Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 06:56 AM JST

PDB ID	:	7F4N
Title	:	Crystal structure of SAH-bound MTA1-p1-p2 complex
Authors	:	Chen, J.; Liu, L.
Deposited on	:	2021-06-21
Resolution	:	3.12 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:

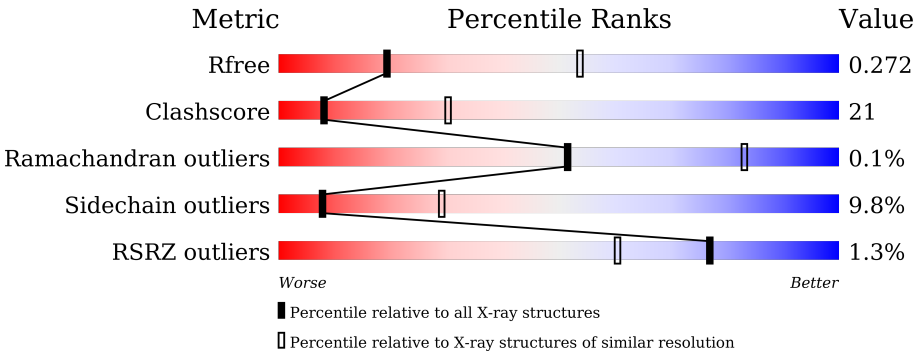
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.12 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	B	142	63% 25% 8%
1	G	142	48% 35% 8% 9%
2	C	247	52% 28% 7% 13%
2	D	247	52% 30% 5% 13%
3	E	309	8% 88%
3	F	309	5% 92%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6202 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 Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	130	Total	C	N	O	S	0	0	0
			1059	672	178	205	4			
1	G	129	Total	C	N	O	S	0	0	0
			1053	667	177	205	4			

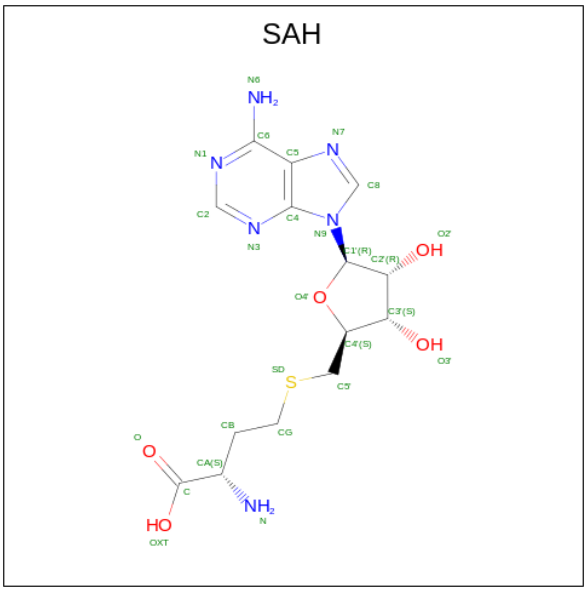
- Molecule 2 is a protein called MT-a70 family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	215	Total	C	N	O	S	0	0	0
			1745	1112	303	320	10			
2	D	216	Total	C	N	O	S	0	0	0
			1742	1111	299	322	10			

- Molecule 3 is a protein called p1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	37	Total	C	N	O	S	0	0	0
			308	196	51	60	1			
3	F	25	Total	C	N	O		0	0	0
			208	134	37	37				

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O S 26 14 6 5 1	0	0
4	D	1	Total C N O S 26 14 6 5 1	0	0

- Molecule 5 is water.

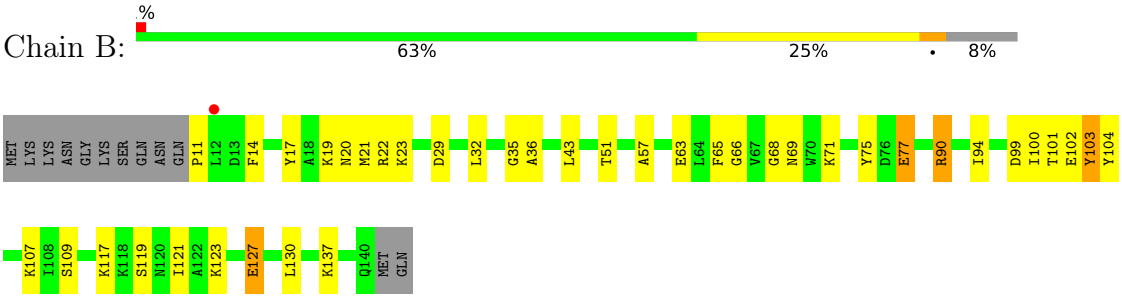
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	6	Total O 6 6	0	0
5	C	12	Total O 12 12	0	0
5	D	12	Total O 12 12	0	0
5	E	2	Total O 2 2	0	0
5	G	3	Total O 3 3	0	0

3 Residue-property plots (i)

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

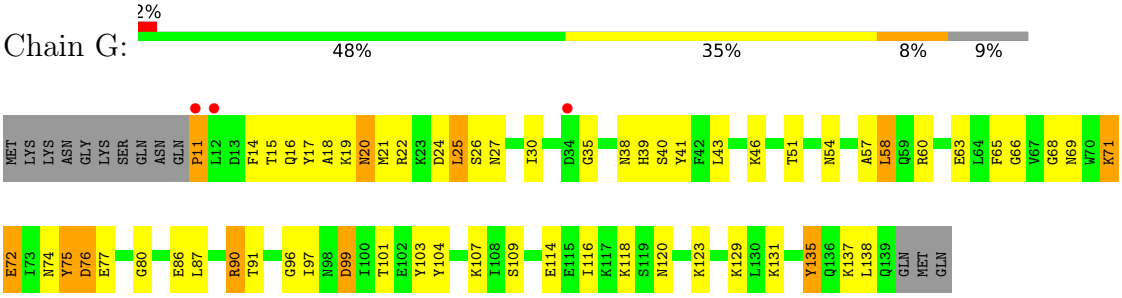
• Molecule 1: Transmembrane protein, putative

Chain B:



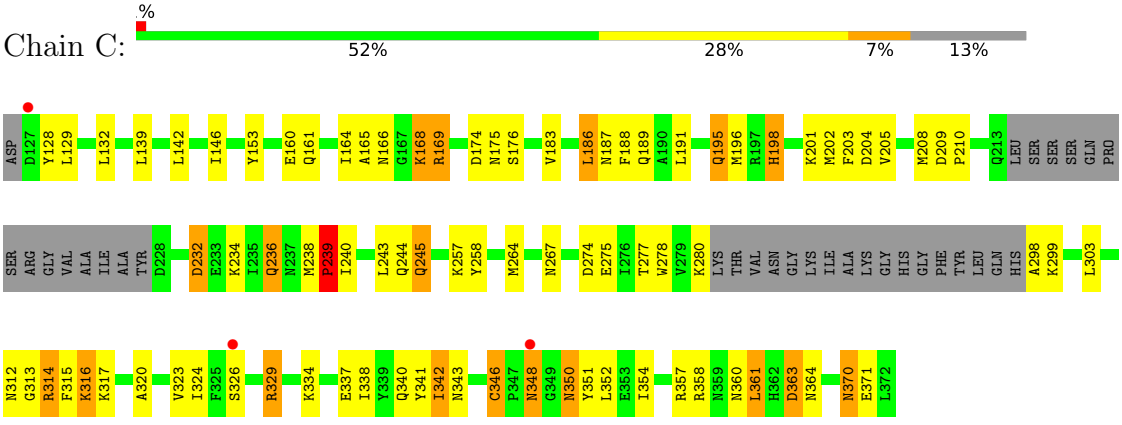
• Molecule 1: Transmembrane protein, putative

Chain G:



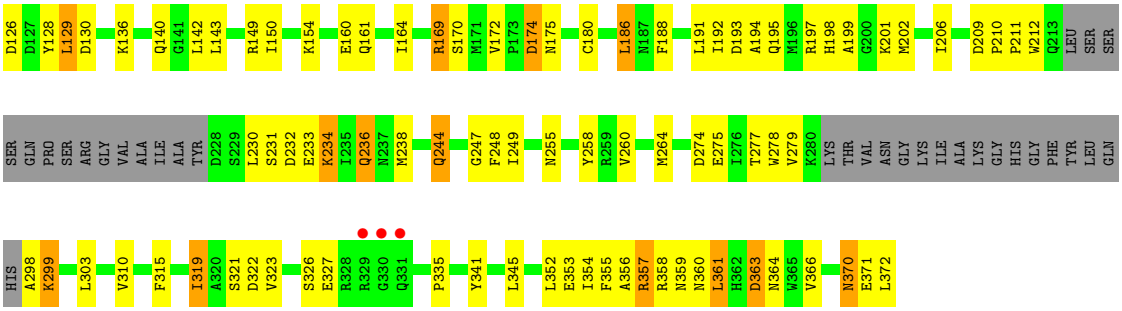
• Molecule 2: MT-a70 family protein

Chain C:



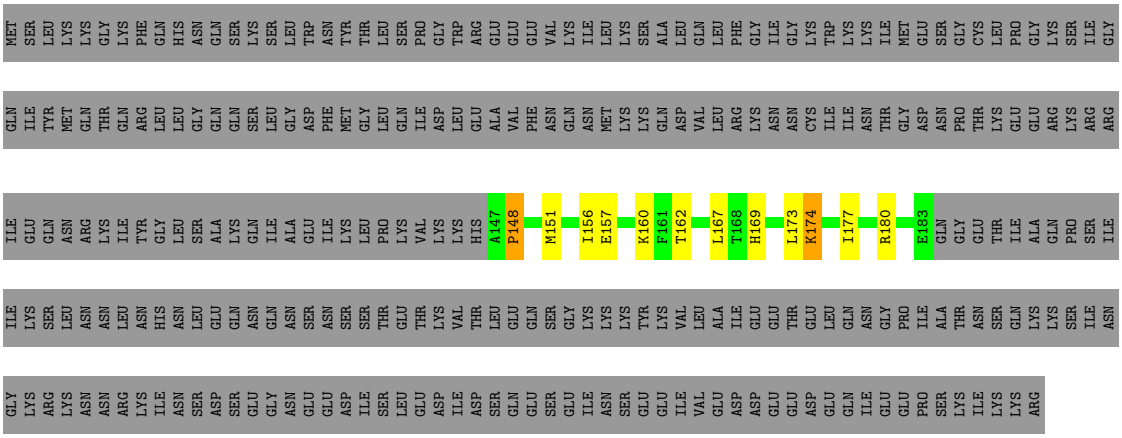
• Molecule 2: MT-a70 family protein

Chain D:



• Molecule 3: p1 protein

Chain E: 8% 88%



• Molecule 3: p1 protein

Chain F: 5% 92%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.62Å 84.85Å 160.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.17 – 3.12 45.17 – 3.12	Depositor EDS
% Data completeness (in resolution range)	72.0 (45.17-3.12) 71.9 (45.17-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.242 , 0.272 0.242 , 0.272	Depositor DCC
R_{free} test set	718 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	47.2	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , -2.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.064 for k,h,-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	6202	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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

