	A	418	SER
1	A	423	ASP
1	A	466	SER
1	A	593	GLU
1	A	626	ASN
1	A	640	GLN
1	A	1107	VAL
1	A	1378	GLN
1	A	1403	GLU
1	A	1404	GLU
1	A	1437	GLY

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Mol	Chain	Res	Type
2	B	164	LYS
2	B	250	PHE
2	B	367	LEU
2	B	531	GLN
2	B	575	PRO
2	B	907	GLY
2	B	932	HIS
2	B	1156	ASP
2	B	1157	ALA
3	C	142	VAL
3	C	161	LYS
3	C	174	ALA
3	C	267	GLN
4	D	15	LEU
4	D	16	LYS
5	E	172	GLU
7	G	153	GLN
10	J	2	ILE
12	L	55	ILE
1	A	42	ASP
1	A	57	ARG
1	A	63	ARG
1	A	146	MET
1	A	188	ASP
1	A	251	SER
1	A	314	ALA
1	A	335	ARG
1	A	410	GLY
1	A	453	MET
1	A	595	THR
1	A	953	ASN
1	A	1221	LYS
2	B	148	LYS
2	B	161	GLU
2	B	221	ASN
2	B	711	GLU
2	B	751	VAL
2	B	778	MET
2	B	925	LEU
2	B	935	ARG
2	B	1046	PRO
2	B	1169	MET

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Mol	Chain	Res	Type
2	B	1185	CYS
3	C	90	ASP
3	C	149	LYS
3	C	243	VAL
4	D	18	VAL
4	D	198	LEU
5	E	3	GLN
5	E	115	ASN
7	G	63	PRO
7	G	154	VAL
8	H	83	GLN
8	H	108	SER
8	H	129	TYR
10	J	15	GLY
1	A	61	ILE
1	A	76	GLU
1	A	131	SER
1	A	156	ASP
1	A	283	GLY
1	A	332	LYS
1	A	424	ILE
1	A	1112	LYS
1	A	1115	SER
1	A	1365	TYR
2	B	81	SER
2	B	146	GLU
2	B	198	ASP
2	B	441	ASP
2	B	831	SER
2	B	889	THR
2	B	923	GLU
2	B	951	GLN
2	B	1108	ARG
2	B	1186	ASP
2	B	1215	ARG
4	D	8	PHE
4	D	20	GLU
5	E	104	ASN
6	F	72	LYS
7	G	120	THR
8	H	17	PRO
10	J	6	ARG

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Mol	Chain	Res	Type
12	L	45	ALA
12	L	59	ALA
1	A	35	ILE
1	A	54	ASN
1	A	158	PRO
1	A	465	TYR
1	A	958	VAL
1	A	1080	THR
1	A	1206	ASP
1	A	1377	THR
2	B	943	SER
3	C	215	GLU
4	D	11	ARG
4	D	17	LYS
4	D	169	SER
4	D	199	ASN
6	F	78	GLN
10	J	10	CYS
2	B	442	PHE
2	B	727	LYS
2	B	881	ASN
1	A	250	ILE
1	A	311	GLN
2	B	1045	SER
1	A	59	GLY
1	A	568	PRO
1	A	1089	VAL
1	A	1388	GLY
2	B	144	GLY
2	B	1017	ILE
1	A	308	ILE
1	A	1156	PRO
2	B	251	ILE
2	B	1109	GLY
1	A	334	GLY
2	B	163	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1244/1520 (82%)	1139 (92%)	105 (8%)	10	33
2	B	996/1061 (94%)	917 (92%)	79 (8%)	11	35
3	C	233/274 (85%)	215 (92%)	18 (8%)	12	36
4	D	156/200 (78%)	145 (93%)	11 (7%)	13	39
5	E	196/197 (100%)	184 (94%)	12 (6%)	17	42
6	F	77/137 (56%)	74 (96%)	3 (4%)	28	51
7	G	152/160 (95%)	143 (94%)	9 (6%)	18	43
8	H	118/128 (92%)	114 (97%)	4 (3%)	32	55
9	I	107/114 (94%)	105 (98%)	2 (2%)	50	67
10	J	60/65 (92%)	53 (88%)	7 (12%)	5	21
11	K	99/102 (97%)	92 (93%)	7 (7%)	13	39
12	L	38/57 (67%)	31 (82%)	7 (18%)	1	11
All	All	3476/4015 (87%)	3212 (92%)	264 (8%)	12	37

