Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 09:57 AM EDT

PDB ID	:	3KU1
Title	:	Crystal structure of Streptococcus pneumoniae Sp1610, a putative tRNA (m1A22) methyltransferase, in complex with S-adenosyl-L-methionine
Authors	:	Ta, M.H.; Kim, K.K.
Deposited on	:	2009-11-26
Resolution	:	3.00 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:

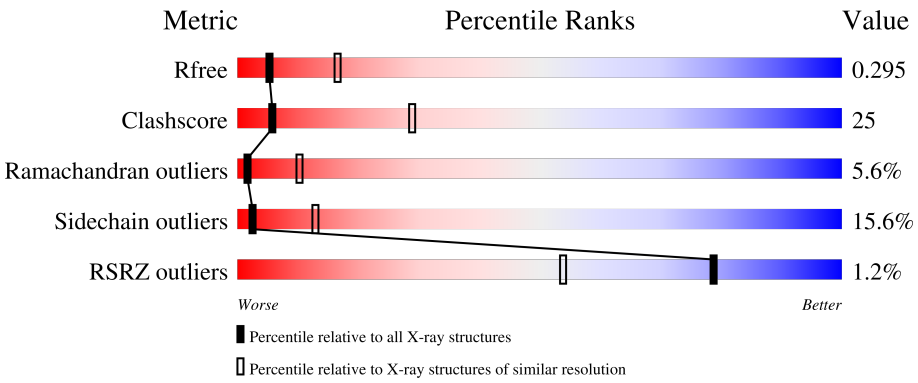
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	225	52% 34% 8% • 5%
1	B	225	% 46% 36% 11% • 5%
1	C	225	48% 42% • • 5%
1	D	225	2% 46% 35% 13% • 5%
1	E	225	2% 52% 31% 12% • 5%

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Mol	Chain	Length	Quality of chain
1	F	225	2% 46% 38% 10% • 5%
1	G	225	55% 34% 6% • 5%
1	H	225	58% 30% 6% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SAM	C	226	-	-	X	-
2	SAM	G	226	-	-	X	-

2 Entry composition (i)

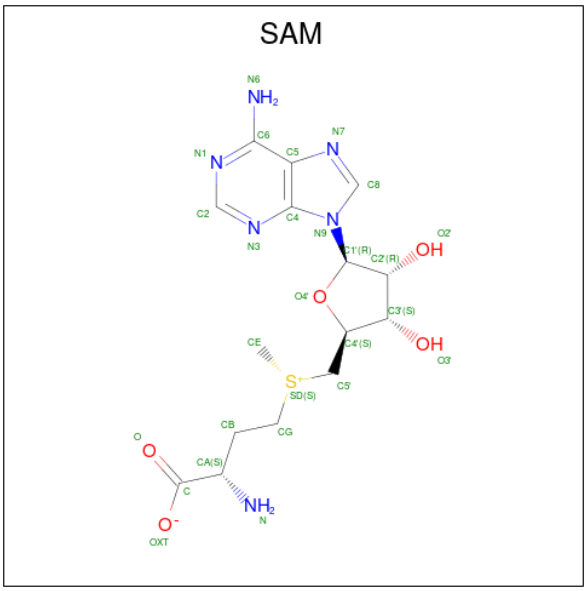
There are 2 unique types of molecules in this entry. The entry contains 13482 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SAM-dependent methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1663	1064	283	313	3	0	0	0
1	B	214	1673	1069	286	315	3	0	0	0
1	C	214	1673	1069	286	315	3	0	0	0
1	D	214	1673	1069	286	315	3	0	0	0
1	E	214	1673	1069	286	315	3	0	0	0
1	F	214	1673	1069	286	315	3	0	0	0
1	G	214	1673	1069	286	315	3	0	0	0
1	H	214	1673	1069	286	315	3	0	0	0

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



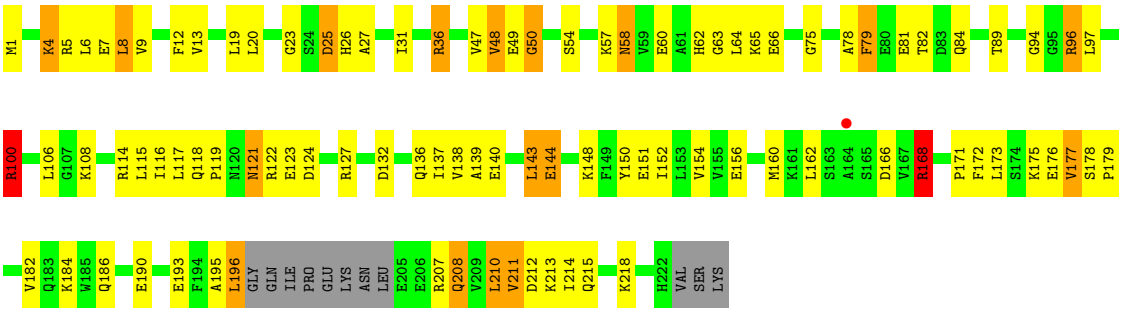
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	G	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	H	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

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.

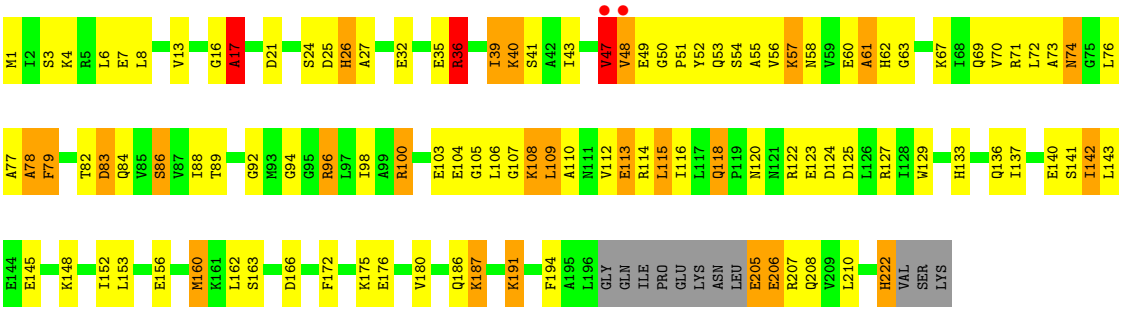
• Molecule 1: SAM-dependent methyltransferase

Chain A: 52% 34% 8% • 5%



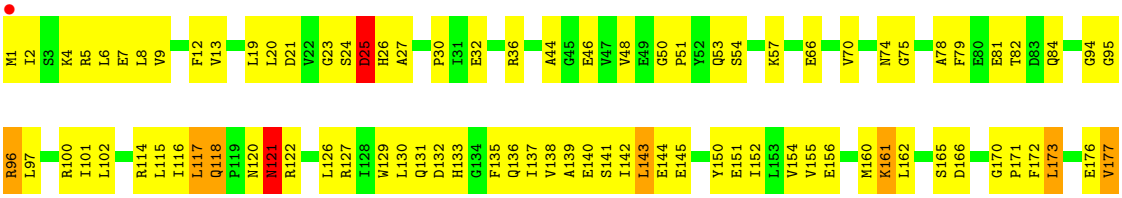
• Molecule 1: SAM-dependent methyltransferase

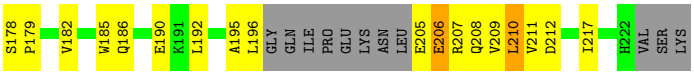
Chain B: % 46% 36% 11% • 5%



• Molecule 1: SAM-dependent methyltransferase

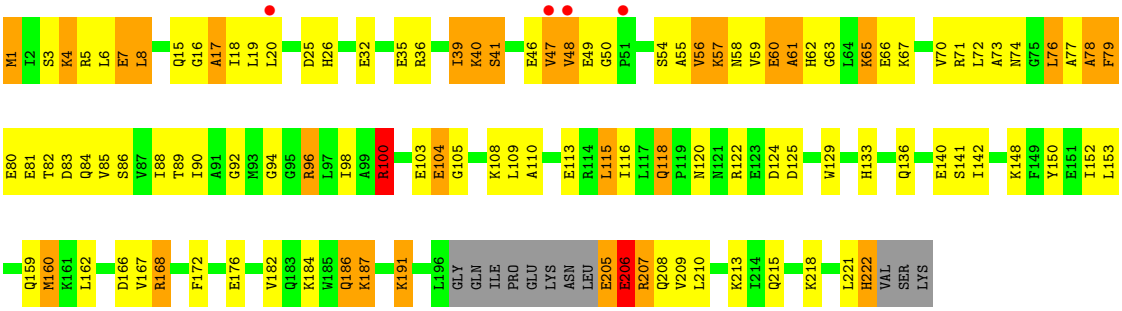
Chain C: 48% 42% • • 5%





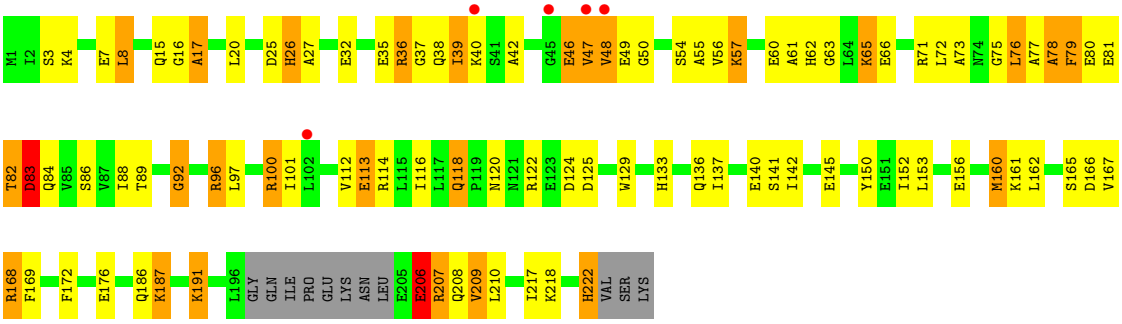
• Molecule 1: SAM-dependent methyltransferase

Chain D:



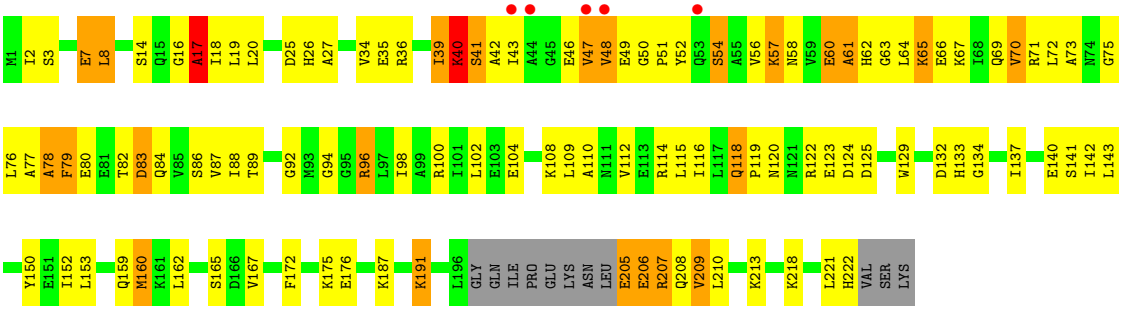
• Molecule 1: SAM-dependent methyltransferase

Chain E:



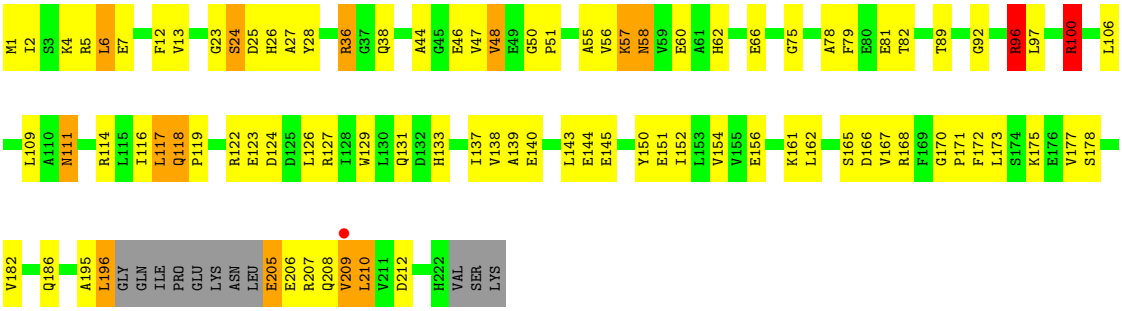
• Molecule 1: SAM-dependent methyltransferase

Chain F:



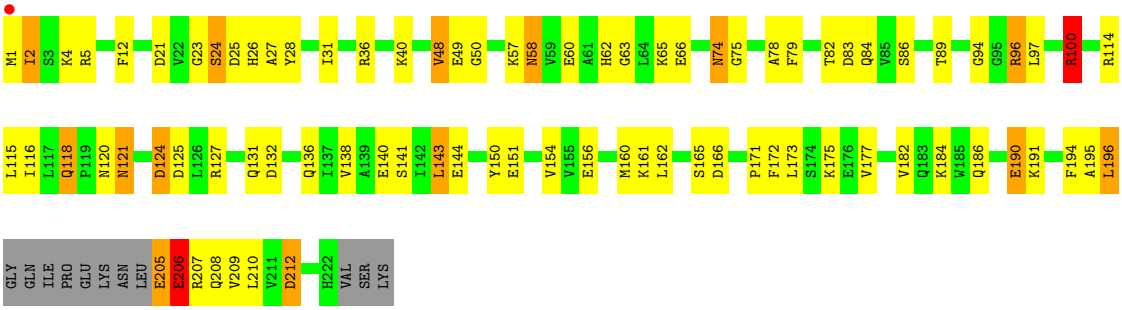
• Molecule 1: SAM-dependent methyltransferase