5.1 Standard geometry

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

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	B	0.74	5/1075 (0.5%)	0.81	7/1439 (0.5%)
1	G	0.51	0/1069	0.68	1/1432 (0.1%)
2	C	0.59	1/1779 (0.1%)	0.77	2/2394 (0.1%)
2	D	0.52	0/1776	0.67	1/2393 (0.0%)
3	E	0.61	0/311	0.80	1/419 (0.2%)
3	F	0.43	0/210	0.65	0/283
All	All	0.59	6/6220 (0.1%)	0.73	12/8360 (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
2	C	0	1
2	D	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	TYR	CG-CD1	9.51	1.51	1.39
1	B	75	TYR	CE1-CZ	-8.42	1.27	1.38
1	B	75	TYR	CD1-CE1	-8.07	1.27	1.39
1	B	75	TYR	CD2-CE2	-7.01	1.28	1.39
1	B	75	TYR	CB-CG	-5.50	1.43	1.51
2	C	239	PRO	N-CD	5.22	1.55	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	75	TYR	CB-CG-CD2	-9.73	115.16	121.00
1	B	75	TYR	CG-CD2-CE2	-7.90	114.98	121.30
1	B	75	TYR	OH-CZ-CE2	-7.08	100.98	120.10
1	B	75	TYR	CA-CB-CG	-6.78	100.52	113.40
1	B	75	TYR	CE1-CZ-CE2	6.27	129.83	119.80
1	B	75	TYR	CD1-CE1-CZ	-5.99	114.41	119.80
3	E	148	PRO	N-CA-CB	5.92	110.40	103.30
1	B	11	PRO	N-CA-CB	5.88	110.36	103.30
2	C	238	MET	C-N-CD	5.75	140.47	128.40
1	G	11	PRO	N-CA-CB	5.72	110.16	103.30
2	D	129	LEU	CA-CB-CG	5.34	127.59	115.30
2	C	232	ASP	CB-CG-OD2	5.14	122.92	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	166	ASN	Peptide
2	D	321	SER	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	B	1059	0	1050	32	0
1	G	1053	0	1041	65	0
2	C	1745	0	1730	96	0
2	D	1742	0	1715	88	0
3	E	308	0	305	9	0
3	F	208	0	213	8	0
4	C	26	0	19	5	0
4	D	26	0	19	6	0
5	B	6	0	0	4	0
5	C	12	0	0	2	0
5	D	12	0	0	2	0
5	E	2	0	0	0	0
5	G	3	0	0	0	0
All	All	6202	0	6092	261	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (261) 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:C:169:ARG:NH2	2:C:174:ASP:OD2	1.64	1.30
2:C:201:LYS:NZ	2:C:314:ARG:NH2	1.83	1.25
2:C:201:LYS:HZ1	2:C:314:ARG:NH2	1.34	1.25
2:C:360:ASN:ND2	4:C:401:SAH:O	1.72	1.23
2:D:360:ASN:ND2	4:D:401:SAH:O	1.78	1.17
2:C:188:PHE:CE1	2:C:239:PRO:HD2	1.86	1.09
2:C:188:PHE:HD1	2:C:239:PRO:HG2	1.06	1.09
2:C:188:PHE:CD1	2:C:239:PRO:HG2	1.91	1.06
2:C:201:LYS:NZ	2:C:314:ARG:HH22	1.49	1.04
2:C:160:GLU:O	2:C:164:ILE:HG13	1.60	1.01
2:C:245:GLN:HB2	5:C:501:HOH:O	1.61	0.99
1:B:43:LEU:HD12	2:C:164:ILE:HG23	1.45	0.98
2:C:329:ARG:HG2	2:C:329:ARG:HH11	1.26	0.97
1:B:23:LYS:HE3	5:B:201:HOH:O	1.70	0.92
1:G:63:GLU:HG3	1:G:109:SER:HA	1.53	0.90
2:C:188:PHE:CD1	2:C:239:PRO:CG	2.54	0.90
2:C:201:LYS:HZ2	2:C:314:ARG:NH2	1.69	0.89
2:D:209:ASP:OD2	4:D:401:SAH:N	2.06	0.89
1:B:20:ASN:HB3	2:C:198:HIS:CD2	2.11	0.86
1:B:43:LEU:HD11	2:C:168:LYS:HB3	1.60	0.84
2:C:188:PHE:HD1	2:C:239:PRO:CG	1.88	0.83
2:D:231:SER:O	2:D:233:GLU:HG3	1.79	0.82
2:C:236:GLN:HG3	2:C:264:MET:HE2	1.60	0.82
1:B:102:GLU:OE2	1:B:137:LYS:NZ	2.13	0.81
1:B:43:LEU:CD1	2:C:164:ILE:HG23	2.10	0.81
1:B:22:ARG:NH1	1:B:35:GLY:O	2.14	0.81
2:D:211:PRO:HG3	4:D:401:SAH:C8	2.11	0.80
2:C:320:ALA:O	2:C:341:TYR:CE1	2.35	0.80
2:D:353:GLU:HG2	2:D:356:ALA:HB2	1.64	0.80
2:C:320:ALA:O	2:C:341:TYR:HE1	1.64	0.79
1:B:35:GLY:HA3	5:B:201:HOH:O	1.83	0.79
2:C:346:CYS:O	2:C:351:TYR:OH	2.00	0.78
2:C:209:ASP:OD2	2:C:334:LYS:NZ	2.17	0.77
2:D:231:SER:O	2:D:233:GLU:N	2.15	0.77
1:G:17:TYR:CE2	1:G:21:MET:HG3	2.20	0.76
2:D:364:ASN:CG	1:G:14:PHE:CD1	2.60	0.75
2:C:324:ILE:HD11	2:C:337:GLU:HB2	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:LYS:H	1:G:71:LYS:HD3	1.54	0.73
2:C:169:ARG:NH2	2:C:174:ASP:CG	2.42	0.73
2:D:180:CYS:SG	1:G:46:LYS:NZ	2.57	0.73
2:C:204:ASP:OD2	2:C:314:ARG:NH1	2.22	0.72
2:D:198:HIS:CD2	1:G:20:ASN:CB	2.72	0.72
2:C:240:ILE:HA	2:C:243:LEU:HD12	1.70	0.72
2:C:202:MET:HB2	2:C:245:GLN:HG2	1.72	0.72
2:D:236:GLN:HG3	2:D:264:MET:HG2	1.72	0.71
2:D:198:HIS:CD2	1:G:20:ASN:HB3	2.26	0.71
2:D:186:LEU:HD21	2:D:188:PHE:CE2	2.25	0.71
2:D:360:ASN:CG	4:D:401:SAH:O	2.28	0.71
1:G:15:THR:O	1:G:19:LYS:HG3	1.91	0.70
2:C:188:PHE:CD1	2:C:239:PRO:HD2	2.26	0.70
2:D:364:ASN:HB3	1:G:14:PHE:HE1	1.56	0.70
2:D:211:PRO:HG3	4:D:401:SAH:H8	1.76	0.67
1:G:18:ALA:O	1:G:22:ARG:N	2.17	0.67
2:C:232:ASP:OD2	2:C:257:LYS:NZ	2.22	0.67
2:C:360:ASN:HD21	4:C:401:SAH:C	1.98	0.67
2:C:280:LYS:HD2	2:C:298:ALA:HB1	1.78	0.66
1:G:71:LYS:H	1:G:71:LYS:CD	2.08	0.65
2:C:188:PHE:CD1	2:C:239:PRO:CD	2.80	0.64
2:D:364:ASN:HB3	1:G:14:PHE:CE1	2.33	0.64
3:E:156:ILE:HD13	3:E:169:HIS:HB3	1.79	0.64
2:D:230:LEU:O	2:D:234:LYS:HB2	1.98	0.64
2:D:175:ASN:HB2	2:D:363:ASP:HB3	1.80	0.63
2:D:370:ASN:HD22	2:D:370:ASN:C	2.02	0.63
2:C:188:PHE:CE1	2:C:239:PRO:CD	2.73	0.62
