



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:28 PM UTC

PDB ID : 6JPL / pdb_00006jpl
Title : The X-ray structure of yeast tRNA methyltransferase Trm7-Trm734 in complex with S-adenosyl-L-methionine
Authors : Hirata, A.; Okada, K.; Yoshii, K.; Shiraisi, H.; Saijo, S.; Yonezawa, K.; Shimizu, N.; Hori, H.
Deposited on : 2019-03-27
Resolution : 2.32 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

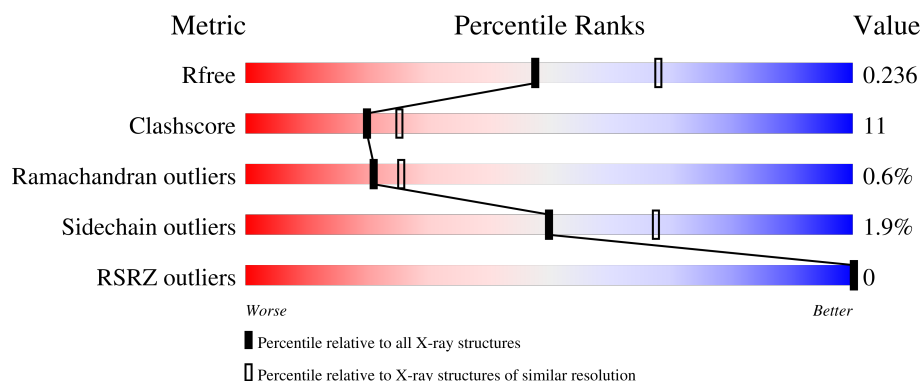
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

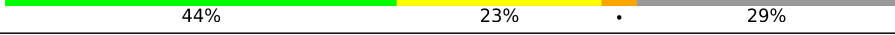
The reported resolution of this entry is 2.32 Å.

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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	1028	
1	C	1028	
2	B	325	
2	D	325	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20155 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
1	A	998	Total	C	N	O	S	0	0	0
			7951	5074	1328	1517	32			
1	C	998	Total	C	N	O	S	0	0	0
			7951	5074	1328	1517	32			

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
2	B	231	Total	C	N	O	S	0	0	0
			1829	1158	318	342	11			
2	D	231	Total	C	N	O	S	0	0	0
			1829	1158	318	342	11			

There are 30 discrepancies between the modelled and reference sequences:

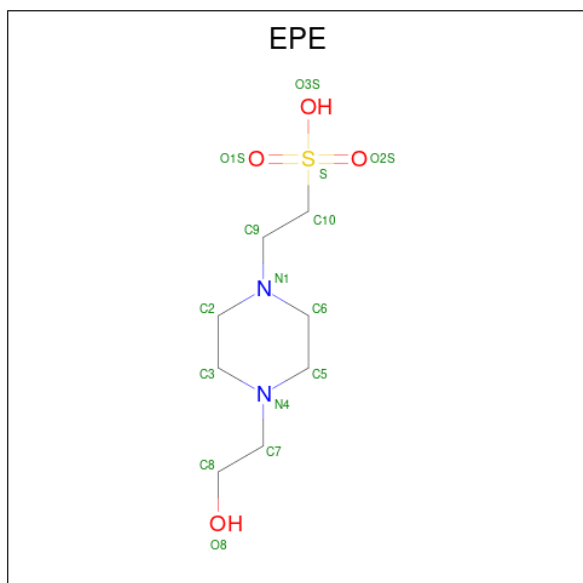
Chain	Residue	Modelled	Actual	Comment	Reference
B	311	LEU	-	expression tag	UNP P38238
B	312	GLU	-	expression tag	UNP P38238
B	313	VAL	-	expression tag	UNP P38238
B	314	LEU	-	expression tag	UNP P38238
B	315	PHE	-	expression tag	UNP P38238
B	316	GLN	-	expression tag	UNP P38238
B	317	GLY	-	expression tag	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 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



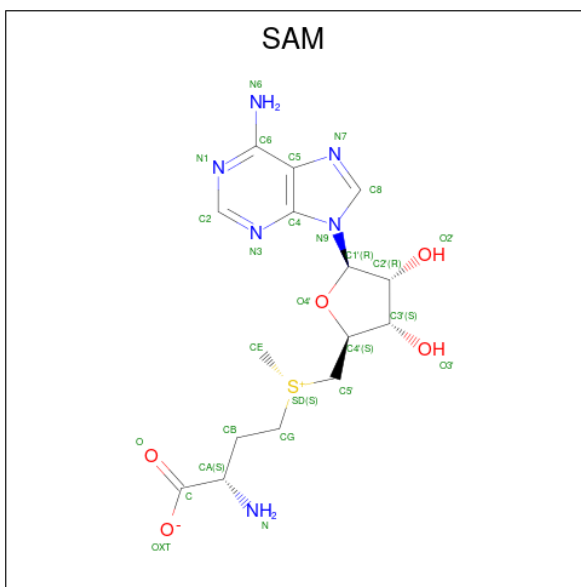
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 27	C 15	N 6	O 5	S 1	0	0
5	D	1	Total 27	C 15	N 6	O 5	S 1	0	0

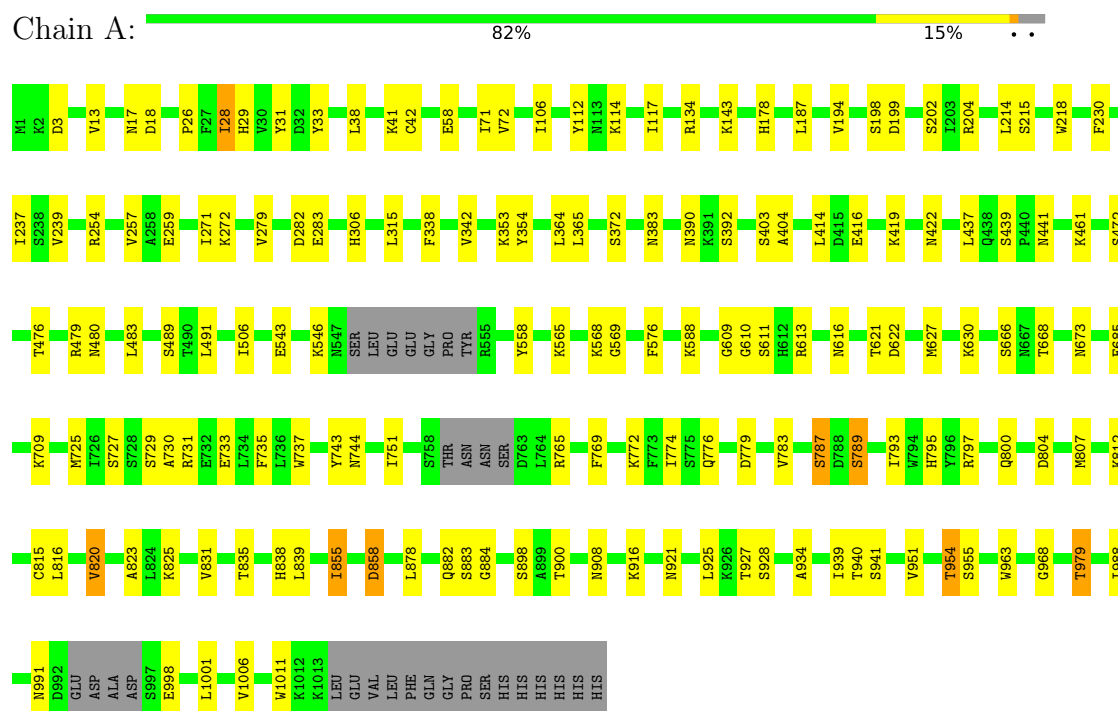
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	213	Total O 213 213	0	0
6	B	19	Total O 19 19	0	0
6	C	208	Total O 208 208	0	0
6	D	21	Total O 21 21	0	0

