



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:49 AM UTC

PDB ID : 4BP3 / pdb_00004bp3
Title : Crystal Structure of Plasmodium Falciparum Spermidine Synthase in Complex with DECARBOXYLATED S-ADENOSYLMETHIONINE5' AND 4-METHYLANILINE
Authors : Sprenger, J.; Halander, J.C.; Svensson, B.; Al-Karadaghi, S.; Persson, L.
Deposited on : 2013-05-23
Resolution : 1.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

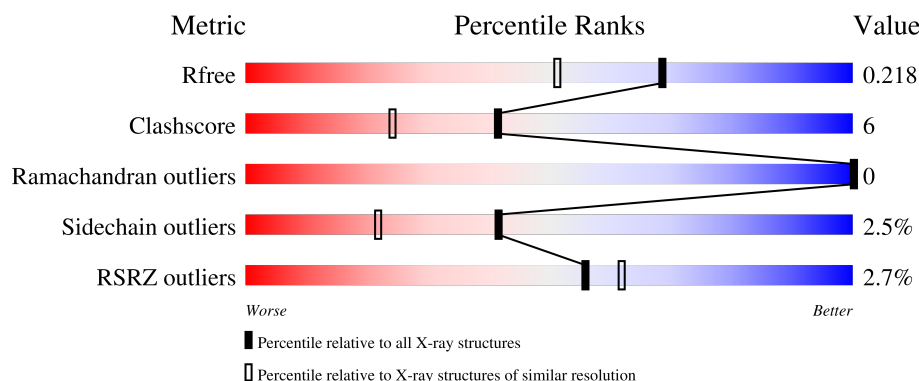
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	283	4% 81% 18% ..
1	B	283	4% 82% 14% ..
1	C	283	% 81% 17% ..

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	1PG	C	602	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7288 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.

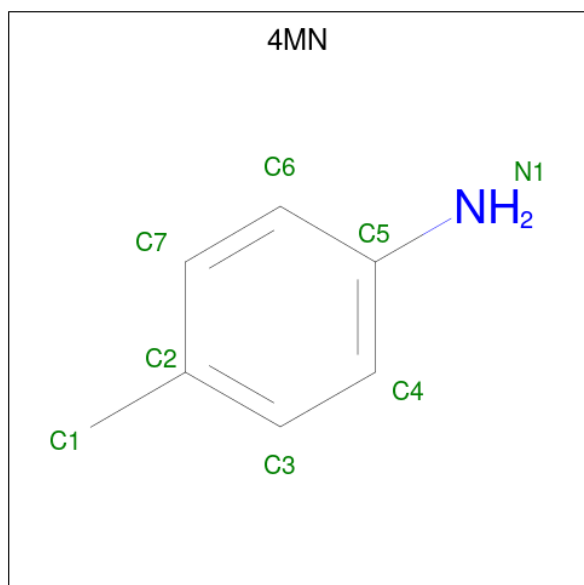
- Molecule 1 is a protein called SPERMIDINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	2	0
			2251	1462	351	423	15			
1	B	280	Total	C	N	O	S	0	3	0
			2253	1464	350	425	14			
1	C	281	Total	C	N	O	S	0	1	0
			2257	1465	352	426	14			

There are 3 discrepancies between the modelled and reference sequences:

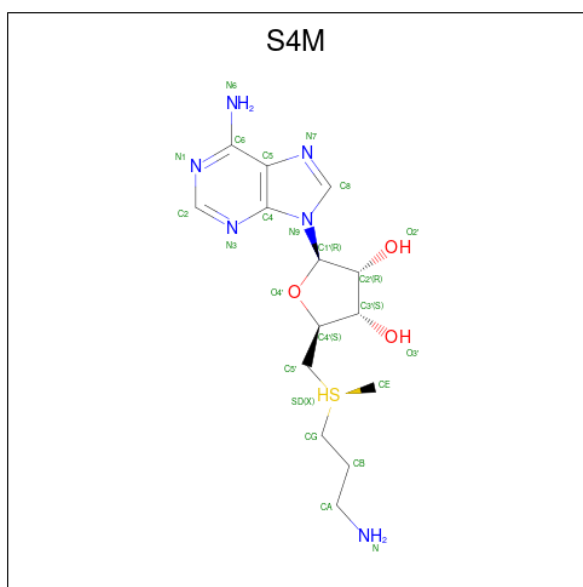
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLY	-	expression tag	UNP Q8II73
B	39	GLY	-	expression tag	UNP Q8II73
C	39	GLY	-	expression tag	UNP Q8II73