Chain G:



- Molecule 1: SAM-dependent methyltransferase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	142.75Å 142.75Å 148.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.46 – 3.00 46.73 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.46-3.00) 99.8 (46.73-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.296 0.242 , 0.295	Depositor DCC
R_{free} test set	3411 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	82.0	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.479 for -h,-k,l 0.480 for h,-h-k,-l 0.479 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13482	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: SAM

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	0.87	2/1685 (0.1%)	0.97	6/2271 (0.3%)
1	B	0.92	0/1695	0.96	2/2283 (0.1%)
1	C	0.88	2/1695 (0.1%)	1.00	6/2283 (0.3%)
1	D	0.94	4/1695 (0.2%)	0.98	2/2283 (0.1%)
1	E	0.91	1/1695 (0.1%)	0.94	0/2283
1	F	0.91	0/1695	0.93	0/2283
1	G	0.90	2/1695 (0.1%)	1.00	6/2283 (0.3%)
1	H	0.88	0/1695	0.98	1/2283 (0.0%)
All	All	0.90	11/13550 (0.1%)	0.97	23/18252 (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	B	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	H	0	1
All	All	0	5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	7	GLU	CG-CD	8.93	1.65	1.51
1	G	81	GLU	CB-CG	5.55	1.62	1.52
1	C	100	ARG	CG-CD	5.51	1.65	1.51
1	A	100	ARG	CG-CD	5.46	1.65	1.51
1	D	159	GLN	CG-CD	5.43	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	GLU	CB-CG	5.42	1.62	1.52
1	E	206	GLU	CD-OE2	5.36	1.31	1.25
1	C	81	GLU	CB-CG	5.34	1.62	1.52
1	G	100	ARG	CG-CD	5.28	1.65	1.51
1	D	191	LYS	CE-NZ	5.21	1.62	1.49
1	D	191	LYS	CD-CE	5.07	1.64	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	100	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	H	100	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	G	96	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	100	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	D	191	LYS	CD-CE-NZ	-6.73	96.23	111.70
1	C	100	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	25	ASP	CB-CA-C	6.29	122.98	110.40
1	G	117	LEU	CA-CB-CG	6.07	129.25	115.30
1	G	100	ARG	CA-CB-CG	5.84	126.24	113.40
1	A	25	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	D	100	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	100	ARG	CA-CB-CG	5.65	125.83	113.40
1	A	117	LEU	CA-CB-CG	5.56	128.09	115.30
1	B	36	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	A	100	ARG	CA-CB-CG	5.42	125.31	113.40
1	C	117	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	168	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	G	117	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	G	96	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	C	173	LEU	CA-CB-CG	5.29	127.47	115.30
1	C	100	ARG	CD-NE-CZ	5.16	130.82	123.60
1	B	106	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	117	LEU	CB-CG-CD1	-5.09	102.34	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	17	ALA	Peptide
1	D	206	GLU	Peptide
1	E	206	GLU	Peptide
1	F	17	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	H	206	GLU	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	1663	0	1705	85	1
1	B	1673	0	1720	98	1
1	C	1673	0	1720	87	0
1	D	1673	0	1720	100	0
1	E	1673	0	1720	100	0
1	F	1673	0	1720	88	1
1	G	1673	0	1720	90	0
1	H	1673	0	1720	62	1
2	A	27	0	22	7	0
2	C	27	0	22	9	0
2	G	27	0	21	18	0
2	H	27	0	22	6	0
All	All	13482	0	13832	693	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (693) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:HH11	1:A:96:ARG:CB	1.16	1.57
1:A:96:ARG:HB2	1:A:96:ARG:NH1	1.18	1.51
1:G:96:ARG:CB	1:G:96:ARG:HH11	1.28	1.45
1:H:96:ARG:HB2	1:H:96:ARG:NH1	1.31	1.43
1:C:96:ARG:NH1	1:C:96:ARG:HB2	1.22	1.40
1:G:96:ARG:NH1	1:G:96:ARG:HB2	1.06	1.38
1:C:96:ARG:NH1	1:C:96:ARG:CB	1.98	1.25
1:C:96:ARG:CB	1:C:96:ARG:HH11	1.53	1.20
1:G:96:ARG:CB	1:G:96:ARG:NH1	1.95	1.19
1:E:161:LYS:HD3	1:G:57:LYS:CG	1.75	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:LYS:HD3	1:G:57:LYS:HG3	1.21	1.14
1:H:96:ARG:NH1	1:H:96:ARG:CB	2.12	1.12
1:A:168:ARG:HG3	1:A:168:ARG:HH11	1.12	1.11
1:G:96:ARG:HH22	1:G:122:ARG:HD2	1.14	1.11
1:E:96:ARG:HH12	1:E:122:ARG:HD3	1.02	1.09
1:H:96:ARG:HB2	1:H:96:ARG:CZ	1.74	1.09
1:A:96:ARG:HH11	1:A:96:ARG:CG	1.67	1.08
1:E:206:GLU:C	1:E:208:GLN:H	1.62	1.02
1:G:75:GLY:H	2:G:226:SAM:HN62	1.04	1.02
1:H:206:GLU:C	1:H:208:GLN:H	1.64	1.01
1:C:96:ARG:HB2	1:C:96:ARG:CZ	1.92	1.00
1:A:23:GLY:HA2	2:A:226:SAM:H8	1.45	0.99
1:H:75:GLY:H	2:H:226:SAM:HN62	1.02	0.98
1:G:96:ARG:HB2	1:G:96:ARG:CZ	1.94	0.97
1:C:96:ARG:HH11	1:C:96:ARG:CG	1.78	0.95
1:E:96:ARG:HH12	1:E:122:ARG:CD	1.79	0.95
1:A:177:VAL:HG12	1:A:177:VAL:O	1.64	0.95
1:H:23:GLY:HA2	2:H:226:SAM:H8	1.48	0.94
1:E:96:ARG:NH1	1:E:122:ARG:HD3	1.81	0.93
1:B:205:GLU:HG3	1:B:206:GLU:H	1.33	0.92
1:C:75:GLY:H	2:C:226:SAM:HN62	1.12	0.92
1:A:75:GLY:H	2:A:226:SAM:HN62	1.00	0.91
1:G:92:GLY:O	2:G:226:SAM:HE2	1.72	0.90
1:E:161:LYS:CD	1:G:57:LYS:HG3	2.00	0.90
1:B:88:ILE:HD12	1:B:112:VAL:HG11	1.54	0.90
1:F:47:VAL:HA	1:F:73:ALA:O	1.70	0.90
1:G:96:ARG:HH22	1:G:122:ARG:CD	1.84	0.90
1:A:23:GLY:HA2	2:A:226:SAM:C8	2.02	0.89
1:B:206:GLU:C	1:B:208:GLN:H	1.74	0.89
1:C:5:ARG:HH11	1:C:118:GLN:NE2	1.69	0.89
1:H:23:GLY:O	2:H:226:SAM:N	2.05	0.89
1:C:21:ASP:OD2	1:C:24:SER:HB3	1.74	0.88
1:E:46:GLU:OE1	1:E:46:GLU:HA	1.73	0.87
1:G:75:GLY:N	2:G:226:SAM:N6	2.22	0.87
1:G:96:ARG:NH2	1:G:122:ARG:HD2	1.89	0.86
1:D:96:ARG:NH1	1:D:125:ASP:OD2	2.09	0.85
1:A:168:ARG:HG3	1:A:168:ARG:NH1	1.89	0.85
1:G:100:ARG:CB	1:G:100:ARG:HH11	1.89	0.85
1:E:88:ILE:HD12	1:E:112:VAL:HG11	1.58	0.84
1:G:100:ARG:HH11	1:G:100:ARG:HB3	1.39	0.84
1:H:96:ARG:CB	1:H:96:ARG:HH11	1.85	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:GLY:O	2:G:226:SAM:CE	2.26	0.84
1:B:96:ARG:NH1	1:B:125:ASP:OD2	2.12	0.83
1:D:72:LEU:HD22	1:E:65:LYS:HD3	1.62	0.82
1:G:58:ASN:HD21	1:G:62:HIS:CE1	1.97	0.82
1:C:206:GLU:O	1:C:206:GLU:HG2	1.80	0.82
1:D:129:TRP:O	1:D:133:HIS:HD2	1.61	0.82
1:D:100:ARG:HG2	1:D:100:ARG:HH11	1.45	0.81
1:C:120:ASN:O	1:C:121:ASN:HB3	1.80	0.81
1:H:206:GLU:C	1:H:208:GLN:N	2.32	0.81
1:H:96:ARG:CB	1:H:96:ARG:CZ	2.56	0.80
1:B:48:VAL:HG22	1:B:49:GLU:H	1.47	0.80
1:B:73:ALA:CB	1:B:78:ALA:H	1.95	0.80
1:D:40:LYS:O	1:D:41:SER:HB3	1.82	0.80
1:C:23:GLY:HA2	2:C:226:SAM:H8	1.62	0.79
1:A:96:ARG:CB	1:A:96:ARG:NH1	1.95	0.79
1:A:25:ASP:O	1:A:27:ALA:N	2.15	0.79
1:B:73:ALA:HB1	1:B:77:ALA:HB3	1.64	0.79
1:D:206:GLU:C	1:D:208:GLN:H	1.84	0.78
1:E:96:ARG:HH22	1:E:122:ARG:CD	1.97	0.78
1:F:129:TRP:O	1:F:133:HIS:HD2	1.67	0.78
1:E:206:GLU:C	1:E:208:GLN:N	2.32	0.78
1:A:140:GLU:HB2	1:A:172:PHE:HB2	1.66	0.77
1:G:6:LEU:HD21	2:G:226:SAM:OXT	1.84	0.77
1:E:47:VAL:HA	1:E:73:ALA:O	1.84	0.77
1:F:108:LYS:O	1:F:110:ALA:N	2.18	0.77
1:H:58:ASN:HD21	1:H:62:HIS:CE1	2.03	0.77
1:F:47:VAL:O	1:F:72:LEU:HD21	1.85	0.77
1:H:120:ASN:O	1:H:121:ASN:HB3	1.84	0.77
1:H:140:GLU:HB2	1:H:172:PHE:HB2	1.66	0.77
1:E:96:ARG:HH22	1:E:122:ARG:HD2	1.50	0.76
1:C:96:ARG:HH21	1:D:62:HIS:HA	1.51	0.76
1:F:96:ARG:HH22	1:F:122:ARG:HG3	1.48	0.76
1:D:187:LYS:O	1:D:191:LYS:HG3	1.87	0.75
1:F:60:GLU:O	1:F:63:GLY:N	2.19	0.75
1:A:96:ARG:HH22	1:A:122:ARG:HD2	1.52	0.74
1:B:187:LYS:O	1:B:191:LYS:HD3	1.88	0.74
1:G:96:ARG:HH11	1:G:96:ARG:CG	2.00	0.74
1:C:96:ARG:NH2	1:D:62:HIS:HA	2.02	0.73
1:H:25:ASP:O	1:H:27:ALA:N	2.20	0.73
1:C:4:LYS:O	1:C:7:GLU:HB3	1.88	0.73
1:H:23:GLY:HA2	2:H:226:SAM:C8	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:ARG:HG2	1:H:115:LEU:H	1.50	0.73
1:E:73:ALA:CB	1:E:78:ALA:H	2.02	0.73
1:B:206:GLU:O	1:B:208:GLN:N	2.22	0.73
1:F:73:ALA:CB	1:F:78:ALA:H	2.02	0.73
1:A:96:ARG:NH1	1:A:96:ARG:CG	2.34	0.73
1:B:96:ARG:HH22	1:B:122:ARG:HG3	1.55	0.72
1:B:206:GLU:C	1:B:208:GLN:N	2.41	0.72
1:B:108:LYS:O	1:B:110:ALA:N	2.22	0.72
1:C:12:PHE:CD1	1:C:154:VAL:HG21	2.25	0.72
1:G:100:ARG:HB3	1:G:100:ARG:NH1	2.05	0.72
1:D:47:VAL:HG22	1:D:74:ASN:HA	1.70	0.72
1:F:46:GLU:HA	1:F:46:GLU:OE1	1.90	0.71
1:B:71:ARG:NH1	1:B:83:ASP:OD2	2.19	0.71
1:E:100:ARG:HH11	1:E:100:ARG:HG2	1.55	0.71
1:C:5:ARG:HH11	1:C:118:GLN:HE21	1.37	0.70
1:D:47:VAL:CG2	1:D:74:ASN:HA	2.21	0.70
1:G:25:ASP:O	1:G:27:ALA:N	2.22	0.70
1:H:143:LEU:HD23	1:H:150:TYR:HB2	1.73	0.70
1:E:161:LYS:HD3	1:G:57:LYS:HG2	1.70	0.70
