



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:53 AM UTC

PDB ID : 3CJQ / pdb_00003cjq
Title : Ribosomal protein L11 methyltransferase (PrmA) in complex with dimethylated ribosomal protein L11 in space group P212121
Authors : Demirci, H.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2008-03-13
Resolution : 2.70 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

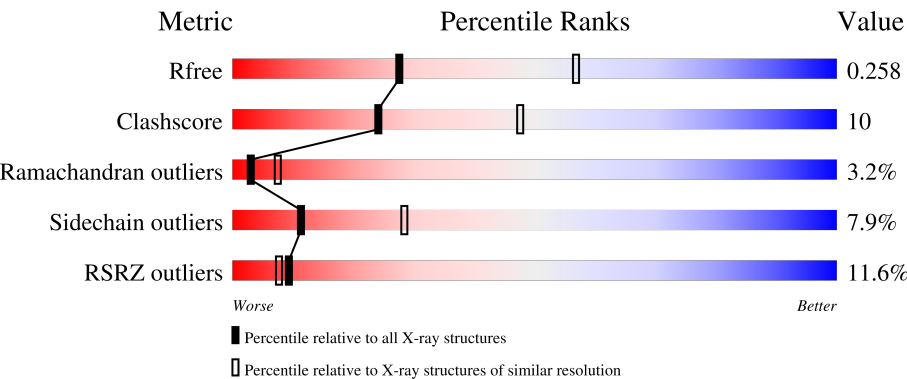
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	254	2% 71% 26% .
1	D	254	3% 77% 18% ..
1	G	254	4% 70% 26% ...
2	B	146	25% 55% 23% 5% 17%
2	E	146	25% 51% 25% . 21%

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Mol	Chain	Length	Quality of chain
2	H	146	

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
5	2MM	E	1	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8801 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 Ribosomal protein L11 methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1949	1265	338	342	4			
1	D	252	Total	C	N	O	S	0	1	0
			1954	1270	338	342	4			
1	G	252	Total	C	N	O	S	5	0	0
			1941	1261	337	339	4			

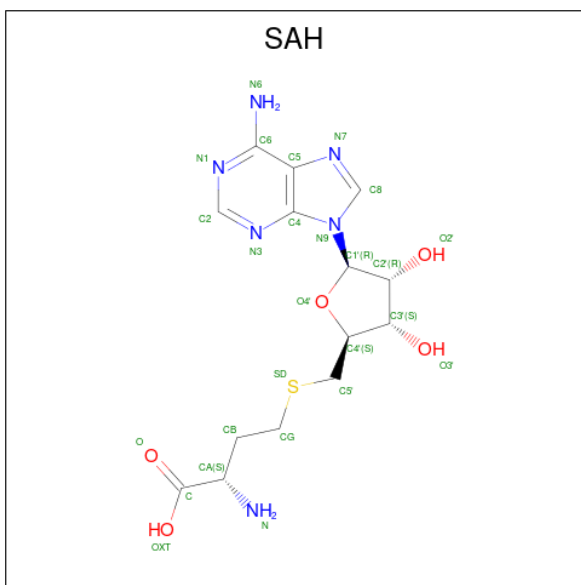
- Molecule 2 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			884	566	150	163	5			
2	E	115	Total	C	N	O	S	0	0	0
			838	540	143	150	5			
2	H	121	Total	C	N	O	S	0	0	0
			884	566	150	163	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	39	ALA	LYS	engineered mutation	UNP P36238
E	39	ALA	LYS	engineered mutation	UNP P36238
H	39	ALA	LYS	engineered mutation	UNP P36238

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).

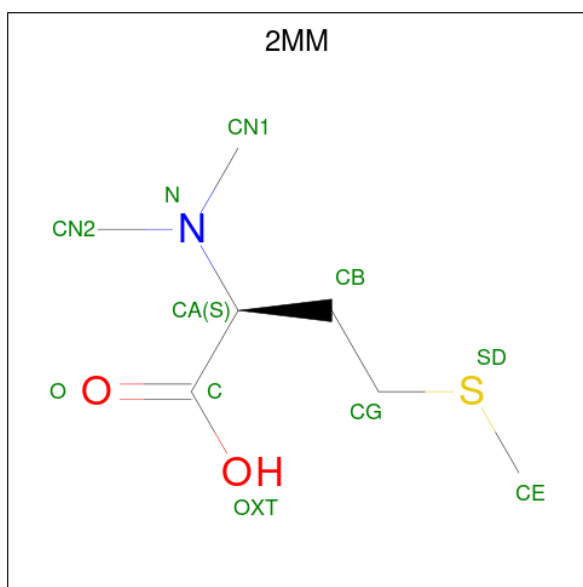


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	G	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	I	0	0
			1	1		
4	H	1	Total	I	0	0
			1	1		

- Molecule 5 is N,N-dimethyl-L-methionine (CCD ID: 2MM) (formula: C₇H₁₅NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			10	7	1	1	1		
5	E	1	Total	C	N	O	S	0	0
			10	7	1	1	1		
5	H	1	Total	C	N	O	S	0	0
			10	7	1	1	1		

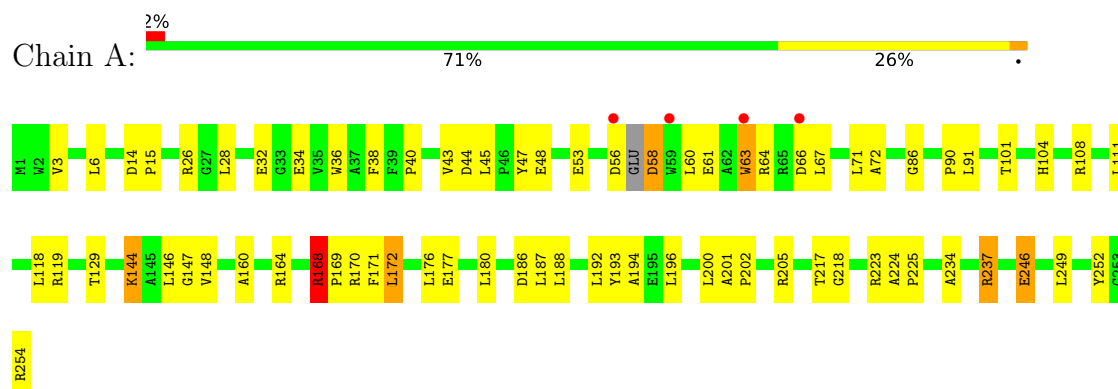
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total	O	0	0
			75	75		
6	B	10	Total	O	0	0
			10	10		
6	D	88	Total	O	0	0
			88	88		
6	E	16	Total	O	0	0
			16	16		
6	G	48	Total	O	0	0
			48	48		
6	H	4	Total	O	0	0
			4	4		

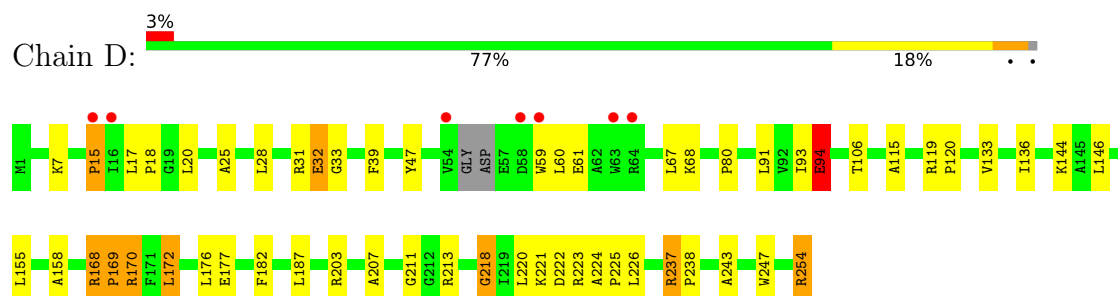
3 Residue-property plots [i](#)

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.