- Molecule 2 is 4-METHYLANILINE (CCD ID: 4MN) (formula: C₇H₉N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			8	7	1		
2	B	1	Total	C	N	0	0
			8	7	1		
2	C	1	Total	C	N	0	0
			8	7	1		

- Molecule 3 is 5'-[(S)-(3-AMINOPROPYL)(METHYL)-LAMBDA 4 -SULFANYL]-5'-DEOXYADENOSINE (CCD ID: S4M) (formula: $C_{14}H_{24}N_6O_3S$).



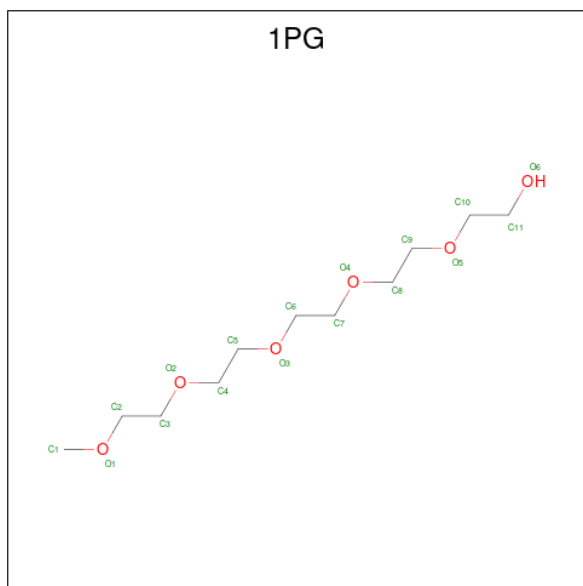
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
3	B	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
3	C	1	Total	C	N	O	S	0	0
			24	14	6	3	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (CCD ID: 1PG) (formula: $C_{11}H_{24}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			17	11	6		
5	C	1	Total	C	O	0	0
			17	11	6		

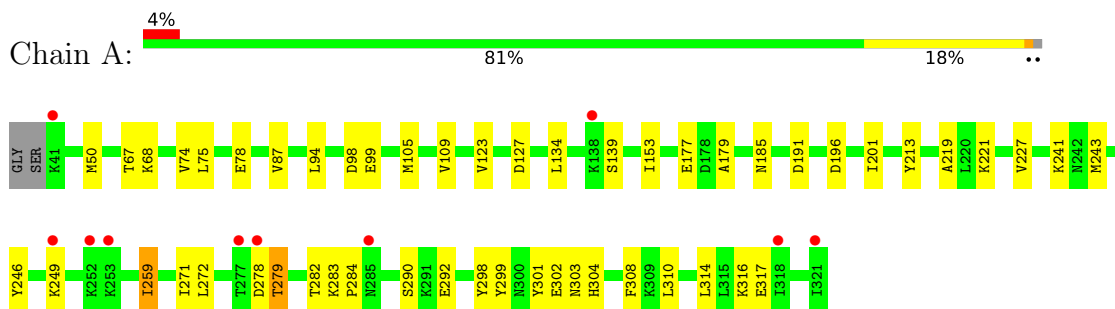
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	84	Total 84	O 84	0	0
6	B	147	Total 147	O 147	0	0
6	C	160	Total 160	O 160	0	0