1:D:77:ALA:O	1:D:79:PHE:N	2.25	0.70
1:C:206:GLU:C	1:C:208:GLN:H	1.95	0.70
1:G:75:GLY:N	2:G:226:SAM:HN62	1.85	0.70
1:H:166:ASP:O	1:H:171:PRO:HD3	1.91	0.69
1:C:25:ASP:HB2	1:C:51:PRO:HB3	1.73	0.69
1:B:82:THR:O	1:B:84:GLN:HG2	1.92	0.69
1:D:7:GLU:OE1	1:D:36:ARG:NH2	2.24	0.69
1:E:60:GLU:O	1:E:63:GLY:N	2.24	0.69
1:G:205:GLU:O	1:G:208:GLN:HB2	1.92	0.69
1:B:73:ALA:HB1	1:B:78:ALA:H	1.56	0.69
1:E:168:ARG:HH11	1:E:168:ARG:CG	2.05	0.69
1:G:75:GLY:H	2:G:226:SAM:HN61	1.37	0.69
1:B:40:LYS:HE2	1:B:40:LYS:HA	1.72	0.69
1:E:206:GLU:O	1:E:208:GLN:N	2.25	0.69
1:G:111:ASN:N	1:G:111:ASN:HD22	1.90	0.69
1:B:47:VAL:O	1:B:72:LEU:HD21	1.92	0.69
1:D:129:TRP:O	1:D:133:HIS:CD2	2.46	0.69
1:C:114:ARG:HH11	1:C:154:VAL:HG11	1.58	0.68
1:E:96:ARG:CZ	1:E:96:ARG:HB2	2.24	0.68
1:B:210:LEU:HD12	1:B:210:LEU:H	1.58	0.68
1:H:114:ARG:NH1	1:H:154:VAL:HG11	2.08	0.68
1:F:75:GLY:O	1:F:77:ALA:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASN:HD21	1:A:62:HIS:CE1	2.11	0.68
1:F:205:GLU:HG3	1:F:206:GLU:OE1	1.93	0.68
1:B:88:ILE:HD11	1:B:112:VAL:HG21	1.74	0.68
1:H:4:LYS:NZ	1:H:144:GLU:O	2.27	0.68
1:F:73:ALA:HB3	1:F:78:ALA:HB2	1.76	0.68
1:B:73:ALA:CB	1:B:78:ALA:N	2.56	0.68
1:H:206:GLU:O	1:H:206:GLU:HG2	1.93	0.67
1:A:168:ARG:HH21	1:A:213:LYS:HE2	1.58	0.67
1:D:168:ARG:HH11	1:D:168:ARG:HG2	1.60	0.67
1:E:71:ARG:HH22	1:E:83:ASP:CG	1.97	0.67
1:H:151:GLU:HG2	1:H:173:LEU:HD11	1.77	0.67
1:B:205:GLU:CG	1:B:206:GLU:H	2.08	0.67
1:E:73:ALA:HB1	1:E:78:ALA:H	1.60	0.67
1:F:206:GLU:C	1:F:208:GLN:H	1.98	0.67
1:B:113:GLU:O	1:B:156:GLU:HG2	1.95	0.67
1:B:108:LYS:C	1:B:110:ALA:H	1.99	0.66
1:D:73:ALA:CB	1:D:78:ALA:H	2.07	0.66
1:D:168:ARG:HH11	1:D:168:ARG:CG	2.08	0.66
1:F:73:ALA:HB1	1:F:78:ALA:H	1.60	0.66
1:G:96:ARG:HH11	1:G:96:ARG:CA	2.05	0.66
1:C:166:ASP:HB3	1:C:171:PRO:HD3	1.78	0.66
1:H:12:PHE:CD1	1:H:154:VAL:HG21	2.31	0.66
1:F:96:ARG:HB2	1:F:96:ARG:CZ	2.24	0.66
1:E:48:VAL:HG22	1:E:49:GLU:H	1.59	0.66
1:D:191:LYS:HE2	1:F:191:LYS:HB2	1.76	0.66
1:A:4:LYS:O	1:A:7:GLU:HB3	1.96	0.65
1:B:72:LEU:HD23	1:B:73:ALA:N	2.10	0.65
1:H:143:LEU:CD2	1:H:150:TYR:HB2	2.26	0.65
1:C:48:VAL:HG23	1:C:51:PRO:HD2	1.77	0.65
1:B:89:THR:HG22	1:B:116:ILE:HB	1.78	0.65
1:C:206:GLU:C	1:C:208:GLN:N	2.49	0.65
1:D:108:LYS:O	1:D:110:ALA:N	2.29	0.65
1:G:12:PHE:CD1	1:G:154:VAL:HG21	2.31	0.65
1:E:96:ARG:NH1	1:E:125:ASP:OD2	2.30	0.65
1:C:5:ARG:NH1	1:C:118:GLN:NE2	2.45	0.65
1:G:5:ARG:NH2	2:G:226:SAM:O	2.30	0.65
1:B:92:GLY:H	1:B:118:GLN:HE21	1.44	0.64
1:G:48:VAL:HG22	1:G:51:PRO:HD2	1.79	0.64
1:G:114:ARG:NH1	1:G:154:VAL:HG11	2.13	0.64
1:B:205:GLU:HG3	1:B:206:GLU:N	2.10	0.64
1:A:23:GLY:CA	2:A:226:SAM:C8	2.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:ALA:HB1	1:F:77:ALA:HB3	1.79	0.64
1:G:209:VAL:HG23	1:G:210:LEU:HG	1.80	0.64
1:D:209:VAL:HG22	1:D:210:LEU:HD12	1.79	0.64
1:A:177:VAL:O	1:A:177:VAL:CG1	2.36	0.64
1:A:100:ARG:HH11	1:A:100:ARG:CB	2.10	0.63
1:C:21:ASP:OD2	1:C:24:SER:CB	2.45	0.63
1:C:75:GLY:N	2:C:226:SAM:HN62	1.92	0.63
1:G:46:GLU:HA	2:G:226:SAM:H8	1.80	0.63
1:A:178:SER:HB2	1:A:179:PRO:HD2	1.80	0.63
1:D:73:ALA:HB1	1:D:77:ALA:HB3	1.80	0.63
1:F:49:GLU:O	1:F:52:TYR:HB3	1.99	0.63
1:F:137:ILE:HD12	1:F:160:MET:HE1	1.79	0.63
1:E:8:LEU:HG	1:E:152:ILE:HD13	1.81	0.63
1:A:12:PHE:CD1	1:A:154:VAL:HG21	2.32	0.63
1:C:140:GLU:HB2	1:C:172:PHE:HB2	1.80	0.63
1:D:206:GLU:C	1:D:208:GLN:N	2.47	0.63
1:D:80:GLU:OE1	1:D:80:GLU:HA	1.98	0.63
1:H:96:ARG:HH11	1:H:96:ARG:CG	2.12	0.63
1:A:166:ASP:O	1:A:171:PRO:HD3	1.99	0.63
1:D:60:GLU:O	1:D:63:GLY:N	2.29	0.63
1:E:71:ARG:HD2	1:E:78:ALA:O	1.98	0.63
1:B:60:GLU:O	1:B:63:GLY:N	2.22	0.62
1:F:129:TRP:O	1:F:133:HIS:CD2	2.52	0.62
1:A:143:LEU:HD23	1:A:150:TYR:HB2	1.80	0.62
1:A:151:GLU:OE2	1:A:184:LYS:NZ	2.32	0.62
1:E:168:ARG:HH11	1:E:168:ARG:HG3	1.64	0.62
1:D:65:LYS:HD3	1:E:72:LEU:HD22	1.80	0.62
1:A:75:GLY:N	2:A:226:SAM:HN62	1.85	0.62
1:H:114:ARG:HG2	1:H:115:LEU:N	2.14	0.62
1:A:96:ARG:NH2	1:A:122:ARG:HD2	2.14	0.62
1:A:138:VAL:O	1:A:172:PHE:CZ	2.53	0.62
1:D:142:ILE:HG23	1:D:142:ILE:O	2.00	0.62
1:A:31:ILE:HD13	1:A:58:ASN:ND2	2.15	0.61
1:G:151:GLU:HG2	1:G:173:LEU:HD11	1.81	0.61
1:E:15:GLN:NE2	1:E:38:GLN:HA	2.15	0.61
1:F:40:LYS:O	1:F:41:SER:HB3	2.00	0.61
1:H:5:ARG:HE	1:H:118:GLN:NE2	1.98	0.61
1:D:73:ALA:HB1	1:D:78:ALA:H	1.65	0.61
1:A:151:GLU:HG2	1:A:173:LEU:HD11	1.83	0.61
1:D:82:THR:O	1:D:84:GLN:HG2	2.00	0.61
1:E:73:ALA:HB1	1:E:77:ALA:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:ARG:NH1	1:F:125:ASP:OD2	2.33	0.61
1:B:100:ARG:HG2	1:B:100:ARG:HH11	1.65	0.61
1:A:31:ILE:HD13	1:A:58:ASN:HD22	1.66	0.61
1:C:23:GLY:HA2	2:C:226:SAM:C8	2.30	0.61
1:D:46:GLU:O	1:D:72:LEU:HG	2.00	0.61
1:D:100:ARG:HH11	1:D:100:ARG:CG	2.13	0.61
1:E:26:HIS:ND1	1:E:54:SER:OG	2.26	0.60
1:B:137:ILE:HD12	1:B:160:MET:HE1	1.83	0.60
1:D:1:MET:HE1	1:D:62:HIS:NE2	2.16	0.60
1:E:137:ILE:HD12	1:E:160:MET:HE1	1.84	0.60
1:E:161:LYS:CD	1:G:57:LYS:CG	2.64	0.60
1:D:39:ILE:HG13	1:D:41:SER:H	1.67	0.60
1:E:86:SER:O	1:E:113:GLU:HG3	2.01	0.60
1:A:114:ARG:HH11	1:A:154:VAL:HG11	1.67	0.59
1:E:89:THR:HA	1:E:116:ILE:O	2.03	0.59
1:E:113:GLU:O	1:E:156:GLU:HG2	2.02	0.59
1:G:140:GLU:HB2	1:G:172:PHE:HB2	1.84	0.59
1:B:88:ILE:HB	1:B:115:LEU:HD12	1.84	0.59
1:B:96:ARG:NH2	1:B:122:ARG:HG3	2.16	0.59
1:D:54:SER:O	1:D:57:LYS:HB2	2.03	0.59
1:E:129:TRP:O	1:E:133:HIS:HD2	1.86	0.59
1:C:96:ARG:NH1	1:C:96:ARG:CG	2.46	0.59
1:D:205:GLU:HG3	1:D:206:GLU:H	1.67	0.59
1:D:142:ILE:O	1:D:142:ILE:CG2	2.50	0.59
1:E:71:ARG:NH1	1:E:83:ASP:OD2	2.32	0.59
1:E:96:ARG:NH2	1:E:122:ARG:HD2	2.16	0.59
1:A:182:VAL:O	1:A:186:GLN:HB2	2.02	0.58
1:D:124:ASP:OD1	1:D:125:ASP:N	2.33	0.58
1:F:73:ALA:CB	1:F:78:ALA:N	2.66	0.58
1:H:205:GLU:CD	1:H:206:GLU:N	2.56	0.58
1:C:96:ARG:HH11	1:C:96:ARG:HG3	1.66	0.58
1:D:1:MET:CE	1:D:62:HIS:NE2	2.67	0.58
1:A:23:GLY:O	2:A:226:SAM:HB1	2.04	0.58
1:E:47:VAL:O	1:E:72:LEU:HD21	2.02	0.58
1:G:4:LYS:O	1:G:7:GLU:HB3	2.04	0.58
1:G:162:LEU:HD22	1:G:171:PRO:HG3	1.85	0.58
1:A:138:VAL:HG11	1:A:156:GLU:OE1	2.04	0.58
1:C:205:GLU:CD	1:C:206:GLU:N	2.56	0.58
1:C:205:GLU:O	1:C:208:GLN:HB2	2.04	0.58
1:E:209:VAL:HG13	1:E:210:LEU:HD12	1.84	0.58
1:G:100:ARG:HH11	1:G:100:ARG:HB2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ALA:O	1:D:59:VAL:HG23	2.04	0.58
1:E:168:ARG:HD3	1:E:169:PHE:CZ	2.39	0.58
1:F:26:HIS:O	1:F:27:ALA:HB3	2.04	0.58
1:G:166:ASP:O	1:G:171:PRO:HD3	2.04	0.58
1:A:114:ARG:HG2	1:A:115:LEU:N	2.19	0.57
1:D:35:GLU:OE2	1:D:62:HIS:HD2	1.87	0.57
1:F:72:LEU:HD23	1:F:73:ALA:N	2.19	0.57
1:A:208:GLN:NE2	1:A:212:ASP:OD1	2.37	0.57
1:H:131:GLN:OE1	1:H:161:LYS:HA	2.05	0.57
1:B:88:ILE:CD1	1:B:112:VAL:HG21	2.35	0.57
1:F:52:TYR:CE1	1:F:70:VAL:HG11	2.39	0.57
1:B:73:ALA:HB1	1:B:77:ALA:CB	2.35	0.57
1:E:4:LYS:O	1:E:7:GLU:HB3	2.05	0.57
1:C:114:ARG:NH1	1:C:154:VAL:HG11	2.20	0.57
1:E:210:LEU:HD12	1:E:210:LEU:H	1.70	0.57
1:C:94:GLY:HA2	1:C:121:ASN:ND2	2.20	0.56
1:A:215:GLN:HE22	1:A:218:LYS:HE2	1.71	0.56
1:C:117:LEU:HD13	1:C:126:LEU:HD21	1.87	0.56
1:G:13:VAL:HG23	1:G:116:ILE:HD13	1.86	0.56
1:H:136:GLN:HA	1:H:160:MET:SD	2.45	0.56
1:B:47:VAL:HG12	1:B:48:VAL:H	1.69	0.56
1:D:8:LEU:HG	1:D:152:ILE:HD13	1.88	0.56
1:A:94:GLY:HA2	1:A:121:ASN:ND2	2.21	0.56
1:D:96:ARG:HB2	1:D:96:ARG:CZ	2.35	0.56
1:B:210:LEU:HD12	1:B:210:LEU:N	2.19	0.56
1:D:88:ILE:HB	1:D:115:LEU:HD12	1.88	0.56
1:G:58:ASN:ND2	1:G:62:HIS:CE1	2.71	0.56
1:B:84:GLN:OE1	1:B:84:GLN:HA	2.06	0.56
1:G:111:ASN:N	1:G:111:ASN:ND2	2.53	0.56
1:E:136:GLN:HA	1:E:160:MET:HG2	1.88	0.56
1:B:52:TYR:CE1	1:B:70:VAL:HG11	2.41	0.56
1:B:73:ALA:HB3	1:B:78:ALA:H	1.69	0.56
1:F:51:PRO:HA	1:F:54:SER:HB3	1.87	0.56
1:F:88:ILE:HD11	1:F:112:VAL:HG21	1.88	0.56
1:H:58:ASN:ND2	1:H:62:HIS:CE1	2.74	0.56
1:H:208:GLN:NE2	1:H:212:ASP:OD1	2.40	0.55
1:A:75:GLY:N	2:A:226:SAM:N6	2.47	0.55
1:D:47:VAL:O	1:D:72:LEU:HD21	2.06	0.55
1:H:138:VAL:HG11	1:H:156:GLU:OE1	2.06	0.55
1:D:19:LEU:HG	1:D:20:LEU:N	2.21	0.55
1:F:71:ARG:NH1	1:F:83:ASP:OD2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:PRO:HG2	1:G:123:GLU:HG3	1.89	0.55
1:B:92:GLY:HA2	1:B:120:ASN:OD1	2.06	0.55
1:F:80:GLU:OE1	1:F:80:GLU:HA	2.06	0.55
1:D:8:LEU:HG	1:D:152:ILE:CD1	2.37	0.55
1:E:96:ARG:NH1	1:E:122:ARG:CD	2.55	0.55
1:F:206:GLU:C	1:F:208:GLN:N	2.60	0.55
1:D:96:ARG:HH12	1:D:122:ARG:HD2	1.71	0.55
1:F:8:LEU:HG	1:F:152:ILE:HD13	1.88	0.55