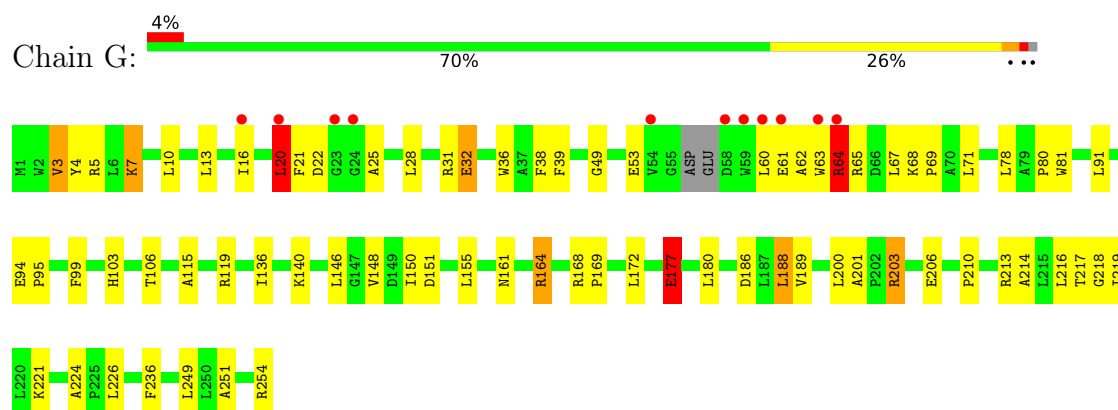
- Molecule 1: Ribosomal protein L11 methyltransferase



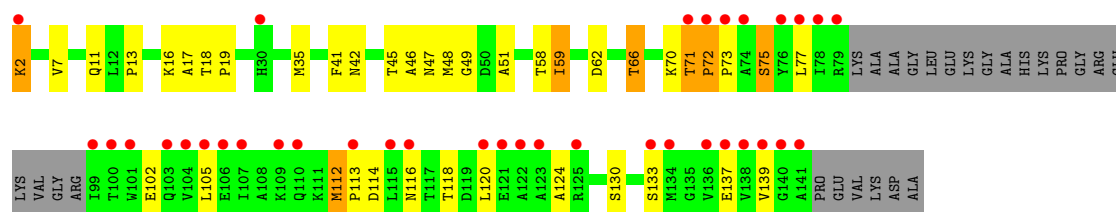
- Molecule 1: Ribosomal protein L11 methyltransferase



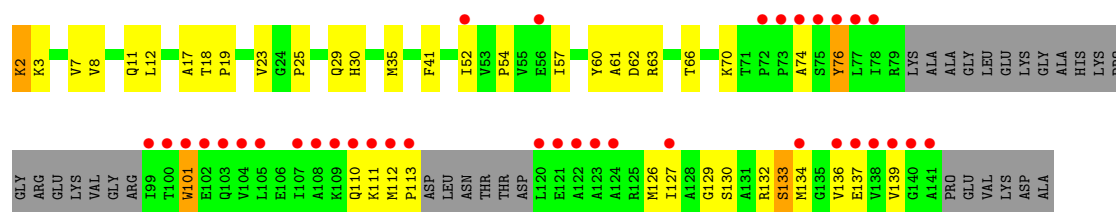
- Molecule 1: Ribosomal protein L11 methyltransferase



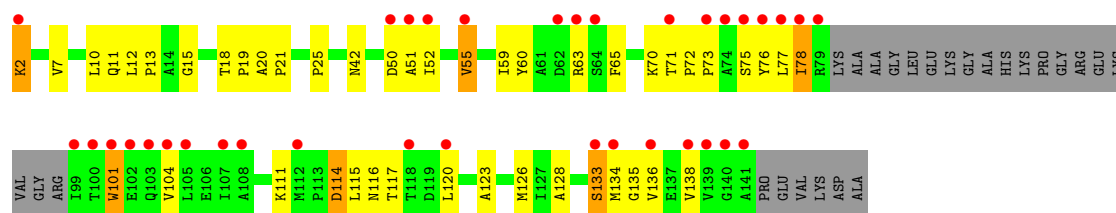
- Molecule 2: 50S ribosomal protein L11



- Molecule 2: 50S ribosomal protein L11



- Molecule 2: 50S ribosomal protein L11



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.53Å 164.98Å 180.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.09 – 2.70 29.09 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.09-2.70) 99.8 (29.09-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.271 0.195 , 0.258	Depositor DCC
R_{free} test set	2207 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8801	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, 2MM, IOD

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	1.47	12/2005 (0.6%)	1.37	12/2732 (0.4%)
1	D	1.48	15/2010 (0.7%)	1.35	20/2739 (0.7%)
1	G	1.41	13/1997 (0.7%)	1.27	12/2721 (0.4%)
2	B	1.14	0/900	1.29	10/1226 (0.8%)
2	E	1.30	4/853 (0.5%)	1.29	6/1159 (0.5%)
2	H	1.38	7/900 (0.8%)	1.39	4/1226 (0.3%)
All	All	1.40	51/8665 (0.6%)	1.33	64/11803 (0.5%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	133	SER	CB-OG	13.33	1.68	1.42
2	E	113	PRO	C-O	10.70	1.45	1.23
1	D	170	ARG	CA-C	8.39	1.64	1.52
1	G	20	LEU	C-O	7.80	1.33	1.24
2	H	72	PRO	CA-C	7.49	1.59	1.52
2	E	133	SER	C-O	7.37	1.33	1.24
1	D	170	ARG	C-O	6.73	1.32	1.23
1	A	56	ASP	CG-OD1	6.59	1.37	1.25
1	D	144	LYS	CA-C	-6.57	1.44	1.52
1	D	169	PRO	N-CA	-6.50	1.39	1.47
1	A	169	PRO	C-N	6.45	1.42	1.33
2	H	114	ASP	CG-OD1	6.45	1.37	1.25
1	D	169	PRO	CA-CB	6.26	1.62	1.53
1	G	136	ILE	CA-CB	-5.92	1.47	1.54
1	A	144	LYS	CE-NZ	5.92	1.67	1.49
1	G	169	PRO	CA-C	-5.82	1.45	1.52
1	D	170	ARG	CA-CB	-5.80	1.43	1.53
1	D	136	ILE	CA-CB	-5.79	1.47	1.54
1	A	111	LEU	C-O	5.77	1.30	1.24
1	G	115	ALA	C-O	-5.75	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	ASP	N-CA	5.73	1.53	1.46
1	A	56	ASP	CG-OD2	5.73	1.36	1.25
1	A	187	LEU	N-CA	-5.71	1.39	1.46
2	H	133	SER	C-O	5.69	1.31	1.24
1	G	177	GLU	CG-CD	5.68	1.66	1.52
1	A	194	ALA	CA-CB	-5.67	1.44	1.53
1	D	158	ALA	CA-CB	-5.65	1.44	1.53
1	G	210	PRO	N-CA	5.63	1.53	1.47
2	E	61	ALA	CA-CB	-5.60	1.43	1.53
1	A	90	PRO	C-O	-5.55	1.17	1.23
1	D	115	ALA	CA-CB	-5.55	1.44	1.53
1	A	252	TYR	C-O	-5.54	1.17	1.23
2	H	2	LYS	CD-CE	5.53	1.69	1.52
1	A	217	THR	C-O	5.50	1.29	1.24
1	G	22	ASP	C-O	5.46	1.30	1.23
1	G	119	ARG	CZ-NH1	5.40	1.40	1.32
2	H	114	ASP	CG-OD2	5.40	1.35	1.25
1	G	177	GLU	CB-CG	5.32	1.68	1.52
1	D	68	LYS	CA-C	5.30	1.59	1.52
1	D	94	GLU	CB-CG	5.29	1.68	1.52
1	D	133	VAL	N-CA	-5.28	1.40	1.46
1	D	177	GLU	CG-CD	5.28	1.65	1.52
1	G	251	ALA	CA-CB	-5.14	1.45	1.53
2	H	133	SER	C-N	5.13	1.40	1.33
1	A	118	LEU	C-O	-5.12	1.17	1.24
1	G	214	ALA	CA-C	-5.11	1.46	1.52
1	G	140	LYS	C-O	-5.04	1.17	1.24
1	G	99	PHE	CA-C	5.04	1.59	1.52
1	D	168	ARG	CG-CD	5.03	1.67	1.52
1	D	207	ALA	CA-CB	-5.02	1.44	1.53
2	E	57	ILE	N-CA	5.02	1.52	1.46

