Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 01:48 AM EDT

PDB ID	:	6JP6
Title	:	The X-ray structure of yeast tRNA methyltransferase complex of Trm7 and Trm734 essential for 2'-O-methylation at the first position of anticodon in specific tRNAs
Authors	:	Hirata, A.; Okada, K.; Yoshii, K.; Shiraisi, H.; Saijo, S.; Yonezawa, K.; Sihimzu, N.; Hori, H.
Deposited on	:	2019-03-26
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

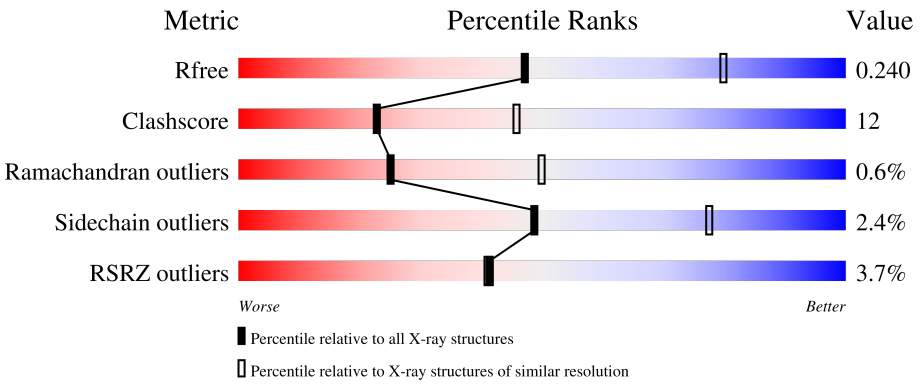
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	1028	% 80% 16% • •
1	C	1028	% 80% 15% • •
2	B	325	11% 44% 24% • • 29%
2	D	325	12% 41% 27% • • 29%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19867 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 tRNA (guanosine(34)-2'-O)-methyltransferase non-catalytic subunit TRM734.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	998	7951	5074	1328	1517	32	0	0	0
1	C	998	7951	5074	1328	1517	32	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1014	LEU	-	expression tag	UNP Q08924
A	1015	GLU	-	expression tag	UNP Q08924
A	1016	VAL	-	expression tag	UNP Q08924
A	1017	LEU	-	expression tag	UNP Q08924
A	1018	PHE	-	expression tag	UNP Q08924
A	1019	GLN	-	expression tag	UNP Q08924
A	1020	GLY	-	expression tag	UNP Q08924
A	1021	PRO	-	expression tag	UNP Q08924
A	1022	SER	-	expression tag	UNP Q08924
A	1023	HIS	-	expression tag	UNP Q08924
A	1024	HIS	-	expression tag	UNP Q08924
A	1025	HIS	-	expression tag	UNP Q08924
A	1026	HIS	-	expression tag	UNP Q08924
A	1027	HIS	-	expression tag	UNP Q08924
A	1028	HIS	-	expression tag	UNP Q08924
C	1014	LEU	-	expression tag	UNP Q08924
C	1015	GLU	-	expression tag	UNP Q08924
C	1016	VAL	-	expression tag	UNP Q08924
C	1017	LEU	-	expression tag	UNP Q08924
C	1018	PHE	-	expression tag	UNP Q08924
C	1019	GLN	-	expression tag	UNP Q08924
C	1020	GLY	-	expression tag	UNP Q08924
C	1021	PRO	-	expression tag	UNP Q08924
C	1022	SER	-	expression tag	UNP Q08924

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1023	HIS	-	expression tag	UNP Q08924
C	1024	HIS	-	expression tag	UNP Q08924
C	1025	HIS	-	expression tag	UNP Q08924
C	1026	HIS	-	expression tag	UNP Q08924
C	1027	HIS	-	expression tag	UNP Q08924
C	1028	HIS	-	expression tag	UNP Q08924

- Molecule 2 is a protein called tRNA (cytidine(34)/guanosine(34)-2'-O)-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	231	1829	1158	318	342	11	0	0	0
2	D	231	1829	1158	318	342	11	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	311	LEU	-	expression tag	UNP P38238
B	312	GLU	-	expression tag	UNP P38238
B	313	VAL	-	expression tag	UNP P38238
B	314	LEU	-	expression tag	UNP P38238
B	315	PHE	-	expression tag	UNP P38238
B	316	GLN	-	expression tag	UNP P38238
B	317	GLY	-	expression tag	UNP P38238
B	318	PRO	-	expression tag	UNP P38238
B	319	SER	-	expression tag	UNP P38238
B	320	HIS	-	expression tag	UNP P38238
B	321	HIS	-	expression tag	UNP P38238
B	322	HIS	-	expression tag	UNP P38238
B	323	HIS	-	expression tag	UNP P38238
B	324	HIS	-	expression tag	UNP P38238
B	325	HIS	-	expression tag	UNP P38238
D	311	LEU	-	expression tag	UNP P38238
D	312	GLU	-	expression tag	UNP P38238
D	313	VAL	-	expression tag	UNP P38238
D	314	LEU	-	expression tag	UNP P38238
D	315	PHE	-	expression tag	UNP P38238
D	316	GLN	-	expression tag	UNP P38238
D	317	GLY	-	expression tag	UNP P38238
D	318	PRO	-	expression tag	UNP P38238
D	319	SER	-	expression tag	UNP P38238

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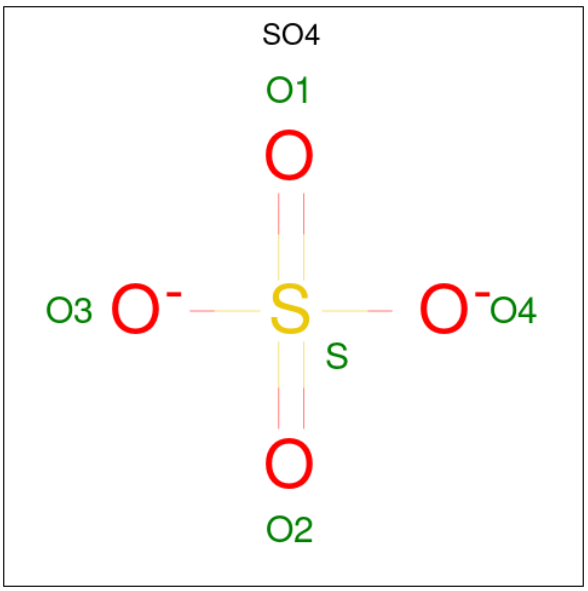
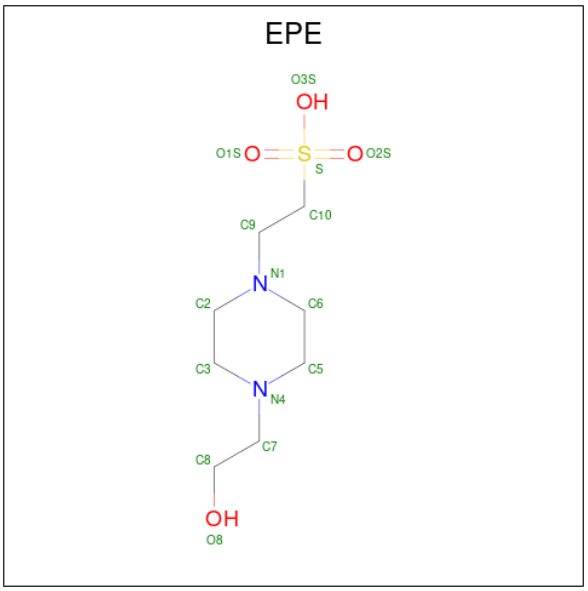
Chain	Residue	Modelled	Actual	Comment	Reference
D	320	HIS	-	expression tag	UNP P38238
D	321	HIS	-	expression tag	UNP P38238
D	322	HIS	-	expression tag	UNP P38238
D	323	HIS	-	expression tag	UNP P38238
D	324	HIS	-	expression tag	UNP P38238
D	325	HIS	-	expression tag	UNP P38238

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	S		0	0
			5	4	1			
3	A	1	Total	O	S		0	0
			5	4	1			
3	C	1	Total	O	S		0	0
			5	4	1			
3	C	1	Total	O	S		0	0
			5	4	1			

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
4	C	1	15	8	2	4	1	0	0

- Molecule 5 is water.