1:E:142:ILE:HG13	1:E:150:TYR:O	2.07	0.54
1:D:94:GLY:O	1:D:98:ILE:HG13	2.07	0.54
1:C:23:GLY:CA	2:C:226:SAM:C8	2.86	0.54
1:C:114:ARG:HH11	1:C:154:VAL:CG1	2.20	0.54
1:D:205:GLU:HG3	1:D:206:GLU:OE1	2.08	0.54
1:F:26:HIS:ND1	1:F:54:SER:OG	2.40	0.54
1:F:94:GLY:O	1:F:98:ILE:HG13	2.08	0.54
1:B:47:VAL:HG12	1:B:48:VAL:N	2.23	0.54
1:B:96:ARG:HH12	1:B:122:ARG:HG3	1.72	0.54
1:C:162:LEU:HD22	1:C:171:PRO:HG3	1.89	0.54
1:D:58:ASN:HA	1:D:61:ALA:HB3	1.90	0.54
1:E:89:THR:HG22	1:E:116:ILE:HB	1.89	0.54
1:H:96:ARG:NH1	1:H:96:ARG:CG	2.70	0.54
1:A:96:ARG:NH1	1:A:96:ARG:HG3	2.19	0.54
1:C:114:ARG:HG2	1:C:115:LEU:H	1.72	0.54
1:E:35:GLU:OE2	1:E:62:HIS:HD2	1.91	0.53
1:A:60:GLU:O	1:A:63:GLY:N	2.39	0.53
1:A:100:ARG:NH1	1:A:100:ARG:HB3	2.23	0.53
1:G:58:ASN:ND2	1:G:62:HIS:ND1	2.56	0.53
1:C:136:GLN:HA	1:C:160:MET:SD	2.49	0.53
1:D:46:GLU:O	1:D:72:LEU:HA	2.09	0.53
1:D:136:GLN:HA	1:D:160:MET:HG2	1.90	0.53
1:F:88:ILE:HD12	1:F:112:VAL:HG11	1.89	0.53
1:B:4:LYS:O	1:B:7:GLU:HB3	2.09	0.53
1:E:92:GLY:H	1:E:118:GLN:HE21	1.55	0.53
1:C:46:GLU:HA	2:C:226:SAM:H8	1.89	0.53
1:C:75:GLY:N	2:C:226:SAM:N6	2.43	0.53
1:D:16:GLY:O	1:D:17:ALA:C	2.46	0.53
1:F:108:LYS:C	1:F:110:ALA:H	2.11	0.53
1:F:34:VAL:HG11	1:F:64:LEU:HD22	1.90	0.53
1:H:23:GLY:CA	2:H:226:SAM:C8	2.86	0.53
1:D:71:ARG:NH1	1:D:83:ASP:OD2	2.32	0.53
1:B:94:GLY:O	1:B:98:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:CD2	1:C:150:TYR:HB2	2.39	0.52
1:E:88:ILE:CD1	1:E:112:VAL:HG21	2.39	0.52
1:A:96:ARG:NH2	1:B:62:HIS:HA	2.24	0.52
1:F:142:ILE:HG13	1:F:150:TYR:O	2.09	0.52
1:C:114:ARG:HG2	1:C:115:LEU:N	2.24	0.52
1:B:47:VAL:CG2	1:B:74:ASN:HA	2.40	0.52
1:F:39:ILE:HG13	1:F:41:SER:H	1.75	0.52
1:F:92:GLY:H	1:F:118:GLN:HE21	1.56	0.52
1:A:100:ARG:HH11	1:A:100:ARG:HB3	1.73	0.52
1:A:100:ARG:HH11	1:A:100:ARG:HB2	1.72	0.52
1:A:114:ARG:HG2	1:A:115:LEU:H	1.75	0.52
1:A:193:GLU:HG3	1:A:214:ILE:HD13	1.90	0.52
1:D:73:ALA:CB	1:D:78:ALA:N	2.71	0.52
1:D:96:ARG:HH22	1:D:122:ARG:HG3	1.75	0.52
1:E:96:ARG:NH1	1:E:96:ARG:HB2	2.25	0.52
1:G:139:ALA:HB3	1:G:154:VAL:HB	1.90	0.52
1:B:16:GLY:O	1:B:17:ALA:C	2.47	0.52
1:B:194:PHE:CD1	1:E:191:LYS:HE3	2.45	0.52
1:C:192:LEU:O	1:C:195:ALA:HB3	2.10	0.52
1:F:60:GLU:C	1:F:62:HIS:N	2.63	0.52
1:F:134:GLY:HA2	1:F:159:GLN:NE2	2.24	0.52
1:F:209:VAL:HG22	1:F:210:LEU:HD12	1.92	0.52
1:C:177:VAL:HG12	1:C:177:VAL:O	2.09	0.52
1:C:151:GLU:HG2	1:C:173:LEU:HD11	1.92	0.52
1:D:206:GLU:CA	1:D:208:GLN:H	2.23	0.52
1:E:96:ARG:NH2	1:E:122:ARG:CD	2.68	0.52
1:F:48:VAL:HG13	1:F:49:GLU:H	1.74	0.51
1:C:143:LEU:HD23	1:C:150:TYR:HB2	1.92	0.51
1:B:108:LYS:C	1:B:110:ALA:N	2.64	0.51
1:G:25:ASP:O	1:G:26:HIS:C	2.48	0.51
1:A:162:LEU:HD22	1:A:171:PRO:HG3	1.91	0.51
1:B:83:ASP:N	1:B:83:ASP:OD1	2.43	0.51
1:E:161:LYS:CE	1:G:57:LYS:HG3	2.39	0.51
1:C:139:ALA:HB3	1:C:154:VAL:HB	1.92	0.51
1:G:4:LYS:HB3	1:G:145:GLU:OE2	2.10	0.51
1:B:86:SER:O	1:B:113:GLU:HG3	2.10	0.51
1:C:25:ASP:O	1:C:27:ALA:N	2.43	0.51
1:B:72:LEU:HD23	1:B:72:LEU:C	2.31	0.51
1:B:123:GLU:OE1	1:B:123:GLU:N	2.40	0.51
1:D:100:ARG:HG2	1:D:100:ARG:NH1	2.20	0.51
1:E:73:ALA:CB	1:E:78:ALA:N	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:ILE:HG21	1:H:62:HIS:CD2	2.46	0.51
1:A:114:ARG:HH11	1:A:154:VAL:CG1	2.22	0.51
1:B:107:GLY:O	1:B:110:ALA:HB2	2.11	0.51
1:E:160:MET:HE2	1:E:162:LEU:HD21	1.93	0.51
1:F:77:ALA:O	1:F:79:PHE:N	2.44	0.51
1:F:58:ASN:HA	1:F:61:ALA:HB3	1.93	0.50
1:A:143:LEU:CD2	1:A:150:TYR:HB2	2.40	0.50
1:F:210:LEU:HD12	1:F:210:LEU:H	1.76	0.50
1:G:24:SER:O	1:G:25:ASP:C	2.50	0.50
1:E:140:GLU:HB2	1:E:172:PHE:HB2	1.93	0.50
1:F:92:GLY:HA2	1:F:120:ASN:OD1	2.12	0.50
1:B:112:VAL:HG12	1:B:114:ARG:H	1.76	0.50
1:B:222:HIS:ND1	1:B:222:HIS:C	2.63	0.50
1:F:60:GLU:O	1:F:62:HIS:N	2.44	0.50
1:F:71:ARG:HH22	1:F:83:ASP:CG	2.14	0.50
1:H:124:ASP:O	1:H:127:ARG:N	2.44	0.50
1:H:206:GLU:O	1:H:209:VAL:HG12	2.12	0.50
1:E:16:GLY:O	1:E:17:ALA:C	2.49	0.50
1:B:32:GLU:O	1:B:36:ARG:HG2	2.12	0.50
1:H:83:ASP:O	1:H:84:GLN:HB2	2.12	0.50
1:H:182:VAL:O	1:H:186:GLN:HB2	2.12	0.50
1:A:195:ALA:O	1:A:196:LEU:C	2.50	0.50
1:B:124:ASP:OD1	1:B:125:ASP:N	2.45	0.50
1:D:32:GLU:O	1:D:36:ARG:HG2	2.11	0.50
1:F:71:ARG:HD2	1:F:78:ALA:O	2.12	0.50
1:E:77:ALA:O	1:E:79:PHE:N	2.45	0.50
1:C:8:LEU:HD23	1:C:152:ILE:HD12	1.93	0.49
1:G:58:ASN:C	1:G:58:ASN:HD22	2.14	0.49
1:H:74:ASN:HD22	1:H:74:ASN:C	2.15	0.49
1:B:140:GLU:HB2	1:B:172:PHE:HB2	1.94	0.49
1:D:209:VAL:O	1:D:213:LYS:HG3	2.11	0.49
1:F:18:ILE:H	1:F:18:ILE:HD12	1.77	0.49
1:B:71:ARG:HD2	1:B:78:ALA:O	2.12	0.49
1:D:118:GLN:HG3	1:D:118:GLN:O	2.12	0.49
1:B:77:ALA:O	1:B:79:PHE:N	2.45	0.49
1:B:47:VAL:CG1	1:B:48:VAL:N	2.75	0.49
1:E:92:GLY:HA2	1:E:120:ASN:OD1	2.12	0.49
1:G:23:GLY:O	2:G:226:SAM:N	2.45	0.49
1:D:65:LYS:CD	1:E:72:LEU:HD22	2.41	0.49
1:G:58:ASN:HD21	1:G:62:HIS:HE1	1.53	0.49
1:B:205:GLU:CG	1:B:206:GLU:N	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:LYS:NZ	1:D:4:LYS:HB3	2.28	0.49
1:D:48:VAL:HG13	1:D:49:GLU:N	2.28	0.49
1:G:138:VAL:HG11	1:G:156:GLU:OE1	2.12	0.49
1:B:89:THR:HA	1:B:116:ILE:O	2.12	0.49
1:B:206:GLU:C	1:B:206:GLU:CD	2.71	0.49
1:C:96:ARG:CB	1:C:96:ARG:CZ	2.65	0.49
1:H:151:GLU:OE2	1:H:184:LYS:NZ	2.44	0.49
1:B:26:HIS:O	1:B:27:ALA:HB3	2.13	0.48
1:G:92:GLY:O	2:G:226:SAM:HE3	2.10	0.48
1:H:75:GLY:N	2:H:226:SAM:N6	2.51	0.48
1:A:114:ARG:HD3	1:A:154:VAL:HG13	1.95	0.48
1:E:88:ILE:HD11	1:E:112:VAL:HG21	1.95	0.48
1:F:71:ARG:HH12	1:F:83:ASP:CG	2.15	0.48
1:B:129:TRP:O	1:B:133:HIS:HD2	1.96	0.48
1:D:92:GLY:HA2	1:D:120:ASN:OD1	2.14	0.48
1:A:13:VAL:HG22	1:A:116:ILE:CD1	2.43	0.48
1:B:17:ALA:O	1:B:39:ILE:HB	2.13	0.48
1:F:124:ASP:HB2	1:F:167:VAL:HG12	1.95	0.48
1:G:60:GLU:OE2	1:G:60:GLU:HA	2.13	0.48
1:G:23:GLY:HA2	2:G:226:SAM:H8	1.95	0.48
1:G:36:ARG:NH1	1:G:38:GLN:OE1	2.41	0.48
1:C:44:ALA:O	1:C:70:VAL:HA	2.14	0.48
1:C:95:GLY:H	1:C:121:ASN:ND2	2.11	0.48
1:B:73:ALA:HB3	1:B:78:ALA:N	2.27	0.48
1:E:26:HIS:O	1:E:27:ALA:HB3	2.13	0.48
1:A:19:LEU:HD11	1:A:89:THR:HG23	1.96	0.48
1:B:49:GLU:OE2	1:B:53:GLN:NE2	2.40	0.48
1:C:4:LYS:HB2	1:C:145:GLU:OE2	2.14	0.48
1:H:206:GLU:CA	1:H:208:GLN:H	2.25	0.48
1:F:123:GLU:OE1	1:F:123:GLU:N	2.45	0.48
1:F:221:LEU:O	1:F:222:HIS:C	2.53	0.48
1:D:89:THR:HA	1:D:116:ILE:O	2.14	0.47
1:E:20:LEU:HD23	1:E:88:ILE:HG12	1.96	0.47
1:F:102:LEU:HD22	1:F:115:LEU:HD21	1.95	0.47
1:A:89:THR:HG22	1:A:116:ILE:HB	1.96	0.47
1:B:58:ASN:HA	1:B:61:ALA:HB3	1.95	0.47
1:D:162:LEU:HD22	1:D:166:ASP:HB3	1.95	0.47
1:B:3:SER:HB2	1:B:145:GLU:OE1	2.14	0.47
1:C:21:ASP:CG	1:C:24:SER:HB3	2.32	0.47
1:D:73:ALA:HB3	1:D:78:ALA:H	1.79	0.47
1:F:89:THR:HG22	1:F:116:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:SER:O	1:B:57:LYS:HB3	2.14	0.47
1:B:96:ARG:NH1	1:B:122:ARG:HG3	2.29	0.47
1:H:25:ASP:O	1:H:26:HIS:C	2.51	0.47
1:B:210:LEU:H	1:B:210:LEU:CD1	2.25	0.47
1:A:8:LEU:HB3	1:A:152:ILE:HD12	1.96	0.47
1:C:96:ARG:NH2	1:C:122:ARG:HD2	2.29	0.47
1:D:72:LEU:C	1:D:72:LEU:HD23	2.35	0.47
1:E:206:GLU:C	1:E:206:GLU:CD	2.73	0.47
1:E:222:HIS:ND1	1:E:222:HIS:C	2.68	0.47
1:F:48:VAL:O	1:F:72:LEU:HD11	2.15	0.47
1:G:23:GLY:HA2	2:G:226:SAM:H1'	1.97	0.47
1:E:80:GLU:HA	1:E:80:GLU:OE1	2.12	0.47
1:F:35:GLU:OE2	1:F:62:HIS:HD2	1.97	0.47
1:F:89:THR:HA	1:F:116:ILE:O	2.15	0.47
1:B:1:MET:O	1:B:1:MET:HG2	2.14	0.47
1:E:217:ILE:O	1:E:218:LYS:C	2.53	0.47
1:G:2:ILE:CD1	1:G:28:TYR:HB3	2.45	0.47
1:A:5:ARG:HG3	1:A:143:LEU:HD21	1.96	0.47
1:B:76:LEU:HD11	1:B:109:LEU:HD21	1.97	0.47
1:B:162:LEU:HD22	1:B:166:ASP:HB3	1.96	0.47
1:E:46:GLU:OE1	1:E:46:GLU:CA	2.55	0.47
1:G:124:ASP:HB2	1:G:167:VAL:HG12	1.97	0.47
1:A:160:MET:CE	1:A:162:LEU:HD11	2.45	0.46
1:D:89:THR:HG22	1:D:116:ILE:HB	1.97	0.46
1:H:100:ARG:HH11	1:H:100:ARG:HB2	1.80	0.46
1:B:71:ARG:HH22	1:B:83:ASP:CG	2.18	0.46
1:C:138:VAL:HG11	1:C:156:GLU:OE1	2.15	0.46
1:G:4:LYS:CB	1:G:145:GLU:OE2	2.63	0.46
1:F:143:LEU:HD23	1:F:143:LEU:H	1.80	0.46
1:F:209:VAL:O	1:F:213:LYS:HG3	2.16	0.46
1:H:2:ILE:HD11	1:H:28:TYR:HB3	1.96	0.46
1:D:210:LEU:HD12	1:D:210:LEU:N	2.30	0.46
1:F:43:ILE:HD11	1:F:83:ASP:HB3	1.98	0.46
1:G:143:LEU:HD23	1:G:150:TYR:HB2	1.97	0.46
1:A:210:LEU:O	1:A:211:VAL:C	2.54	0.46
1:B:142:ILE:HD13	1:B:180:VAL:HG12	1.97	0.46
1:C:170:GLY:HA2	1:C:171:PRO:HD2	1.70	0.46
1:E:124:ASP:OD1	1:E:125:ASP:N	2.48	0.46
1:F:98:ILE:HD12	1:F:119:PRO:HB3	1.98	0.46
1:F:96:ARG:HH12	1:F:122:ARG:HG3	1.81	0.46