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	LYS	CA-C-N	-17.39	90.39	121.70
2	H	2	LYS	C-N-CA	-17.39	90.39	121.70
1	A	168	ARG	CA-C-N	12.34	132.31	119.85
1	A	168	ARG	C-N-CA	12.34	132.31	119.85
1	D	168	ARG	N-CA-C	10.53	126.65	108.75
2	E	2	LYS	CA-C-N	-9.40	104.79	121.70
2	E	2	LYS	C-N-CA	-9.40	104.79	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	168	ARG	CA-C-N	9.38	129.96	119.92
1	D	168	ARG	C-N-CA	9.38	129.96	119.92
2	B	71	THR	CA-C-N	9.11	129.76	120.38
2	B	71	THR	C-N-CA	9.11	129.76	120.38
1	G	224	ALA	CA-C-N	-9.07	109.57	119.19
1	G	224	ALA	C-N-CA	-9.07	109.57	119.19
1	D	168	ARG	N-CA-CB	-8.59	99.62	110.79
2	H	2	LYS	O-C-N	8.28	136.25	123.00
2	B	112	MET	CA-C-N	-8.27	109.50	119.84
2	B	112	MET	C-N-CA	-8.27	109.50	119.84
1	D	169	PRO	CA-C-O	-8.18	111.72	121.95
1	A	237	ARG	CB-CA-C	7.94	118.84	109.47
1	G	68	LYS	CA-C-N	-7.73	111.82	119.78
1	G	68	LYS	C-N-CA	-7.73	111.82	119.78
1	A	119	ARG	CA-C-N	-7.44	112.31	119.90
1	A	119	ARG	C-N-CA	-7.44	112.31	119.90
1	D	211	GLY	N-CA-C	-6.77	105.84	114.37
1	A	45	LEU	CA-C-N	-6.75	113.94	120.83
1	A	45	LEU	C-N-CA	-6.75	113.94	120.83
1	D	170	ARG	N-CA-C	-6.47	101.38	110.50
1	D	172	LEU	N-CA-C	6.39	118.89	109.24
1	G	146	LEU	CA-C-N	-6.34	116.83	122.73
1	G	146	LEU	C-N-CA	-6.34	116.83	122.73
2	B	2	LYS	CA-C-N	-6.32	110.33	121.70
2	B	2	LYS	C-N-CA	-6.32	110.33	121.70
2	E	137	GLU	N-CA-C	6.19	117.86	110.19
1	D	218	GLY	N-CA-C	-6.13	105.63	115.08
2	E	130	SER	N-CA-C	-6.07	106.20	113.97
2	B	137	GLU	N-CA-C	6.01	119.31	110.59
1	G	155	LEU	CA-C-N	-5.92	112.60	119.47
1	G	155	LEU	C-N-CA	-5.92	112.60	119.47
1	A	129	THR	N-CA-C	5.81	118.39	111.71
1	A	186	ASP	N-CA-C	-5.79	106.38	113.50
1	D	169	PRO	CA-N-CD	5.78	120.10	112.00
1	D	25	ALA	N-CA-C	5.70	118.85	110.30
1	D	170	ARG	NE-CZ-NH1	-5.62	115.88	121.50
2	B	59	ILE	CB-CA-C	-5.58	103.99	110.91
2	E	132	ARG	N-CA-C	-5.56	103.05	111.56
1	A	249	LEU	N-CA-C	-5.51	99.45	108.76
1	D	155	LEU	O-C-N	5.49	124.72	120.38
2	B	51	ALA	N-CA-C	5.47	116.98	110.19
1	D	47	TYR	N-CA-C	5.43	119.89	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	VAL	N-CA-C	-5.37	100.69	108.36
1	D	68	LYS	CB-CA-C	5.36	117.18	109.09
2	B	105	LEU	N-CA-C	-5.32	106.76	113.20
1	D	39	PHE	CA-C-N	-5.32	114.19	119.56
1	D	39	PHE	C-N-CA	-5.32	114.19	119.56
1	G	186	ASP	N-CA-C	-5.28	106.97	113.41
1	D	94	GLU	CA-C-N	-5.23	113.30	119.84
1	D	94	GLU	C-N-CA	-5.23	113.30	119.84
1	A	218	GLY	N-CA-C	-5.21	108.06	115.30
1	A	101	THR	N-CA-C	-5.17	106.82	113.23
1	D	93	ILE	CB-CA-C	-5.17	103.08	110.12
2	H	59	ILE	N-CA-C	5.13	115.36	108.17
1	G	201	ALA	CA-C-N	-5.08	114.38	119.56
1	G	201	ALA	C-N-CA	-5.08	114.38	119.56
1	G	53	GLU	N-CA-C	5.01	117.07	108.90

There are no chirality outliers.

There are no planarity outliers.