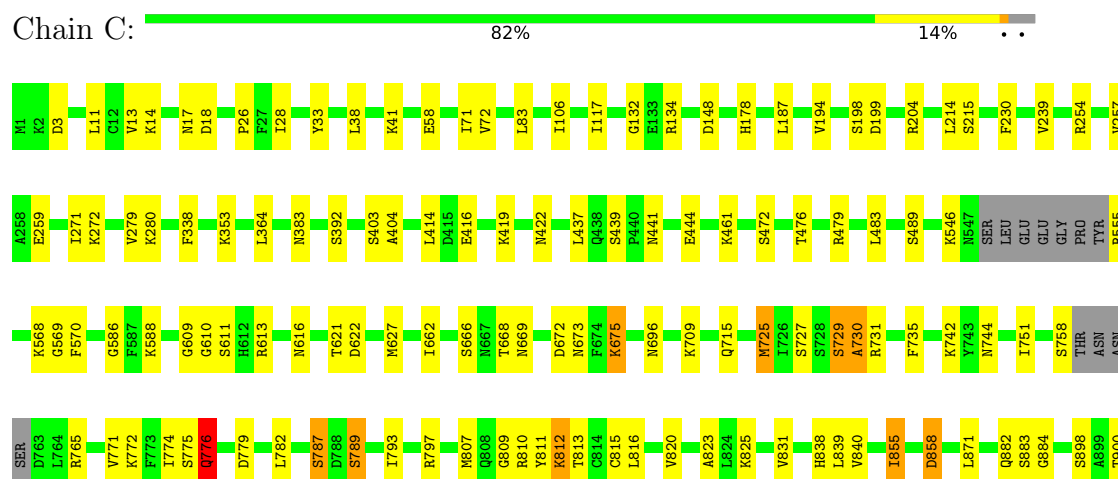
3 Residue-property plots

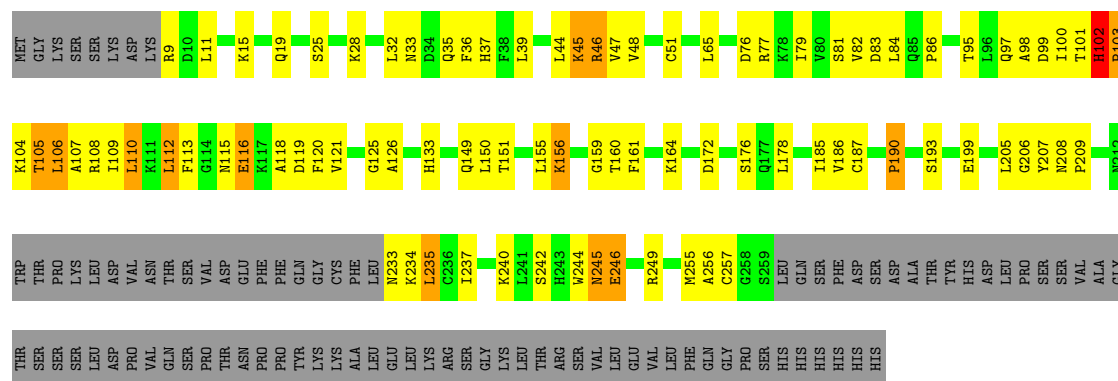
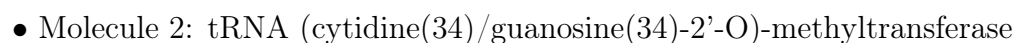
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	253.56Å 110.67Å 133.56Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	47.41 – 2.32 47.41 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.41-2.32) 99.8 (47.41-2.32)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.203 , 0.235 0.206 , 0.236	Depositor DCC
R_{free} test set	7997 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.487 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20155	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.42	0/8110	0.64	1/10972 (0.0%)
1	C	0.43	0/8110	0.66	8/10972 (0.1%)
2	B	0.49	0/1865	0.87	4/2516 (0.2%)
2	D	0.60	4/1865 (0.2%)	1.02	11/2516 (0.4%)
All	All	0.45	4/19950 (0.0%)	0.72	24/26976 (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	1
2	D	0	2
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	116	GLU	CB-CG	-6.31	1.33	1.52
2	D	46	ARG	NE-CZ	-6.10	1.26	1.33
2	D	46	ARG	CB-CG	-5.49	1.35	1.52
2	D	110	LEU	CG-CD2	-5.08	1.35	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	105	THR	CA-C-N	-11.22	100.87	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	105	THR	C-N-CA	-11.22	100.87	121.52
2	D	106	LEU	CB-CG-CD1	-10.18	80.17	110.70
2	D	246	GLU	N-CA-C	8.63	123.05	110.28
1	A	855	ILE	N-CA-C	8.31	120.75	108.45
2	D	46	ARG	NE-CZ-NH1	-8.15	113.35	121.50
1	C	675	LYS	CB-CG-CD	7.90	129.46	111.30
1	C	813	THR	N-CA-C	7.87	123.95	113.72
2	B	246	GLU	N-CA-C	7.75	121.59	109.96
1	C	855	ILE	N-CA-C	7.40	119.41	108.45
1	C	675	LYS	CD-CE-NZ	-7.26	88.66	111.90
1	C	675	LYS	CA-CB-CG	-6.29	101.53	114.10
2	D	106	LEU	CD1-CG-CD2	-6.24	97.07	110.80
2	B	116	GLU	CB-CG-CD	-6.18	102.08	112.60
2	D	149	GLN	CA-CB-CG	6.09	126.28	114.10
2	D	235	LEU	CA-CB-CG	5.93	137.07	116.30
1	C	730	ALA	N-CA-C	-5.93	100.41	108.24
1	C	675	LYS	CG-CD-CE	5.75	124.52	111.30
2	B	112	LEU	CA-CB-CG	5.52	135.63	116.30
2	D	110	LEU	CB-CG-CD2	-5.49	94.22	110.70
2	B	110	LEU	CA-CB-CG	5.25	134.66	116.30
2	D	45	LYS	CB-CA-C	5.24	120.85	110.42
2	D	116	GLU	CB-CG-CD	-5.16	103.84	112.60
1	C	729	SER	N-CA-C	5.15	116.98	108.48

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	776	GLN	Peptide
1	A	855	ILE	Peptide
2	B	245	ASN	Peptide
1	C	776	GLN	Peptide
1	C	855	ILE	Peptide
2	D	102	HIS	Peptide
2	D	245	ASN	Peptide

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	7951	0	7901	127	0
1	C	7951	0	7901	111	1
2	B	1829	0	1829	108	1
2	D	1829	0	1829	117	0
3	A	15	0	17	3	0
3	C	15	0	17	0	0
4	A	25	0	0	1	0
4	C	25	0	0	1	0
5	B	27	0	22	7	0
5	D	27	0	22	7	0
6	A	213	0	0	11	0
6	B	19	0	0	1	0
6	C	208	0	0	5	0
6	D	21	0	0	2	0
All	All	20155	0	19538	446	1