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	57	ARG
1	A	58	LEU
1	A	66	LYS
1	A	69	THR
1	A	70	CYS
1	A	93	VAL
1	A	103	CYS
1	A	110	CYS
1	A	114	LEU
1	A	115	LEU
1	A	120	GLU
1	A	152	VAL
1	A	164	ARG
1	A	187	LYS
1	A	276	LEU
1	A	279	LEU
1	A	323	LYS
1	A	329	LEU

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Mol	Chain	Res	Type
1	A	333	GLU
1	A	353	ILE
1	A	385	ILE
1	A	415	LEU
1	A	447	GLN
1	A	461	LYS
1	A	463	ILE
1	A	469	ARG
1	A	470	LEU
1	A	485	ASP
1	A	495	GLU
1	A	511	ILE
1	A	518	LYS
1	A	523	ILE
1	A	524	VAL
1	A	527	THR
1	A	528	LEU
1	A	536	LEU
1	A	542	GLU
1	A	546	VAL
1	A	582	ILE
1	A	593	GLU
1	A	595	THR
1	A	597	LEU
1	A	598	LEU
1	A	618	GLU
1	A	635	ARG
1	A	657	LEU
1	A	666	ILE
1	A	677	ARG
1	A	685	GLU
1	A	701	LEU
1	A	732	LEU
1	A	734	GLU
1	A	738	LYS
1	A	743	VAL
1	A	845	LEU
1	A	860	LEU
1	A	878	ILE
1	A	913	LEU
1	A	919	ILE
1	A	963	ILE

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Mol	Chain	Res	Type
1	A	981	LEU
1	A	983	ILE
1	A	988	LEU
1	A	995	GLU
1	A	998	LEU
1	A	1006	ILE
1	A	1016	THR
1	A	1017	LEU
1	A	1034	GLU
1	A	1037	LEU
1	A	1048	ASN
1	A	1058	VAL
1	A	1067	LEU
1	A	1074	GLU
1	A	1077	THR
1	A	1098	VAL
1	A	1110	ASN
1	A	1111	MET
1	A	1116	LEU
1	A	1120	LEU
1	A	1186	ASP
1	A	1193	LEU
1	A	1224	LEU
1	A	1227	ILE
1	A	1233	ASP
1	A	1242	VAL
1	A	1244	ARG
1	A	1277	GLU
1	A	1291	VAL
1	A	1303	GLU
1	A	1306	LEU
1	A	1323	ASP
1	A	1354	ASN
1	A	1356	ILE
1	A	1359	ASP
1	A	1366	ARG
1	A	1371	LEU
1	A	1381	LEU
1	A	1394	THR
1	A	1403	GLU
1	A	1406	VAL
1	A	1409	LEU

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Mol	Chain	Res	Type
1	A	1426	GLU
1	A	1436	ILE
2	B	26	THR
2	B	28	GLU
2	B	63	ILE
2	B	66	ASP
2	B	95	ILE
2	B	112	LEU
2	B	115	GLN
2	B	167	ILE
2	B	178	ASN
2	B	217	ARG
2	B	225	VAL
2	B	228	LYS
2	B	251	ILE
2	B	273	LEU
2	B	282	ILE
2	B	298	LEU
2	B	324	ILE
2	B	333	PHE
2	B	341	LEU
2	B	356	LEU
2	B	361	LEU
2	B	364	ILE
2	B	396	ASP
2	B	401	PHE
2	B	424	LEU
2	B	437	GLU
2	B	438	GLU
2	B	461	LEU
2	B	485	ARG
2	B	497	ARG
2	B	510	LYS
2	B	522	VAL
2	B	529	GLU
2	B	539	LEU
2	B	549	THR
2	B	555	ILE
2	B	566	LEU
2	B	616	ILE
2	B	619	ILE
2	B	624	LEU