1:G:206:GLU:C	1:G:208:GLN:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:ASN:C	1:H:74:ASN:ND2	2.68	0.46
1:H:162:LEU:HD22	1:H:171:PRO:HG3	1.98	0.46
1:B:73:ALA:HB1	1:B:78:ALA:N	2.23	0.46
1:C:142:ILE:CG1	1:C:143:LEU:N	2.78	0.46
1:E:15:GLN:HE22	1:E:38:GLN:HA	1.79	0.46
1:E:118:GLN:O	1:E:118:GLN:HG3	2.16	0.46
1:D:83:ASP:HB2	1:D:85:VAL:HG23	1.97	0.45
1:D:168:ARG:CG	1:D:168:ARG:NH1	2.74	0.45
1:E:112:VAL:HG12	1:E:114:ARG:H	1.81	0.45
1:G:89:THR:HG22	1:G:116:ILE:HB	1.98	0.45
1:B:35:GLU:OE2	1:B:62:HIS:HD2	1.99	0.45
1:D:140:GLU:HB2	1:D:172:PHE:HB2	1.97	0.45
1:F:16:GLY:O	1:F:17:ALA:O	2.34	0.45
1:F:92:GLY:C	1:F:120:ASN:HD21	2.20	0.45
1:B:92:GLY:N	1:B:118:GLN:HE21	2.13	0.45
1:B:136:GLN:HA	1:B:160:MET:HG2	1.99	0.45
1:D:6:LEU:HD23	1:D:6:LEU:HA	1.69	0.45
1:E:88:ILE:HD12	1:E:112:VAL:CG1	2.38	0.45
1:C:210:LEU:O	1:C:211:VAL:C	2.54	0.45
1:G:24:SER:HB2	1:G:44:ALA:HB1	1.97	0.45
1:G:13:VAL:CG2	1:G:116:ILE:CD1	2.95	0.45
1:A:79:PHE:O	1:A:108:LYS:HE2	2.17	0.45
1:B:21:ASP:O	1:B:24:SER:HB2	2.16	0.45
1:D:41:SER:HB2	1:D:67:LYS:O	2.17	0.45
1:D:81:GLU:OE2	1:D:108:LYS:HA	2.17	0.45
1:D:182:VAL:O	1:D:186:GLN:HB2	2.17	0.45
1:H:166:ASP:OD1	1:H:171:PRO:HA	2.16	0.45
1:A:31:ILE:CD1	1:A:58:ASN:HD22	2.28	0.45
1:B:41:SER:HB2	1:B:67:LYS:O	2.17	0.45
1:E:82:THR:C	1:E:84:GLN:N	2.70	0.45
1:E:129:TRP:O	1:E:133:HIS:CD2	2.68	0.45
1:F:39:ILE:HD11	1:F:42:ALA:HB2	1.99	0.45
1:G:131:GLN:OE1	1:G:161:LYS:HA	2.16	0.45
1:C:178:SER:HB2	1:C:179:PRO:HD2	1.99	0.45
1:F:16:GLY:O	1:F:17:ALA:C	2.55	0.45
1:F:19:LEU:HG	1:F:20:LEU:N	2.31	0.45
1:C:97:LEU:HD21	2:C:226:SAM:H2	1.99	0.45
1:E:3:SER:HB2	1:E:145:GLU:OE1	2.17	0.45
1:H:196:LEU:HA	1:H:196:LEU:HD13	1.55	0.45
1:B:143:LEU:H	1:B:143:LEU:HD23	1.81	0.44
1:F:96:ARG:NH2	1:F:122:ARG:HG3	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:GLU:HB2	1:F:172:PHE:HB2	1.99	0.44
1:G:117:LEU:HD13	1:G:126:LEU:HD21	1.99	0.44
1:F:112:VAL:HG12	1:F:114:ARG:H	1.82	0.44
1:A:58:ASN:ND2	1:A:62:HIS:CE1	2.82	0.44
1:A:62:HIS:O	1:A:64:LEU:HG	2.17	0.44
1:C:32:GLU:O	1:C:36:ARG:HG3	2.18	0.44
1:D:48:VAL:HG22	1:D:49:GLU:H	1.82	0.44
1:C:13:VAL:CG2	1:C:116:ILE:CD1	2.95	0.44
1:C:5:ARG:NH1	1:C:118:GLN:HE21	2.10	0.44
1:G:129:TRP:O	1:G:133:HIS:HD2	2.01	0.44
1:C:74:ASN:C	1:C:74:ASN:ND2	2.71	0.44
1:H:206:GLU:HA	1:H:208:GLN:HB3	1.99	0.44
1:A:106:LEU:HD12	1:A:106:LEU:O	2.18	0.44
1:E:82:THR:O	1:E:84:GLN:HG2	2.17	0.44
1:A:127:ARG:HG2	1:A:137:ILE:HD11	2.00	0.44
1:C:19:LEU:HG	1:C:20:LEU:N	2.33	0.44
1:D:76:LEU:CD1	1:D:105:GLY:HA3	2.48	0.44
1:E:124:ASP:HB2	1:E:167:VAL:HG12	1.99	0.44
1:F:96:ARG:HH12	1:F:122:ARG:CG	2.30	0.44
1:H:60:GLU:O	1:H:63:GLY:N	2.47	0.44
1:A:12:PHE:CG	1:A:154:VAL:HG21	2.53	0.43
1:A:124:ASP:O	1:A:127:ARG:N	2.48	0.43
1:C:13:VAL:HG22	1:C:116:ILE:HD12	1.99	0.43
1:C:205:GLU:CD	1:C:206:GLU:H	2.19	0.43
1:G:48:VAL:CG2	1:G:51:PRO:HD2	2.46	0.43
1:B:8:LEU:HG	1:B:152:ILE:HD12	2.00	0.43
1:C:131:GLN:OE1	1:C:161:LYS:HA	2.18	0.43
1:C:178:SER:HB2	1:C:179:PRO:CD	2.47	0.43
1:F:160:MET:HE2	1:F:162:LEU:HD21	2.00	0.43
1:A:25:ASP:C	1:A:27:ALA:H	2.19	0.43
1:B:194:PHE:CG	1:E:191:LYS:HE3	2.53	0.43
1:D:56:VAL:HG22	1:D:70:VAL:HG21	2.00	0.43
1:E:133:HIS:CD2	1:E:133:HIS:N	2.86	0.43
1:F:88:ILE:CD1	1:F:112:VAL:HG21	2.48	0.43
1:A:8:LEU:HB3	1:A:152:ILE:CD1	2.49	0.43
1:A:121:ASN:N	1:A:121:ASN:HD22	2.16	0.43
1:C:130:LEU:HD22	1:C:155:VAL:HG21	1.99	0.43
1:D:72:LEU:HD23	1:D:73:ALA:N	2.33	0.43
1:E:35:GLU:OE2	1:E:62:HIS:CD2	2.71	0.43
1:A:97:LEU:HA	1:A:100:ARG:HD3	2.00	0.43
1:C:142:ILE:HG13	1:C:143:LEU:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:GLN:H	1:F:69:GLN:HG2	1.70	0.43
1:A:119:PRO:HG2	1:A:123:GLU:HG3	2.00	0.43
1:C:130:LEU:O	1:C:135:PHE:HB2	2.19	0.43
1:D:118:GLN:O	1:D:118:GLN:CG	2.66	0.43
1:G:206:GLU:C	1:G:208:GLN:H	2.22	0.43
1:G:97:LEU:HD21	2:G:226:SAM:H2	2.00	0.43
1:H:94:GLY:HA2	1:H:121:ASN:OD1	2.19	0.43
1:A:160:MET:HE3	1:A:162:LEU:HD11	2.01	0.43
1:C:6:LEU:HD21	2:C:226:SAM:O	2.18	0.43
1:D:74:ASN:H	1:D:77:ALA:HB3	1.83	0.43
1:E:161:LYS:NZ	1:G:57:LYS:HG3	2.33	0.43
1:E:187:LYS:HD2	1:E:187:LYS:HA	1.91	0.43
1:G:196:LEU:HD13	1:G:196:LEU:HA	1.85	0.43
1:A:136:GLN:HA	1:A:160:MET:SD	2.59	0.43
1:D:5:ARG:HD2	1:D:150:TYR:CD1	2.54	0.43
1:D:47:VAL:HG12	1:D:48:VAL:N	2.34	0.43
1:F:17:ALA:O	1:F:39:ILE:HB	2.19	0.43
1:G:170:GLY:HA2	1:G:171:PRO:HD2	1.83	0.43
1:A:210:LEU:H	1:A:210:LEU:HG	1.58	0.43
1:G:55:ALA:O	1:G:56:VAL:C	2.57	0.43
1:A:4:LYS:NZ	1:A:144:GLU:O	2.52	0.42
1:A:36:ARG:H	1:A:36:ARG:HG3	1.71	0.42
1:C:182:VAL:O	1:C:186:GLN:HB2	2.18	0.42
1:D:83:ASP:O	1:D:84:GLN:HB2	2.19	0.42
1:A:121:ASN:HD22	1:A:121:ASN:H	1.67	0.42
1:D:35:GLU:OE2	1:D:62:HIS:CD2	2.71	0.42
1:E:73:ALA:HB3	1:E:78:ALA:HB2	2.00	0.42
1:F:60:GLU:C	1:F:62:HIS:H	2.23	0.42
1:G:127:ARG:HG2	1:G:137:ILE:HD11	2.02	0.42
1:D:17:ALA:O	1:D:39:ILE:HB	2.18	0.42
1:D:221:LEU:O	1:D:222:HIS:C	2.57	0.42
1:G:23:GLY:HA2	2:G:226:SAM:C8	2.50	0.42
1:C:185:TRP:HB3	1:C:217:ILE:HG23	2.02	0.42
1:D:108:LYS:C	1:D:110:ALA:H	2.21	0.42
1:E:32:GLU:O	1:E:36:ARG:HG2	2.19	0.42
1:A:96:ARG:HH12	1:A:122:ARG:HG3	1.85	0.42
1:D:124:ASP:HB2	1:D:167:VAL:HG12	2.02	0.42
1:G:5:ARG:HG3	1:G:143:LEU:HD21	2.01	0.42
1:H:89:THR:HG22	1:H:116:ILE:HB	2.01	0.42
1:B:105:GLY:O	1:B:108:LYS:HG3	2.20	0.42
1:F:87:VAL:HG22	1:F:114:ARG:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:GLU:HG3	1:F:206:GLU:H	1.85	0.42
1:B:1:MET:CE	1:B:62:HIS:NE2	2.82	0.42
1:B:6:LEU:HD23	1:B:6:LEU:HA	1.86	0.42
1:E:71:ARG:HH11	1:E:79:PHE:HA	1.85	0.42
1:F:3:SER:O	1:F:7:GLU:HB2	2.20	0.42
1:H:195:ALA:O	1:H:196:LEU:C	2.58	0.42
1:D:73:ALA:HB3	1:D:78:ALA:CA	2.50	0.42
1:G:106:LEU:HA	1:G:109:LEU:HD12	2.01	0.42
1:B:40:LYS:HA	1:B:40:LYS:CE	2.42	0.42
1:C:94:GLY:HA2	1:C:121:ASN:HD21	1.85	0.42
1:F:82:THR:C	1:F:84:GLN:N	2.74	0.42
1:G:13:VAL:HG22	1:G:116:ILE:CD1	2.50	0.42
1:D:16:GLY:O	1:D:17:ALA:O	2.38	0.42
1:E:75:GLY:O	1:E:77:ALA:N	2.52	0.42
1:G:75:GLY:N	2:G:226:SAM:HN61	2.05	0.42
1:C:129:TRP:O	1:C:133:HIS:HD2	2.02	0.41
1:E:161:LYS:CD	1:G:57:LYS:HG2	2.45	0.41
1:H:48:VAL:CG2	1:H:49:GLU:N	2.83	0.41
1:H:97:LEU:HA	1:H:100:ARG:HD3	2.02	0.41
1:H:190:GLU:O	1:H:194:PHE:HB2	2.20	0.41
1:C:129:TRP:CE3	1:C:130:LEU:HA	2.55	0.41
1:E:162:LEU:HD22	1:E:166:ASP:HB3	2.02	0.41
1:F:124:ASP:OD1	1:F:125:ASP:N	2.49	0.41
1:G:195:ALA:O	1:G:196:LEU:C	2.58	0.41
1:E:3:SER:O	1:E:7:GLU:HB2	2.20	0.41
1:F:40:LYS:O	1:F:41:SER:CB	2.69	0.41
1:G:5:ARG:HB2	1:G:145:GLU:OE1	2.20	0.41
1:A:47:VAL:HG13	1:A:48:VAL:HG12	2.03	0.41
1:E:39:ILE:HD11	1:E:42:ALA:HB2	2.01	0.41
1:A:19:LEU:HG	1:A:20:LEU:N	2.36	0.41
1:C:208:GLN:O	1:C:212:ASP:OD1	2.38	0.41
1:D:96:ARG:HH12	1:D:122:ARG:CD	2.33	0.41
1:D:210:LEU:HD12	1:D:210:LEU:H	1.85	0.41
1:A:178:SER:CB	1:A:179:PRO:HD2	2.50	0.41
1:B:127:ARG:HG2	1:B:137:ILE:HD11	2.02	0.41
1:C:53:GLN:O	1:C:54:SER:C	2.59	0.41
2:G:226:SAM:HG2	2:G:226:SAM:H4'	1.92	0.41
1:A:139:ALA:HB3	1:A:154:VAL:HB	2.03	0.41
1:C:51:PRO:HD3	1:D:15:GLN:OE1	2.21	0.41
1:E:97:LEU:O	1:E:101:ILE:HG13	2.20	0.41
1:C:101:ILE:HG22	1:C:102:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ARG:HG2	1:C:137:ILE:HD11	2.02	0.41
1:G:182:VAL:O	1:G:186:GLN:HB2	2.20	0.41
1:A:49:GLU:O	1:A:50:GLY:C	2.59	0.41
1:B:43:ILE:HA	1:B:69:GLN:O	2.21	0.41
1:D:54:SER:O	1:D:55:ALA:C	2.59	0.41
1:E:82:THR:O	1:E:84:GLN:N	2.54	0.41
1:E:118:GLN:O	1:E:118:GLN:CG	2.68	0.41
1:F:122:ARG:HA	1:F:122:ARG:HD3	1.58	0.41
1:F:206:GLU:H	1:F:206:GLU:CD	2.24	0.41
1:B:92:GLY:C	1:B:120:ASN:HD21	2.25	0.41
1:C:21:ASP:OD2	1:C:30:PRO:HD3	2.22	0.41
1:D:96:ARG:NH2	1:D:122:ARG:HG3	2.34	0.41
1:D:208:GLN:OE1	1:D:208:GLN:HA	2.20	0.41
1:E:72:LEU:HD23	1:E:73:ALA:N	2.36	0.41
1:H:25:ASP:C	1:H:27:ALA:N	2.72	0.41
1:B:160:MET:HE2	1:B:162:LEU:HD21	2.02	0.40
1:D:103:GLU:C	1:D:105:GLY:H	2.25	0.40
1:G:118:GLN:HB3	1:G:152:ILE:HG12	2.03	0.40
1:B:16:GLY:O	1:B:17:ALA:O	2.38	0.40
1:F:137:ILE:H	1:F:160:MET:CE	2.34	0.40
1:H:65:LYS:HE2	1:H:65:LYS:HB3	1.92	0.40
1:E:168:ARG:CG	1:E:168:ARG:NH1	2.77	0.40
1:G:46:GLU:HA	2:G:226:SAM:C8	2.49	0.40
1:C:196:LEU:HA	1:C:196:LEU:HD13	1.63	0.40
1:E:76:LEU:HD23	1:E:76:LEU:N	2.36	0.40
1:G:100:ARG:CB	1:G:100:ARG:NH1	2.68	0.40
1:H:21:ASP:OD2	1:H:24:SER:OG	2.33	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CE	1:B:96:ARG:CD[2_655]	1.87	0.33
1:F:132:ASP:OD1	1:H:58:ASN:OD1[1_554]	2.15	0.05