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

All (446) 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)
2:B:102:HIS:ND1	2:B:103:PRO:CD	1.97	1.26
2:B:246:GLU:HG3	2:B:247:GLU:OE2	1.33	1.23
2:B:102:HIS:ND1	2:B:103:PRO:HD3	1.56	1.18
2:B:102:HIS:ND1	2:B:103:PRO:HD2	1.66	1.10
1:A:479:ARG:HG3	1:A:480:ASN:H	1.12	1.08
2:D:104:LYS:O	2:D:108:ARG:N	1.92	1.02
2:B:246:GLU:CG	2:B:247:GLU:OE2	2.08	1.02
2:D:106:LEU:HD12	2:D:106:LEU:C	1.87	0.98
2:D:45:LYS:NZ	2:D:46:ARG:HH12	1.61	0.98
2:D:100:ILE:O	2:D:150:LEU:HD21	1.65	0.97
2:D:45:LYS:HZ1	2:D:46:ARG:HH12	1.12	0.94
1:A:730:ALA:CB	1:A:765:ARG:HG2	1.99	0.93
2:B:35:GLN:NE2	2:B:257:CYS:SG	2.41	0.93
2:B:104:LYS:O	2:B:108:ARG:N	2.03	0.90
1:C:882:GLN:HE21	2:D:256:ALA:H	1.13	0.89
1:A:28:ILE:HB	6:A:1273:HOH:O	1.74	0.87
1:A:479:ARG:HG3	1:A:480:ASN:N	1.90	0.86
1:A:479:ARG:CG	1:A:480:ASN:H	1.89	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ARG:HH12	2:B:76:ASP:HB3	1.41	0.83
2:D:110:LEU:HD12	2:D:115:ASN:OD1	1.77	0.83
1:C:730:ALA:CB	1:C:765:ARG:HG2	2.09	0.83
2:B:102:HIS:CG	2:B:103:PRO:HD2	2.14	0.82
2:D:103:PRO:HG2	2:D:104:LYS:H	1.45	0.81
1:A:898:SER:HB3	1:A:916:LYS:HG3	1.60	0.81
2:D:107:ALA:HA	2:D:110:LEU:HD21	1.62	0.80
2:B:45:LYS:HZ3	2:B:119:ASP:N	1.80	0.80
2:D:104:LYS:HA	2:D:107:ALA:HB3	1.64	0.80
1:A:673:ASN:ND2	1:A:744:ASN:O	2.15	0.80
1:C:898:SER:HB3	1:C:916:LYS:HG3	1.64	0.79
1:C:416:GLU:OE2	1:C:461:LYS:NZ	2.14	0.77
1:C:673:ASN:ND2	1:C:744:ASN:O	2.19	0.76
2:B:100:ILE:O	2:B:150:LEU:HD11	1.85	0.76
2:D:103:PRO:CG	2:D:104:LYS:H	1.94	0.76
2:B:73:ASP:OD1	2:B:73:ASP:N	2.18	0.75
2:D:45:LYS:HZ1	2:D:46:ARG:NH1	1.84	0.75
1:C:422:ASN:ND2	1:C:472:SER:O	2.21	0.74
1:C:730:ALA:HB2	1:C:765:ARG:HG2	1.70	0.74
2:D:103:PRO:HD2	2:D:105:THR:HG23	1.68	0.74
2:B:104:LYS:HA	2:B:107:ALA:HB3	1.68	0.74
1:A:729:SER:O	6:A:1201:HOH:O	2.06	0.73
2:B:103:PRO:HG2	2:B:104:LYS:H	1.54	0.73
1:A:988:ILE:HG12	1:A:1001:LEU:HD22	1.69	0.73
1:A:134:ARG:HG2	2:B:233:ASN:HA	1.69	0.72
1:A:630:LYS:NZ	6:A:1202:HOH:O	2.21	0.72
1:C:825:LYS:NZ	1:C:921:ASN:OD1	2.19	0.72
2:D:108:ARG:O	2:D:112:LEU:HD13	1.90	0.72
1:C:882:GLN:HE22	2:D:255:MET:HA	1.55	0.71
2:D:39:LEU:HD23	2:D:44:LEU:CD2	2.20	0.71
1:A:730:ALA:HB2	1:A:765:ARG:HG2	1.72	0.70
2:D:106:LEU:HD12	2:D:106:LEU:O	1.91	0.70
1:C:730:ALA:CB	1:C:765:ARG:CG	2.70	0.70
1:A:282:ASP:OD2	1:A:283:GLU:HG3	1.92	0.69
2:B:107:ALA:O	2:B:110:LEU:HB3	1.91	0.69
1:C:672:ASP:O	1:C:675:LYS:HG2	1.92	0.69
1:C:882:GLN:NE2	2:D:255:MET:HA	2.07	0.69
2:D:39:LEU:HD23	2:D:44:LEU:HD21	1.73	0.69
1:C:882:GLN:NE2	2:D:256:ALA:H	1.89	0.68
1:C:999:LYS:NZ	4:C:1104:SO4:O2	2.26	0.68
1:C:729:SER:OG	1:C:730:ALA:N	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:988:ILE:HG12	1:C:1001:LEU:HD22	1.75	0.68
2:B:102:HIS:CG	2:B:103:PRO:CD	2.74	0.68
1:C:134:ARG:HG3	2:D:233:ASN:HA	1.76	0.67
2:D:104:LYS:HG2	2:D:108:ARG:HB2	1.75	0.67
2:B:85:GLN:NE2	2:B:86:PRO:O	2.28	0.67
1:C:26:PRO:HD3	1:C:979:THR:HG21	1.76	0.67
5:B:401:SAM:N	6:B:501:HOH:O	2.28	0.66
2:B:35:GLN:C	2:B:37:HIS:H	2.04	0.66
2:D:36:PHE:HE2	2:D:257:CYS:SG	2.18	0.66
2:D:107:ALA:HA	2:D:110:LEU:CD2	2.26	0.66
2:B:246:GLU:CD	2:B:247:GLU:OE2	2.38	0.66
2:D:36:PHE:HE2	2:D:257:CYS:HG	1.42	0.66
1:C:669:ASN:OD1	1:C:742:LYS:NZ	2.29	0.66
1:C:925:LEU:O	1:C:926:LYS:HD2	1.96	0.66
2:B:9:ARG:HH22	2:D:9:ARG:NH2	1.94	0.65
1:A:271:ILE:HG13	1:A:272:LYS:HB3	1.78	0.65
2:D:99:ASP:OD1	2:D:101:THR:OG1	2.15	0.65
1:A:422:ASN:ND2	1:A:472:SER:O	2.30	0.65
1:A:282:ASP:OD2	1:A:283:GLU:N	2.29	0.64
1:A:609:GLY:O	1:A:611:SER:N	2.30	0.64
2:D:33:ASN:ND2	2:D:39:LEU:H	1.96	0.64
2:D:208:ASN:HB3	2:D:209:PRO:HD2	1.78	0.64
1:C:616:ASN:HB3	1:C:627:MET:HE3	1.79	0.64
2:B:208:ASN:HB3	2:B:209:PRO:HD2	1.79	0.64
2:D:103:PRO:HD2	2:D:105:THR:H	1.63	0.64
1:A:730:ALA:HB1	1:A:765:ARG:HG2	1.80	0.63
2:D:103:PRO:CG	2:D:104:LYS:N	2.61	0.63
2:B:104:LYS:HG2	2:B:108:ARG:HB2	1.80	0.63
1:A:729:SER:OG	1:A:730:ALA:N	2.25	0.63
1:C:898:SER:CB	1:C:916:LYS:HG3	2.30	0.62
1:A:26:PRO:HD3	1:A:979:THR:HG21	1.81	0.62
2:B:125:GLY:HA2	5:B:401:SAM:HG1	1.82	0.62
2:B:208:ASN:HB3	2:B:209:PRO:CD	2.29	0.62
2:D:208:ASN:HB3	2:D:209:PRO:CD	2.29	0.62
1:A:991:ASN:ND2	1:A:998:GLU:HG2	2.14	0.62
1:A:882:GLN:NE2	2:B:255:MET:HA	2.14	0.62
2:B:45:LYS:HE2	2:B:46:ARG:HB2	1.82	0.62
1:C:730:ALA:O	1:C:731:ARG:HB2	1.99	0.62
1:A:616:ASN:HB3	1:A:627:MET:HE3	1.81	0.61
2:D:237:ILE:HG13	2:D:240:LYS:HD3	1.81	0.61
1:A:568:LYS:HD2	1:A:569:GLY:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:ARG:NH1	2:D:116:GLU:OE2	2.34	0.61
1:A:735:PHE:HB3	1:A:751:ILE:HD11	1.83	0.61
2:B:174:LEU:O	2:B:178:LEU:HB2	2.01	0.61
2:D:45:LYS:HG2	2:D:46:ARG:NH1	2.17	0.60
2:D:46:ARG:HG2	2:D:113:PHE:CD1	2.37	0.60
1:C:725:MET:HE1	1:C:727:SER:HB3	1.84	0.59
2:D:106:LEU:HB3	2:D:150:LEU:HD13	1.84	0.59
2:B:46:ARG:HH12	2:B:76:ASP:CB	2.11	0.59
1:C:38:LEU:HD21	1:C:41:LYS:HG3	1.84	0.59
2:B:190:PRO:HD2	2:B:193:SER:HB2	1.85	0.59