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Mol	Chain	Res	Type
2	B	633	VAL
2	B	651	LEU
2	B	658	ILE
2	B	698	GLU
2	B	711	GLU
2	B	743	ILE
2	B	795	ILE
2	B	797	TYR
2	B	817	LEU
2	B	825	VAL
2	B	841	MET
2	B	854	LEU
2	B	868	MET
2	B	875	GLU
2	B	891	ASP
2	B	899	ILE
2	B	911	ILE
2	B	931	TYR
2	B	953	LEU
2	B	955	THR
2	B	959	ASP
2	B	964	VAL
2	B	965	LYS
2	B	971	THR
2	B	983	ARG
2	B	1007	VAL
2	B	1028	GLU
2	B	1031	LEU
2	B	1087	PHE
2	B	1093	GLN
2	B	1147	LEU
2	B	1150	ARG
2	B	1159	ARG
2	B	1162	ILE
2	B	1165	ILE
2	B	1166	CYS
2	B	1191	ILE
2	B	1202	LEU
2	B	1215	ARG
3	C	19	ASP
3	C	22	LEU
3	C	43	THR

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Mol	Chain	Res	Type
3	C	44	LEU
3	C	52	GLU
3	C	55	THR
3	C	56	THR
3	C	72	LEU
3	C	101	LEU
3	C	133	ILE
3	C	138	GLU
3	C	140	ASN
3	C	142	VAL
3	C	186	LEU
3	C	203	GLN
3	C	240	VAL
3	C	245	VAL
3	C	258	ILE
4	D	15	LEU
4	D	38	ILE
4	D	50	LEU
4	D	57	LEU
4	D	120	GLU
4	D	134	THR
4	D	139	LYS
4	D	164	ILE
4	D	187	THR
4	D	214	LEU
4	D	218	GLU
5	E	14	ARG
5	E	33	GLU
5	E	37	LEU
5	E	39	LEU
5	E	58	MET
5	E	80	VAL
5	E	92	THR
5	E	116	ILE
5	E	123	LEU
5	E	144	ILE
5	E	149	LEU
5	E	175	LEU
6	F	79	ARG
6	F	111	LEU
6	F	132	LEU
7	G	13	LEU

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Mol	Chain	Res	Type
7	G	39	THR
7	G	45	ILE
7	G	57	GLN
7	G	64	THR
7	G	119	LEU
7	G	134	GLU
7	G	154	VAL
7	G	171	ILE
8	H	27	GLU
8	H	111	LEU
8	H	125	LEU
8	H	126	GLU
9	I	3	THR
9	I	68	LEU
10	J	3	VAL
10	J	22	LEU
10	J	24	LEU
10	J	49	MET
10	J	51	LEU
10	J	57	ILE
10	J	64	ASN
11	K	12	LEU
11	K	42	LEU
11	K	47	ARG
11	K	49	GLU
11	K	51	LEU
11	K	75	ILE
11	K	114	LEU
12	L	27	LEU
12	L	33	GLU
12	L	37	LYS
12	L	40	LEU
12	L	43	THR
12	L	57	LEU
12	L	64	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	18	GLN
1	A	68	GLN

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	273	ASN
1	A	358	ASN
1	A	447	GLN
1	A	471	ASN
1	A	515	GLN
1	A	525	GLN
1	A	648	ASN
1	A	660	ASN
1	A	767	GLN
1	A	877	HIS
1	A	906	HIS
1	A	1009	ASN
1	A	1033	GLN
1	A	1128	GLN
1	A	1171	GLN
1	A	1265	ASN
1	A	1312	ASN
1	A	1330	ASN
1	A	1354	ASN
2	B	103	ASN
2	B	115	GLN
2	B	215	GLN
2	B	255	GLN
2	B	300	HIS
2	B	325	GLN
2	B	363	HIS
2	B	531	GLN
2	B	592	ASN
2	B	706	GLN
2	B	770	GLN
2	B	776	GLN
2	B	835	GLN
2	B	843	GLN
2	B	975	GLN
2	B	1065	GLN
2	B	1141	HIS
2	B	1179	GLN
2	B	1211	ASN
3	C	7	GLN
3	C	131	HIS
3	C	151	GLN