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	1949	0	1948	31	1
1	D	1954	0	1957	41	0
1	G	1941	0	1944	46	0
2	B	884	0	906	15	0
2	E	838	0	865	21	0
2	H	884	0	906	31	0
3	A	26	0	19	0	0
3	D	26	0	19	1	0
3	G	26	0	19	0	0
4	B	1	0	0	0	0
4	H	1	0	0	1	0
5	B	10	0	14	3	0
5	E	10	0	14	6	0
5	H	10	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	75	0	0	2	0
6	B	10	0	0	0	0
6	D	88	0	0	3	0
6	E	16	0	0	1	1
6	G	48	0	0	6	0
6	H	4	0	0	0	0
All	All	8801	0	8625	169	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (169) 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:H:133:SER:CB	2:H:133:SER:OG	1.68	1.38
2:H:71:THR:CG2	2:H:114:ASP:HB3	1.73	1.16
2:H:71:THR:HG21	2:H:114:ASP:HB3	1.24	1.15
2:H:78:ILE:HD11	2:H:134:MET:SD	1.87	1.14
2:B:13:PRO:HG2	2:B:16:LYS:HD2	1.55	0.88
1:G:80:PRO:HG3	1:G:164:ARG:HH12	1.40	0.87
1:G:249:LEU:HA	6:G:350:HOH:O	1.74	0.86
2:H:71:THR:HG22	2:H:114:ASP:HB3	1.59	0.85
1:A:168:ARG:HG2	1:D:120:PRO:HB2	1.58	0.82
1:G:203:ARG:HH11	1:G:203:ARG:HG3	1.42	0.82
2:H:2:LYS:CA	5:H:1:2MM:C	2.60	0.79
1:G:7:LYS:HB2	1:G:7:LYS:NZ	1.98	0.78
1:A:146:LEU:HD11	1:A:172:LEU:HD22	1.66	0.78
1:A:164:ARG:HD3	6:A:343:HOH:O	1.88	0.74
1:G:28:LEU:HB2	2:H:11:GLN:HB2	1.71	0.72
2:H:71:THR:HG21	2:H:114:ASP:CB	2.13	0.72
1:G:69:PRO:HB3	1:G:78:LEU:HD23	1.71	0.72
1:G:216:LEU:O	6:G:350:HOH:O	2.07	0.72
1:G:80:PRO:CG	1:G:164:ARG:HH12	2.05	0.70
1:D:221:LYS:HE3	6:D:371:HOH:O	1.91	0.69
2:H:101:TRP:HE3	2:H:101:TRP:H	1.40	0.69
1:G:80:PRO:HG3	1:G:164:ARG:NH1	2.08	0.68
2:E:3:LYS:HE2	5:E:1:2MM:HEA	1.74	0.68
1:G:7:LYS:HB2	1:G:7:LYS:HZ2	1.58	0.67
1:A:28:LEU:HB2	2:B:11:GLN:HB3	1.75	0.66
1:A:148:VAL:HG12	1:A:172:LEU:CD2	2.26	0.66
1:D:94:GLU:HA	1:D:94:GLU:OE1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:LYS:HG2	2:B:16:LYS:O	1.98	0.64
1:G:177:GLU:HB3	6:G:331:HOH:O	1.97	0.64
1:D:170:ARG:HH11	1:D:170:ARG:HG3	1.64	0.63
2:E:2:LYS:CA	5:E:1:2MM:C	2.76	0.63
2:B:2:LYS:CA	5:B:1:2MM:C	2.76	0.62
1:A:58:ASP:OD2	1:A:58:ASP:N	2.31	0.62
1:D:15:PRO:HA	2:E:134:MET:HE2	1.80	0.62
2:E:3:LYS:CE	5:E:1:2MM:HEA	2.29	0.62
2:E:12:LEU:HD13	2:E:17:ALA:HB2	1.81	0.62
2:H:104:VAL:HG11	2:H:128:ALA:HB2	1.81	0.62
1:D:146:LEU:CD1	1:D:170:ARG:HB3	2.32	0.60
1:D:60:LEU:HD11	2:E:35:MET:HE3	1.84	0.59
1:G:61:GLU:HG3	1:G:64:ARG:NH2	2.17	0.59
1:D:170:ARG:HG3	1:D:170:ARG:NH1	2.17	0.59
1:G:103:HIS:HD2	6:G:325:HOH:O	1.85	0.59
2:H:12:LEU:HD12	2:H:55:VAL:HG11	1.85	0.59
1:G:148:VAL:HG12	1:G:172:LEU:HB3	1.85	0.59
1:D:247:TRP:CH2	5:E:1:2MM:HEB	2.38	0.58
1:G:16:ILE:O	1:G:20:LEU:HB2	2.03	0.58
2:B:58:THR:HB	2:B:66:THR:HG22	1.86	0.58
1:D:146:LEU:HD13	1:D:170:ARG:HB3	1.86	0.58
2:E:62:ASP:O	2:E:63:ARG:HB2	2.03	0.58
1:G:203:ARG:HG3	1:G:203:ARG:NH1	2.16	0.56
2:H:123:ALA:HA	2:H:126:MET:HE2	1.87	0.56
1:A:61:GLU:HG3	6:A:363:HOH:O	2.06	0.55
1:D:170:ARG:HH11	1:D:170:ARG:CG	2.18	0.55
1:A:205:ARG:HD2	1:A:234:ALA:O	2.05	0.55
2:B:2:LYS:N	5:B:1:2MM:CA	2.68	0.55
1:D:176:LEU:HD23	1:D:203:ARG:HB3	1.88	0.55
1:D:170:ARG:HD3	1:D:182:PHE:CE2	2.43	0.54
2:E:2:LYS:N	6:E:149:HOH:O	2.40	0.54
1:A:246:GLU:H	1:A:246:GLU:CD	2.16	0.53
2:H:134:MET:H	2:H:135:GLY:HA2	1.74	0.53
1:G:161:ASN:HA	1:G:164:ARG:HD2	1.91	0.53
1:A:144:LYS:HG2	1:D:119:ARG:HD2	1.91	0.53
2:H:18:THR:C	2:H:20:ALA:H	2.17	0.52
1:G:63:TRP:C	1:G:65:ARG:H	2.17	0.52
1:A:3:VAL:HG22	1:A:38:PHE:CE2	2.45	0.52
2:B:42:ASN:O	2:B:46:ALA:N	2.43	0.52
2:H:133:SER:CB	2:H:133:SER:HG	2.12	0.52
2:E:18:THR:HB	2:E:19:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:ALA:HB2	1:G:39:PHE:CZ	2.45	0.52
1:G:13:LEU:HD22	1:G:16:ILE:HD11	1.91	0.51
1:A:14:ASP:HB3	1:A:15:PRO:HD3	1.93	0.51
1:A:148:VAL:HG12	1:A:172:LEU:HD23	1.91	0.51
1:D:31:ARG:O	1:D:32:GLU:C	2.54	0.51
1:D:67:LEU:HD23	2:E:63:ARG:CZ	2.41	0.51
2:H:2:LYS:HE2	2:H:60:TYR:CZ	2.46	0.51
1:G:203:ARG:NE	1:G:206:GLU:OE1	2.36	0.51
1:D:247:TRP:CZ3	5:E:1:2MM:HEB	2.46	0.51
1:G:31:ARG:O	1:G:32:GLU:C	2.54	0.51
1:G:3:VAL:HG22	1:G:5:ARG:HG3	1.92	0.51
2:B:47:ASN:O	2:B:49:GLY:N	2.42	0.50
1:D:106:THR:HG21	1:D:218:GLY:HA2	1.93	0.50
1:A:192:LEU:HD13	1:A:196:LEU:HD23	1.92	0.50
1:G:94:GLU:HG3	1:G:95:PRO:HD2	1.94	0.50
1:G:106:THR:HG21	1:G:218:GLY:HA2	1.94	0.50
1:D:237:ARG:NH2	1:G:168:ARG:HH21	2.10	0.49
2:H:134:MET:H	2:H:135:GLY:CA	2.26	0.49
2:B:18:THR:HB	2:B:19:PRO:HD2	1.94	0.49
1:A:58:ASP:HB2	1:A:60:LEU:H	1.77	0.49
1:A:72:ALA:HB2	1:A:108:ARG:HG2	1.94	0.48
2:H:2:LYS:HA	5:H:1:2MM:C	2.42	0.48
1:G:36:TRP:HE3	1:G:38:PHE:CZ	2.31	0.48
1:D:237:ARG:NH2	1:G:168:ARG:NH2	2.62	0.48
2:B:47:ASN:C	2:B:49:GLY:H	2.21	0.47
1:A:6:LEU:O	1:A:34:GLU:HA	2.14	0.47
1:D:254:ARG:HH11	1:D:254:ARG:HG3	1.79	0.47
2:E:2:LYS:HB3	2:E:60:TYR:CE1	2.49	0.47
1:G:94:GLU:HG3	1:G:95:PRO:CD	2.44	0.47
1:A:148:VAL:HG12	1:A:172:LEU:HD21	1.97	0.47
1:A:63:TRP:CZ3	1:A:64:ARG:HG2	2.50	0.47
1:D:170:ARG:NH1	1:D:170:ARG:CG	2.77	0.47
1:G:7:LYS:NZ	1:G:7:LYS:CB	2.74	0.46
1:G:67:LEU:HD23	2:H:63:ARG:NE	2.30	0.46
1:A:170:ARG:HG3	1:A:170:ARG:HH11	1.80	0.46
1:D:223:ARG:O	1:D:226:LEU:HB2	2.16	0.46
1:D:15:PRO:HA	2:E:134:MET:CE	2.46	0.46
1:D:59:TRP:CZ2	2:E:25:PRO:HB3	2.50	0.46
2:B:71:THR:HA	2:B:72:PRO:HD3	1.71	0.46
2:E:29:GLN:HG3	2:E:30:HIS:ND1	2.31	0.46
2:H:120:LEU:HD23	2:H:120:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:LEU:N	1:D:18:PRO:CD	2.79	0.45
1:D:119:ARG:HD3	6:D:364:HOH:O	2.15	0.45
1:D:222:ASP:OD2	1:D:222:ASP:N	2.49	0.45
1:G:67:LEU:HD23	2:H:63:ARG:HE	1.80	0.45
1:G:219:ILE:HD12	6:G:350:HOH:O	2.16	0.45
2:B:45:THR:C	2:B:47:ASN:N	2.73	0.45
1:D:17:LEU:HA	1:D:20:LEU:HD12	1.98	0.45
1:A:104:HIS:HB2	2:B:62:ASP:HB3	1.98	0.45
1:A:147:GLY:O	1:A:171:PHE:HA	2.16	0.45
1:A:47:TYR:O	1:A:48:GLU:HB2	2.17	0.45
1:G:217:THR:HA	6:G:350:HOH:O	2.16	0.45
1:G:236:PHE:CE2	1:G:254:ARG:HB3	2.52	0.45
1:G:4:TYR:OH	1:G:49:GLY:N	2.51	0.44
1:G:63:TRP:CZ3	1:G:64:ARG:HG3	2.52	0.44
2:H:21:PRO:HA	2:H:25:PRO:HD2	2.00	0.44
1:G:151:ASP:OD1	1:G:151:ASP:C	2.59	0.44
1:A:201:ALA:HB3	1:A:202:PRO:HD3	1.99	0.44
1:D:146:LEU:HD12	1:D:170:ARG:HB3	1.99	0.44
1:G:36:TRP:HB3	1:G:38:PHE:CE1	2.53	0.44
2:H:2:LYS:N	4:H:148:IOD:I	3.21	0.44
1:A:160:ALA:O	1:A:164:ARG:HG3	2.17	0.44
2:H:117:THR:HG21	2:H:123:ALA:HB2	2.00	0.43
1:D:28:LEU:HB2	2:E:11:GLN:HB2	2.00	0.43
2:H:65:PHE:C	2:H:65:PHE:CD1	2.96	0.43
1:A:3:VAL:HG11	1:A:36:TRP:CE3	2.53	0.43
1:G:63:TRP:CH2	1:G:81:TRP:CH2	3.06	0.43
1:D:224:ALA:N	1:D:225:PRO:CD	2.82	0.43
1:D:168:ARG:HA	1:D:169:PRO:HD2	1.88	0.43
1:D:119:ARG:NH1	6:D:364:HOH:O	2.09	0.43
2:H:10:LEU:HB2	2:H:55:VAL:HG13	2.00	0.43
1:D:254:ARG:HG3	1:D:254:ARG:O	2.18	0.42
1:G:39:PHE:CD1	1:G:39:PHE:N	2.87	0.42
1:G:62:ALA:HA	1:G:65:ARG:CZ	2.49	0.42
2:H:134:MET:N	2:H:135:GLY:HA2	2.33	0.42
2:B:72:PRO:HB3	2:B:73:PRO:HD3	2.01	0.42
2:H:111:LYS:O	2:H:115:LEU:HG	2.18	0.42
1:A:176:LEU:HA	1:A:176:LEU:HD12	1.73	0.42
2:E:3:LYS:O	2:E:60:TYR:HA	2.19	0.42
1:G:3:VAL:HG21	1:G:36:TRP:CE3	2.54	0.42
1:A:26:ARG:HH21	1:A:40:PRO:HG3	1.85	0.42
1:A:170:ARG:HG3	1:A:170:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:ARG:O	1:D:33:GLY:N	2.52	0.42
3:D:303:SAH:HB3'	2:E:2:LYS:HD2	2.02	0.42
2:B:17:ALA:HB2	2:B:41:PHE:CD2	2.55	0.42
1:D:237:ARG:HA	1:D:238:PRO:HD3	1.92	0.42
2:E:41:PHE:CD2	2:E:41:PHE:C	2.98	0.41
1:G:21:PHE:CE1	2:H:52:ILE:HG21	2.55	0.41
1:A:193:TYR:HB3	5:B:1:2MM:HB	2.02	0.41
1:G:188:LEU:HD12	1:G:189:VAL:N	2.36	0.41
2:E:18:THR:O	2:E:23:VAL:HB	2.20	0.41
1:D:220:LEU:HG	5:E:1:2MM:HE	2.02	0.41
1:D:243:ALA:HA	1:D:247:TRP:O	2.21	0.41
1:G:63:TRP:HH2	1:G:81:TRP:CH2	2.37	0.41
1:A:224:ALA:N	1:A:225:PRO:CD	2.83	0.41
2:H:15:GLY:HA2	2:H:42:ASN:HA	2.03	0.40
1:D:17:LEU:N	1:D:18:PRO:HD2	2.37	0.40
2:E:52:ILE:HD12	2:E:76:TYR:HB2	2.03	0.40
2:H:13:PRO:HA	2:H:51:ALA:O	2.21	0.40
1:D:187[B]:LEU:HD13	1:D:213:ARG:HB2	2.02	0.40
2:E:54:PRO:HG2	2:E:70:LYS:HB3	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLU:OE1	6:E:149:HOH:O[3_554]	2.16	0.04