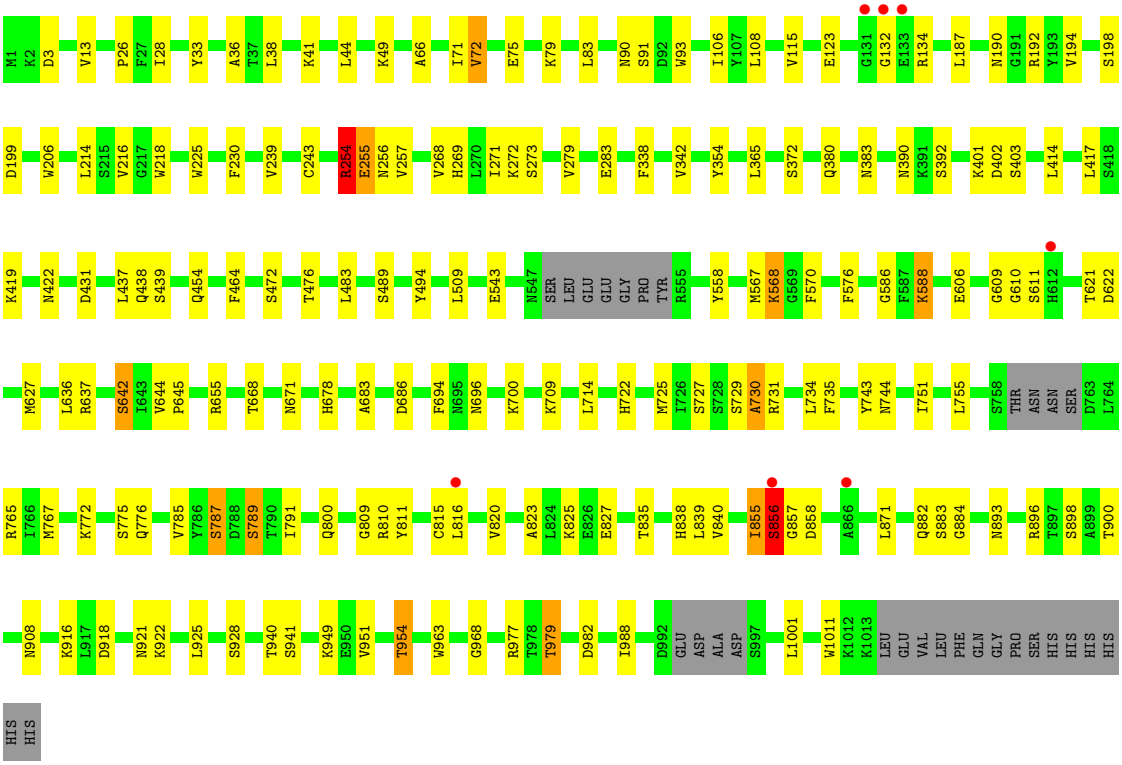
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	121	121	121	0	0
			Total	O		
5	B	10	10	10	0	0
			Total	O		
5	C	114	114	114	0	0
			Total	O		
5	D	12	12	12	0	0

3 Residue-property plots (i)

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.

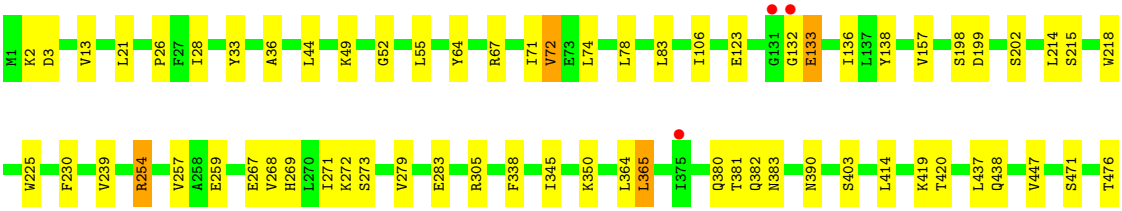
• Molecule 1: tRNA (guanosine(34)-2'-O)-methyltransferase non-catalytic subunit TRM734

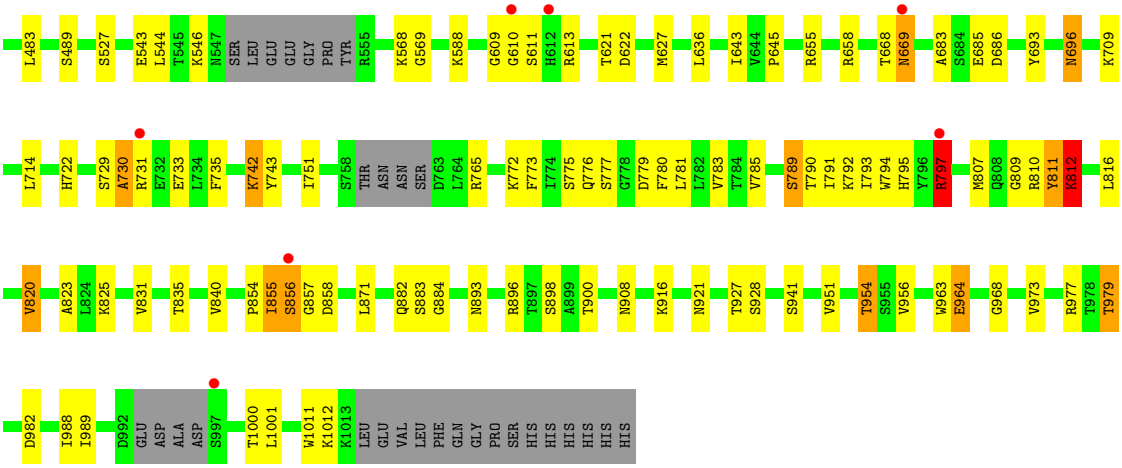
Chain A:



• Molecule 1: tRNA (guanosine(34)-2'-O)-methyltransferase non-catalytic subunit TRM734

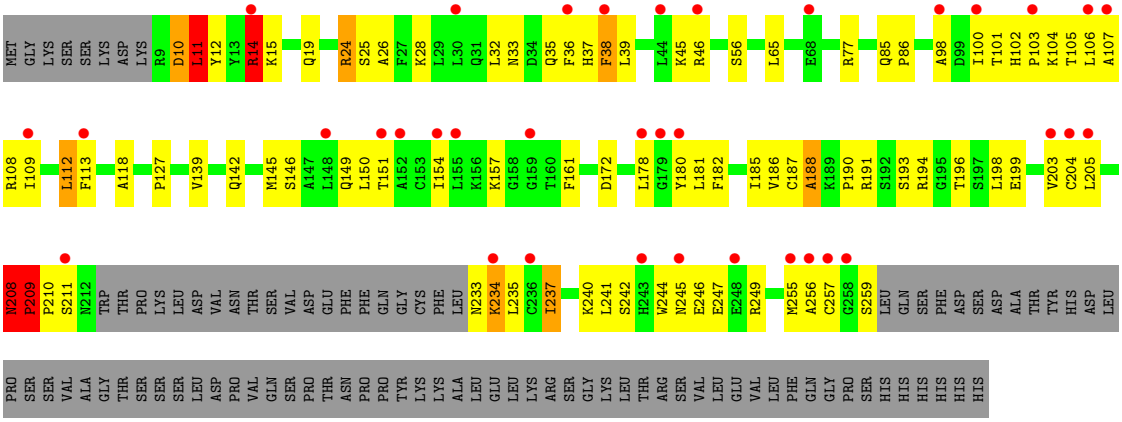
Chain C:





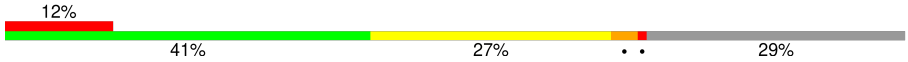
- Molecule 2: tRNA (cytidine(34)/guanosine(34)-2'-O)-methyltransferase

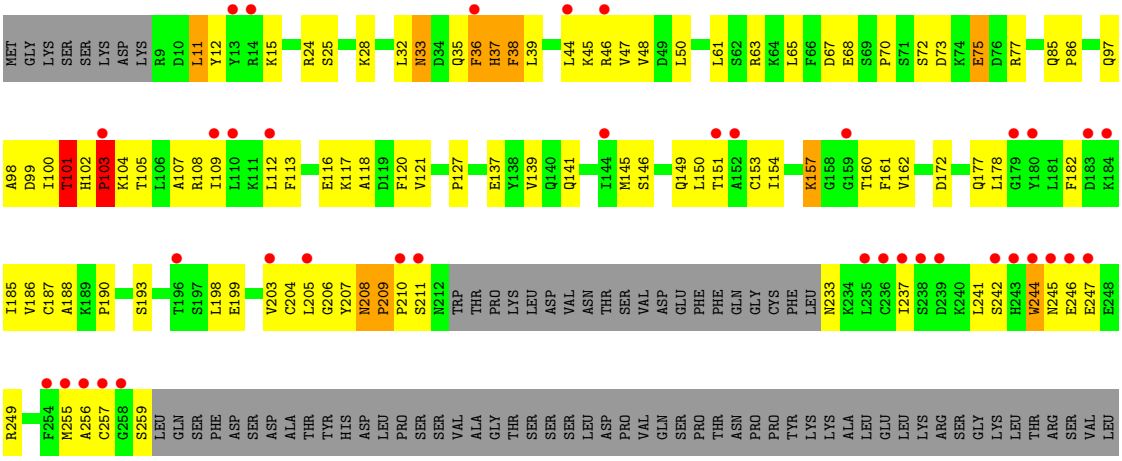
Chain B:



- Molecule 2: tRNA (cytidine(34)/guanosine(34)-2'-O)-methyltransferase

Chain D:





GLU
VAL
LEU
PHE
GLN
GLY
PRO
SER
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	253.64Å 110.35Å 133.50Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	36.43 – 2.70 36.43 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.43-2.70) 99.6 (36.43-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.194 , 0.239 0.197 , 0.240	Depositor DCC
R_{free} test set	5048 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 22.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19867	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EPE

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	0.60	8/8110 (0.1%)	0.71	3/10972 (0.0%)
1	C	0.53	1/8110 (0.0%)	0.71	6/10972 (0.1%)
2	B	0.58	2/1865 (0.1%)	0.87	8/2516 (0.3%)
2	D	0.60	0/1865	0.85	8/2516 (0.3%)
All	All	0.57	11/19950 (0.1%)	0.74	25/26976 (0.1%)

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
1	C	0	2
2	B	0	4
2	D	0	2
All	All	0	10

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	ARG	NE-CZ	-7.90	1.22	1.33
1	A	588	LYS	CA-CB	-7.43	1.37	1.53
1	A	254	ARG	CZ-NH2	-6.75	1.24	1.33
1	A	254	ARG	CZ-NH1	-6.46	1.24	1.33
1	A	255	GLU	CD-OE1	6.31	1.32	1.25
1	A	254	ARG	CG-CD	-6.00	1.36	1.51
1	A	642	SER	CB-OG	-5.28	1.35	1.42
1	A	218	TRP	CE3-CZ3	-5.24	1.29	1.38
1	C	133	GLU	CD-OE1	-5.20	1.20	1.25
2	B	210	PRO	N-CD	5.10	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	209	PRO	N-CD	5.05	1.54	1.47

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	254	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	C	797	ARG	CD-NE-CZ	8.72	135.81	123.60
1	C	812	LYS	N-CA-C	-7.71	90.19	111.00
2	B	11	LEU	CA-CB-CG	7.60	132.77	115.30
2	D	11	LEU	CB-CG-CD2	7.13	123.12	111.00
2	D	36	PHE	CB-CA-C	-6.66	97.08	110.40
2	D	103	PRO	CA-N-CD	-6.66	102.18	111.50
2	D	75	GLU	CA-CB-CG	-6.54	99.02	113.40
2	B	235	LEU	CA-CB-CG	6.40	130.01	115.30
2	D	11	LEU	CA-CB-CG	6.34	129.88	115.30
2	B	208	ASN	C-N-CD	6.32	141.66	128.40
1	C	964	GLU	CB-CA-C	6.21	122.82	110.40
2	D	208	ASN	C-N-CD	6.06	141.12	128.40
2	D	209	PRO	C-N-CD	6.04	141.08	128.40
1	C	811	TYR	CB-CA-C	6.03	122.46	110.40
2	B	10	ASP	CB-CG-OD1	-5.95	112.94	118.30
2	B	209	PRO	C-N-CD	5.85	140.68	128.40
2	B	237	ILE	CG1-CB-CG2	-5.64	99.00	111.40
2	B	14	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	568	LYS	CB-CG-CD	5.41	125.67	111.60
2	B	14	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	C	797	ARG	CB-CG-CD	5.34	125.49	111.60
1	A	254	ARG	CA-CB-CG	5.26	124.97	113.40
1	C	742	LYS	CD-CE-NZ	5.10	123.43	111.70
2	D	101	THR	C-N-CA	5.01	134.23	121.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	855	ILE	Peptide
1	A	856	SER	Peptide
2	B	101	THR	Peptide
2	B	11	LEU	Mainchain
2	B	188	ALA	Peptide
2	B	245	ASN	Peptide
1	C	797	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	855	ILE	Peptide
2	D	101	THR	Peptide
2	D	245	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7951	0	7901	119	0
1	C	7951	0	7901	130	0
2	B	1829	0	1829	103	0
2	D	1829	0	1829	117	0
3	A	10	0	0	0	0
3	C	10	0	0	0	0
4	A	15	0	17	2	0
4	C	15	0	17	1	0
5	A	121	0	0	8	0
5	B	10	0	0	0	0
5	C	114	0	0	7	0
5	D	12	0	0	0	0
All	All	19867	0	19494	451	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 12.