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	210/225 (93%)	174 (83%)	24 (11%)	12 (6%)	1 10
1	B	210/225 (93%)	176 (84%)	20 (10%)	14 (7%)	1 6
1	C	210/225 (93%)	185 (88%)	17 (8%)	8 (4%)	3 18
1	D	210/225 (93%)	174 (83%)	23 (11%)	13 (6%)	1 8
1	E	210/225 (93%)	168 (80%)	26 (12%)	16 (8%)	1 5
1	F	210/225 (93%)	171 (81%)	24 (11%)	15 (7%)	1 5
1	G	210/225 (93%)	175 (83%)	28 (13%)	7 (3%)	4 21
1	H	210/225 (93%)	179 (85%)	22 (10%)	9 (4%)	2 15
All	All	1680/1800 (93%)	1402 (84%)	184 (11%)	94 (6%)	2 10

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
1	B	17	ALA
1	B	50	GLY
1	B	78	ALA
1	B	109	LEU
1	B	207	ARG
1	C	177	VAL
1	C	207	ARG
1	D	17	ALA
1	D	26	HIS
1	D	41	SER
1	D	78	ALA
1	D	109	LEU
1	E	26	HIS
1	E	65	LYS
1	E	78	ALA
1	E	207	ARG

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Mol	Chain	Res	Type
1	F	17	ALA
1	F	25	ASP
1	F	41	SER
1	F	48	VAL
1	F	57	LYS
1	F	76	LEU
1	F	78	ALA
1	F	109	LEU
1	G	177	VAL
1	H	78	ALA
1	H	175	LYS
1	H	177	VAL
1	A	26	HIS
1	A	50	GLY
1	A	78	ALA
1	A	175	LYS
1	B	13	VAL
1	B	25	ASP
1	B	55	ALA
1	C	50	GLY
1	C	121	ASN
1	D	50	GLY
1	D	57	LYS
1	D	65	LYS
1	E	17	ALA
1	E	55	ALA
1	E	57	LYS
1	F	40	LYS
1	F	54	SER
1	F	61	ALA
1	F	207	ARG
1	G	50	GLY
1	G	78	ALA
1	G	207	ARG
1	G	209	VAL
1	H	50	GLY
1	H	121	ASN
1	H	207	ARG
1	A	132	ASP
1	A	208	GLN
1	B	51	PRO
1	C	26	HIS

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Mol	Chain	Res	Type
1	C	78	ALA
1	C	132	ASP
1	D	25	ASP
1	D	61	ALA
1	D	104	GLU
1	D	207	ARG
1	E	25	ASP
1	E	76	LEU
1	E	83	ASP
1	F	50	GLY
1	G	6	LEU
1	G	175	LYS
1	H	125	ASP
1	H	132	ASP
1	A	176	GLU
1	D	48	VAL
1	E	61	ALA
1	F	47	VAL
1	F	65	LYS
1	H	124	ASP
1	A	6	LEU
1	A	9	VAL
1	A	211	VAL
1	B	26	HIS
1	B	48	VAL
1	B	61	ALA
1	B	104	GLU
1	E	48	VAL
1	E	50	GLY
1	A	207	ARG
1	C	9	VAL
1	E	47	VAL
1	B	47	VAL
1	E	37	GLY
1	E	92	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	176/188 (94%)	153 (87%)	23 (13%)	4 18
1	B	178/188 (95%)	147 (83%)	31 (17%)	2 10
1	C	178/188 (95%)	157 (88%)	21 (12%)	5 22
1	D	178/188 (95%)	142 (80%)	36 (20%)	1 6
1	E	178/188 (95%)	149 (84%)	29 (16%)	2 11
1	F	178/188 (95%)	144 (81%)	34 (19%)	1 8
1	G	178/188 (95%)	156 (88%)	22 (12%)	4 20
1	H	178/188 (95%)	152 (85%)	26 (15%)	3 15
All	All	1422/1504 (94%)	1200 (84%)	222 (16%)	2 13

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	8	LEU
1	A	36	ARG
1	A	48	VAL
1	A	54	SER
1	A	57	LYS
1	A	58	ASN
1	A	65	LYS
1	A	66	GLU
1	A	79	PHE
1	A	82	THR
1	A	84	GLN
1	A	96	ARG
1	A	100	ARG
1	A	118	GLN
1	A	121	ASN
1	A	143	LEU
1	A	144	GLU
1	A	148	LYS
1	A	168	ARG
1	A	190	GLU
1	A	196	LEU
1	A	210	LEU
1	B	36	ARG
1	B	39	ILE

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Mol	Chain	Res	Type
1	B	40	LYS
1	B	47	VAL
1	B	56	VAL
1	B	57	LYS
1	B	74	ASN
1	B	79	PHE
1	B	83	ASP
1	B	86	SER
1	B	96	ARG
1	B	100	ARG
1	B	103	GLU
1	B	108	LYS
1	B	113	GLU
1	B	115	LEU
1	B	118	GLN
1	B	141	SER
1	B	142	ILE
1	B	148	LYS
1	B	153	LEU
1	B	160	MET
1	B	163	SER
1	B	175	LYS
1	B	176	GLU
1	B	186	GLN
1	B	187	LYS
1	B	191	LYS
1	B	205	GLU
1	B	206	GLU
1	B	222	HIS
1	C	1	MET
1	C	2	ILE
1	C	25	ASP
1	C	57	LYS
1	C	66	GLU
1	C	79	PHE
1	C	82	THR
1	C	84	GLN
1	C	96	ARG
1	C	118	GLN
1	C	121	ASN
1	C	141	SER
1	C	143	LEU