1:A:611:SER:HA	1:C:810:ARG:CZ	2.32	0.59
1:A:797:ARG:NH1	1:A:804:ASP:OD1	2.35	0.59
1:A:611:SER:HA	1:C:810:ARG:NH2	2.17	0.59
1:A:991:ASN:HD21	1:A:998:GLU:HG2	1.68	0.58
1:C:991:ASN:OD1	1:C:998:GLU:HG2	2.03	0.58
1:C:772:LYS:HE2	1:C:823:ALA:HB2	1.83	0.58
2:D:11:LEU:CD2	2:D:15:LYS:HD3	2.34	0.58
1:A:414:LEU:HD12	1:A:437:LEU:HD23	1.85	0.58
1:C:730:ALA:HB1	1:C:765:ARG:HG3	1.84	0.58
2:D:242:SER:O	2:D:246:GLU:HB2	2.04	0.58
1:A:898:SER:CB	1:A:916:LYS:HG3	2.33	0.57
1:C:609:GLY:O	1:C:611:SER:N	2.37	0.57
2:D:98:ALA:HB1	2:D:105:THR:HG21	1.86	0.57
1:A:795:HIS:CE1	1:A:797:ARG:HD3	2.39	0.57
2:D:45:LYS:NZ	2:D:46:ARG:NH1	2.43	0.57
1:C:730:ALA:HB1	1:C:765:ARG:CG	2.33	0.57
1:C:271:ILE:HG13	1:C:272:LYS:HB3	1.86	0.57
1:A:772:LYS:HE2	1:A:823:ALA:HB2	1.86	0.56
1:A:858:ASP:OD2	1:A:858:ASP:N	2.38	0.56
1:C:815:CYS:N	6:C:1207:HOH:O	2.38	0.56
1:C:882:GLN:HE21	2:D:256:ALA:N	1.95	0.56
2:B:102:HIS:CB	2:B:103:PRO:HD2	2.36	0.56
2:B:99:ASP:HB3	2:B:102:HIS:HB2	1.87	0.56
1:C:71:ILE:HD11	1:C:106:ILE:HD13	1.88	0.56
2:D:125:GLY:HA2	5:D:401:SAM:HG1	1.88	0.56
2:D:190:PRO:HD2	2:D:193:SER:HB2	1.88	0.56
1:A:71:ILE:HD11	1:A:106:ILE:HD13	1.88	0.55
1:A:38:LEU:HD21	1:A:41:LYS:HG3	1.89	0.55
2:D:35:GLN:C	2:D:37:HIS:H	2.15	0.55
1:A:797:ARG:HH21	1:A:800:GLN:HE22	1.53	0.55
1:A:198:SER:OG	1:A:199:ASP:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLU:OE2	1:A:461:LYS:NZ	2.26	0.55
1:C:882:GLN:HE22	2:D:255:MET:CA	2.19	0.55
1:A:441:ASN:HB2	6:A:1215:HOH:O	2.07	0.55
2:D:11:LEU:HD21	2:D:15:LYS:HD3	1.88	0.55
2:B:151:THR:HG21	2:B:161:PHE:CD1	2.41	0.55
1:A:143:LYS:HZ2	1:A:187:LEU:HB2	1.72	0.55
2:B:46:ARG:NH1	2:B:76:ASP:O	2.40	0.54
2:B:109:ILE:HG23	2:B:113:PHE:HE1	1.72	0.54
1:C:669:ASN:OD1	1:C:669:ASN:N	2.40	0.54
2:D:100:ILE:O	2:D:150:LEU:CD2	2.48	0.54
5:D:401:SAM:N	6:D:501:HOH:O	2.33	0.54
1:C:72:VAL:CG2	1:C:83:LEU:HD13	2.36	0.54
2:D:47:VAL:HG12	2:D:120:PHE:HD1	1.70	0.54
2:B:119:ASP:HA	2:B:156:LYS:HE2	1.89	0.54
2:B:146:SER:O	2:B:149:GLN:NE2	2.41	0.54
1:C:198:SER:OG	1:C:199:ASP:N	2.39	0.54
2:B:99:ASP:OD1	2:B:101:THR:OG1	2.21	0.54
1:C:441:ASN:HB2	6:C:1302:HOH:O	2.08	0.54
2:B:126:ALA:H	5:B:401:SAM:HE3	1.73	0.54
1:C:414:LEU:HD12	1:C:437:LEU:HD23	1.89	0.54
2:B:84:LEU:HD21	2:B:99:ASP:HB2	1.89	0.53
2:B:246:GLU:OE1	2:B:246:GLU:HA	2.07	0.53
1:C:132:GLY:O	2:D:233:ASN:HB2	2.09	0.53
1:C:18:ASP:H	1:C:280:LYS:NZ	2.06	0.53
2:D:102:HIS:CG	2:D:103:PRO:HD3	2.44	0.53
2:B:45:LYS:HD3	2:B:46:ARG:H	1.73	0.53
1:A:730:ALA:HB2	6:A:1201:HOH:O	2.07	0.53
1:A:254:ARG:H	1:A:254:ARG:CD	2.21	0.53
1:C:928:SER:OG	1:C:968:GLY:O	2.25	0.53
2:D:84:LEU:HD21	2:D:99:ASP:HB2	1.90	0.52
1:A:254:ARG:H	1:A:254:ARG:HD2	1.75	0.52
2:B:35:GLN:HG3	2:B:257:CYS:O	2.10	0.52
2:D:120:PHE:HD2	2:D:160:THR:OG1	1.91	0.52
1:A:733:GLU:HG2	1:A:735:PHE:CZ	2.45	0.52
1:A:568:LYS:HD2	1:A:569:GLY:H	1.75	0.52
2:D:33:ASN:HD21	2:D:39:LEU:H	1.57	0.52
1:A:338:PHE:CD1	1:A:383:ASN:HA	2.45	0.52
1:C:134:ARG:HG2	2:D:233:ASN:OD1	2.10	0.52
2:D:19:GLN:HG2	6:D:505:HOH:O	2.10	0.52
2:D:48:VAL:HB	2:D:121:VAL:HG22	1.92	0.52
2:B:86:PRO:HG3	2:B:97:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:SER:OG	2:D:199:GLU:OE1	2.21	0.51
1:A:820:VAL:HG12	1:A:831:VAL:HB	1.93	0.51
1:C:568:LYS:HG3	1:C:588:LYS:HG2	1.92	0.51
2:D:126:ALA:H	5:D:401:SAM:HE3	1.75	0.51
1:C:858:ASP:N	1:C:858:ASP:OD2	2.43	0.51
2:D:100:ILE:HG12	5:D:401:SAM:N1	2.26	0.51
1:A:730:ALA:HB1	1:A:765:ARG:CG	2.41	0.51
1:C:215:SER:HB2	1:C:259:GLU:HA	1.93	0.51
1:C:730:ALA:HB2	1:C:765:ARG:CG	2.36	0.51
1:C:568:LYS:HD2	1:C:569:GLY:N	2.26	0.51
1:A:134:ARG:NH1	2:B:236:CYS:SG	2.83	0.50
1:A:735:PHE:HB3	1:A:751:ILE:CD1	2.41	0.50
1:C:353:LYS:HE3	1:C:404:ALA:HB3	1.93	0.50
2:D:35:GLN:HB2	2:D:257:CYS:O	2.12	0.50
2:B:103:PRO:CG	2:B:104:LYS:H	2.13	0.50
2:B:35:GLN:C	2:B:37:HIS:N	2.68	0.50
1:C:134:ARG:CG	2:D:233:ASN:HA	2.41	0.50
1:C:838:HIS:HD2	6:C:1259:HOH:O	1.94	0.50
2:D:39:LEU:HD23	2:D:44:LEU:HD22	1.94	0.50
2:B:33:ASN:C	2:B:35:GLN:H	2.19	0.50
2:B:36:PHE:HZ	2:B:186:VAL:HG11	1.76	0.50
2:D:246:GLU:OE1	2:D:246:GLU:HA	2.11	0.50
1:A:565:LYS:NZ	6:A:1214:HOH:O	2.44	0.49
1:C:709:LYS:HD3	1:C:735:PHE:CZ	2.47	0.49
2:D:45:LYS:HA	2:D:77:ARG:HG2	1.94	0.49
1:A:114:LYS:NZ	2:B:233:ASN:OD1	2.45	0.49
1:A:838:HIS:HD2	6:A:1292:HOH:O	1.94	0.49
2:B:45:LYS:HD3	2:B:119:ASP:OD1	2.13	0.49
2:D:36:PHE:HD1	2:D:205:LEU:HD11	1.76	0.49
1:A:928:SER:OG	1:A:968:GLY:O	2.29	0.49
1:A:883:SER:OG	1:A:884:GLY:N	2.45	0.49
1:A:364:LEU:HB3	1:A:365:LEU:HD23	1.94	0.49
2:B:45:LYS:HA	2:B:77:ARG:HG2	1.95	0.49
1:C:26:PRO:HD3	1:C:979:THR:CG2	2.42	0.49
2:D:186:VAL:CG1	2:D:255:MET:HB2	2.42	0.49
1:A:42:CYS:HB3	6:A:1273:HOH:O	2.12	0.49
1:A:882:GLN:HE21	2:B:255:MET:HA	1.78	0.49
2:B:45:LYS:O	2:B:77:ARG:HA	2.12	0.49
2:B:86:PRO:HB2	2:D:86:PRO:HB2	1.95	0.49
1:A:951:VAL:HB	1:A:963:TRP:HB2	1.95	0.49
2:B:103:PRO:HG2	2:B:104:LYS:N	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:666:SER:HB2	1:C:668:THR:HG22	1.95	0.49