All (451) 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:C:669:ASN:HD21	1:C:742:LYS:CE	1.15	1.59
2:D:11:LEU:HD22	2:D:15:LYS:NZ	1.22	1.40
1:C:669:ASN:ND2	1:C:742:LYS:CE	1.94	1.28
2:D:11:LEU:CD2	2:D:15:LYS:HZ2	1.51	1.23
1:C:789:SER:CB	1:C:812:LYS:O	1.89	1.21
2:D:117:LYS:NZ	2:D:153:CYS:O	1.87	1.07
1:C:669:ASN:ND2	1:C:742:LYS:HE2	1.70	1.06
2:D:137:GLU:O	2:D:141:GLN:NE2	1.89	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:669:ASN:HD21	1:C:742:LYS:HE3	0.94	1.04
1:C:669:ASN:ND2	1:C:742:LYS:CD	2.21	1.03
2:B:85:GLN:OE1	2:B:86:PRO:O	1.80	1.00
1:C:898:SER:HB3	1:C:916:LYS:HD2	1.40	0.99
1:C:669:ASN:HD21	1:C:742:LYS:HE2	1.24	0.98
1:A:898:SER:HB3	1:A:916:LYS:HD2	1.40	0.98
1:C:795:HIS:HE1	1:C:797:ARG:NH1	1.62	0.98
2:B:208:ASN:HB3	2:B:209:PRO:CD	1.95	0.97
1:C:789:SER:HB3	1:C:812:LYS:O	1.65	0.96
1:C:795:HIS:CE1	1:C:797:ARG:NH1	2.34	0.95
1:A:642:SER:OG	1:A:644:VAL:O	1.86	0.93
1:A:856:SER:HA	1:A:896:ARG:HD2	1.49	0.93
1:C:669:ASN:HD21	1:C:742:LYS:CD	1.80	0.92
2:D:11:LEU:CD2	2:D:15:LYS:NZ	2.16	0.92
1:C:643:ILE:HD12	1:C:643:ILE:H	1.34	0.91
2:B:36:PHE:HE1	2:B:257:CYS:HG	1.19	0.91
2:D:104:LYS:O	2:D:108:ARG:N	2.04	0.89
2:D:11:LEU:HD22	2:D:15:LYS:HZ3	1.32	0.88
1:C:669:ASN:ND2	1:C:742:LYS:HE3	1.76	0.86
1:A:730:ALA:HB1	1:A:765:ARG:HG2	1.58	0.86
1:C:988:ILE:HG12	1:C:1001:LEU:HD22	1.59	0.85
2:D:157:LYS:H	2:D:157:LYS:HD2	1.42	0.83
1:C:789:SER:HB2	1:C:812:LYS:O	1.78	0.83
2:D:33:ASN:HD21	2:D:37:HIS:HA	1.42	0.82
2:B:11:LEU:O	2:B:14:ARG:HD3	1.79	0.82
1:C:669:ASN:ND2	1:C:742:LYS:HD2	1.96	0.81
2:B:237:ILE:HG22	2:B:241:LEU:HD13	1.63	0.80
2:D:104:LYS:HG3	2:D:107:ALA:HB3	1.62	0.80
1:C:658:ARG:NE	1:C:685:GLU:OE1	2.12	0.80
1:C:882:GLN:NE2	2:D:255:MET:HA	1.97	0.79
1:A:568:LYS:HD2	1:A:588:LYS:HD3	1.63	0.79
2:D:102:HIS:CG	2:D:103:PRO:HD3	2.17	0.79
1:A:123:GLU:OE1	5:A:1202:HOH:O	2.02	0.78
1:A:882:GLN:HE21	2:B:256:ALA:H	1.29	0.78
1:A:730:ALA:CB	1:A:765:ARG:HG2	2.13	0.78
2:D:33:ASN:ND2	2:D:37:HIS:HA	1.99	0.78
2:B:100:ILE:O	2:B:150:LEU:HD11	1.84	0.77
2:B:149:GLN:HA	2:B:237:ILE:HD11	1.64	0.77
1:C:2:LYS:NZ	5:C:1204:HOH:O	2.17	0.77
1:A:882:GLN:NE2	2:B:255:MET:HA	2.00	0.77
2:D:11:LEU:HD22	2:D:15:LYS:CE	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:ARG:NH1	2:B:15:LYS:HB2	2.00	0.76
1:C:825:LYS:NZ	1:C:921:ASN:OD1	2.18	0.76
2:B:208:ASN:HB3	2:B:209:PRO:HD2	1.67	0.76
1:C:668:THR:HG21	1:C:722:HIS:CE1	2.21	0.76
2:B:104:LYS:O	2:B:108:ARG:N	2.13	0.76
2:B:36:PHE:HE1	2:B:257:CYS:SG	2.09	0.74
2:D:246:GLU:OE1	2:D:247:GLU:N	2.19	0.74
1:C:123:GLU:OE1	5:C:1202:HOH:O	2.04	0.74
1:A:988:ILE:HG12	1:A:1001:LEU:HD22	1.70	0.74
1:C:964:GLU:HG2	1:C:973:VAL:HG11	1.70	0.73
2:B:104:LYS:HG2	2:B:107:ALA:HB3	1.70	0.72
1:C:71:ILE:HD11	1:C:106:ILE:HD13	1.72	0.71
2:D:208:ASN:HB3	2:D:209:PRO:HD2	1.72	0.71
1:A:941:SER:HB2	1:A:954:THR:HB	1.72	0.71
2:B:14:ARG:HH12	2:B:15:LYS:HB2	1.53	0.71
2:D:193:SER:OG	2:D:199:GLU:OE1	2.08	0.70
1:A:71:ILE:HD11	1:A:106:ILE:HD13	1.74	0.70
2:D:33:ASN:ND2	2:D:33:ASN:O	2.25	0.69
2:B:108:ARG:HE	2:B:112:LEU:HD11	1.57	0.69
1:C:730:ALA:CB	1:C:765:ARG:HG2	2.22	0.69
1:C:730:ALA:N	5:C:1205:HOH:O	2.25	0.69
2:D:46:ARG:NH1	2:D:116:GLU:HB3	2.08	0.68
1:A:268:VAL:HG23	1:A:269:HIS:HD2	1.59	0.68
1:C:267:GLU:OE2	5:C:1203:HOH:O	2.11	0.67
1:C:882:GLN:HE22	2:D:255:MET:HA	1.59	0.67
1:C:28:ILE:HD12	1:C:44:LEU:HD11	1.75	0.67
2:D:33:ASN:OD1	2:D:39:LEU:HB2	1.94	0.67
1:A:882:GLN:HE22	2:B:255:MET:HA	1.60	0.67
1:A:271:ILE:HG12	1:A:272:LYS:HB3	1.75	0.67
1:C:67:ARG:NH2	2:D:247:GLU:OE1	2.24	0.67
2:D:35:GLN:O	2:D:36:PHE:HD1	1.78	0.67
1:C:730:ALA:HB1	1:C:765:ARG:HG2	1.76	0.67
1:A:825:LYS:NZ	1:A:921:ASN:OD1	2.22	0.66
2:B:36:PHE:HD2	2:B:205:LEU:HD11	1.61	0.66
1:C:669:ASN:HD22	1:C:742:LYS:HD2	1.59	0.65
1:A:940:THR:OG1	1:A:954:THR:HG22	1.96	0.65
1:C:882:GLN:HE21	2:D:256:ALA:H	1.43	0.65
1:A:730:ALA:HB2	5:A:1201:HOH:O	1.97	0.65
1:A:856:SER:HA	1:A:896:ARG:CD	2.25	0.65
1:C:789:SER:OG	1:C:812:LYS:O	2.15	0.64
2:B:98:ALA:HB1	2:B:105:THR:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:ARG:HG2	2:D:113:PHE:CD2	2.32	0.64
2:D:100:ILE:O	2:D:150:LEU:HD11	1.98	0.64
2:B:149:GLN:HG2	2:B:237:ILE:HD12	1.80	0.64
1:A:33:TYR:OH	1:A:283:GLU:OE1	2.12	0.63
1:C:669:ASN:HD22	1:C:742:LYS:CD	2.10	0.63
2:D:150:LEU:N	2:D:150:LEU:HD12	2.14	0.63
2:D:46:ARG:HG2	2:D:113:PHE:HD2	1.63	0.63
1:C:268:VAL:HG23	1:C:269:HIS:HD2	1.64	0.62
1:C:568:LYS:HD2	1:C:569:GLY:N	2.14	0.62
1:C:730:ALA:HB2	5:C:1201:HOH:O	1.98	0.62
2:B:193:SER:OG	2:B:199:GLU:OE1	2.14	0.62
2:B:11:LEU:O	2:B:14:ARG:NH1	2.33	0.62
2:B:36:PHE:CD2	2:B:205:LEU:HD11	2.34	0.62
2:B:15:LYS:HG2	2:B:19:GLN:HE21	1.65	0.62
2:D:35:GLN:O	2:D:36:PHE:HB2	2.00	0.61
1:A:928:SER:OG	1:A:968:GLY:O	2.19	0.61
2:D:105:THR:HG23	2:D:108:ARG:NH2	2.16	0.61
2:B:102:HIS:CD2	2:B:103:PRO:HD2	2.36	0.60
1:C:772:LYS:HE2	1:C:823:ALA:HB2	1.82	0.60
2:B:46:ARG:HD2	2:B:113:PHE:CD2	2.36	0.60
2:B:38:PHE:HD1	2:B:39:LEU:HD13	1.67	0.60
2:D:35:GLN:O	2:D:36:PHE:CD1	2.54	0.60
2:B:46:ARG:HB3	2:B:113:PHE:CE2	2.36	0.60