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	249/254 (98%)	231 (93%)	16 (6%)	2 (1%)	16 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	249/254 (98%)	237 (95%)	10 (4%)	2 (1%)	16	37
1	G	248/254 (98%)	233 (94%)	12 (5%)	3 (1%)	10	27
2	B	117/146 (80%)	86 (74%)	20 (17%)	11 (9%)	0	0
2	E	109/146 (75%)	84 (77%)	15 (14%)	10 (9%)	0	0
2	H	117/146 (80%)	92 (79%)	18 (15%)	7 (6%)	1	2
All	All	1089/1200 (91%)	963 (88%)	91 (8%)	35 (3%)	3	7

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	GLY
2	B	75	SER
2	B	113	PRO
2	B	118	THR
2	B	120	LEU
2	E	112	MET
2	E	127	ILE
2	E	129	GLY
2	E	133	SER
1	G	10	LEU
1	G	64	ARG
2	H	73	PRO
2	H	75	SER
2	H	77	LEU
2	H	78	ILE
2	H	101	TRP
1	A	32	GLU
2	B	48	MET
2	B	124	ALA
2	B	133	SER
2	B	139	VAL
2	E	74	ALA
2	E	136	VAL
2	E	139	VAL
2	B	77	LEU
1	D	32	GLU
2	E	111	LYS
1	G	32	GLU
2	B	112	MET
2	H	19	PRO

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Mol	Chain	Res	Type
2	H	50	ASP
2	E	101	TRP
2	E	126	MET
2	B	72	PRO
1	D	15	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/189 (100%)	170 (90%)	18 (10%)	8	20
1	D	189/189 (100%)	181 (96%)	8 (4%)	26	55
1	G	187/189 (99%)	170 (91%)	17 (9%)	9	22
2	B	90/109 (83%)	80 (89%)	10 (11%)	6	15
2	E	84/109 (77%)	79 (94%)	5 (6%)	17	41
2	H	90/109 (83%)	83 (92%)	7 (8%)	11	29
All	All	828/894 (93%)	763 (92%)	65 (8%)	11	28

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

Mol	Chain	Res	Type
1	A	43	VAL
1	A	53	GLU
1	A	58	ASP
1	A	63	TRP
1	A	66	ASP
1	A	67	LEU
1	A	71	LEU
1	A	91	LEU
1	A	168	ARG
1	A	172	LEU
1	A	177	GLU
1	A	180	LEU
1	A	188	LEU

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Mol	Chain	Res	Type
1	A	200	LEU
1	A	223	ARG
1	A	237	ARG
1	A	246	GLU
1	A	254	ARG
2	B	7	VAL
2	B	35	MET
2	B	59	ILE
2	B	66	THR
2	B	70	LYS
2	B	75	SER
2	B	102	GLU
2	B	114	ASP
2	B	116	ASN
2	B	130	SER
1	D	7	LYS
1	D	61	GLU
1	D	80	PRO
1	D	91	LEU
1	D	94	GLU
1	D	172	LEU
1	D	237	ARG
1	D	254	ARG
2	E	7	VAL
2	E	66	THR
2	E	76	TYR
2	E	101	TRP
2	E	110	GLN
1	G	3	VAL
1	G	7	LYS
1	G	20	LEU
1	G	60	LEU
1	G	64	ARG
1	G	71	LEU
1	G	91	LEU
1	G	150	ILE
1	G	164	ARG
1	G	177	GLU
1	G	180	LEU
1	G	188	LEU
1	G	200	LEU
1	G	203	ARG

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Mol	Chain	Res	Type
1	G	213	ARG
1	G	221	LYS
1	G	226	LEU
2	H	7	VAL
2	H	55	VAL
2	H	70	LYS
2	H	76	TYR
2	H	116	ASN
2	H	136	VAL
2	H	138	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	11	GLN
2	B	47	ASN
1	D	103	HIS
2	E	11	GLN
2	E	30	HIS
2	E	110	GLN
2	H	30	HIS
2	H	110	GLN
2	H	116	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
5	2MM	H	1	2	7,9,10	0.63	0	5,10,12	1.34	1 (20%)
3	SAH	G	303	-	27,28,28	1.90	10 (37%)	36,40,40	2.46	16 (44%)
3	SAH	D	303	-	27,28,28	0.96	1 (3%)	36,40,40	1.95	11 (30%)
5	2MM	E	1	2	7,9,10	0.62	0	5,10,12	0.40	0
5	2MM	B	1	2	7,9,10	0.61	0	5,10,12	0.97	0
3	SAH	A	303	-	27,28,28	1.30	4 (14%)	36,40,40	2.27	13 (36%)