1:G:17:TYR:CE2	1:G:21:MET:CG	2.83	0.62
2:C:299:LYS:NZ	2:D:275:GLU:O	2.32	0.62
2:D:198:HIS:CD2	1:G:20:ASN:HB2	2.33	0.62
2:C:314:ARG:HH11	2:C:314:ARG:CG	2.12	0.62
2:C:314:ARG:HH11	2:C:314:ARG:HG3	1.65	0.62
2:C:188:PHE:HE1	2:C:239:PRO:HD2	1.59	0.61
2:C:201:LYS:HZ1	2:C:314:ARG:HH21	1.42	0.61
2:C:201:LYS:HZ1	2:C:314:ARG:HH22	1.10	0.60
2:C:201:LYS:HZ2	2:C:314:ARG:CZ	2.14	0.60
2:D:255:ASN:HA	2:D:258:TYR:CE2	2.37	0.60
2:D:210:PRO:HG2	2:D:212:TRP:CZ2	2.37	0.60
1:G:87:LEU:O	1:G:91:THR:HG23	2.01	0.60
1:G:22:ARG:HG2	1:G:26:SER:OG	2.01	0.59
2:C:175:ASN:HB2	2:C:363:ASP:HB2	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:ARG:NH2	2:D:174:ASP:OD1	2.36	0.59
2:D:143:LEU:HD11	3:E:174:LYS:HG2	1.85	0.59
2:C:208:MET:HE2	2:C:210:PRO:HG3	1.86	0.58
2:C:329:ARG:HH11	2:C:329:ARG:CG	2.08	0.58
1:B:63:GLU:HG2	1:B:109:SER:HA	1.85	0.57
1:G:21:MET:O	1:G:25:LEU:HD12	2.05	0.57
2:C:191:LEU:O	2:C:195:GLN:HB2	2.04	0.57
2:C:195:GLN:NE2	2:C:201:LYS:O	2.37	0.57
2:D:244:GLN:NE2	2:D:248:PHE:O	2.26	0.56
2:C:299:LYS:HE3	2:D:322:ASP:HB3	1.87	0.56
2:D:260:VAL:HG13	5:D:508:HOH:O	2.04	0.56
1:G:16:GLN:HG3	1:G:20:ASN:OD1	2.05	0.56
2:D:170:SER:HA	1:G:43:LEU:HD21	1.88	0.56
2:D:188:PHE:O	2:D:191:LEU:N	2.38	0.56
1:B:19:LYS:HB3	5:B:201:HOH:O	2.06	0.56
1:G:20:ASN:O	1:G:24:ASP:OD1	2.24	0.55
1:G:57:ALA:HB1	1:G:77:GLU:HB3	1.87	0.55
2:C:280:LYS:HD2	2:C:298:ALA:CB	2.36	0.55
1:G:58:LEU:HD11	1:G:91:THR:HG22	1.88	0.55
2:D:191:LEU:HA	1:G:25:LEU:HD21	1.89	0.55
2:C:205:VAL:HG11	2:C:342:ILE:HD12	1.89	0.55
2:D:197:ARG:HD2	2:D:198:HIS:CE1	2.42	0.55
2:D:211:PRO:HG2	2:D:230:LEU:HD12	1.88	0.55
2:D:150:ILE:O	2:D:154:LYS:HB2	2.07	0.54
1:G:114:GLU:HG3	1:G:118:LYS:HE3	1.88	0.54
2:D:238:MET:CE	2:D:354:ILE:HG21	2.37	0.54
2:D:274:ASP:OD1	2:D:275:GLU:N	2.40	0.54
2:C:142:LEU:HD13	3:F:177:ILE:HD11	1.90	0.54
1:G:17:TYR:O	1:G:21:MET:HG2	2.09	0.53
1:G:123:LYS:HD2	1:G:135:TYR:HE1	1.73	0.53
1:G:22:ARG:O	1:G:26:SER:HB2	2.09	0.53
2:D:126:ASP:CB	2:D:129:LEU:HB2	2.39	0.53
2:D:353:GLU:OE2	5:D:501:HOH:O	2.19	0.53
2:C:258:TYR:HE1	2:C:303:LEU:HD11	1.74	0.53
2:D:234:LYS:HD2	2:D:234:LYS:N	2.24	0.53
2:C:329:ARG:HG2	2:C:329:ARG:NH1	2.05	0.52
2:C:338:ILE:O	2:C:342:ILE:HG12	2.09	0.52
1:G:76:ASP:HB3	1:G:77:GLU:OE1	2.10	0.52
2:C:239:PRO:HG2	2:C:239:PRO:O	2.10	0.52
2:C:363:ASP:OD1	2:C:363:ASP:N	2.33	0.52
2:C:340:GLN:HA	2:C:343:ASN:HB2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:364:ASN:CG	1:G:14:PHE:CE1	2.83	0.51
1:G:69:ASN:HB3	1:G:72:GLU:OE1	2.11	0.51
2:C:357:ARG:O	2:C:360:ASN:N	2.37	0.51
1:G:66:GLY:HA2	1:G:107:LYS:HA	1.92	0.51
1:B:103:TYR:CD2	1:B:103:TYR:N	2.78	0.51
2:C:146:ILE:HD11	3:F:173:LEU:HD22	1.93	0.51
2:C:334:LYS:HG3	4:C:401:SAH:HN2	1.74	0.51
2:D:136:LYS:O	2:D:140:GLN:HG3	2.10	0.51
1:B:121:ILE:HG23	1:B:130:LEU:HD11	1.93	0.51
2:D:358:ARG:O	2:D:361:LEU:HD22	2.11	0.51
1:B:90:ARG:O	1:B:94:ILE:HG13	2.12	0.50
2:C:175:ASN:HB2	2:C:363:ASP:CB	2.41	0.50
2:D:370:ASN:ND2	2:D:371:GLU:HG3	2.26	0.50
2:D:160:GLU:O	2:D:164:ILE:HG13	2.12	0.49
2:C:329:ARG:CG	2:C:329:ARG:NH1	2.72	0.49
2:D:194:ALA:HA	2:D:197:ARG:HE	1.77	0.49
1:G:16:GLN:O	1:G:19:LYS:N	2.45	0.49
1:B:57:ALA:O	1:B:77:GLU:HG2	2.13	0.49
2:C:169:ARG:HH21	2:C:174:ASP:CG	2.15	0.49
2:C:161:GLN:O	2:C:165:ALA:HB2	2.12	0.49
1:B:119:SER:O	1:B:123:LYS:HB2	2.13	0.49
2:C:240:ILE:HG22	2:C:240:ILE:O	2.13	0.49
2:C:129:LEU:HD13	3:F:180:ARG:HH21	1.77	0.49
2:D:364:ASN:OD1	1:G:14:PHE:CD1	2.66	0.48
1:G:22:ARG:NH1	1:G:35:GLY:O	2.46	0.48
1:B:29:ASP:OD2	1:B:51:THR:HG22	2.13	0.48
2:C:186:LEU:HD22	2:C:187:ASN:H	1.79	0.48
2:C:358:ARG:O	2:C:361:LEU:HB2	2.13	0.48
2:C:314:ARG:NH1	2:C:314:ARG:CG	2.73	0.48
1:G:20:ASN:OD1	1:G:20:ASN:N	2.46	0.48
1:B:99:ASP:OD2	1:B:101:THR:OG1	2.22	0.47
1:G:138:LEU:HD23	1:G:138:LEU:HA	1.77	0.47
2:C:274:ASP:OD2	2:C:275:GLU:N	2.47	0.47
1:G:51:THR:H	1:G:54:ASN:HD22	1.61	0.47
1:G:68:GLY:HA2	1:G:104:TYR:CD2	2.49	0.47
2:C:350:ASN:OD1	2:C:350:ASN:N	2.33	0.47
2:D:161:GLN:OE1	1:G:90:ARG:NH2	2.48	0.47
2:D:357:ARG:HE	2:D:359:ASN:HD21	1.63	0.47
1:B:43:LEU:CD1	2:C:168:LYS:HB3	2.38	0.47
2:D:364:ASN:CB	1:G:14:PHE:CE1	2.97	0.47
2:C:209:ASP:OD2	4:C:401:SAH:N	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:PHE:HE2	2:C:348:ASN:HB2	1.80	0.47
1:G:129:LYS:HD2	1:G:129:LYS:HA	1.67	0.47
1:G:30:ILE:HG12	1:G:41:TYR:CE1	2.50	0.47
2:D:188:PHE:O	2:D:192:ILE:HG13	2.15	0.46
1:G:74:ASN:ND2	1:G:80:GLY:HA2	2.31	0.46
2:C:186:LEU:HD22	2:C:187:ASN:N	2.31	0.46
3:F:162:THR:O	3:F:166:ILE:HG13	2.15	0.46
2:C:139:LEU:HD22	3:F:177:ILE:HG23	1.97	0.46