1:A:26:PRO:HD3	1:A:979:THR:HG21	1.82	0.60
2:B:150:LEU:N	2:B:150:LEU:HD12	2.17	0.59
1:A:568:LYS:HD2	1:A:588:LYS:CD	2.31	0.59
2:B:151:THR:HG21	2:B:161:PHE:CD1	2.37	0.59
1:C:271:ILE:HG13	1:C:272:LYS:HB3	1.85	0.58
1:A:38:LEU:HD21	1:A:41:LYS:HG3	1.84	0.58
2:B:46:ARG:HD2	2:B:113:PHE:HD2	1.68	0.58
2:B:109:ILE:HG23	2:B:113:PHE:HE1	1.67	0.58
1:C:733:GLU:HG2	1:C:735:PHE:CZ	2.38	0.58
1:A:134:ARG:HG2	2:B:233:ASN:HA	1.85	0.58
2:B:149:GLN:HA	2:B:237:ILE:CD1	2.32	0.58
2:D:35:GLN:C	2:D:36:PHE:HD1	2.05	0.58
2:D:104:LYS:HG2	2:D:108:ARG:HG3	1.86	0.58
1:C:783:VAL:HB	1:C:793:ILE:HD13	1.85	0.57
2:B:85:GLN:OE1	2:B:86:PRO:C	2.41	0.57
1:C:543:GLU:OE2	1:C:743:TYR:OH	2.18	0.57
2:D:105:THR:HG23	2:D:108:ARG:HH21	1.70	0.57
1:C:568:LYS:HE3	1:C:588:LYS:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:ARG:HH11	2:D:116:GLU:HB3	1.67	0.57
2:D:11:LEU:HD22	2:D:15:LYS:HZ2	0.76	0.57
1:A:731:ARG:HG3	1:A:731:ARG:O	2.05	0.57
1:C:797:ARG:HH11	1:C:797:ARG:HG2	1.70	0.57
2:D:149:GLN:HG2	2:D:237:ILE:HD12	1.87	0.57
1:C:26:PRO:HD3	1:C:979:THR:HG21	1.87	0.56
1:A:134:ARG:CG	2:B:233:ASN:HA	2.35	0.56
1:C:854:PRO:O	1:C:855:ILE:HG13	2.06	0.56
2:D:86:PRO:HG3	2:D:97:GLN:NE2	2.21	0.56
2:B:209:PRO:O	2:B:209:PRO:HG2	2.06	0.56
2:D:149:GLN:HA	2:D:237:ILE:HD12	1.87	0.56
1:A:567:MET:HG2	5:A:1285:HOH:O	2.04	0.56
2:D:241:LEU:HD23	2:D:244:TRP:CZ3	2.40	0.56
2:B:108:ARG:O	2:B:112:LEU:HD13	2.05	0.56
2:D:35:GLN:HG2	2:D:36:PHE:CD1	2.40	0.56
2:D:104:LYS:HG2	2:D:108:ARG:CG	2.36	0.56
1:A:772:LYS:HE2	1:A:823:ALA:HB2	1.86	0.56
2:D:36:PHE:CE1	2:D:257:CYS:SG	2.98	0.56
1:A:725:MET:CE	1:A:727:SER:HB3	2.36	0.56
2:B:10:ASP:OD1	2:B:12:TYR:N	2.38	0.56
2:B:240:LYS:HD2	2:B:244:TRP:CZ2	2.41	0.56
1:A:132:GLY:O	2:B:233:ASN:HB2	2.05	0.56
1:A:422:ASN:ND2	1:A:472:SER:O	2.39	0.56
1:C:928:SER:OG	1:C:968:GLY:O	2.23	0.56
2:D:99:ASP:OD1	2:D:101:THR:HG23	2.06	0.56
1:A:380:GLN:HB2	5:A:1317:HOH:O	2.04	0.55
2:B:102:HIS:CG	2:B:103:PRO:HD2	2.42	0.55
2:D:36:PHE:O	2:D:38:PHE:N	2.39	0.55
1:A:893:ASN:ND2	1:A:898:SER:OG	2.39	0.55
1:C:655:ARG:HG3	1:C:686:ASP:HB3	1.88	0.55
2:D:149:GLN:HA	2:D:237:ILE:CD1	2.37	0.55
1:A:810:ARG:HH21	1:C:611:SER:N	2.04	0.55
2:D:35:GLN:HG2	2:D:36:PHE:CE1	2.42	0.55
2:B:98:ALA:HB1	2:B:105:THR:CG2	2.37	0.55
1:A:609:GLY:O	1:A:611:SER:N	2.40	0.55
1:A:856:SER:CA	1:A:896:ARG:HD2	2.32	0.55
1:C:856:SER:HA	1:C:896:ARG:HD2	1.90	0.54
2:D:145:MET:SD	2:D:241:LEU:HD12	2.47	0.54
2:D:35:GLN:C	2:D:36:PHE:CD1	2.80	0.54
1:A:28:ILE:HD12	1:A:44:LEU:HD11	1.88	0.54
2:B:104:LYS:HD3	2:B:108:ARG:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:LEU:CG	2:D:15:LYS:HZ2	2.17	0.54
2:D:151:THR:HG21	2:D:161:PHE:CD1	2.42	0.54
2:B:194:ARG:HB3	2:B:196:THR:HG22	1.88	0.54
2:B:38:PHE:CD1	2:B:39:LEU:HD13	2.42	0.54
1:C:214:LEU:HD22	1:C:257:VAL:HB	1.89	0.54
1:C:893:ASN:ND2	1:C:898:SER:OG	2.40	0.54
2:D:208:ASN:HB3	2:D:209:PRO:CD	2.34	0.54
1:A:800:GLN:N	1:A:800:GLN:OE1	2.41	0.54
1:C:795:HIS:CE1	1:C:797:ARG:HH11	2.19	0.54
1:C:28:ILE:CD1	1:C:44:LEU:HD11	2.37	0.53
1:A:254:ARG:HH21	1:A:255:GLU:CD	2.11	0.53
1:C:772:LYS:HE3	1:C:857:GLY:O	2.08	0.53
2:D:35:GLN:O	2:D:36:PHE:CB	2.55	0.53
2:D:172:ASP:HB2	2:D:249:ARG:HB3	1.90	0.53
2:D:36:PHE:HE1	2:D:257:CYS:SG	2.30	0.53
1:A:214:LEU:HD22	1:A:257:VAL:HB	1.90	0.53
1:C:49:LYS:NZ	1:C:979:THR:HB	2.23	0.53
2:D:108:ARG:O	2:D:112:LEU:HD23	2.07	0.53
2:B:233:ASN:N	2:B:234:LYS:HZ2	2.07	0.53
2:D:127:PRO:HG2	2:D:139:VAL:CG1	2.39	0.53
2:D:177:GLN:HB3	2:D:241:LEU:HD13	1.91	0.53
2:B:149:GLN:HG2	2:B:237:ILE:CD1	2.39	0.53
1:C:921:ASN:ND2	5:C:1207:HOH:O	2.31	0.53
1:A:772:LYS:HE3	1:A:857:GLY:O	2.09	0.52
1:A:882:GLN:HE21	2:B:256:ALA:N	2.03	0.52
2:D:102:HIS:CD2	2:D:103:PRO:HD3	2.44	0.52
1:A:431:ASP:OD1	1:A:454:GLN:NE2	2.43	0.52
1:A:476:THR:HG22	1:A:483:LEU:HB2	1.91	0.52
1:A:543:GLU:OE2	1:A:743:TYR:OH	2.22	0.52
1:C:611:SER:OG	1:C:613:ARG:NH1	2.43	0.52
1:A:338:PHE:CD1	1:A:383:ASN:HA	2.45	0.51
2:D:72:SER:O	2:D:75:GLU:OE1	2.28	0.51
1:C:3:ASP:HA	1:C:1011:TRP:CD1	2.46	0.51
2:D:28:LYS:O	2:D:32:LEU:HG	2.11	0.51
2:B:65:LEU:HB3	2:B:77:ARG:HD3	1.91	0.51
2:D:36:PHE:CD2	2:D:203:VAL:HG11	2.45	0.51
1:A:775:SER:HB2	1:A:776:GLN:NE2	2.24	0.51
1:A:3:ASP:HA	1:A:1011:TRP:CD1	2.46	0.51
1:A:606:GLU:OE1	1:A:637:ARG:NH1	2.38	0.51
2:B:35:GLN:C	2:B:37:HIS:H	2.14	0.51
2:B:109:ILE:O	2:B:113:PHE:HD1	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:45:LYS:HE3	2:D:46:ARG:NH2	2.26	0.51
1:A:49:LYS:NZ	1:A:979:THR:HB	2.26	0.51
1:A:668:THR:HG21	1:A:722:HIS:CD2	2.45	0.51
1:A:951:VAL:HB	1:A:963:TRP:HB2	1.93	0.51
2:D:208:ASN:CB	2:D:209:PRO:HD2	2.38	0.51
1:A:725:MET:HE1	1:A:727:SER:HB3	1.92	0.50
1:C:198:SER:OG	1:C:199:ASP:N	2.43	0.50
1:C:855:ILE:HA	1:C:896:ARG:HD3	1.93	0.50
1:A:810:ARG:NH2	1:C:611:SER:N	2.60	0.50
2:D:188:ALA:HB1	2:D:257:CYS:SG	2.52	0.50
2:B:180:TYR:HB2	2:B:181:LEU:HD12	1.91	0.50
2:D:103:PRO:CG	2:D:104:LYS:H	2.25	0.50
4:A:1103:EPE:H21	5:A:1286:HOH:O	2.11	0.50
1:A:28:ILE:CD1	1:A:44:LEU:HD11	2.42	0.50
1:C:811:TYR:CE1	1:C:840:VAL:HG21	2.47	0.50