1:C:883:SER:OG	1:C:884:GLY:N	2.46	0.49
2:B:33:ASN:C	2:B:35:GLN:N	2.70	0.48
1:A:797:ARG:HG3	1:A:797:ARG:HH11	1.79	0.48
2:B:45:LYS:NZ	2:B:119:ASP:OD2	2.36	0.48
2:D:106:LEU:O	2:D:110:LEU:HD23	2.13	0.48
1:A:178:HIS:CE1	1:A:204:ARG:HD2	2.48	0.48
2:B:25:SER:HA	2:B:28:LYS:HD2	1.94	0.48
1:A:3:ASP:HA	1:A:1011:TRP:CD1	2.49	0.48
2:B:48:VAL:HB	2:B:121:VAL:HG22	1.96	0.48
1:C:675:LYS:HG2	1:C:675:LYS:H	1.40	0.48
1:C:789:SER:HA	1:C:816:LEU:HG	1.96	0.48
1:A:215:SER:HB2	1:A:259:GLU:HA	1.95	0.48
2:D:36:PHE:CE2	2:D:257:CYS:SG	3.02	0.48
2:D:45:LYS:HZ3	2:D:76:ASP:HB3	1.79	0.47
1:A:576:PHE:HB2	3:A:1101:EPE:H91	1.96	0.47
2:D:98:ALA:HB1	2:D:105:THR:CG2	2.45	0.47
2:B:46:ARG:HB3	2:B:113:PHE:CE2	2.49	0.47
2:D:103:PRO:HG2	2:D:104:LYS:N	2.22	0.47
1:A:112:TYR:CG	1:A:134:ARG:NH2	2.82	0.47
1:C:793:ILE:HB	1:C:807:MET:HB3	1.96	0.47
1:A:779:ASP:CG	1:A:797:ARG:HA	2.39	0.47
1:A:214:LEU:HD22	1:A:257:VAL:HB	1.97	0.47
2:D:15:LYS:HB3	2:D:15:LYS:HE3	1.68	0.47
2:D:35:GLN:HE22	2:D:255:MET:CE	2.28	0.47
2:D:82:VAL:HG21	2:D:109:ILE:HD11	1.97	0.47
2:B:45:LYS:HG3	2:B:46:ARG:NH2	2.29	0.47
1:C:14:LYS:HE3	6:C:1347:HOH:O	2.13	0.47
1:C:546:LYS:HB2	1:C:546:LYS:HE3	1.72	0.47
1:C:918:ASP:OD2	1:C:922:LYS:HG2	2.14	0.47
3:A:1101:EPE:H21	6:A:1328:HOH:O	2.14	0.47
1:C:178:HIS:CE1	1:C:204:ARG:HD2	2.49	0.47
1:C:820:VAL:HG12	1:C:831:VAL:HB	1.96	0.47
2:D:47:VAL:CG2	2:D:79:ILE:HG12	2.45	0.47
2:B:117:LYS:CD	2:B:157:LYS:HZ1	2.28	0.47
2:B:126:ALA:HB2	2:B:164:LYS:HE2	1.97	0.47
1:C:730:ALA:HA	1:C:765:ARG:HG2	1.96	0.47
2:B:186:VAL:CG1	2:B:255:MET:HB2	2.45	0.47
2:B:36:PHE:CD2	2:B:203:VAL:HG11	2.50	0.46
1:A:709:LYS:HD3	1:A:735:PHE:CZ	2.51	0.46
2:B:120:PHE:HD2	2:B:160:THR:OG1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ASP:HA	1:C:33:TYR:CE2	2.51	0.46
1:C:364:LEU:HD12	1:C:364:LEU:HA	1.74	0.46
1:C:476:THR:HG22	1:C:483:LEU:HB2	1.96	0.46
2:B:28:LYS:O	2:B:32:LEU:HG	2.14	0.46
2:B:45:LYS:HG2	2:B:46:ARG:NE	2.30	0.46
1:C:214:LEU:HD22	1:C:257:VAL:HB	1.98	0.46
2:D:45:LYS:N	2:D:119:ASP:OD1	2.45	0.46
1:C:672:ASP:O	1:C:675:LYS:CD	2.64	0.46
1:C:774:ILE:HG22	1:C:774:ILE:O	2.14	0.46
2:D:45:LYS:CE	2:D:46:ARG:HH12	2.27	0.46
1:A:774:ILE:O	1:A:774:ILE:HG22	2.15	0.46
2:B:183:ASP:OD2	2:B:208:ASN:ND2	2.42	0.46
1:A:479:ARG:CG	1:A:480:ASN:N	2.61	0.46
2:B:237:ILE:HA	2:B:240:LYS:HG2	1.98	0.46
1:A:825:LYS:HZ3	1:A:921:ASN:HD21	1.63	0.46
1:C:72:VAL:HG22	1:C:83:LEU:HD13	1.96	0.46
1:C:951:VAL:HB	1:C:963:TRP:HB2	1.97	0.46
2:D:45:LYS:NZ	2:D:76:ASP:HB3	2.30	0.46
1:A:33:TYR:OH	1:A:283:GLU:OE1	2.28	0.45
1:A:730:ALA:CA	1:A:765:ARG:HG2	2.45	0.45
1:A:1006:VAL:HG21	2:B:133:HIS:CE1	2.51	0.45
2:B:243:HIS:ND1	2:B:244:TRP:HD1	2.14	0.45
1:C:3:ASP:HA	1:C:1011:TRP:CD1	2.51	0.45
1:A:372:SER:OG	1:A:390:ASN:OD1	2.21	0.45
1:A:793:ILE:HB	1:A:807:MET:HB3	1.98	0.45
1:A:940:THR:OG1	1:A:954:THR:HG23	2.16	0.45
2:B:36:PHE:CD1	2:B:205:LEU:HD11	2.51	0.45
2:B:96:LEU:HD22	2:B:108:ARG:CZ	2.47	0.45
2:B:98:ALA:HB1	2:B:105:THR:OG1	2.17	0.45
1:A:730:ALA:CB	1:A:765:ARG:CG	2.83	0.45
2:B:180:TYR:CE2	2:B:244:TRP:HE3	2.34	0.45
1:C:271:ILE:HA	1:C:272:LYS:HA	1.40	0.45
2:D:28:LYS:HE2	2:D:199:GLU:OE1	2.16	0.45
1:A:353:LYS:HB2	1:A:364:LEU:HD22	1.99	0.45
1:A:797:ARG:NH2	1:A:800:GLN:HE22	2.15	0.45
2:B:102:HIS:CB	2:B:103:PRO:CD	2.95	0.45
1:C:811:TYR:CE1	1:C:840:VAL:HG21	2.51	0.45
1:A:353:LYS:HE3	1:A:404:ALA:HB3	1.99	0.45
2:D:86:PRO:HG3	2:D:97:GLN:NE2	2.32	0.45
2:D:159:GLY:O	2:D:207:TYR:HB2	2.16	0.45
1:A:939:ILE:HA	1:A:955:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:LYS:CD	2:B:119:ASP:CG	2.89	0.45
1:C:230:PHE:CD2	1:C:279:VAL:HG11	2.51	0.45
1:A:825:LYS:NZ	1:A:921:ASN:HD21	2.15	0.45
2:B:35:GLN:CG	2:B:257:CYS:O	2.65	0.45
1:C:148:ASP:OD1	6:C:1201:HOH:O	2.21	0.45
1:C:338:PHE:CD1	1:C:383:ASN:HA	2.52	0.45
2:B:45:LYS:HD3	2:B:119:ASP:CG	2.42	0.44
1:A:725:MET:HE1	1:A:727:SER:HB3	1.99	0.44
2:D:125:GLY:HA2	5:D:401:SAM:H5'2	1.98	0.44
1:A:17:ASN:O	1:A:18:ASP:HB2	2.17	0.44
1:C:419:LYS:O	1:C:439:SER:HB2	2.18	0.44
1:C:839:LEU:HB3	1:C:925:LEU:HD21	2.00	0.44
1:A:479:ARG:NH1	1:A:546:LYS:HD3	2.33	0.44
2:B:157:LYS:HZ3	2:B:157:LYS:HG2	1.60	0.44
1:A:546:LYS:HE3	1:A:546:LYS:HB2	1.67	0.44
2:B:126:ALA:N	5:B:401:SAM:HE3	2.33	0.44
2:D:28:LYS:O	2:D:32:LEU:HG	2.16	0.44
2:D:118:ALA:O	2:D:156:LYS:HB3	2.18	0.44
1:A:730:ALA:HA	1:A:765:ARG:HG2	1.99	0.44
2:B:36:PHE:CE2	2:B:203:VAL:HG11	2.53	0.44
2:B:106:LEU:HD12	2:B:106:LEU:O	2.17	0.44
2:B:117:LYS:CE	2:B:157:LYS:HZ1	2.31	0.44
1:C:730:ALA:CA	1:C:765:ARG:HG2	2.47	0.44
2:D:176:SER:HB2	2:D:245:ASN:OD1	2.17	0.44
1:A:568:LYS:HG3	1:A:588:LYS:HG2	1.99	0.44
2:D:102:HIS:ND1	2:D:103:PRO:CD	2.81	0.44
1:A:26:PRO:HD3	1:A:979:THR:CG2	2.47	0.44
1:A:306:HIS:HE1	6:A:1322:HOH:O	2.01	0.44
1:A:543:GLU:O	1:A:558:TYR:HA	2.18	0.44
2:B:100:ILE:HG12	5:B:401:SAM:N1	2.32	0.44
1:A:187:LEU:HD22	1:A:194:VAL:HG22	2.00	0.43