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Mol	Chain	Res	Type
4	D	9	GLN
4	D	51	ASN
4	D	150	ASN
4	D	179	GLN
5	E	106	GLN
5	E	115	ASN
6	F	78	GLN
7	G	53	ASN
8	H	33	GLN
8	H	43	ASN
8	H	134	ASN
8	H	137	GLN
8	H	139	ASN
9	I	46	HIS
9	I	51	ASN
9	I	60	GLN
9	I	83	ASN
9	I	87	GLN
10	J	64	ASN
11	K	44	ASN
11	K	96	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	7/9 (77%)	2 (28%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	3	C
13	R	6	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1434/1733 (82%)	0.25	43 (2%) 52 37	75, 183, 269, 300	0
2	B	1158/1224 (94%)	0.36	39 (3%) 48 34	84, 195, 283, 300	0
3	C	265/318 (83%)	0.30	6 (2%) 61 43	119, 190, 255, 297	0
4	D	178/221 (80%)	0.32	5 (2%) 55 39	115, 201, 273, 300	0
5	E	214/215 (99%)	0.36	11 (5%) 33 26	131, 218, 277, 294	0
6	F	87/155 (56%)	0.01	2 (2%) 61 43	91, 156, 211, 261	0
7	G	171/179 (95%)	0.24	6 (3%) 47 33	117, 184, 232, 300	0
8	H	135/146 (92%)	0.36	5 (3%) 45 33	150, 236, 291, 300	0
9	I	114/120 (95%)	0.57	7 (6%) 27 23	156, 234, 282, 300	0
10	J	65/70 (92%)	0.31	2 (3%) 51 36	114, 197, 266, 287	0
11	K	115/120 (95%)	0.28	2 (1%) 69 49	113, 189, 252, 273	0
12	L	44/70 (62%)	0.77	2 (4%) 38 29	155, 219, 273, 300	0
13	R	9/9 (100%)	1.11	2 (22%) 2 4	230, 267, 300, 300	0
14	S	13/53 (24%)	3.66	13 (100%) 0 0	20, 167, 300, 300	0
15	U	27/53 (50%)	2.48	18 (66%) 0 1	160, 198, 300, 300	0
All	All	4029/4686 (85%)	0.34	163 (4%) 42 31	20, 193, 276, 300	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1081	LEU	5.1
15	U	10	DA	5.1
15	U	5	DC	4.9
14	S	28	DG	4.8
14	S	38	DA	4.7
15	U	8	DA	4.7
14	S	36	DG	4.6