1:C:820:VAL:HG12	1:C:831:VAL:HB	1.93	0.49
1:A:372:SER:OG	1:A:390:ASN:OD1	2.18	0.49
2:B:11:LEU:HD22	2:B:12:TYR:CZ	2.47	0.49
1:C:643:ILE:H	1:C:643:ILE:CD1	2.07	0.49
1:C:775:SER:HB2	1:C:776:GLN:NE2	2.27	0.49
1:A:709:LYS:HE2	5:A:1292:HOH:O	2.12	0.49
1:A:729:SER:O	1:A:730:ALA:HB2	2.12	0.49
2:B:127:PRO:HG2	2:B:139:VAL:CG1	2.42	0.49
1:A:75:GLU:OE2	1:A:79:LYS:NZ	2.27	0.49
2:B:109:ILE:O	2:B:113:PHE:CD1	2.66	0.49
1:A:655:ARG:HG3	1:A:686:ASP:HB3	1.94	0.49
2:B:118:ALA:N	2:B:154:ILE:O	2.38	0.49
2:D:104:LYS:O	2:D:108:ARG:HG3	2.12	0.48
2:D:178:LEU:HB3	2:D:185:ILE:CD1	2.43	0.48
1:A:751:ILE:HG21	5:A:1292:HOH:O	2.12	0.48
1:A:72:VAL:HG22	1:A:83:LEU:HD13	1.95	0.48
2:D:242:SER:O	2:D:246:GLU:HB2	2.13	0.48
1:C:941:SER:HB2	1:C:954:THR:HB	1.95	0.48
1:A:225:TRP:CD1	1:A:273:SER:HB3	2.48	0.48
1:A:883:SER:OG	1:A:884:GLY:N	2.46	0.48
2:D:32:LEU:O	2:D:35:GLN:O	2.30	0.48
1:A:187:LEU:HD22	1:A:194:VAL:HG22	1.96	0.48
1:A:882:GLN:NE2	2:B:255:MET:CA	2.74	0.48
1:C:132:GLY:O	2:D:233:ASN:HB2	2.14	0.48
1:C:783:VAL:HB	1:C:793:ILE:CD1	2.43	0.48
1:C:989:ILE:HG22	1:C:1000:THR:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:LEU:HB3	2:D:77:ARG:HD3	1.95	0.48
1:A:835:THR:HA	1:A:884:GLY:HA2	1.96	0.48
2:B:15:LYS:NZ	2:B:19:GLN:HE22	2.12	0.48
1:A:811:TYR:CE1	1:A:840:VAL:HG21	2.48	0.48
2:B:237:ILE:HD13	2:B:237:ILE:HG21	1.62	0.48
1:C:33:TYR:OH	1:C:283:GLU:OE1	2.19	0.47
1:C:305:ARG:CD	1:C:643:ILE:HG12	2.44	0.47
1:C:789:SER:HA	1:C:816:LEU:HG	1.95	0.47
2:D:103:PRO:HD2	2:D:108:ARG:HH22	1.78	0.47
1:C:898:SER:CB	1:C:916:LYS:HD2	2.28	0.47
2:D:104:LYS:NZ	2:D:108:ARG:HG2	2.29	0.47
1:C:136:ILE:O	1:C:157:VAL:HG23	2.14	0.47
1:C:609:GLY:O	1:C:611:SER:N	2.47	0.47
1:A:767:MET:HG3	1:A:815:CYS:SG	2.55	0.47
2:B:46:ARG:CD	2:B:113:PHE:HD2	2.27	0.47
1:C:792:LYS:HD3	1:C:794:TRP:CZ2	2.49	0.47
2:D:208:ASN:CB	2:D:209:PRO:CD	2.92	0.47
1:A:785:VAL:HG12	1:A:791:ILE:HG12	1.97	0.47
2:B:180:TYR:HB2	2:B:181:LEU:CD1	2.44	0.47
2:D:157:LYS:HD2	2:D:157:LYS:N	2.22	0.47
1:A:268:VAL:HG23	1:A:269:HIS:CD2	2.46	0.47
1:A:671:ASN:ND2	1:A:744:ASN:HA	2.30	0.47
1:C:254:ARG:H	1:C:254:ARG:CD	2.28	0.47
1:C:338:PHE:CD1	1:C:383:ASN:HA	2.50	0.47
2:D:25:SER:HA	2:D:28:LYS:HD2	1.97	0.47
2:B:106:LEU:HD12	2:B:106:LEU:O	2.15	0.47
1:C:476:THR:HG22	1:C:483:LEU:HB2	1.97	0.47
2:B:146:SER:HA	2:B:149:GLN:HG3	1.97	0.47
1:A:198:SER:OG	1:A:199:ASP:N	2.47	0.46
2:B:33:ASN:C	2:B:35:GLN:H	2.18	0.46
2:B:45:LYS:O	2:B:77:ARG:HA	2.16	0.46
1:C:669:ASN:CG	1:C:742:LYS:HE2	2.29	0.46
1:C:790:THR:HG22	1:C:810:ARG:HD2	1.97	0.46
4:C:1103:EPE:H51	4:C:1103:EPE:H81	1.52	0.46
2:D:11:LEU:HD22	2:D:15:LYS:CD	2.45	0.46
1:C:735:PHE:HB3	1:C:751:ILE:CD1	2.45	0.46
1:C:793:ILE:HB	1:C:807:MET:HB3	1.98	0.46
1:C:898:SER:HB3	1:C:916:LYS:CD	2.28	0.46
1:A:855:ILE:HA	1:A:896:ARG:HD3	1.97	0.46
1:A:271:ILE:HA	1:A:272:LYS:HA	1.48	0.46
1:A:342:VAL:HB	1:A:354:TYR:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:PRO:HB2	2:D:86:PRO:HB2	1.98	0.46
2:D:47:VAL:HG11	2:D:61:LEU:HD13	1.97	0.46
1:A:734:LEU:HB3	1:A:755:LEU:HB2	1.97	0.46
1:C:72:VAL:HG22	1:C:83:LEU:HD13	1.98	0.46
2:B:178:LEU:HB3	2:B:185:ILE:CD1	2.46	0.46
2:D:109:ILE:HG23	2:D:113:PHE:HE1	1.80	0.46
1:A:621:THR:O	1:A:622:ASP:HB2	2.15	0.46
1:A:855:ILE:HB	5:A:1290:HOH:O	2.16	0.46
2:D:102:HIS:CD2	2:D:103:PRO:CD	3.00	0.45
2:D:104:LYS:HG3	2:D:107:ALA:CB	2.39	0.45
1:A:225:TRP:NE1	1:A:273:SER:HB3	2.31	0.45
1:C:21:LEU:HD22	1:C:55:LEU:HD11	1.99	0.45
2:D:102:HIS:CG	2:D:103:PRO:CD	2.97	0.45
1:A:230:PHE:CD2	1:A:279:VAL:HG11	2.51	0.45
2:D:146:SER:HA	2:D:149:GLN:HG3	1.99	0.45
2:D:15:LYS:HZ3	2:D:15:LYS:HG3	1.53	0.45
2:D:127:PRO:HG2	2:D:139:VAL:HG12	1.98	0.45
2:B:11:LEU:HD22	2:B:12:TYR:CE2	2.51	0.45
1:C:883:SER:OG	1:C:884:GLY:N	2.49	0.45
2:B:172:ASP:HB2	2:B:249:ARG:HB3	1.98	0.45
1:A:190:ASN:CG	1:A:192:ARG:HG3	2.37	0.45
1:A:735:PHE:HB3	1:A:751:ILE:CD1	2.47	0.45
2:B:188:ALA:HB1	2:B:257:CYS:SG	2.57	0.45
1:A:827:GLU:OE2	1:A:921:ASN:ND2	2.50	0.45
2:B:11:LEU:HG	2:B:14:ARG:NH2	2.32	0.45
2:B:157:LYS:H	2:B:157:LYS:HD3	1.82	0.45
1:C:627:MET:HG2	1:C:636:LEU:HD23	1.99	0.45
2:B:46:ARG:HG3	2:B:46:ARG:HH11	1.82	0.44
1:A:789:SER:HA	1:A:816:LEU:HG	1.99	0.44
1:C:381:THR:HG23	1:C:382:GLN:HG2	1.99	0.44
2:D:162:VAL:HG22	2:D:203:VAL:HG13	1.98	0.44
2:B:11:LEU:C	2:B:14:ARG:NH1	2.71	0.44
2:B:28:LYS:HE2	2:B:199:GLU:OE1	2.18	0.44
1:C:268:VAL:HG23	1:C:269:HIS:CD2	2.48	0.44
1:C:621:THR:O	1:C:622:ASP:HB2	2.17	0.44
1:A:36:ALA:HB2	1:A:645:PRO:HG2	1.98	0.44
1:A:982:ASP:OD1	2:B:198:LEU:HD21	2.17	0.44
1:A:419:LYS:O	1:A:439:SER:HB2	2.18	0.44
1:A:678:HIS:CD2	1:A:696:ASN:HD21	2.36	0.44
1:C:202:SER:HB3	1:C:218:TRP:CZ3	2.53	0.44
1:C:225:TRP:NE1	1:C:273:SER:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:GLN:HG3	2:B:36:PHE:N	2.33	0.44
2:B:157:LYS:H	2:B:157:LYS:CD	2.31	0.44
2:D:33:ASN:C	2:D:35:GLN:H	2.21	0.44
2:D:186:VAL:HG12	2:D:187:CYS:N	2.33	0.44
1:C:225:TRP:CD1	1:C:273:SER:HB3	2.52	0.44
1:C:271:ILE:HA	1:C:272:LYS:HA	1.48	0.44