1:A:611:SER:OG	1:A:613:ARG:NE	2.51	0.43
2:B:149:GLN:OE1	2:B:150:LEU:HD12	2.18	0.43
2:B:172:ASP:HB2	2:B:249:ARG:HB3	2.00	0.43
2:D:46:ARG:HG2	2:D:113:PHE:HD1	1.79	0.43
1:A:18:ASP:HA	1:A:33:TYR:CE2	2.54	0.43
1:A:613:ARG:NH2	4:A:1106:SO4:O1	2.51	0.43
1:A:825:LYS:NZ	1:A:921:ASN:ND2	2.66	0.43
2:D:45:LYS:NZ	2:D:76:ASP:CB	2.81	0.43
1:A:58:GLU:HB2	6:A:1229:HOH:O	2.18	0.43
1:A:419:LYS:O	1:A:439:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:ASP:HB3	5:B:401:SAM:N	2.33	0.43
2:B:186:VAL:HG12	2:B:187:CYS:N	2.34	0.43
1:C:662:ILE:HG13	1:C:987:GLU:HG2	2.00	0.43
1:C:1006:VAL:HG21	2:D:133:HIS:CE1	2.53	0.43
1:A:117:ILE:HD12	1:A:117:ILE:N	2.33	0.43
2:D:172:ASP:HB2	2:D:249:ARG:HB3	2.01	0.43
1:A:230:PHE:CE1	1:A:237:ILE:HB	2.54	0.43
1:A:271:ILE:HA	1:A:272:LYS:HA	1.39	0.43
1:C:672:ASP:O	1:C:675:LYS:CG	2.63	0.43
1:C:441:ASN:HB3	1:C:444:GLU:HG3	2.00	0.43
2:D:45:LYS:HE3	2:D:46:ARG:HH22	1.83	0.43
1:C:797:ARG:HE	1:C:797:ARG:HB3	1.18	0.43
2:D:81:SER:OG	2:D:95:THR:HG22	2.19	0.43
2:D:44:LEU:HD23	2:D:65:LEU:HD11	1.99	0.43
2:D:86:PRO:HG3	2:D:97:GLN:HE22	1.83	0.43
1:A:991:ASN:ND2	1:A:998:GLU:O	2.51	0.43
2:B:46:ARG:CZ	2:B:116:GLU:OE1	2.66	0.43
2:B:193:SER:OG	2:B:199:GLU:OE1	2.23	0.43
2:D:151:THR:HG21	2:D:161:PHE:CD1	2.53	0.43
1:C:479:ARG:NH1	1:C:546:LYS:HD3	2.34	0.42
2:D:178:LEU:O	2:D:185:ILE:HD11	2.19	0.42
1:A:941:SER:N	1:A:954:THR:HG22	2.35	0.42
2:B:17:LYS:HA	2:B:17:LYS:HD3	1.88	0.42
2:B:82:VAL:HG21	2:B:109:ILE:HD11	2.01	0.42
1:A:769:PHE:HA	1:A:783:VAL:O	2.19	0.42
2:B:164:LYS:HD2	2:B:199:GLU:HG3	2.01	0.42
1:C:765:ARG:H	1:C:787:SER:HG	1.65	0.42
1:C:809:GLY:HA3	1:C:871:LEU:HB3	2.02	0.42
2:D:102:HIS:HB3	2:D:103:PRO:HD3	2.00	0.42
2:D:155:LEU:HD21	2:D:159:GLY:O	2.20	0.42
1:A:621:THR:O	1:A:622:ASP:HB2	2.19	0.42
1:C:666:SER:CB	1:C:668:THR:HG22	2.50	0.42
1:C:811:TYR:O	1:C:812:LYS:HG2	2.20	0.42
1:A:666:SER:HB2	1:A:668:THR:HG22	2.01	0.42
1:A:934:ALA:HB3	1:A:939:ILE:HD11	2.02	0.42
2:B:159:GLY:O	2:B:207:TYR:HB2	2.18	0.42
1:C:187:LEU:HD22	1:C:194:VAL:HG22	2.02	0.42
1:C:742:LYS:HE3	1:C:742:LYS:HB3	1.77	0.42
2:D:126:ALA:HB2	2:D:164:LYS:HE2	2.01	0.42
1:A:685:GLU:O	1:A:685:GLU:HG2	2.20	0.42
2:B:100:ILE:O	2:B:150:LEU:CD1	2.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:LEU:HD23	2:B:198:LEU:HA	1.91	0.42
2:D:36:PHE:CD1	2:D:205:LEU:HD11	2.54	0.42
2:D:83:ASP:O	2:D:97:GLN:HA	2.20	0.42
1:C:775:SER:OG	1:C:776:GLN:N	2.53	0.42
2:B:241:LEU:HD23	2:B:241:LEU:HA	1.87	0.42
2:D:102:HIS:CB	2:D:103:PRO:HD3	2.50	0.42
1:A:765:ARG:H	1:A:787:SER:HG	1.66	0.41
1:C:570:PHE:O	1:C:586:GLY:HA3	2.19	0.41
1:C:758:SER:O	1:C:758:SER:OG	2.37	0.41
1:C:254:ARG:HA	1:C:254:ARG:HD3	1.78	0.41
1:C:715:GLN:HG3	1:C:729:SER:O	2.21	0.41
3:A:1101:EPE:H101	3:A:1101:EPE:H22	1.79	0.41
1:C:17:ASN:O	1:C:18:ASP:HB2	2.20	0.41
1:C:977:ARG:HH11	1:C:977:ARG:HG2	1.84	0.41
1:A:315:LEU:HD12	1:A:315:LEU:HA	1.89	0.41
2:B:148:LEU:HD23	2:B:148:LEU:HA	1.85	0.41
1:A:29:HIS:HB3	1:A:31:TYR:CE1	2.55	0.41
1:C:621:THR:O	1:C:622:ASP:HB2	2.20	0.41
1:C:735:PHE:HB3	1:C:751:ILE:CD1	2.51	0.41
2:D:35:GLN:O	2:D:36:PHE:HB2	2.20	0.41
2:D:46:ARG:CZ	2:D:116:GLU:OE2	2.68	0.41
2:D:103:PRO:CD	2:D:105:THR:HG23	2.44	0.41
2:D:186:VAL:HG12	2:D:187:CYS:N	2.35	0.41
2:D:240:LYS:HE2	2:D:244:TRP:CH2	2.56	0.41
2:B:28:LYS:HE2	2:B:199:GLU:OE1	2.20	0.41
2:D:106:LEU:HB3	2:D:150:LEU:CD1	2.50	0.41
1:A:783:VAL:HB	1:A:793:ILE:HD13	2.03	0.41
1:A:491:LEU:HD22	1:A:506:ILE:HD12	2.03	0.41
2:B:53:ALA:HB3	5:B:401:SAM:O3'	2.21	0.41
1:C:117:ILE:N	1:C:117:ILE:HD12	2.36	0.41
1:C:555:ARG:HA	1:C:555:ARG:HD3	1.91	0.41
2:D:84:LEU:HD12	5:D:401:SAM:C6	2.51	0.41
1:A:725:MET:CE	1:A:737:TRP:CD1	3.04	0.41
1:A:815:CYS:O	1:A:835:THR:HG23	2.22	0.41
1:C:779:ASP:CG	1:C:797:ARG:HA	2.47	0.41
2:D:234:LYS:HG2	2:D:235:LEU:N	2.36	0.41
1:A:476:THR:HG22	1:A:483:LEU:HB2	2.02	0.40
1:A:839:LEU:HB3	1:A:925:LEU:HD21	2.03	0.40
1:A:878:LEU:HD21	1:A:927:THR:HB	2.02	0.40
2:B:178:LEU:O	2:B:185:ILE:HD11	2.21	0.40
2:B:209:PRO:HA	2:B:210:PRO:HD2	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:960:ILE:O	1:C:975:LYS:HA	2.21	0.40
1:A:342:VAL:HB	1:A:354:TYR:HB3	2.03	0.40
1:A:725:MET:HE2	1:A:737:TRP:CD1	2.56	0.40
2:B:44:LEU:HA	2:B:119:ASP:OD1	2.21	0.40
2:B:172:ASP:CG	2:B:249:ARG:HB3	2.46	0.40
1:C:771:VAL:HG12	1:C:782:LEU:HD12	2.03	0.40
2:B:46:ARG:NE	2:B:116:GLU:OE1	2.54	0.40
2:D:36:PHE:HZ	2:D:186:VAL:HG11	1.87	0.40
2:D:102:HIS:ND1	2:D:103:PRO:N	2.69	0.40
2:D:234:LYS:N	2:D:234:LYS:HD3	2.36	0.40
1:A:202:SER:HB3	1:A:218:TRP:CZ3	2.56	0.40
1:A:789:SER:HA	1:A:816:LEU:HG	2.04	0.40
1:C:611:SER:OG	1:C:613:ARG:NH1	2.55	0.40
2:D:25:SER:HA	2:D:28:LYS:HD2	2.02	0.40
2:D:51:CYS:HB3	5:D:401:SAM:O4'	2.21	0.40
1:A:230:PHE:CD2	1:A:279:VAL:HG11	2.56	0.40
1:A:543:GLU:OE2	1:A:743:TYR:OH	2.29	0.40
1:A:725:MET:HE2	1:A:737:TRP:HD1	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:SER:OG	1:C:58:GLU:OE2[4_445]	2.19	0.01