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Mol	Chain	Res	Type	RSRZ
14	S	31	DT	4.6
8	H	45	GLU	4.4
2	B	880	THR	4.4
1	A	1080	THR	4.2
15	U	13	DC	4.0
2	B	266	ALA	3.9
15	U	28	DA	3.8
1	A	145	LYS	3.8
2	B	929	THR	3.7
15	U	15	DG	3.7
14	S	35	DG	3.7
1	A	2	VAL	3.7
15	U	7	DG	3.6
15	U	12	DG	3.6
14	S	34	DC	3.5
1	A	1086	PHE	3.5
2	B	1049	ASP	3.5
14	S	39	DG	3.4
1	A	1084	PHE	3.4
6	F	69	LEU	3.4
13	R	2	U	3.3
5	E	93	MET	3.3
1	A	1091	SER	3.3
15	U	14	DA	3.2
2	B	246	LYS	3.2
2	B	926	GLY	3.2
14	S	32	DA	3.2
14	S	30	DT	3.2
1	A	69	THR	3.2
2	B	249	ARG	3.2
2	B	932	HIS	3.1
15	U	17	DC	3.1
1	A	1087	ALA	3.1
2	B	962	LYS	3.1
14	S	33	DT	3.1
14	S	29	DC	3.1
1	A	1093	LYS	3.0
15	U	11	DA	3.0
15	U	2	DC	3.0
2	B	863	GLU	3.0
14	S	37	DT	3.0
2	B	930	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	561	TRP	2.9
10	J	65	PRO	2.9
9	I	2	THR	2.9
1	A	43	GLU	2.9
1	A	368	LYS	2.9
1	A	252	PHE	2.9
1	A	1280	GLU	2.9
2	B	448	ILE	2.9
4	D	117	GLU	2.9
15	U	3	DT	2.8
1	A	1090	ALA	2.8
5	E	139	ALA	2.8
2	B	879	ARG	2.8
3	C	52	GLU	2.8
1	A	1092	LYS	2.8
1	A	479	ASN	2.8
15	U	6	DC	2.8
13	R	10	A	2.8
15	U	4	DA	2.8
2	B	251	ILE	2.7
14	S	27	DT	2.7
3	C	219	PHE	2.7
2	B	341	LEU	2.7
1	A	601	LYS	2.7
5	E	101	GLN	2.7
9	I	28	GLU	2.7
6	F	155	LEU	2.7
8	H	82	PRO	2.6
2	B	790	ASP	2.6
2	B	730	ARG	2.6
1	A	1085	HIS	2.6
9	I	105	SER	2.6
2	B	965	LYS	2.6
1	A	13	THR	2.6
5	E	207	ARG	2.6
1	A	84	ILE	2.5
15	U	9	DT	2.5
5	E	13	TRP	2.5
2	B	925	LEU	2.5
1	A	626	ASN	2.5
7	G	128	PRO	2.5
1	A	65	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	596	THR	2.5
1	A	1361	SER	2.5
2	B	860	MET	2.5
7	G	42	PHE	2.4
11	K	64	GLU	2.4
2	B	1124	ARG	2.4
1	A	70	CYS	2.4
5	E	152	LYS	2.3
9	I	59	VAL	2.3
12	L	68	GLU	2.3
7	G	171	ILE	2.3
3	C	183	TRP	2.3
2	B	241	ARG	2.3
3	C	185	LYS	2.3
1	A	994	GLN	2.3
4	D	31	GLN	2.3
9	I	4	PHE	2.3
3	C	93	ASP	2.3
2	B	199	MET	2.3
1	A	179	LEU	2.3
1	A	1290	LYS	2.3
15	U	16	DA	2.2
2	B	471	LYS	2.2
4	D	6	SER	2.2
12	L	27	LEU	2.2
5	E	115	ASN	2.2
15	U	18	DG	2.2
1	A	557	ASP	2.2
8	H	137	GLN	2.2
2	B	444	MET	2.2
1	A	1185	PHE	2.2
5	E	125	PRO	2.2
4	D	16	LYS	2.2
2	B	931	TYR	2.2
2	B	214	ALA	2.1
8	H	140	ALA	2.1
4	D	4	SER	2.1
2	B	1071	VAL	2.1
5	E	132	ILE	2.1
2	B	277	LYS	2.1
1	A	976	THR	2.1
2	B	539	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	1009	ASP	2.1
7	G	41	LYS	2.1
1	A	1218	GLN	2.1
1	A	22	PHE	2.1
5	E	124	VAL	2.1
11	K	115	ALA	2.1
1	A	1175	SER	2.1
2	B	1050	ILE	2.1
1	A	45	GLN	2.1
2	B	77	HIS	2.1
7	G	88	ASP	2.1
2	B	247	GLY	2.1
1	A	1099	PRO	2.1
3	C	55	THR	2.1
9	I	16	PRO	2.1
1	A	226	GLU	2.1
1	A	830	LYS	2.1
2	B	506	GLY	2.0
1	A	635	ARG	2.0
1	A	1254	ALA	2.0
1	A	1339	LEU	2.0
9	I	57	GLY	2.0
2	B	785	TYR	2.0
7	G	127	PRO	2.0
8	H	56	THR	2.0
2	B	629	ASP	2.0
1	A	159	THR	2.0
2	B	252	SER	2.0
5	E	62	ALA	2.0
10	J	28	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.