1:A:918:ASP:OD2	1:A:922:LYS:HG2	2.18	0.43
2:B:10:ASP:OD2	2:B:24:ARG:NE	2.51	0.43
2:D:50:LEU:HD22	2:D:100:ILE:HG22	2.00	0.43
2:D:63:ARG:O	2:D:68:GLU:HG3	2.18	0.43
1:A:254:ARG:HD2	1:A:255:GLU:H	1.83	0.43
1:C:36:ALA:HB2	1:C:645:PRO:HG2	2.00	0.43
2:D:207:TYR:CD1	2:D:208:ASN:N	2.85	0.43
1:A:90:ASN:ND2	1:A:91:SER:H	2.16	0.43
1:A:922:LYS:O	1:A:922:LYS:HG3	2.17	0.43
2:B:182:PHE:CG	2:B:204:CYS:HB3	2.53	0.43
2:B:15:LYS:HG2	2:B:19:GLN:NE2	2.32	0.43
2:B:237:ILE:CG2	2:B:241:LEU:HD13	2.41	0.43
2:B:172:ASP:OD1	2:B:172:ASP:N	2.51	0.43
1:C:364:LEU:HB3	1:C:365:LEU:HD23	2.00	0.43
1:A:134:ARG:HG2	2:B:233:ASN:OD1	2.18	0.43
1:A:576:PHE:HB2	4:A:1103:EPE:H91	2.00	0.43
2:B:109:ILE:CG2	2:B:113:PHE:HE1	2.31	0.43
1:C:74:LEU:O	1:C:78:LEU:HD23	2.19	0.43
2:D:48:VAL:HB	2:D:121:VAL:HG22	2.00	0.43
1:A:216:VAL:HG21	2:D:67:ASP:HB3	2.01	0.43
1:A:489:SER:HB3	1:A:509:LEU:H	1.83	0.43
1:C:345:ILE:HA	1:C:350:LYS:O	2.18	0.43
1:C:809:GLY:HA3	1:C:871:LEU:HB3	2.00	0.43
2:B:104:LYS:O	2:B:104:LYS:HD3	2.18	0.43
2:B:186:VAL:HG12	2:B:187:CYS:N	2.33	0.43
1:C:215:SER:HB2	1:C:259:GLU:HA	2.00	0.43
1:C:964:GLU:CG	1:C:973:VAL:HG11	2.44	0.43
2:D:109:ILE:O	2:D:113:PHE:CD1	2.72	0.43
2:D:109:ILE:O	2:D:113:PHE:HD1	2.02	0.43
2:D:70:PRO:O	2:D:73:ASP:OD1	2.37	0.43
1:A:683:ALA:HB1	1:A:714:LEU:HG	1.99	0.43
1:A:839:LEU:HB3	1:A:925:LEU:HD21	2.01	0.43
1:C:438:GLN:HE22	1:C:471:SER:HA	1.83	0.43
2:D:98:ALA:HB1	2:D:105:THR:CG2	2.49	0.43
2:D:118:ALA:N	2:D:154:ILE:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LEU:HD12	1:A:437:LEU:HD23	2.00	0.42
2:D:150:LEU:N	2:D:150:LEU:CD1	2.81	0.42
2:B:36:PHE:CD2	2:B:203:VAL:HG11	2.54	0.42
2:B:150:LEU:N	2:B:150:LEU:CD1	2.82	0.42
1:C:380:GLN:NE2	5:C:1206:HOH:O	2.26	0.42
1:C:835:THR:HA	1:C:884:GLY:HA2	2.01	0.42
2:D:172:ASP:OD1	2:D:172:ASP:N	2.52	0.42
1:A:709:LYS:HD3	1:A:735:PHE:CZ	2.54	0.42
1:A:949:LYS:HD3	1:A:949:LYS:HA	1.78	0.42
2:B:208:ASN:HB3	2:B:209:PRO:HD3	1.96	0.42
1:A:765:ARG:H	1:A:787:SER:HG	1.63	0.42
2:D:103:PRO:HG2	2:D:104:LYS:H	1.85	0.42
2:B:28:LYS:O	2:B:32:LEU:HG	2.20	0.42
2:B:102:HIS:CD2	2:B:103:PRO:CD	3.02	0.42
1:C:683:ALA:HB1	1:C:714:LEU:HG	2.01	0.42
1:C:855:ILE:CG2	1:C:856:SER:H	2.33	0.42
2:D:38:PHE:HD1	2:D:39:LEU:HG	1.84	0.42
1:A:809:GLY:HA3	1:A:871:LEU:HB3	2.02	0.42
2:B:127:PRO:HG2	2:B:139:VAL:HG12	2.01	0.42
1:C:390:ASN:HA	1:C:420:THR:O	2.20	0.42
2:D:85:GLN:HA	2:D:86:PRO:HD3	1.95	0.42
2:D:120:PHE:HD2	2:D:160:THR:OG1	2.02	0.42
1:C:414:LEU:HD12	1:C:437:LEU:HD23	2.01	0.42
1:A:627:MET:HG2	1:A:636:LEU:CD2	2.49	0.42
2:B:45:LYS:HA	2:B:77:ARG:HG2	2.02	0.42
1:C:546:LYS:HE2	1:C:546:LYS:HB2	1.91	0.42
2:D:182:PHE:CG	2:D:204:CYS:HB3	2.54	0.41
2:D:39:LEU:HD23	2:D:44:LEU:HD21	2.03	0.41
1:C:951:VAL:HB	1:C:963:TRP:HB2	2.02	0.41
1:A:66:ALA:HA	1:A:93:TRP:CE3	2.55	0.41
2:B:178:LEU:HB3	2:B:185:ILE:HD11	2.02	0.41
1:C:527:SER:HA	1:C:544:LEU:O	2.21	0.41
1:C:781:LEU:HD23	1:C:795:HIS:HA	2.02	0.41
2:D:12:TYR:HA	2:D:15:LYS:NZ	2.36	0.41
1:A:26:PRO:HD3	1:A:979:THR:CG2	2.50	0.41
1:A:464:PHE:HB3	1:A:494:TYR:CE1	2.55	0.41
1:A:543:GLU:O	1:A:558:TYR:HA	2.20	0.41
2:B:145:MET:SD	2:B:241:LEU:HD22	2.61	0.41
1:C:49:LYS:HZ3	1:C:979:THR:HB	1.84	0.41
2:D:45:LYS:O	2:D:77:ARG:HA	2.21	0.41
1:A:194:VAL:HB	1:A:206:TRP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:729:SER:O	1:C:730:ALA:HB2	2.21	0.41
2:D:178:LEU:HB3	2:D:185:ILE:HD11	2.02	0.41
2:B:242:SER:O	2:B:246:GLU:HB2	2.21	0.41
1:C:709:LYS:HD3	1:C:735:PHE:CZ	2.56	0.41
2:D:186:VAL:CG1	2:D:255:MET:HB2	2.50	0.41
1:A:401:LYS:HG3	1:A:402:ASP:N	2.36	0.41
1:A:417:LEU:HD22	1:A:439:SER:HB3	2.03	0.41
1:A:570:PHE:O	1:A:586:GLY:HA3	2.21	0.41
1:A:694:PHE:HA	1:A:700:LYS:O	2.21	0.41
2:B:25:SER:HA	2:B:28:LYS:HD2	2.03	0.41
2:B:246:GLU:CD	2:B:247:GLU:H	2.24	0.41
1:C:52:GLY:HA3	1:C:64:TYR:CE1	2.55	0.41
1:C:138:TYR:CE1	1:C:157:VAL:HG22	2.56	0.41
1:C:230:PHE:CD2	1:C:279:VAL:HG11	2.56	0.41
1:C:730:ALA:O	1:C:731:ARG:C	2.59	0.41
1:C:773:PHE:CD1	1:C:780:PHE:HB3	2.56	0.41
1:A:243:CYS:SG	1:A:272:LYS:O	2.73	0.40
2:B:26:ALA:HB2	2:B:56:SER:HB2	2.02	0.40
2:B:139:VAL:O	2:B:142:GLN:HB2	2.21	0.40
1:A:108:LEU:O	1:A:115:VAL:HA	2.20	0.40
1:A:977:ARG:HH11	1:A:977:ARG:HG2	1.86	0.40
1:C:785:VAL:HG12	1:C:791:ILE:HG12	2.02	0.40
1:C:982:ASP:OD1	2:D:198:LEU:HD21	2.21	0.40
2:D:149:GLN:HB2	2:D:150:LEU:HD12	2.03	0.40
2:D:208:ASN:O	2:D:210:PRO:HD3	2.22	0.40
1:A:438:GLN:HG3	1:A:439:SER:N	2.36	0.40
1:C:777:SER:OG	1:C:779:ASP:HB2	2.21	0.40
2:D:186:VAL:HG13	2:D:255:MET:HB2	2.02	0.40
2:D:208:ASN:O	2:D:210:PRO:CD	2.70	0.40
2:B:14:ARG:HH11	2:B:15:LYS:H	1.69	0.40
1:C:414:LEU:HD13	1:C:447:VAL:HG11	2.04	0.40
1:C:696:ASN:ND2	1:C:1012:LYS:NZ	2.69	0.40
1:C:977:ARG:HH11	1:C:977:ARG:HG2	1.87	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	990/1028 (96%)	943 (95%)	44 (4%)	3 (0%)	41	66
1	C	990/1028 (96%)	942 (95%)	45 (4%)	3 (0%)	41	66
2	B	227/325 (70%)	211 (93%)	13 (6%)	3 (1%)	12	30
2	D	227/325 (70%)	206 (91%)	16 (7%)	5 (2%)	6	17
All	All	2434/2706 (90%)	2302 (95%)	118 (5%)	14 (1%)	25	50