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%)	944 (95%)	44 (4%)	2 (0%)	43 53
1	C	990/1028 (96%)	942 (95%)	46 (5%)	2 (0%)	43 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	227/325 (70%)	209 (92%)	12 (5%)	6 (3%)	4	3
2	D	227/325 (70%)	210 (92%)	13 (6%)	4 (2%)	6	5
All	All	2434/2706 (90%)	2305 (95%)	115 (5%)	14 (1%)	21	25

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	610	GLY
2	B	103	PRO
1	C	610	GLY
2	D	103	PRO
2	B	34	ASP
2	B	210	PRO
2	B	245	ASN
1	A	812	LYS
2	B	190	PRO
1	C	812	LYS
2	D	190	PRO
2	B	206	GLY
2	D	102	HIS
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%)	884 (98%)	16 (2%)	51	69
1	C	900/927 (97%)	881 (98%)	19 (2%)	47	65
2	B	203/289 (70%)	199 (98%)	4 (2%)	48	66
2	D	203/289 (70%)	201 (99%)	2 (1%)	68	81
All	All	2206/2432 (91%)	2165 (98%)	41 (2%)	50	67

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	28	ILE
1	A	72	VAL
1	A	239	VAL
1	A	392	SER
1	A	403	SER
1	A	489	SER
1	A	731	ARG
1	A	787	SER
1	A	789	SER
1	A	820	VAL
1	A	858	ASP
1	A	900	THR
1	A	908	ASN
1	A	954	THR
1	A	979	THR
2	B	15	LYS
2	B	73	ASP
2	B	112	LEU
2	B	181	LEU
1	C	11	LEU
1	C	13	VAL
1	C	28	ILE
1	C	239	VAL
1	C	392	SER
1	C	403	SER
1	C	489	SER
1	C	696	ASN
1	C	725	MET
1	C	776	GLN
1	C	787	SER
1	C	789	SER
1	C	858	ASP
1	C	900	THR
1	C	908	ASN
1	C	927	THR
1	C	954	THR
1	C	979	THR
1	C	997	SER
2	D	112	LEU
2	D	156	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	HIS
1	A	454	GLN
1	A	462	HIS
1	A	481	HIS
1	A	547	ASN
1	A	635	HIS
1	A	678	HIS
1	A	696	ASN
1	A	800	GLN
1	A	921	ASN
1	A	991	ASN
2	B	35	GLN
2	B	245	ASN
2	B	250	ASN
1	C	306	HIS
1	C	481	HIS
1	C	635	HIS
1	C	702	GLN
1	C	882	GLN
1	C	946	ASN
2	D	33	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
4	SO4	C	1104	-	4,4,4	0.26	0	6,6,6	0.24	0
3	EPE	A	1101	-	15,15,15	0.66	0	19,20,20	1.65	2 (10%)
4	SO4	C	1105	-	4,4,4	0.27	0	6,6,6	0.18	0
4	SO4	C	1102	-	4,4,4	0.25	0	6,6,6	0.31	0
4	SO4	A	1106	-	4,4,4	0.32	0	6,6,6	0.09	0
4	SO4	C	1106	-	4,4,4	0.26	0	6,6,6	0.21	0
4	SO4	A	1102	-	4,4,4	0.28	0	6,6,6	0.15	0
5	SAM	B	401	-	27,29,29	1.22	3 (11%)	34,42,42	2.21	9 (26%)
4	SO4	A	1104	-	4,4,4	0.24	0	6,6,6	0.33	0
4	SO4	A	1105	-	4,4,4	0.34	0	6,6,6	0.12	0
3	EPE	C	1101	-	15,15,15	0.75	1 (6%)	19,20,20	1.90	4 (21%)
4	SO4	C	1103	-	4,4,4	0.17	0	6,6,6	0.44	0
5	SAM	D	401	-	27,29,29	1.21	4 (14%)	34,42,42	2.20	10 (29%)
4	SO4	A	1103	-	4,4,4	0.36	0	6,6,6	0.30	0

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
3	EPE	A	1101	-	-	6/9/19/19	0/1/1/1
5	SAM	D	401	-	-	2/17/33/33	0/3/3/3
5	SAM	B	401	-	-	4/17/33/33	0/3/3/3
3	EPE	C	1101	-	-	6/9/19/19	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	SAM	C2-N3	3.03	1.39	1.33
5	B	401	SAM	C2-N3	3.02	1.39	1.33
5	D	401	SAM	C2-N1	2.84	1.39	1.33
5	B	401	SAM	C2-N1	2.73	1.38	1.33
5	D	401	SAM	C8-N7	2.52	1.36	1.31
5	B	401	SAM	C8-N7	2.50	1.36	1.31
3	C	1101	EPE	C10-S	2.49	1.81	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	SAM	OXT-C	-2.01	1.24	1.30

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	SAM	N3-C2-N1	-5.42	120.38	128.58
5	B	401	SAM	C5-C4-N3	-5.34	119.36	126.72
5	D	401	SAM	N3-C2-N1	-5.31	120.54	128.58
5	D	401	SAM	C5-C4-N3	-5.31	119.41	126.72
3	C	1101	EPE	C5-N4-C3	5.16	119.95	108.84
3	A	1101	EPE	C5-N4-C3	4.53	118.60	108.84
5	D	401	SAM	N9-C8-N7	-4.09	108.13	113.94
5	D	401	SAM	C5-N7-C8	3.95	109.66	103.45
5	B	401	SAM	C5-N7-C8	3.94	109.64	103.45
5	B	401	SAM	N9-C8-N7	-3.91	108.39	113.94
5	B	401	SAM	C2-N3-C4	3.87	121.28	111.83
5	D	401	SAM	C2-N3-C4	3.82	121.16	111.83
5	B	401	SAM	O4'-C1'-N9	3.54	114.89	108.09
5	D	401	SAM	O4'-C1'-N9	3.43	114.68	108.09
5	D	401	SAM	N3-C4-N9	3.26	132.71	127.17
5	B	401	SAM	C4-C5-N7	-3.24	106.88	110.58
5	B	401	SAM	N3-C4-N9	3.23	132.66	127.17
5	D	401	SAM	C4-C5-N7	-3.23	106.89	110.58
3	C	1101	EPE	C7-N4-C3	3.17	119.69	111.24
3	C	1101	EPE	C7-N4-C5	3.17	119.67	111.24
3	C	1101	EPE	O1S-S-C10	2.48	110.47	106.73
5	B	401	SAM	OXT-C-O	-2.47	118.47	124.08
5	D	401	SAM	OXT-C-O	-2.33	118.78	124.08
3	A	1101	EPE	C9-N1-C6	-2.33	105.02	111.24
5	D	401	SAM	C6-C5-C4	2.02	119.94	117.18

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	EPE	C9-C10-S-O1S
3	A	1101	EPE	N4-C7-C8-O8
3	C	1101	EPE	C9-C10-S-O3S
3	C	1101	EPE	C8-C7-N4-C3
3	A	1101	EPE	C10-C9-N1-C2
3	C	1101	EPE	C10-C9-N1-C2
3	A	1101	EPE	C9-C10-S-O2S

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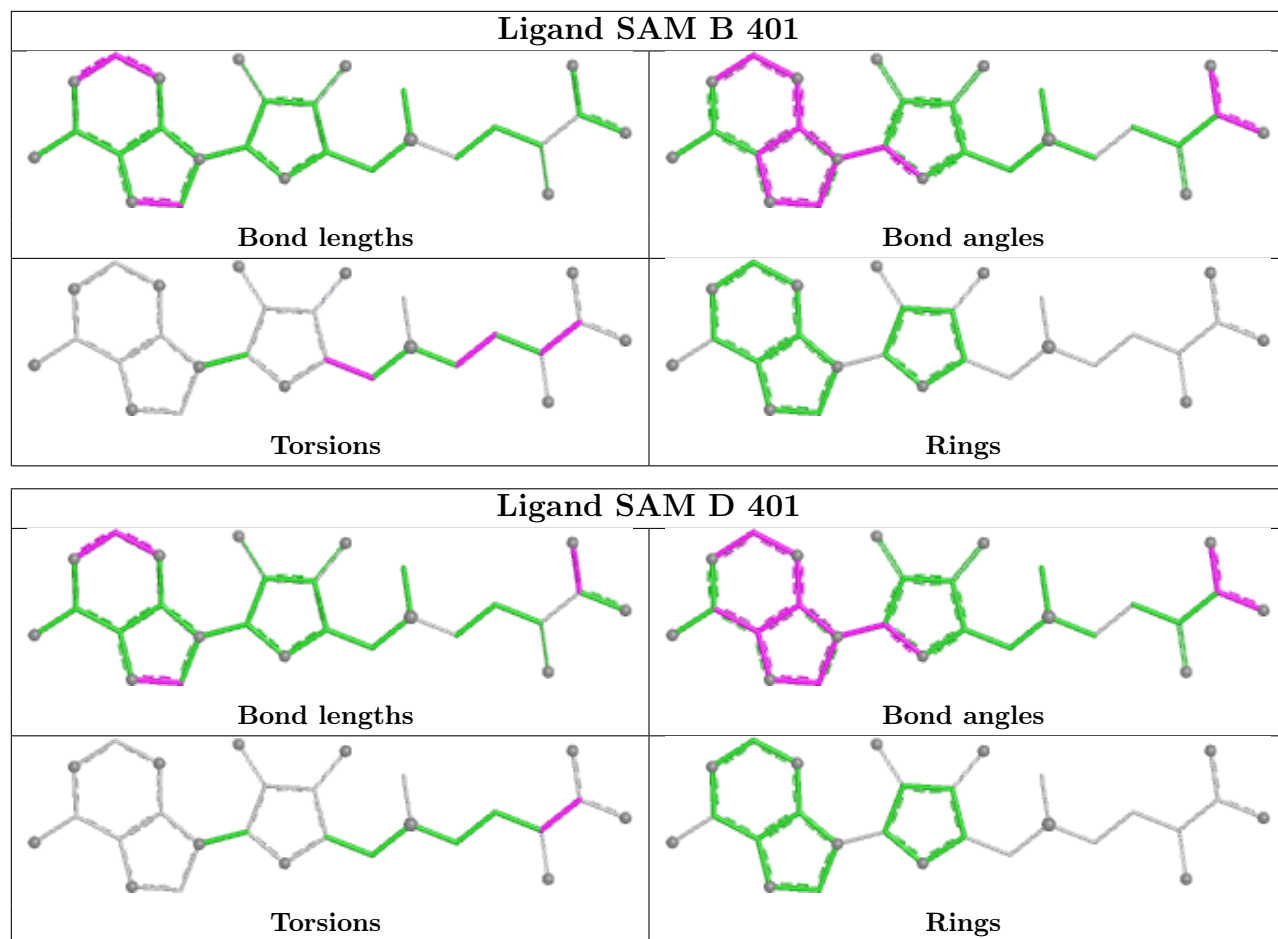
Mol	Chain	Res	Type	Atoms
3	C	1101	EPE	C9-C10-S-O1S
3	C	1101	EPE	C9-C10-S-O2S
3	A	1101	EPE	S-C10-C9-N1
5	B	401	SAM	CA-CB-CG-SD
5	B	401	SAM	O4'-C4'-C5'-SD
3	C	1101	EPE	C10-C9-N1-C6
3	A	1101	EPE	C9-C10-S-O3S
5	D	401	SAM	O-C-CA-N
5	D	401	SAM	OXT-C-CA-N
5	B	401	SAM	OXT-C-CA-N
5	B	401	SAM	O-C-CA-N