2:C:357:ARG:H	2:C:360:ASN:HB2	1.80	0.46
3:E:151:MET:HE1	3:E:156:ILE:HA	1.98	0.46
1:G:97:ILE:HA	1:G:135:TYR:HB3	1.98	0.46
2:D:358:ARG:HA	2:D:372:LEU:HD23	1.98	0.45
1:G:75:TYR:HD2	1:G:75:TYR:HA	1.53	0.45
1:B:71:LYS:HE2	1:B:71:LYS:HB2	1.86	0.45
1:G:38:ASN:OD1	1:G:40:SER:OG	2.29	0.45
2:C:142:LEU:O	2:C:146:ILE:HG13	2.15	0.45
1:G:86:GLU:O	1:G:90:ARG:HB2	2.17	0.45
2:D:299:LYS:HE3	2:D:299:LYS:HB3	1.86	0.45
1:G:18:ALA:O	1:G:22:ARG:HB2	2.17	0.45
2:C:153:TYR:O	3:F:167:LEU:HD11	2.17	0.45
1:B:66:GLY:HA2	1:B:107:LYS:HA	1.98	0.45
2:C:183:VAL:HG22	4:C:401:SAH:N1	2.32	0.45
1:G:17:TYR:O	1:G:21:MET:CG	2.65	0.45
2:D:172:VAL:HG22	2:D:361:LEU:HD21	1.98	0.45
1:G:96:GLY:HA3	1:G:120:ASN:HB2	1.98	0.45
2:D:370:ASN:HD22	2:D:371:GLU:HG3	1.82	0.45
2:D:363:ASP:OD1	2:D:363:ASP:N	2.49	0.44
2:C:363:ASP:O	2:C:364:ASN:HB2	2.17	0.44
2:D:193:ASP:O	2:D:197:ARG:HG2	2.17	0.44
3:E:173:LEU:O	3:E:177:ILE:HG12	2.17	0.44
2:D:186:LEU:CD2	2:D:188:PHE:CE2	2.97	0.44
1:G:65:PHE:CE1	1:G:72:GLU:HB3	2.52	0.44
1:B:23:LYS:CE	5:B:201:HOH:O	2.46	0.44
2:C:361:LEU:HA	2:C:361:LEU:HD12	1.63	0.44
2:D:174:ASP:O	1:G:22:ARG:NH2	2.51	0.44
1:G:63:GLU:O	1:G:107:LYS:HB3	2.18	0.44
2:D:186:LEU:HD21	2:D:188:PHE:HE2	1.76	0.44
1:G:103:TYR:HE1	1:G:116:ILE:HG21	1.83	0.44
2:D:126:ASP:N	3:E:180:ARG:HH22	2.15	0.44
2:D:143:LEU:HD12	2:D:143:LEU:HA	1.63	0.44
2:C:316:LYS:N	2:C:316:LYS:HD2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:329:ARG:HD3	2:C:329:ARG:HA	1.65	0.43
2:C:358:ARG:HA	2:C:361:LEU:HD22	2.00	0.43
2:D:149:ARG:HD3	3:E:157:GLU:OE2	2.17	0.43
2:D:230:LEU:HD23	2:D:230:LEU:HA	1.84	0.43
2:D:275:GLU:HG3	2:D:303:LEU:HD13	1.99	0.43
3:F:181:LEU:HD23	3:F:181:LEU:HA	1.75	0.43
1:B:94:ILE:O	1:B:117:LYS:HB2	2.18	0.43
1:B:32:LEU:O	1:B:35:GLY:N	2.31	0.43
1:B:43:LEU:CD1	2:C:168:LYS:HD2	2.48	0.43
2:D:201:LYS:NZ	2:D:202:MET:O	2.52	0.43
2:D:231:SER:O	2:D:232:ASP:HB2	2.19	0.43
2:C:315:PHE:C	2:C:316:LYS:HD2	2.38	0.43
2:D:231:SER:C	2:D:233:GLU:N	2.72	0.43
1:B:68:GLY:HA3	1:B:104:TYR:CE1	2.54	0.43
2:D:319:ILE:HG13	2:D:341:TYR:HE2	1.84	0.43
2:C:278:TRP:HZ2	2:C:326:SER:HG	1.66	0.42
2:C:370:ASN:HD22	2:C:371:GLU:N	2.17	0.42
1:G:103:TYR:CE1	1:G:116:ILE:HG21	2.54	0.42
2:D:238:MET:CE	2:D:354:ILE:HD13	2.50	0.42
5:C:504:HOH:O	2:D:298:ALA:HB3	2.19	0.42
2:D:198:HIS:HD2	1:G:20:ASN:CB	2.29	0.42
2:C:323:VAL:HG22	2:D:299:LYS:HB2	2.01	0.42
2:D:199:ALA:O	1:G:11:PRO:N	2.52	0.42
3:E:167:LEU:HD23	3:E:167:LEU:HA	1.82	0.42
2:C:323:VAL:CG2	2:D:299:LYS:HB2	2.50	0.42
2:D:170:SER:HB3	1:G:39:HIS:ND1	2.34	0.42
2:D:352:LEU:HD12	2:D:366:VAL:O	2.19	0.42
1:B:17:TYR:O	1:B:21:MET:HG2	2.20	0.42
2:C:203:PHE:O	2:C:244:GLN:HG3	2.20	0.41
2:D:319:ILE:HB	2:D:341:TYR:HE2	1.84	0.41
2:D:354:ILE:HG22	2:D:355:PHE:H	1.84	0.41
3:E:173:LEU:HD23	3:E:173:LEU:HA	1.83	0.41
4:D:401:SAH:H4'	4:D:401:SAH:HG2	1.43	0.41
1:B:102:GLU:HB2	1:B:103:TYR:CD2	2.56	0.41
2:C:245:GLN:HG2	2:C:245:GLN:H	1.58	0.41
2:C:313:GLY:O	2:C:316:LYS:HE3	2.21	0.41
1:G:17:TYR:CD2	1:G:21:MET:CG	3.04	0.41
1:G:30:ILE:O	1:G:38:ASN:HB3	2.20	0.41
1:G:99:ASP:OD2	1:G:101:THR:OG1	2.39	0.41
1:B:127:GLU:H	1:B:127:GLU:HG2	1.54	0.41
2:D:247:GLY:HA2	2:D:315:PHE:CZ	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:353:GLU:CG	2:D:356:ALA:HB2	2.44	0.41
1:B:65:PHE:O	1:B:69:ASN:ND2	2.50	0.41
2:D:206:ILE:O	2:D:249:ILE:HA	2.20	0.41
2:D:278:TRP:CE2	2:D:335:PRO:HG3	2.56	0.41
2:D:326:SER:HA	2:D:327:GLU:HA	1.80	0.41
3:E:151:MET:CE	3:E:156:ILE:HA	2.51	0.41
1:G:27:ASN:HB2	1:G:30:ILE:HG13	2.02	0.41
1:B:100:ILE:HG21	1:B:100:ILE:HD13	1.86	0.41
2:C:132:LEU:HD23	2:C:132:LEU:HA	1.76	0.41
2:D:128:TYR:CD2	2:D:129:LEU:HD23	2.56	0.41
2:D:198:HIS:NE2	1:G:20:ASN:HB3	2.36	0.41
2:D:238:MET:HE1	2:D:354:ILE:HD13	2.03	0.41
1:B:22:ARG:HH12	1:B:36:ALA:HA	1.84	0.40
2:C:277:THR:HG21	2:D:277:THR:HG21	2.02	0.40
1:G:60:ARG:HH21	1:G:77:GLU:HG2	1.85	0.40
2:C:352:LEU:HD21	2:C:354:ILE:HD11	2.03	0.40
2:D:238:MET:HE1	2:D:354:ILE:HG21	2.03	0.40
3:F:174:LYS:O	3:F:178:VAL:HG23	2.21	0.40
1:G:123:LYS:HD2	1:G:135:TYR:CE1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	128/142 (90%)	126 (98%)	2 (2%)	0	100 100
1	G	127/142 (89%)	124 (98%)	3 (2%)	0	100 100
2	C	209/247 (85%)	203 (97%)	6 (3%)	0	100 100
2	D	210/247 (85%)	198 (94%)	12 (6%)	0	100 100
3	E	35/309 (11%)	33 (94%)	1 (3%)	1 (3%)	4 23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	F	23/309 (7%)	23 (100%)	0	0	100 100
All	All	732/1396 (52%)	707 (97%)	24 (3%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	148	PRO