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	610	GLY
1	A	856	SER
2	B	211	SER
1	C	610	GLY
1	C	730	ALA
1	C	856	SER
2	D	37	HIS
2	D	211	SER
1	A	730	ALA
2	B	208	ASN
2	D	103	PRO
2	B	190	PRO
2	D	190	PRO
2	D	206	GLY

5.3.2 Protein sidechains (i)

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	900/927 (97%)	883 (98%)	17 (2%)	57	82
1	C	900/927 (97%)	878 (98%)	22 (2%)	49	77
2	B	203/289 (70%)	195 (96%)	8 (4%)	32	61
2	D	203/289 (70%)	196 (97%)	7 (3%)	37	66
All	All	2206/2432 (91%)	2152 (98%)	54 (2%)	49	77

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	72	VAL
1	A	239	VAL
1	A	254	ARG
1	A	256	ASN
1	A	365	LEU
1	A	392	SER
1	A	403	SER
1	A	787	SER
1	A	789	SER
1	A	820	VAL
1	A	838	HIS
1	A	858	ASP
1	A	900	THR
1	A	908	ASN
1	A	954	THR
1	A	979	THR
2	B	14	ARG
2	B	24	ARG
2	B	38	PHE
2	B	112	LEU
2	B	191	ARG
2	B	209	PRO
2	B	234	LYS
2	B	259	SER
1	C	13	VAL
1	C	72	VAL
1	C	133	GLU
1	C	239	VAL
1	C	254	ARG
1	C	365	LEU
1	C	403	SER
1	C	419	LYS

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Mol	Chain	Res	Type
1	C	489	SER
1	C	669	ASN
1	C	693	TYR
1	C	696	ASN
1	C	789	SER
1	C	812	LYS
1	C	820	VAL
1	C	858	ASP
1	C	900	THR
1	C	908	ASN
1	C	927	THR
1	C	954	THR
1	C	956	VAL
1	C	979	THR
2	D	24	ARG
2	D	33	ASN
2	D	38	PHE
2	D	157	LYS
2	D	205	LEU
2	D	244	TRP
2	D	259	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	671	ASN
1	A	673	ASN
1	A	776	GLN
1	A	882	GLN
2	B	19	GLN
2	B	35	GLN
2	B	102	HIS
2	B	177	GLN
1	C	669	ASN
1	C	673	ASN
1	C	678	HIS
1	C	696	ASN
1	C	722	HIS
1	C	776	GLN
1	C	795	HIS
1	C	808	GLN

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Mol	Chain	Res	Type
1	C	882	GLN
2	D	33	ASN
2	D	35	GLN
2	D	97	GLN
2	D	102	HIS
2	D	141	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are 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	$\#\|Z\| > 2$
3	SO4	A	1102	-	4,4,4	0.40	0	6,6,6	0.41	0
3	SO4	A	1101	-	4,4,4	0.32	0	6,6,6	0.38	0
3	SO4	C	1102	-	4,4,4	0.23	0	6,6,6	0.30	0
3	SO4	C	1101	-	4,4,4	0.16	0	6,6,6	0.33	0
4	EPE	A	1103	-	15,15,15	0.84	1 (6%)	19,20,20	1.73	3 (15%)
4	EPE	C	1103	-	15,15,15	0.82	1 (6%)	19,20,20	1.98	5 (26%)

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
4	EPE	C	1103	-	-	2/9/19/19	0/1/1/1
4	EPE	A	1103	-	-	4/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1103	EPE	C10-S	2.65	1.81	1.77
4	A	1103	EPE	C10-S	2.56	1.81	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1103	EPE	C5-N4-C3	5.40	120.46	108.84
4	A	1103	EPE	C5-N4-C3	4.83	119.25	108.84
4	A	1103	EPE	C7-N4-C5	3.36	120.19	111.24
4	C	1103	EPE	C7-N4-C3	3.15	119.62	111.24
4	C	1103	EPE	C7-N4-C5	3.00	119.22	111.24
4	C	1103	EPE	O3S-S-C10	2.88	111.64	106.00
4	C	1103	EPE	O2S-S-O1S	-2.17	106.76	113.82
4	A	1103	EPE	O2S-S-C10	2.03	109.80	106.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1103	EPE	C10-C9-N1-C2
4	C	1103	EPE	C8-C7-N4-C5
4	C	1103	EPE	N4-C7-C8-O8
4	A	1103	EPE	C8-C7-N4-C5
4	A	1103	EPE	N4-C7-C8-O8
4	A	1103	EPE	S-C10-C9-N1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1103	EPE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1103	EPE	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	998/1028 (97%)	0.12	7 (0%) 87 89	22, 39, 66, 96	0
1	C	998/1028 (97%)	0.14	10 (1%) 82 83	22, 39, 66, 94	0
2	B	231/325 (71%)	0.87	36 (15%) 2 1	27, 68, 96, 109	0
2	D	231/325 (71%)	0.92	38 (16%) 1 1	26, 68, 96, 106	0
All	All	2458/2706 (90%)	0.27	91 (3%) 41 41	22, 42, 83, 109	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	237	ILE	5.7
2	B	14	ARG	5.3
1	A	856	SER	4.9
2	D	257	CYS	4.9
2	D	235	LEU	4.8
2	B	257	CYS	4.6
2	D	205	LEU	4.4
2	D	258	GLY	4.3
2	D	245	ASN	4.3
2	D	243	HIS	4.3
2	B	255	MET	4.3
2	B	211	SER	4.3
2	B	243	HIS	4.2
2	B	106	LEU	4.2
2	D	255	MET	4.1
1	C	856	SER	3.8
1	C	610	GLY	3.8
2	B	245	ASN	3.8
2	D	196	THR	3.5
2	B	36	PHE	3.4
2	B	205	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	131	GLY	3.4
2	D	236	CYS	3.3
1	A	866	ALA	3.3
2	D	36	PHE	3.3
2	D	256	ALA	3.3
2	B	154	ILE	3.1
2	D	242	SER	3.1
2	D	183	ASP	3.1
1	A	612	HIS	3.0
2	D	44	LEU	3.0
2	B	103	PRO	3.0
2	D	244	TRP	2.9
2	B	258	GLY	2.9
2	B	38	PHE	2.9
2	D	110	LEU	2.8
1	A	133	GLU	2.8
1	C	731	ARG	2.7
2	B	151	THR	2.7
2	D	13	TYR	2.7
2	B	256	ALA	2.7
2	D	180	TYR	2.7
2	D	152	ALA	2.6
2	B	44	LEU	2.6
2	D	239	ASP	2.6
2	B	152	ALA	2.5
2	B	148	LEU	2.5
2	B	109	ILE	2.5
1	A	132	GLY	2.5
2	D	254	PHE	2.4
2	B	180	TYR	2.4
1	C	669	ASN	2.4
2	B	113	PHE	2.4
2	B	248	GLU	2.4
2	D	46	ARG	2.4
2	D	247	GLU	2.3
2	B	234	LYS	2.3
2	D	210	PRO	2.3
1	C	797	ARG	2.3
1	C	612	HIS	2.3
2	D	159	GLY	2.3
1	C	132	GLY	2.3
2	B	98	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	107	ALA	2.3
2	B	179	GLY	2.3
1	C	375	ILE	2.3
2	D	109	ILE	2.3
2	B	178	LEU	2.2
1	C	131	GLY	2.2
2	D	211	SER	2.2
2	D	246	GLU	2.2
2	D	179	GLY	2.2
2	D	203	VAL	2.2
1	C	997	SER	2.2
2	B	159	GLY	2.2
2	B	30	LEU	2.1
2	B	203	VAL	2.1
2	D	112	LEU	2.1
2	B	204	CYS	2.1
2	D	151	THR	2.1
2	D	184	LYS	2.1
1	A	816	LEU	2.1
2	D	103	PRO	2.1
2	B	236	CYS	2.1
2	D	144	ILE	2.0
2	B	46	ARG	2.0
2	B	100	ILE	2.0
2	B	68	GLU	2.0
2	D	14	ARG	2.0
2	D	238	SER	2.0
2	B	155	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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
4	EPE	C	1103	15/15	0.93	0.22	42,50,69,74	0
4	EPE	A	1103	15/15	0.95	0.21	41,50,63,69	0
3	SO4	A	1102	5/5	0.95	0.13	57,59,63,79	0
3	SO4	C	1102	5/5	0.96	0.15	57,59,65,71	0
3	SO4	C	1101	5/5	0.99	0.18	29,34,38,42	0
3	SO4	A	1101	5/5	0.99	0.16	31,36,39,47	0

6.5 Other polymers (i)

There are no such residues in this entry.