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
5	2MM	H	1	2	-	3/9/10/12	-
3	SAH	G	303	-	-	2/15/31/31	0/3/3/3
3	SAH	D	303	-	-	3/15/31/31	0/3/3/3
5	2MM	E	1	2	-	2/9/10/12	-
5	2MM	B	1	2	-	2/9/10/12	-
3	SAH	A	303	-	-	2/15/31/31	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	303	SAH	C2-N3	4.02	1.41	1.33
3	G	303	SAH	C2'-C1'	-3.56	1.42	1.53
3	G	303	SAH	C8-N7	3.49	1.38	1.31
3	G	303	SAH	C2-N1	3.27	1.39	1.33
3	A	303	SAH	C8-N7	2.73	1.36	1.31
3	G	303	SAH	OXT-C	-2.44	1.22	1.30
3	A	303	SAH	C5-N7	-2.36	1.34	1.39
3	G	303	SAH	C5'-SD	2.30	1.89	1.81
3	D	303	SAH	C8-N7	2.29	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	303	SAH	C3'-C4'	-2.22	1.47	1.53
3	G	303	SAH	O3'-C3'	2.18	1.48	1.43
3	G	303	SAH	O2'-C2'	2.14	1.48	1.43
3	A	303	SAH	O4'-C4'	-2.13	1.40	1.45
3	G	303	SAH	C4-N3	2.06	1.38	1.34
3	A	303	SAH	C2-N3	2.06	1.37	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	303	SAH	C4-N9-C8	5.86	111.89	105.74
3	G	303	SAH	N9-C8-N7	-5.73	105.81	113.94
3	D	303	SAH	N3-C2-N1	-5.52	120.23	128.58
3	A	303	SAH	N9-C8-N7	-4.50	107.55	113.94
3	A	303	SAH	C5'-SD-CG	-4.45	89.05	102.26
3	A	303	SAH	C5-C4-N3	-4.44	120.60	126.72
3	D	303	SAH	C5-C4-N3	-4.30	120.80	126.72
3	A	303	SAH	N3-C2-N1	-4.08	122.40	128.58
3	A	303	SAH	OXT-C-O	-4.02	114.95	124.08
3	G	303	SAH	N6-C6-N1	3.84	126.92	118.38
3	G	303	SAH	O3'-C3'-C4'	-3.77	100.24	111.08
3	G	303	SAH	C4-N9-C1'	-3.63	118.15	126.63
3	G	303	SAH	C2'-C3'-C4'	3.44	109.25	102.61
3	G	303	SAH	C5-C6-N6	-3.43	114.80	123.29
3	D	303	SAH	C2-N3-C4	3.34	119.99	111.83
3	A	303	SAH	C5-N7-C8	3.31	108.65	103.45
3	G	303	SAH	C5-N7-C8	3.26	108.57	103.45
3	A	303	SAH	C2-N3-C4	3.17	119.57	111.83
3	A	303	SAH	CB-CG-SD	-3.06	106.61	113.45
3	A	303	SAH	O4'-C1'-N9	-3.05	102.24	108.09
3	G	303	SAH	O2'-C2'-C1'	3.02	120.51	110.10
3	G	303	SAH	O2'-C2'-C3'	-3.01	102.18	111.82
3	G	303	SAH	OXT-C-O	-2.83	117.65	124.08
3	A	303	SAH	C4-C5-N7	-2.80	107.38	110.58
3	G	303	SAH	C5'-C4'-C3'	-2.80	108.05	115.06
3	A	303	SAH	C4-N9-C8	2.68	108.55	105.74
3	D	303	SAH	N9-C8-N7	-2.62	110.21	113.94
3	D	303	SAH	N3-C4-N9	2.62	131.62	127.17
5	H	1	2MM	CE-SD-CG	2.60	113.80	100.32
3	A	303	SAH	N3-C4-N9	2.53	131.47	127.17
3	D	303	SAH	C4'-C5'-SD	-2.51	104.82	113.78
3	G	303	SAH	C4'-O4'-C1'	2.51	115.01	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	303	SAH	N3-C2-N1	-2.47	124.84	128.58
3	D	303	SAH	C5-N7-C8	2.46	107.32	103.45
3	G	303	SAH	C5-C4-N9	-2.36	103.24	105.81
3	D	303	SAH	O4'-C1'-C2'	-2.18	101.95	106.62
3	D	303	SAH	OXT-C-O	-2.17	119.15	124.08
3	D	303	SAH	C2'-C3'-C4'	2.11	106.69	102.61
3	G	303	SAH	O4'-C4'-C3'	-2.11	100.96	105.15
3	D	303	SAH	C2-N1-C6	2.09	122.17	118.73
3	A	303	SAH	C6-C5-C4	2.03	119.95	117.18

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	1	2MM	C-CA-CB-CG
5	H	1	2MM	CB-CG-SD-CE
3	D	303	SAH	C2'-C1'-N9-C8
3	A	303	SAH	CB-CG-SD-C5'
5	B	1	2MM	C-CA-CB-CG
5	E	1	2MM	C-CA-CB-CG
3	D	303	SAH	CB-CG-SD-C5'
3	G	303	SAH	CB-CG-SD-C5'
5	B	1	2MM	CB-CG-SD-CE
3	A	303	SAH	C2'-C1'-N9-C8
5	H	1	2MM	CA-CB-CG-SD
3	G	303	SAH	C2'-C1'-N9-C8
3	D	303	SAH	C2'-C1'-N9-C4
5	E	1	2MM	CB-CG-SD-CE

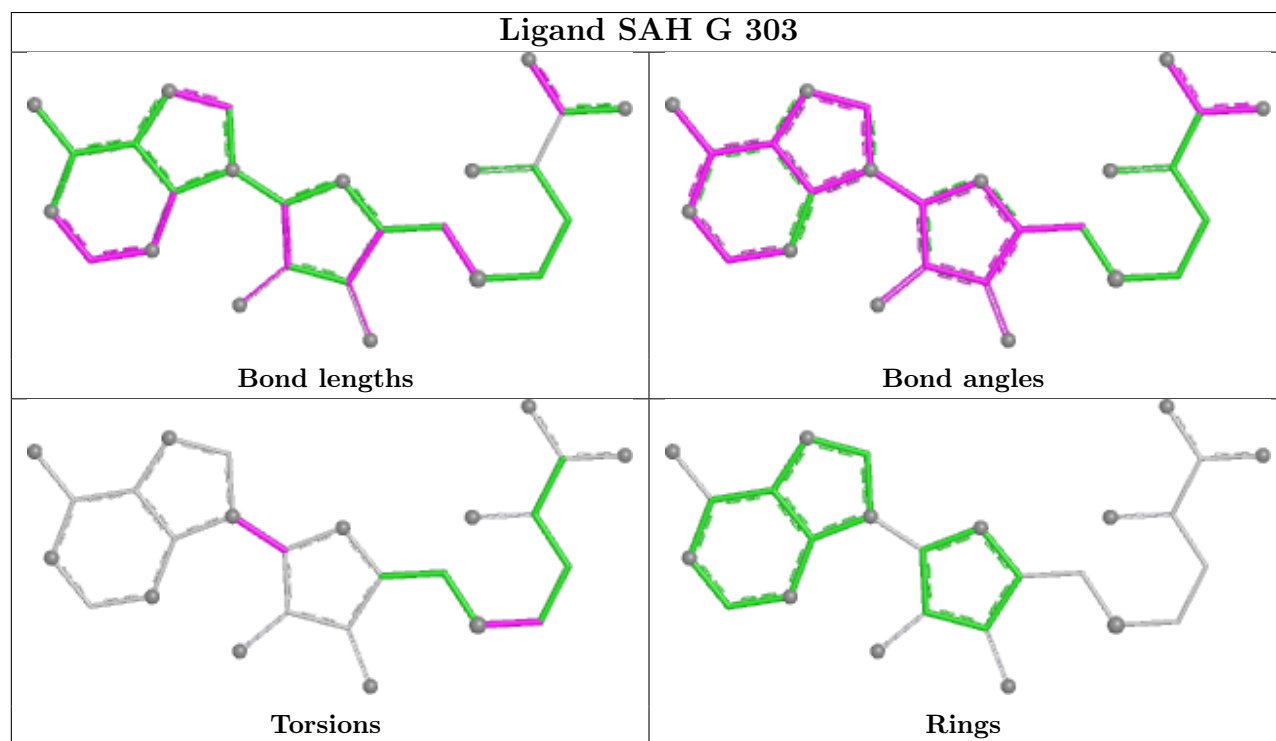
There are no ring outliers.