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1104	SO4	1	0
3	A	1101	EPE	3	0
4	A	1106	SO4	1	0
5	B	401	SAM	7	0
5	D	401	SAM	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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%)	-1.24	0 100 100	29, 44, 67, 95	0
1	C	998/1028 (97%)	-1.23	0 100 100	29, 43, 67, 94	0
2	B	231/325 (71%)	-0.82	0 100 100	34, 72, 97, 106	0
2	D	231/325 (71%)	-0.81	0 100 100	34, 71, 97, 107	0
All	All	2458/2706 (90%)	-1.15	0 100 100	29, 46, 84, 107	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

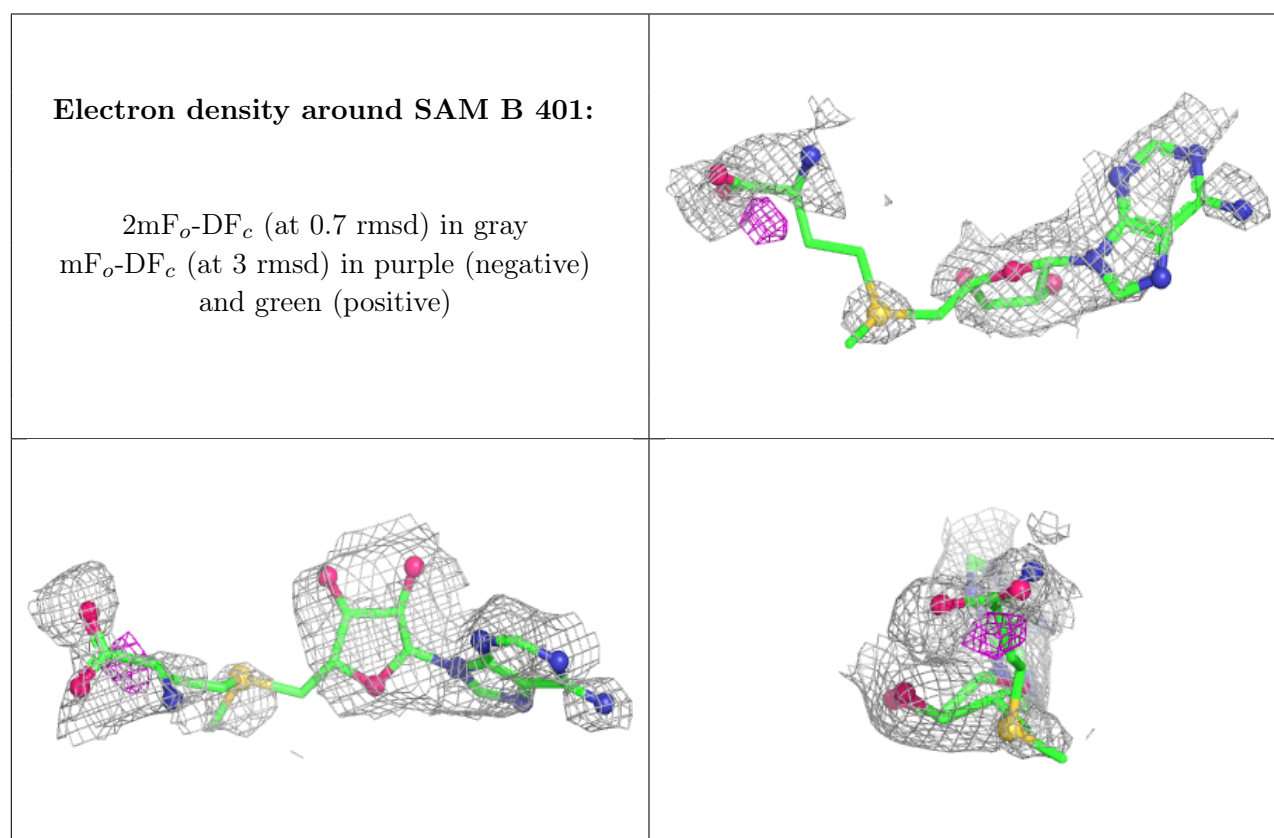
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	1105	5/5	0.97	0.05	71,76,81,84	0
4	SO4	C	1104	5/5	0.98	0.04	73,75,83,86	0
4	SO4	C	1105	5/5	0.98	0.05	76,77,82,85	0
4	SO4	C	1106	5/5	0.98	0.04	71,73,83,86	0

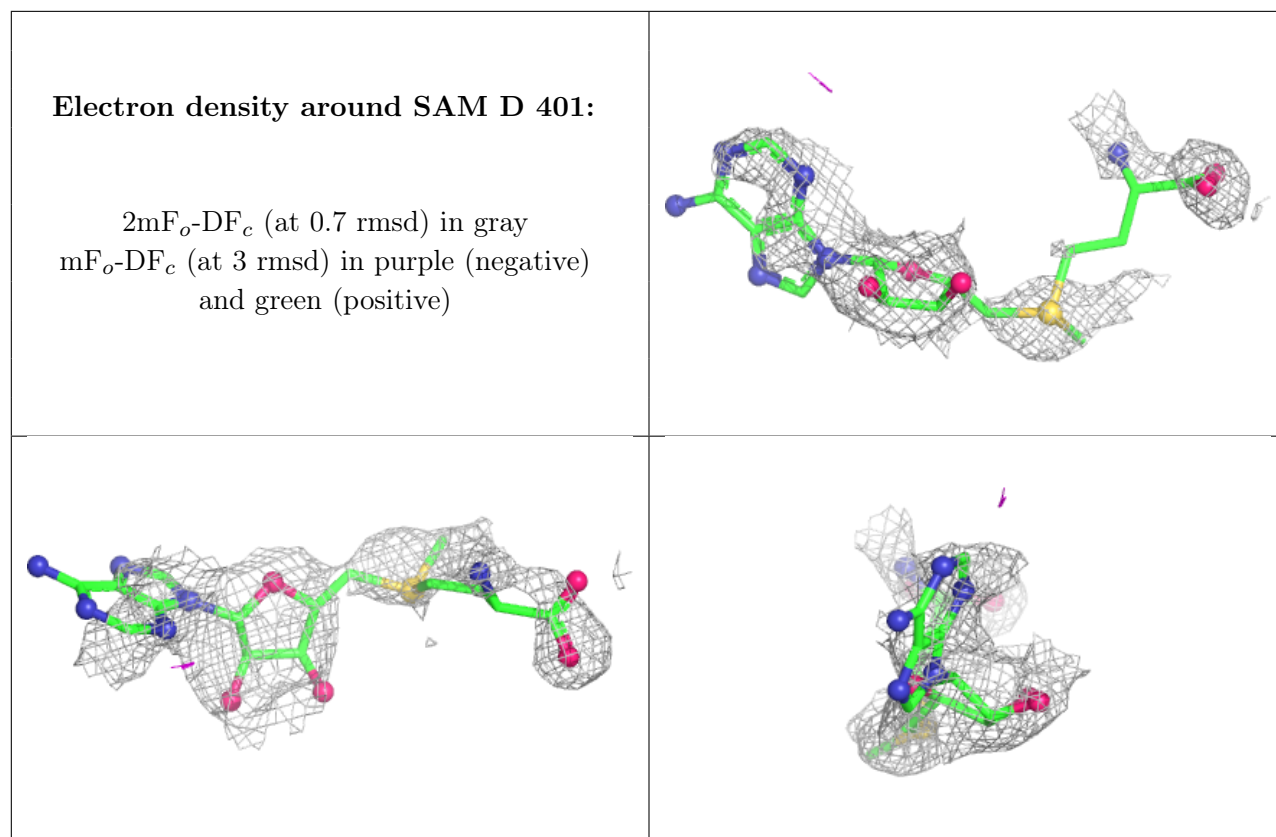
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SAM	B	401	27/27	0.98	0.07	55,74,82,87	0
5	SAM	D	401	27/27	0.98	0.07	55,73,83,85	0
4	SO4	A	1106	5/5	0.99	0.04	71,73,80,84	0
4	SO4	C	1103	5/5	0.99	0.03	59,62,66,74	0
3	EPE	C	1101	15/15	0.99	0.06	54,65,87,90	0
4	SO4	A	1102	5/5	0.99	0.04	38,43,47,47	0
4	SO4	A	1103	5/5	0.99	0.03	58,64,72,76	0
4	SO4	A	1104	5/5	0.99	0.04	77,78,81,83	0
3	EPE	A	1101	15/15	0.99	0.05	51,62,84,91	0
4	SO4	C	1102	5/5	1.00	0.03	37,43,47,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.