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	B	113/127 (89%)	109 (96%)	4 (4%)	36 67
1	G	113/127 (89%)	101 (89%)	12 (11%)	6 25
2	C	190/219 (87%)	164 (86%)	26 (14%)	3 16
2	D	189/219 (86%)	170 (90%)	19 (10%)	7 27
3	E	33/282 (12%)	30 (91%)	3 (9%)	9 33
3	F	22/282 (8%)	21 (96%)	1 (4%)	27 59
All	All	660/1256 (52%)	595 (90%)	65 (10%)	8 29

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	77	GLU
1	B	90	ARG
1	B	103	TYR
1	B	127	GLU
2	C	128	TYR
2	C	168	LYS
2	C	169	ARG
2	C	176	SER
2	C	186	LEU
2	C	189	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	195	GLN
2	C	196	MET
2	C	198	HIS
2	C	234	LYS
2	C	236	GLN
2	C	239	PRO
2	C	245	GLN
2	C	267	ASN
2	C	312	ASN
2	C	314	ARG
2	C	316	LYS
2	C	317	LYS
2	C	329	ARG
2	C	342	ILE
2	C	346	CYS
2	C	348	ASN
2	C	350	ASN
2	C	361	LEU
2	C	363	ASP
2	C	370	ASN
2	D	130	ASP
2	D	142	LEU
2	D	169	ARG
2	D	174	ASP
2	D	186	LEU
2	D	195	GLN
2	D	234	LYS
2	D	236	GLN
2	D	244	GLN
2	D	279	VAL
2	D	299	LYS
2	D	310	VAL
2	D	319	ILE
2	D	323	VAL
2	D	345	LEU
2	D	357	ARG
2	D	361	LEU
2	D	363	ASP
2	D	370	ASN
3	E	160	LYS
3	E	162	THR
3	E	174	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	173	LEU
1	G	20	ASN
1	G	25	LEU
1	G	58	LEU
1	G	71	LYS
1	G	72	GLU
1	G	75	TYR
1	G	76	ASP
1	G	90	ARG
1	G	99	ASP
1	G	131	LYS
1	G	135	TYR
1	G	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	144	GLN
2	C	195	GLN
2	C	236	GLN
2	C	245	GLN
2	C	370	ASN
2	D	152	HIS
2	D	370	ASN
1	G	54	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	SAH	C	401	-	24,28,28	1.17	1 (4%)	25,40,40	1.61	6 (24%)
4	SAH	D	401	-	24,28,28	1.15	2 (8%)	25,40,40	1.40	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAH	C	401	-	-	3/11/31/31	0/3/3/3
4	SAH	D	401	-	-	8/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	SAH	C2'-C1'	-2.77	1.49	1.53
4	D	401	SAH	C2'-C1'	-2.16	1.50	1.53
4	D	401	SAH	OXT-C	-2.14	1.23	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	401	SAH	N3-C2-N1	-3.46	123.26	128.68
4	C	401	SAH	CB-CG-SD	-3.40	105.69	113.31
4	C	401	SAH	C1'-N9-C4	-3.23	120.97	126.64
4	D	401	SAH	N3-C2-N1	-2.95	124.07	128.68
4	D	401	SAH	C2'-C3'-C4'	2.28	107.06	102.64
4	D	401	SAH	C4-C5-N7	-2.23	107.07	109.40
4	C	401	SAH	O3'-C3'-C2'	-2.17	104.81	111.82
4	C	401	SAH	C2-N1-C6	2.12	122.38	118.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	401	SAH	O3'-C3'-C2'	-2.05	105.20	111.82
4	C	401	SAH	C4-C5-N7	-2.03	107.28	109.40