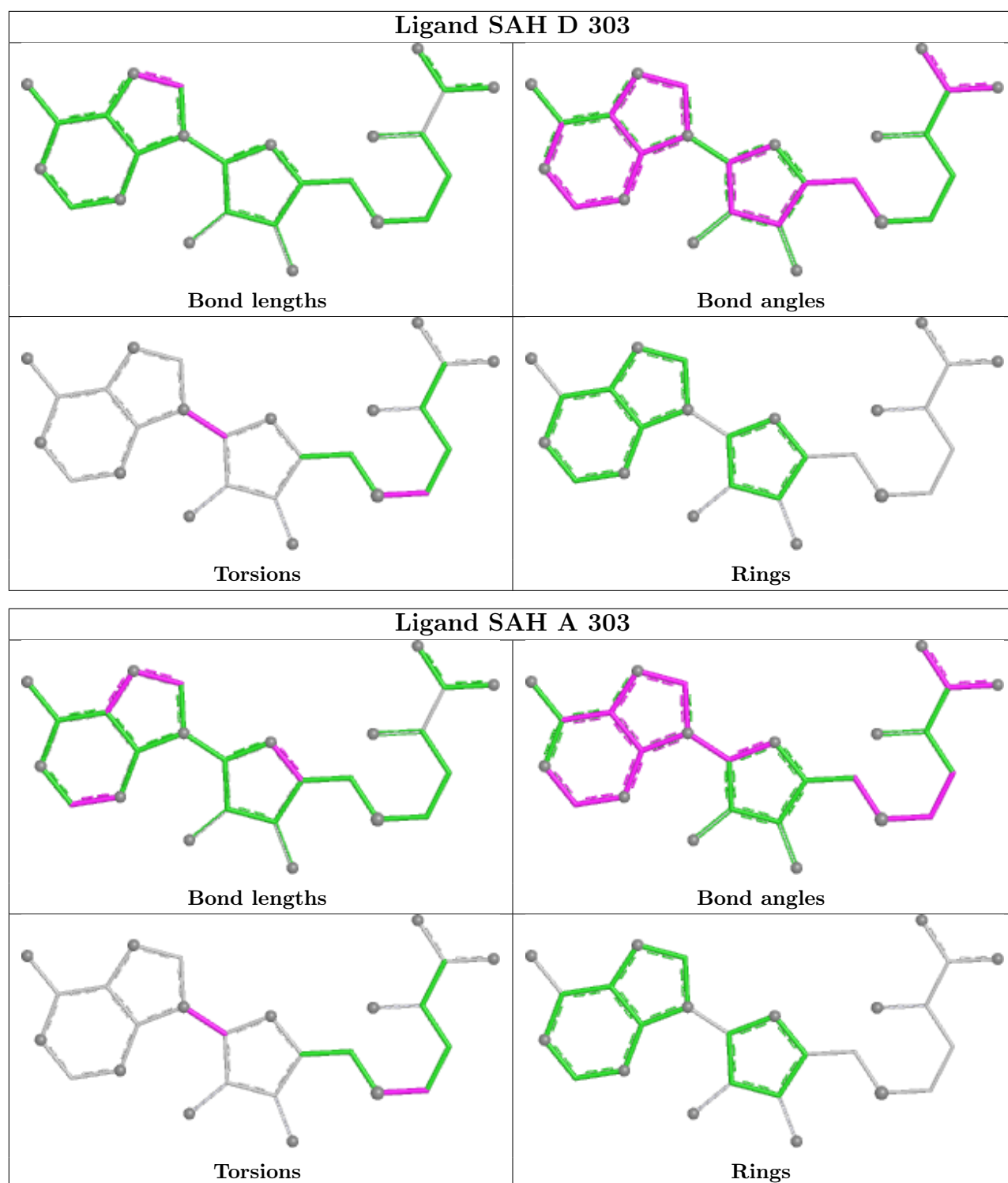
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	2MM	2	0
3	D	303	SAH	1	0
5	E	1	2MM	6	0
5	B	1	2MM	3	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	253/254 (99%)	0.16	4 (1%) 70 68	38, 48, 80, 99	0
1	D	252/254 (99%)	0.18	7 (2%) 55 51	20, 48, 79, 83	1 (0%)
1	G	252/254 (99%)	0.38	11 (4%) 39 35	38, 48, 81, 100	2 (0%)
2	B	121/146 (82%)	1.34	36 (29%) 1 1	34, 62, 80, 96	50 (41%)
2	E	115/146 (78%)	1.64	36 (31%) 1 1	34, 64, 96, 99	37 (32%)
2	H	121/146 (82%)	1.60	35 (28%) 1 1	49, 70, 97, 100	7 (5%)
All	All	1114/1200 (92%)	0.65	129 (11%) 9 8	20, 50, 82, 100	97 (8%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	74	ALA	8.3
2	H	73	PRO	7.3
2	H	77	LEU	7.0
2	H	76	TYR	6.9
2	E	112	MET	6.9
2	H	105	LEU	6.4
2	B	73	PRO	6.3
2	E	113	PRO	6.2
2	H	75	SER	5.7
2	E	78	ILE	5.6
2	E	120	LEU	5.6
2	E	74	ALA	5.5
2	B	72	PRO	5.3
2	H	104	VAL	5.2
2	E	100	THR	5.0
2	B	113	PRO	5.0
2	H	78	ILE	4.9
2	E	99	ILE	4.8
1	A	59	TRP	4.7

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Mol	Chain	Res	Type	RSRZ
2	E	108	ALA	4.6
2	B	104	VAL	4.5
2	B	101	TRP	4.5
2	B	71	THR	4.5
2	E	77	LEU	4.5
2	H	101	TRP	4.5
2	B	76	TYR	4.4
2	E	109	LYS	4.4
2	B	105	LEU	4.4
2	H	52	ILE	4.3
2	H	79	ARG	4.3
2	E	110	GLN	4.2
2	B	115	LEU	4.2
2	E	136	VAL	4.1
2	E	73	PRO	4.0
2	B	125	ARG	4.0
1	G	63	TRP	3.9
2	E	122	ALA	3.9
1	A	63	TRP	3.9
2	E	139	VAL	3.8
2	E	103	GLN	3.8
1	D	54	VAL	3.8
2	E	127	ILE	3.8
2	E	141	ALA	3.8
2	H	141	ALA	3.8
2	E	123	ALA	3.7
2	E	76	TYR	3.7
2	B	79	ARG	3.6
2	B	133	SER	3.6
2	H	102	GLU	3.6
2	E	56	GLU	3.6
1	G	59	TRP	3.5
1	D	63	TRP	3.5
1	G	54	VAL	3.5
2	B	77	LEU	3.4
2	E	134	MET	3.4
2	E	75	SER	3.3
2	E	124	ALA	3.3
2	H	99	ILE	3.3
2	H	103	GLN	3.3
2	H	107	ILE	3.3
2	E	140	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	101	TRP	3.2
2	B	120	LEU	3.2
2	E	111	LYS	3.1
1	G	23	GLY	3.1
1	A	56	ASP	3.1
2	H	138	VAL	3.0
2	B	99	ILE	3.0
2	B	74	ALA	3.0
2	H	140	GLY	2.9
2	B	141	ALA	2.9
1	G	60	LEU	2.9
2	H	2	LYS	2.9
2	E	72	PRO	2.9
2	B	106	GLU	2.8
2	E	121	GLU	2.8
2	H	64	SER	2.8
1	A	66	ASP	2.8
2	H	120	LEU	2.7
2	H	51	ALA	2.7
2	B	116	ASN	2.7
2	B	134	MET	2.6
2	E	102	GLU	2.6
2	H	62	ASP	2.6
2	E	52	ILE	2.6
2	B	30	HIS	2.5
2	B	2	LYS	2.4
2	H	133	SER	2.4
2	B	103	GLN	2.4
2	E	104	VAL	2.4
2	B	121	GLU	2.4
2	H	134	MET	2.4
2	B	78	ILE	2.4
2	H	136	VAL	2.4
1	G	58	ASP	2.4
2	H	139	VAL	2.4
2	B	107	ILE	2.3
2	B	100	THR	2.3
2	E	137	GLU	2.3
1	D	15	PRO	2.3
1	D	64	ARG	2.3
2	H	118	THR	2.3
2	B	137	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	122	ALA	2.3
1	D	58	ASP	2.3
2	B	110	GLN	2.3
2	E	105	LEU	2.3
1	G	16	ILE	2.3
2	B	139	VAL	2.3
1	G	61	GLU	2.2
2	B	138	VAL	2.2
2	E	138	VAL	2.2
2	H	108	ALA	2.2
2	B	136	VAL	2.2
2	H	100	THR	2.2
2	B	140	GLY	2.2
2	B	123	ALA	2.1
2	H	63	ARG	2.1
2	B	109	LYS	2.1
1	G	64	ARG	2.1
1	D	16	ILE	2.1
1	G	24	GLY	2.1
2	H	112	MET	2.1
2	H	71	THR	2.0
2	H	50	ASP	2.0
1	D	59	TRP	2.0
1	G	20	LEU	2.0
2	E	107	ILE	2.0
2	H	55	VAL	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](#)