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Mol	Chain	Res	Type
1	C	144	GLU
1	C	161	LYS
1	C	165	SER
1	C	176	GLU
1	C	190	GLU
1	C	206	GLU
1	C	209	VAL
1	C	210	LEU
1	D	1	MET
1	D	3	SER
1	D	4	LYS
1	D	8	LEU
1	D	18	ILE
1	D	39	ILE
1	D	40	LYS
1	D	47	VAL
1	D	56	VAL
1	D	60	GLU
1	D	66	GLU
1	D	76	LEU
1	D	79	PHE
1	D	86	SER
1	D	90	ILE
1	D	96	ARG
1	D	100	ARG
1	D	104	GLU
1	D	113	GLU
1	D	115	LEU
1	D	118	GLN
1	D	141	SER
1	D	148	LYS
1	D	153	LEU
1	D	160	MET
1	D	168	ARG
1	D	176	GLU
1	D	184	LYS
1	D	186	GLN
1	D	187	LYS
1	D	205	GLU
1	D	206	GLU
1	D	207	ARG
1	D	215	GLN

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Mol	Chain	Res	Type
1	D	218	LYS
1	D	222	HIS
1	E	8	LEU
1	E	36	ARG
1	E	39	ILE
1	E	40	LYS
1	E	46	GLU
1	E	56	VAL
1	E	57	LYS
1	E	66	GLU
1	E	79	PHE
1	E	81	GLU
1	E	82	THR
1	E	83	ASP
1	E	96	ARG
1	E	100	ARG
1	E	113	GLU
1	E	118	GLN
1	E	141	SER
1	E	153	LEU
1	E	160	MET
1	E	165	SER
1	E	168	ARG
1	E	176	GLU
1	E	186	GLN
1	E	187	LYS
1	E	191	LYS
1	E	206	GLU
1	E	207	ARG
1	E	209	VAL
1	E	222	HIS
1	F	2	ILE
1	F	7	GLU
1	F	8	LEU
1	F	14	SER
1	F	36	ARG
1	F	39	ILE
1	F	40	LYS
1	F	56	VAL
1	F	57	LYS
1	F	60	GLU
1	F	65	LYS

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Mol	Chain	Res	Type
1	F	66	GLU
1	F	67	LYS
1	F	70	VAL
1	F	79	PHE
1	F	83	ASP
1	F	86	SER
1	F	96	ARG
1	F	100	ARG
1	F	104	GLU
1	F	118	GLN
1	F	141	SER
1	F	153	LEU
1	F	160	MET
1	F	165	SER
1	F	175	LYS
1	F	176	GLU
1	F	187	LYS
1	F	191	LYS
1	F	205	GLU
1	F	206	GLU
1	F	207	ARG
1	F	209	VAL
1	F	218	LYS
1	G	1	MET
1	G	24	SER
1	G	36	ARG
1	G	47	VAL
1	G	48	VAL
1	G	57	LYS
1	G	58	ASN
1	G	66	GLU
1	G	79	PHE
1	G	82	THR
1	G	96	ARG
1	G	100	ARG
1	G	111	ASN
1	G	118	GLN
1	G	144	GLU
1	G	165	SER
1	G	168	ARG
1	G	178	SER
1	G	196	LEU

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Mol	Chain	Res	Type
1	G	205	GLU
1	G	210	LEU
1	G	212	ASP
1	H	1	MET
1	H	2	ILE
1	H	24	SER
1	H	36	ARG
1	H	40	LYS
1	H	48	VAL
1	H	57	LYS
1	H	58	ASN
1	H	66	GLU
1	H	74	ASN
1	H	79	PHE
1	H	82	THR
1	H	86	SER
1	H	96	ARG
1	H	100	ARG
1	H	118	GLN
1	H	141	SER
1	H	143	LEU
1	H	165	SER
1	H	190	GLU
1	H	191	LYS
1	H	196	LEU
1	H	205	GLU
1	H	206	GLU
1	H	210	LEU
1	H	212	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	69	GLN
1	A	121	ASN
1	A	133	HIS
1	A	215	GLN
1	B	58	ASN
1	B	118	GLN
1	B	133	HIS
1	C	69	GLN

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Mol	Chain	Res	Type
1	C	74	ASN
1	C	118	GLN
1	C	121	ASN
1	C	133	HIS
1	D	53	GLN
1	D	133	HIS
1	E	15	GLN
1	E	62	HIS
1	E	118	GLN
1	E	133	HIS
1	F	118	GLN
1	F	133	HIS
1	F	159	GLN
1	G	58	ASN
1	G	74	ASN
1	G	111	ASN
1	G	133	HIS
1	G	183	GLN
1	H	15	GLN
1	H	58	ASN
1	H	74	ASN
1	H	118	GLN
1	H	133	HIS

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)

4 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	$\#\|Z\| > 2$
2	SAM	A	226	-	24,29,29	1.70	4 (16%)	23,42,42	2.29	10 (43%)
2	SAM	H	226	-	24,29,29	1.62	5 (20%)	23,42,42	2.12	8 (34%)
2	SAM	G	226	-	24,29,29	1.48	7 (29%)	23,42,42	1.61	4 (17%)
2	SAM	C	226	-	24,29,29	1.69	6 (25%)	23,42,42	2.27	9 (39%)

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
2	SAM	A	226	-	-	3/12/33/33	0/3/3/3
2	SAM	H	226	-	-	6/12/33/33	0/3/3/3
2	SAM	G	226	-	-	8/12/33/33	0/3/3/3
2	SAM	C	226	-	-	4/12/33/33	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	226	SAM	C2-N1	4.59	1.42	1.33
2	A	226	SAM	C2-N3	4.40	1.39	1.32
2	H	226	SAM	C2-N1	4.04	1.41	1.33
2	C	226	SAM	C2-N1	4.00	1.41	1.33
2	C	226	SAM	C2-N3	3.87	1.38	1.32
2	H	226	SAM	C2-N3	3.62	1.37	1.32
2	C	226	SAM	C6-C5	-3.38	1.30	1.43
2	H	226	SAM	C6-C5	-3.02	1.32	1.43
2	A	226	SAM	C6-C5	-3.00	1.32	1.43
2	G	226	SAM	C2-N3	2.59	1.36	1.32
2	H	226	SAM	OXT-C	-2.56	1.22	1.30
2	H	226	SAM	C4-N3	-2.55	1.32	1.35
2	G	226	SAM	C6-C5	-2.52	1.33	1.43
2	C	226	SAM	OXT-C	-2.51	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	226	SAM	C4-N3	-2.50	1.32	1.35
2	G	226	SAM	O4'-C4'	-2.38	1.39	1.45
2	A	226	SAM	OXT-C	-2.35	1.22	1.30
2	G	226	SAM	C5-N7	-2.20	1.31	1.39
2	C	226	SAM	C4-N3	-2.16	1.32	1.35
2	G	226	SAM	OXT-C	-2.15	1.23	1.30
2	C	226	SAM	C5-N7	-2.06	1.32	1.39
2	G	226	SAM	C2'-C1'	-2.04	1.50	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	226	SAM	N6-C6-N1	4.77	128.48	118.57
2	A	226	SAM	C5-C6-N6	-4.63	113.32	120.35
2	H	226	SAM	C3'-C2'-C1'	-4.62	94.02	100.98
2	C	226	SAM	C4-C5-N7	4.62	114.22	109.40
2	C	226	SAM	C5-C6-N6	-4.60	113.36	120.35
2	G	226	SAM	N3-C2-N1	-4.57	121.54	128.68
2	C	226	SAM	N6-C6-N1	4.36	127.62	118.57
2	H	226	SAM	N6-C6-N1	4.14	127.16	118.57
2	A	226	SAM	C4-C5-N7	3.95	113.52	109.40
2	H	226	SAM	C5-C6-N6	-3.61	114.87	120.35
2	H	226	SAM	C4-C5-N7	3.60	113.15	109.40
2	C	226	SAM	C3'-C2'-C1'	-3.55	95.64	100.98
2	H	226	SAM	O4'-C1'-C2'	-3.38	101.99	106.93
2	C	226	SAM	OXT-C-O	-3.04	117.19	124.09
2	C	226	SAM	N3-C2-N1	-2.98	124.01	128.68
2	H	226	SAM	N3-C2-N1	-2.96	124.06	128.68
2	A	226	SAM	C1'-N9-C4	2.92	131.78	126.64
2	A	226	SAM	N3-C2-N1	-2.89	124.16	128.68
2	A	226	SAM	C3'-C2'-C1'	-2.77	96.81	100.98
2	C	226	SAM	O4'-C1'-C2'	-2.77	102.88	106.93
2	A	226	SAM	OXT-C-O	-2.62	118.15	124.09
2	A	226	SAM	CB-CA-N	2.53	116.80	110.17
2	G	226	SAM	C1'-N9-C4	2.39	130.84	126.64
2	G	226	SAM	OXT-C-CA	2.34	121.35	113.38
2	H	226	SAM	OXT-C-O	-2.23	119.03	124.09
2	C	226	SAM	C2'-C3'-C4'	2.22	106.95	102.64
2	A	226	SAM	O4'-C1'-C2'	-2.14	103.80	106.93
2	G	226	SAM	N6-C6-N1	2.13	122.99	118.57
2	H	226	SAM	C1'-N9-C4	2.11	130.35	126.64
2	C	226	SAM	OXT-C-CA	2.10	120.53	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	226	SAM	OXT-C-CA	2.08	120.48	113.38

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	226	SAM	C-CA-CB-CG
2	A	226	SAM	O4'-C4'-C5'-SD
2	A	226	SAM	C3'-C4'-C5'-SD
2	C	226	SAM	CB-CG-SD-C5'
2	C	226	SAM	O4'-C4'-C5'-SD
2	C	226	SAM	C3'-C4'-C5'-SD
2	G	226	SAM	O-C-CA-N
2	G	226	SAM	O4'-C4'-C5'-SD
2	G	226	SAM	C3'-C4'-C5'-SD
2	G	226	SAM	OXT-C-CA-N
2	C	226	SAM	CB-CG-SD-CE
2	H	226	SAM	CB-CG-SD-CE
2	G	226	SAM	O-C-CA-CB
2	G	226	SAM	C4'-C5'-SD-CG
2	H	226	SAM	CB-CG-SD-C5'
2	H	226	SAM	O4'-C4'-C5'-SD
2	H	226	SAM	C3'-C4'-C5'-SD
2	H	226	SAM	O-C-CA-CB
2	H	226	SAM	OXT-C-CA-CB
2	G	226	SAM	OXT-C-CA-CB
2	G	226	SAM	N-CA-CB-CG

There are no ring outliers.

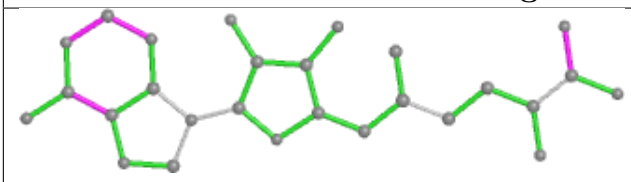
4 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	226	SAM	7	0
2	H	226	SAM	6	0
2	G	226	SAM	18	0
2	C	226	SAM	9	0

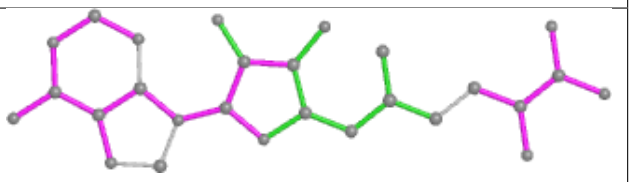
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