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	401	SAH	O-C-CA-N
4	D	401	SAH	O-C-CA-N
4	D	401	SAH	O4'-C4'-C5'-SD
4	D	401	SAH	C3'-C4'-C5'-SD
4	D	401	SAH	CA-CB-CG-SD
4	D	401	SAH	OXT-C-CA-N
4	C	401	SAH	OXT-C-CA-N
4	D	401	SAH	OXT-C-CA-CB
4	D	401	SAH	C4'-C5'-SD-CG
4	D	401	SAH	O-C-CA-CB
4	C	401	SAH	C-CA-CB-CG

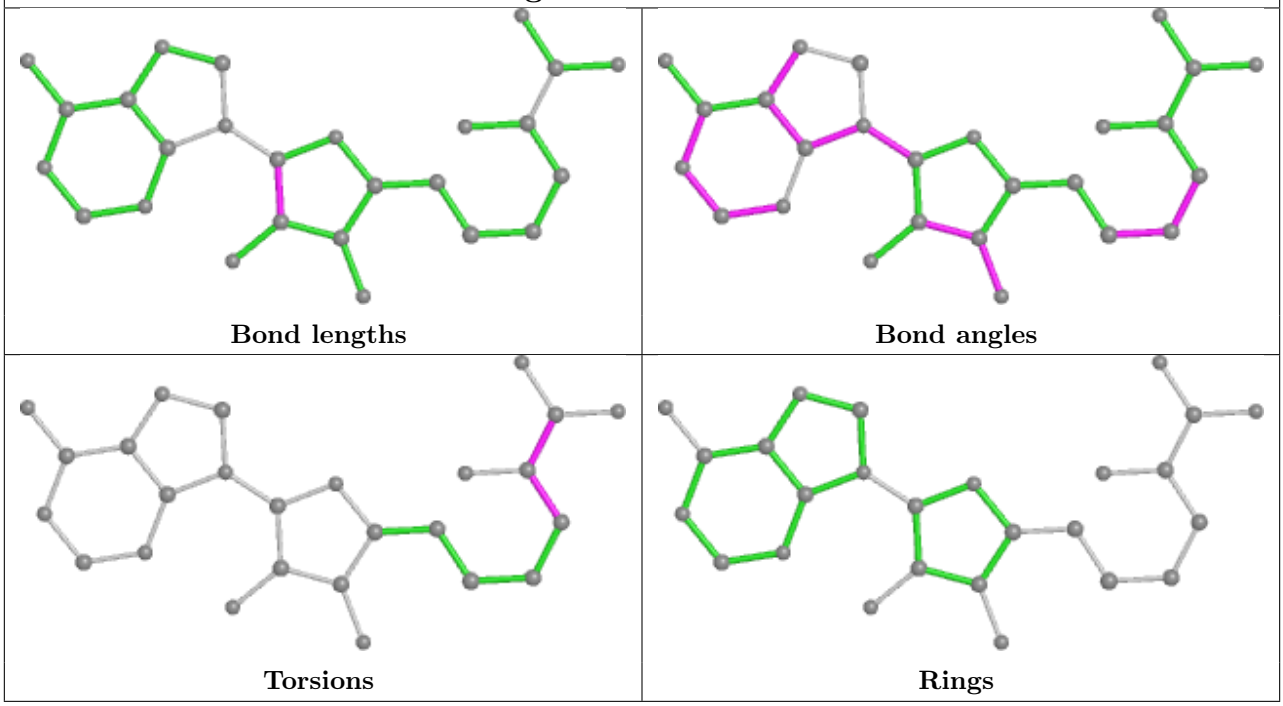
There are no ring outliers.

2 monomers are involved in 11 short contacts:

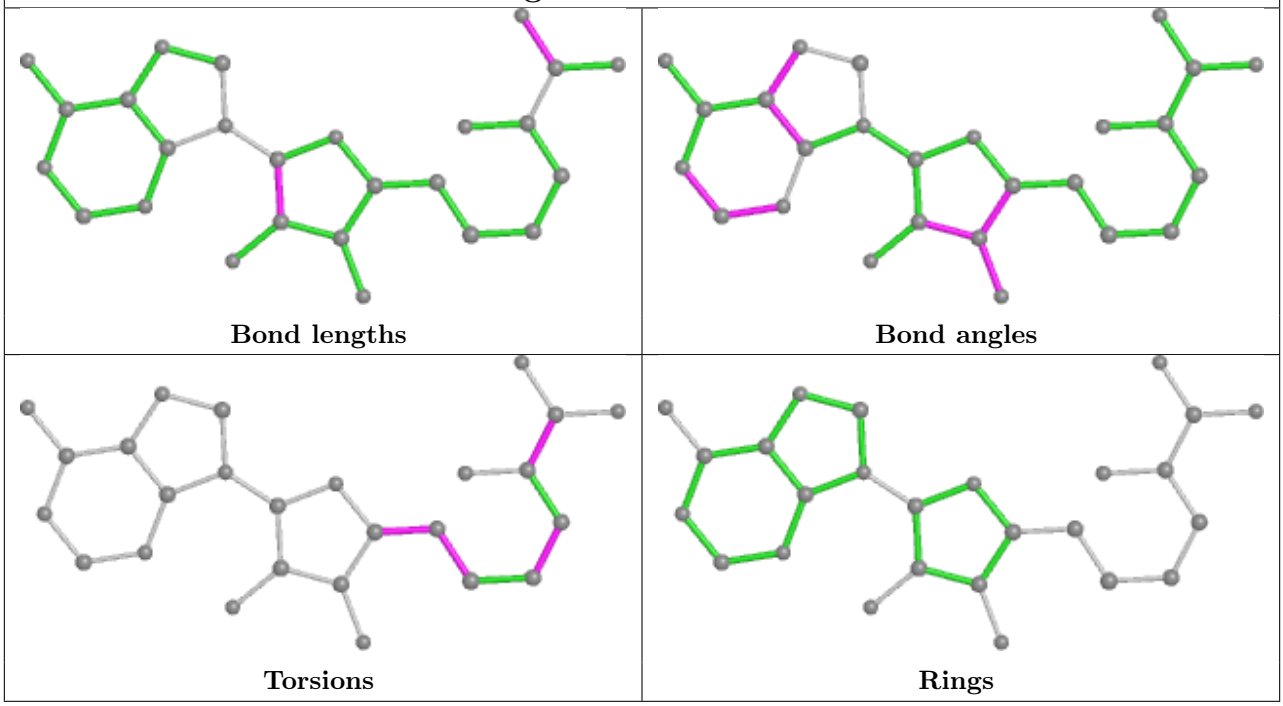
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	SAH	5	0
4	D	401	SAH	6	0