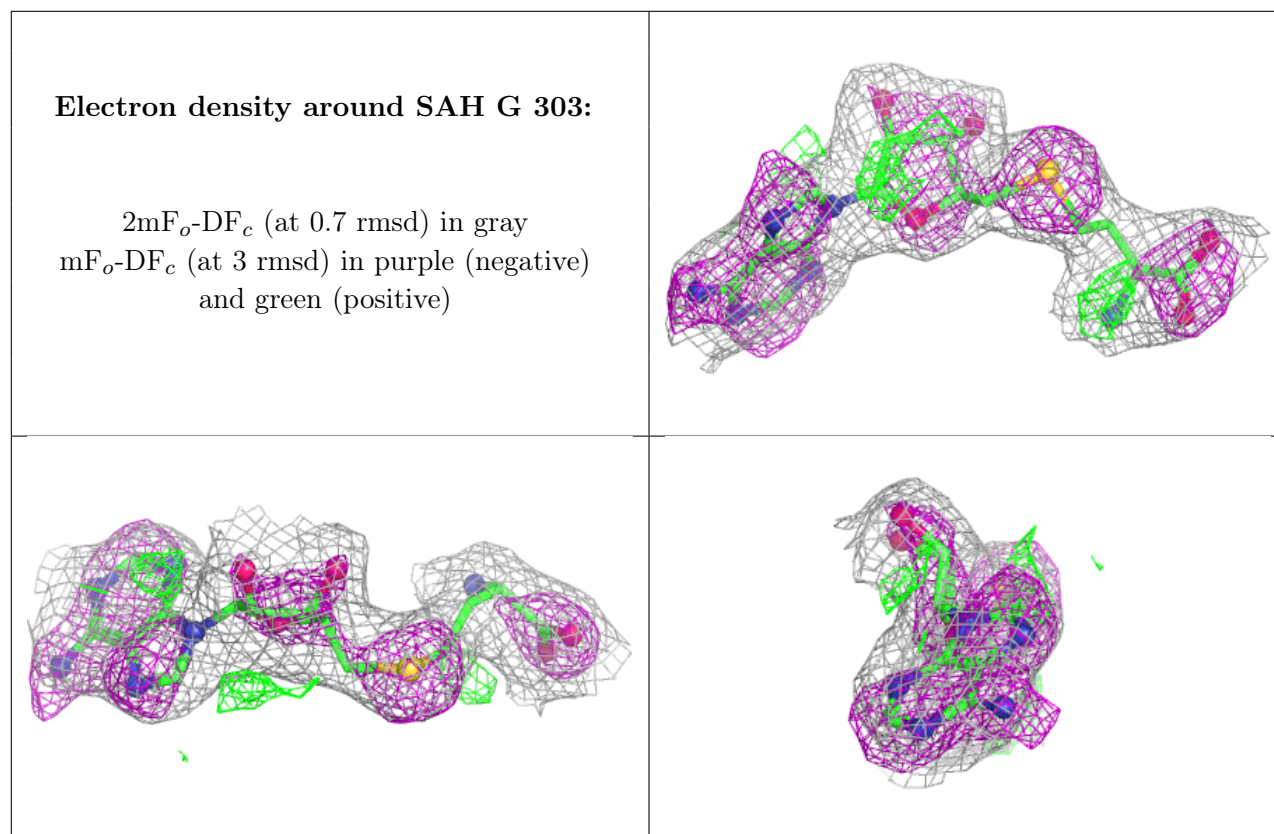
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

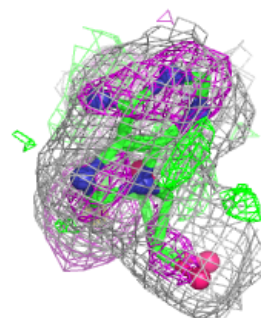
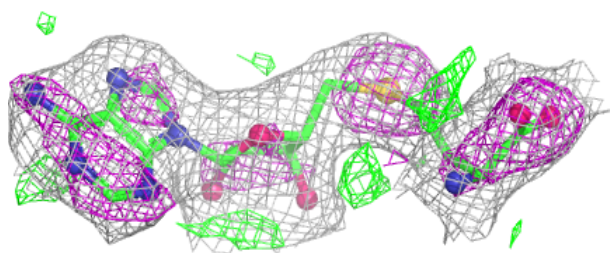
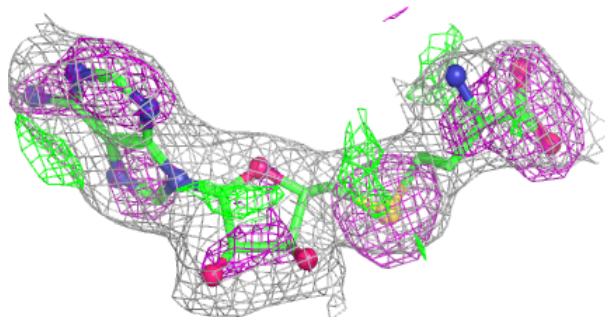
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	2MM	B	1	10/11	0.91	0.18	49,53,66,67	0
3	SAH	G	303	26/26	0.92	0.12	35,39,43,46	0
3	SAH	D	303	26/26	0.92	0.12	32,41,44,47	0
5	2MM	E	1	10/11	0.92	0.18	45,50,57,64	0
3	SAH	A	303	26/26	0.93	0.13	33,42,48,51	0
5	2MM	H	1	10/11	0.93	0.20	51,52,62,64	0
4	IOD	H	148	1/1	0.98	0.13	81,81,81,81	1
4	IOD	B	148	1/1	0.99	0.15	59,59,59,59	1

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.

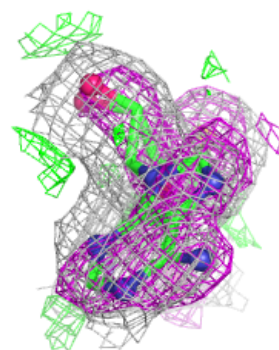
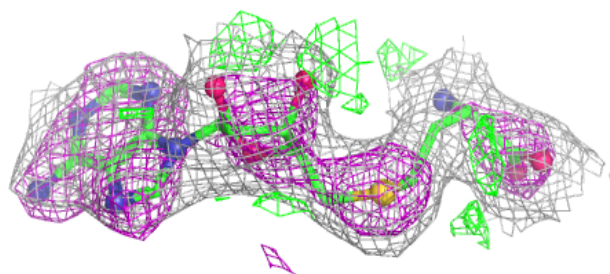
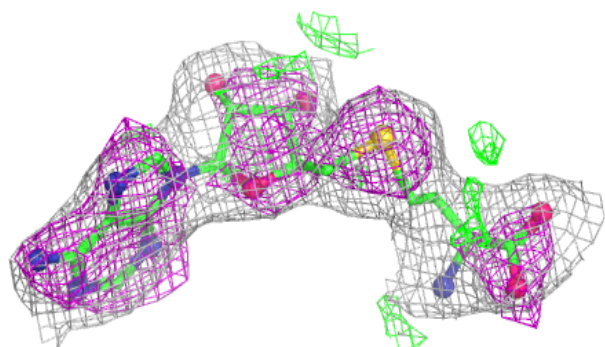


Electron density around SAH D 303:

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

**Electron density around SAH A 303:**

$2mF_o-DF_c$ (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.