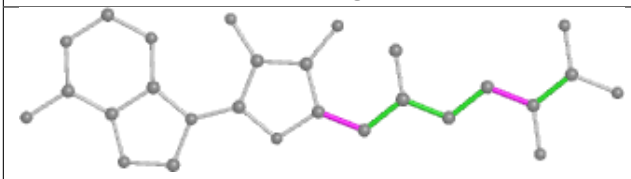
Ligand SAM A 226



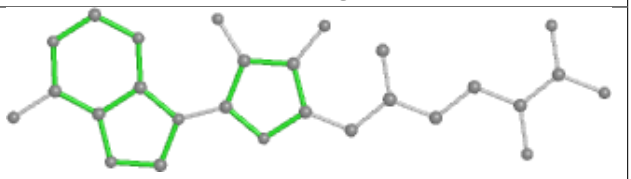
Bond lengths



Bond angles

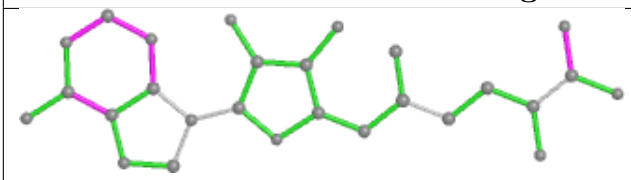


Torsions

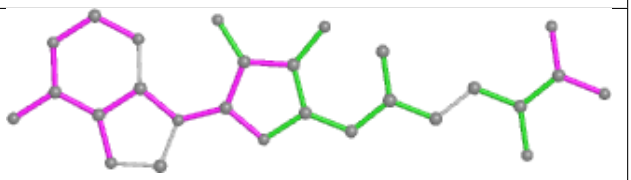


Rings

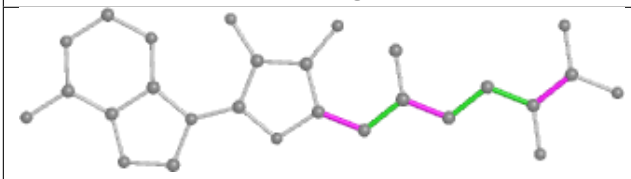
Ligand SAM H 226



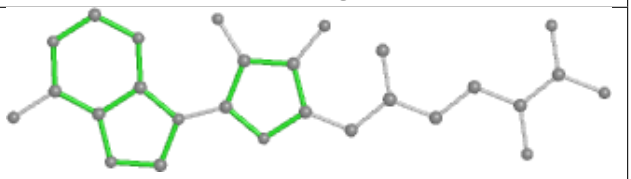
Bond lengths



Bond angles

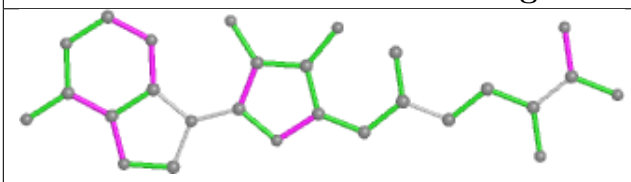


Torsions

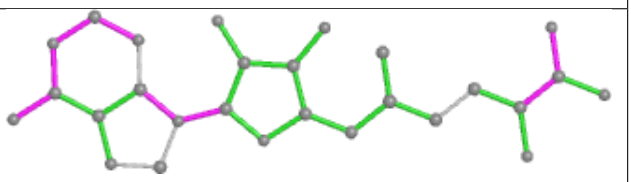


Rings

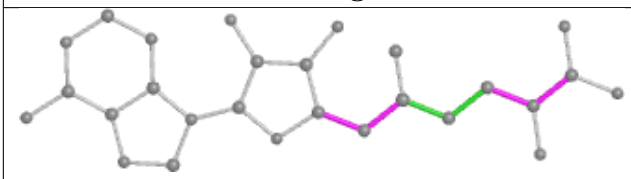
Ligand SAM G 226



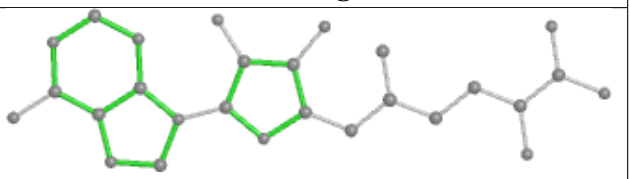
Bond lengths



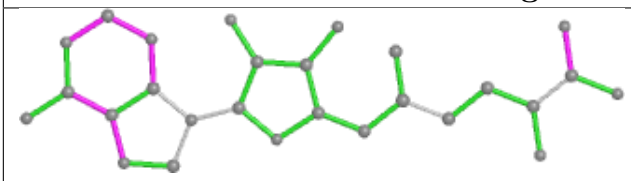
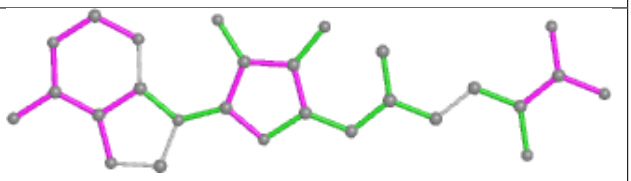
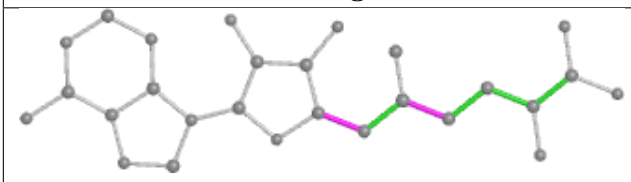
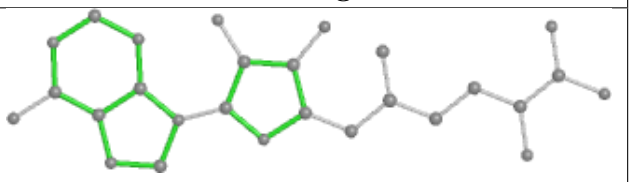
Bond angles



Torsions



Rings

Ligand SAM C 226	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	214/225 (95%)	0.25	1 (0%)	91	75	60, 78, 107, 123	0
1	B	214/225 (95%)	0.26	2 (0%)	84	63	55, 79, 116, 131	0
1	C	214/225 (95%)	0.24	1 (0%)	91	75	60, 78, 109, 125	0
1	D	214/225 (95%)	0.32	4 (1%)	66	37	56, 81, 114, 131	0
1	E	214/225 (95%)	0.34	5 (2%)	60	31	55, 80, 120, 134	0
1	F	214/225 (95%)	0.37	5 (2%)	60	31	54, 80, 120, 134	0
1	G	214/225 (95%)	0.21	1 (0%)	91	75	59, 78, 107, 125	0
1	H	214/225 (95%)	0.21	1 (0%)	91	75	60, 78, 109, 125	0
All	All	1712/1800 (95%)	0.28	20 (1%)	79	54	54, 79, 113, 134	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	48	VAL	5.3
1	F	47	VAL	4.9
1	D	47	VAL	4.1
1	B	47	VAL	3.7
1	B	48	VAL	3.4
1	D	48	VAL	3.2
1	E	48	VAL	2.9
1	F	53	GLN	2.9
1	E	40	LYS	2.9
1	D	20	LEU	2.6
1	E	45	GLY	2.5
1	E	47	VAL	2.5
1	E	102	LEU	2.4
1	G	209	VAL	2.3
1	C	1	MET	2.3
1	F	43	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	1	MET	2.2
1	F	44	ALA	2.2
1	D	51	PRO	2.0
1	A	164	ALA	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)

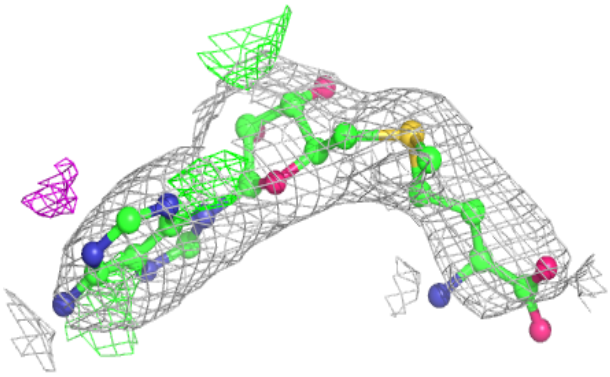
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

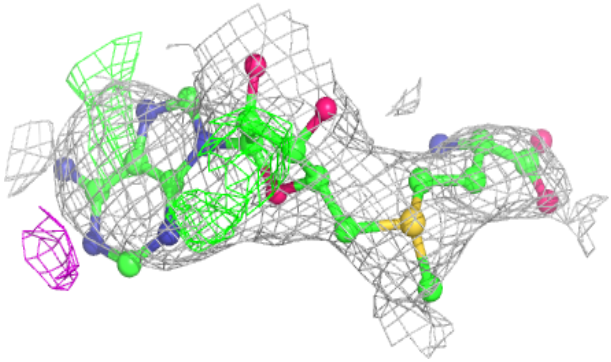
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SAM	G	226	27/27	0.86	0.33	142,147,156,157	0
2	SAM	A	226	27/27	0.93	0.25	64,73,81,81	0
2	SAM	C	226	27/27	0.94	0.27	69,75,81,84	0
2	SAM	H	226	27/27	0.94	0.27	67,77,81,82	0

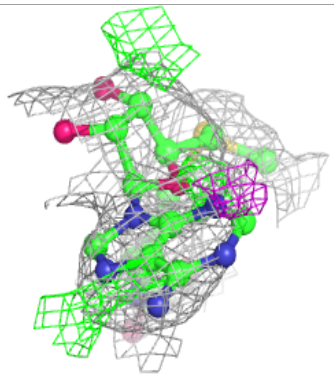
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAM G 226:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

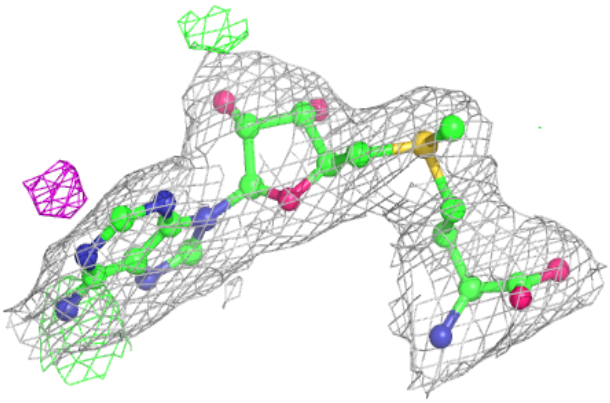


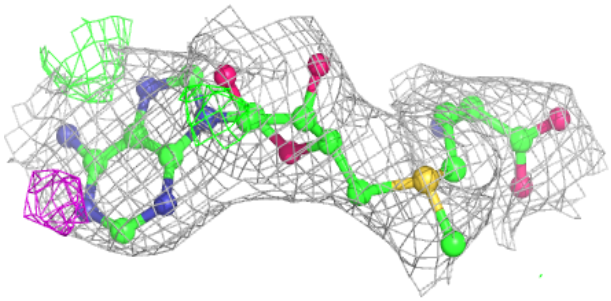


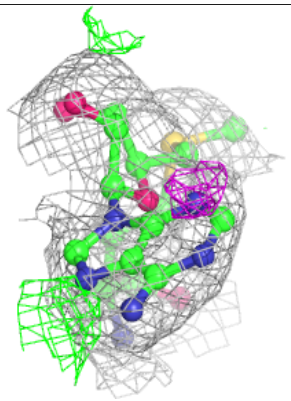


Electron density around SAM A 226:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

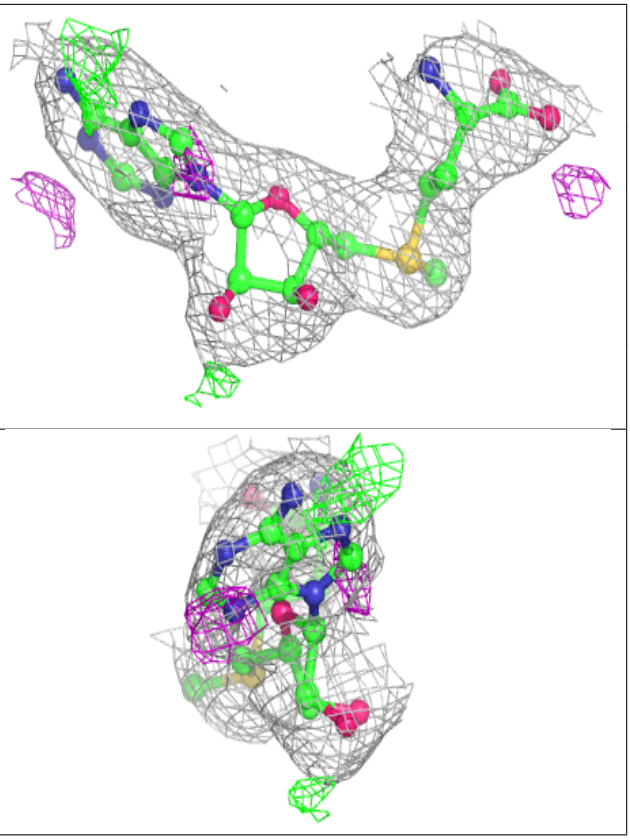






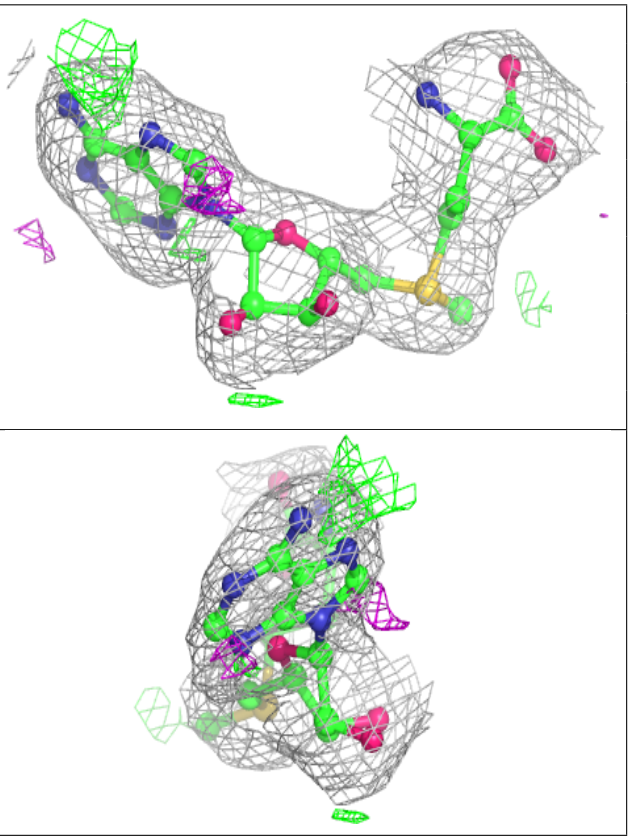
Electron density around SAM C 226:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SAM H 226:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.