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 SAH C 401



Ligand SAH D 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	B	130/142 (91%)	-0.27	1 (0%) 86 74	24, 53, 79, 93	0
1	G	129/142 (90%)	-0.13	3 (2%) 60 39	11, 42, 69, 96	0
2	C	215/247 (87%)	-0.03	3 (1%) 75 58	18, 48, 87, 98	0
2	D	216/247 (87%)	-0.16	3 (1%) 75 58	10, 44, 73, 110	0
3	E	37/309 (11%)	-0.44	0 100 100	9, 23, 47, 52	0
3	F	25/309 (8%)	-0.50	0 100 100	20, 30, 57, 66	0
All	All	752/1396 (53%)	-0.16	10 (1%) 77 60	9, 45, 79, 110	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	11	PRO	4.5
1	G	34	ASP	4.4
2	D	330	GLY	4.2
2	D	331	GLN	3.0
2	D	329	ARG	2.8
1	B	12	LEU	2.4
2	C	348	ASN	2.4
2	C	127	ASP	2.3
2	C	326	SER	2.2
1	G	12	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

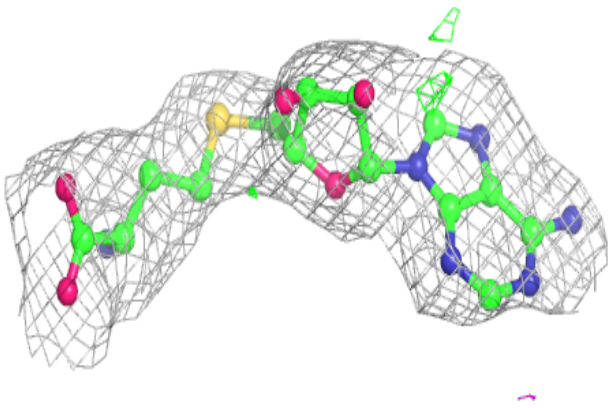
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

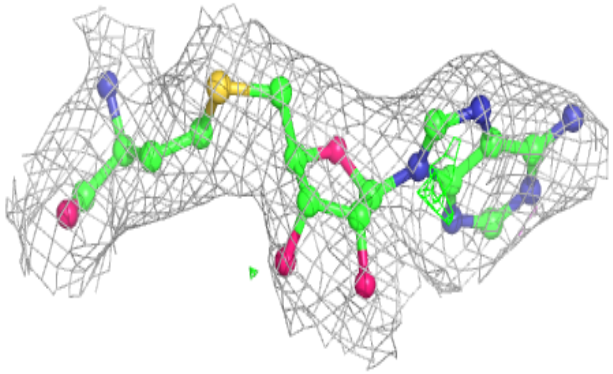
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SAH	D	401	26/26	0.92	0.17	34,41,48,51	0
4	SAH	C	401	26/26	0.96	0.13	26,33,47,49	0

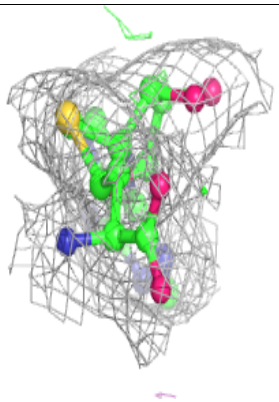
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH D 401:

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

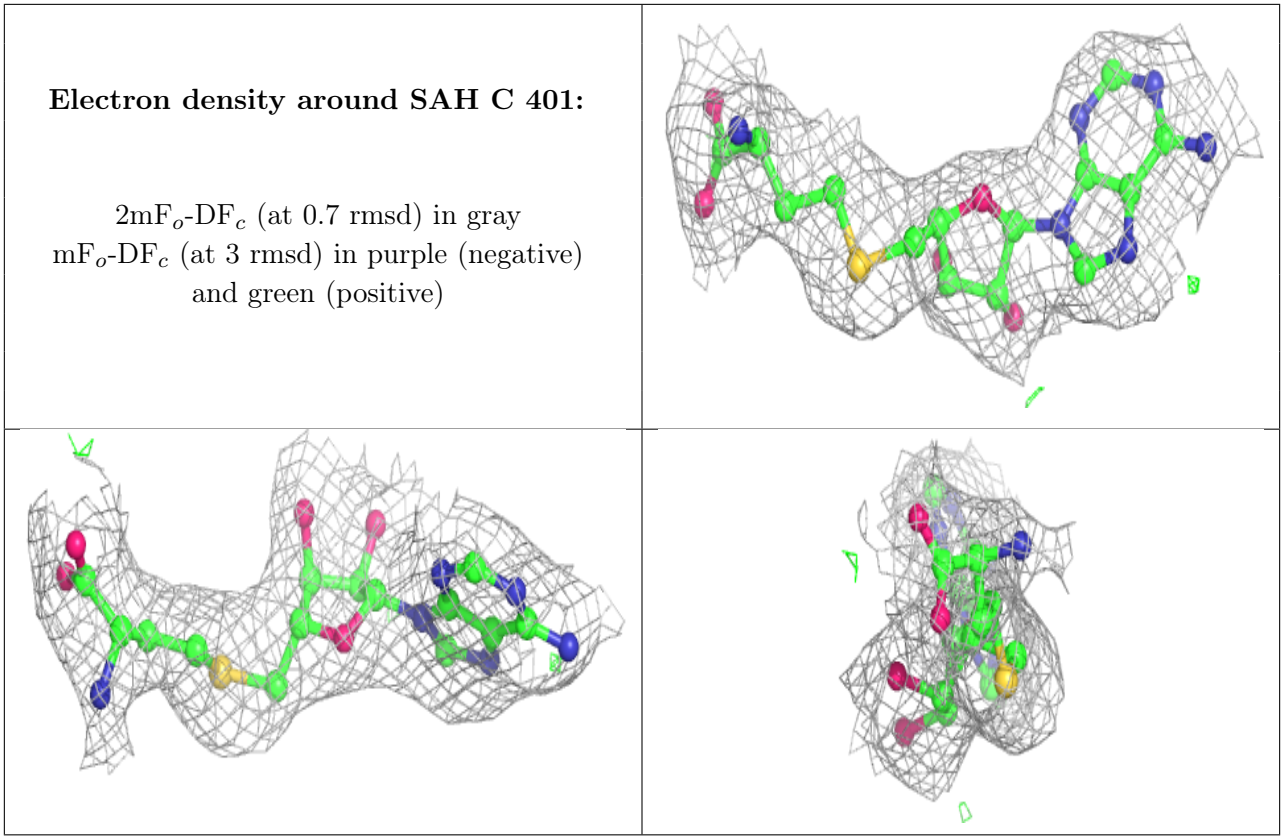






Electron density around SAH C 401:

$2mF_o$-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.