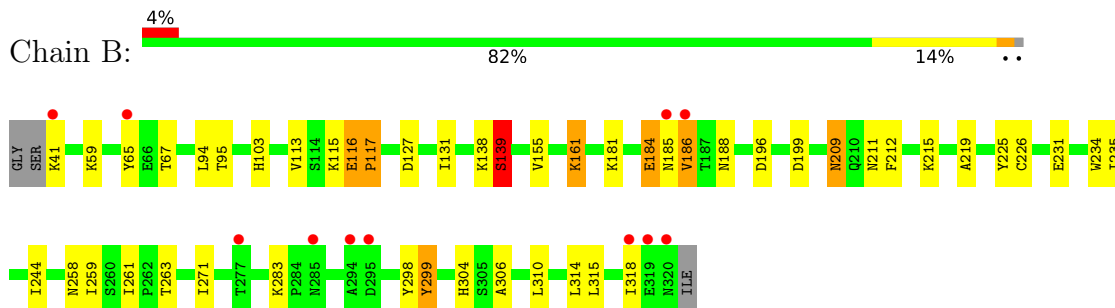
3 Residue-property plots [i](#)

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.

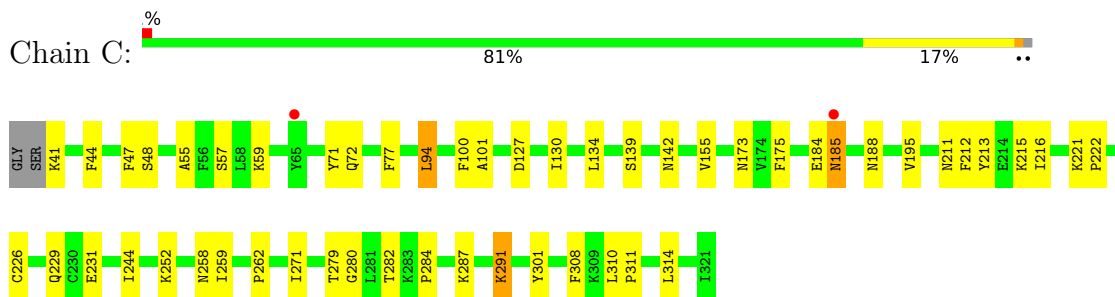
• Molecule 1: SPERMIDINE SYNTHASE



• Molecule 1: SPERMIDINE SYNTHASE



• Molecule 1: SPERMIDINE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.46Å 132.79Å 49.16Å 90.00° 94.86° 90.00°	Depositor
Resolution (Å)	28.66 – 1.75 28.66 – 1.75	Depositor EDS
% Data completeness (in resolution range)	94.1 (28.66-1.75) 94.1 (28.66-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.180 , 0.212 0.187 , 0.218	Depositor DCC
R_{free} test set	6260 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7288	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: GOL, 4MN, S4M, 1PG

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	1.43	9/2306 (0.4%)	1.33	9/3115 (0.3%)
1	B	1.55	15/2312 (0.6%)	1.32	8/3124 (0.3%)
1	C	1.63	13/2310 (0.6%)	1.33	10/3119 (0.3%)
All	All	1.54	37/6928 (0.5%)	1.33	27/9358 (0.3%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	TYR	N-CA	-8.96	1.35	1.46
1	A	283	LYS	C-O	-8.87	1.16	1.25
1	B	116	GLU	C-O	-8.70	1.19	1.23
1	B	235	ILE	C-O	-8.45	1.14	1.24
1	C	175	PHE	CA-C	-8.10	1.43	1.52
1	C	134	LEU	C-O	-7.66	1.15	1.24
1	B	139	SER	CA-CB	7.06	1.65	1.53
1	B	139	SER	CB-OG	7.03	1.56	1.42
1	B	225	TYR	CA-C	-6.82	1.44	1.52
1	B	298	TYR	CA-C	-6.33	1.44	1.52
1	B	131	ILE	N-CA	6.28	1.53	1.46
1	B	244	ILE	N-CA	-6.23	1.39	1.46
1	C	130	ILE	C-O	-6.08	1.17	1.24
1	C	77	PHE	N-CA	-5.99	1.38	1.45
1	A	99	GLU	C-O	-5.77	1.16	1.24
1	C	101	ALA	C-O	-5.74	1.17	1.24
1	A	74	VAL	N-CA	-5.71	1.39	1.46
1	B	184	GLU	CA-C	5.63	1.60	1.52
1	A	227	VAL	CA-CB	-5.61	1.47	1.54
1	C	100	PHE	N-CA	-5.60	1.39	1.46
1	A	219	ALA	CA-C	-5.58	1.44	1.52
1	C	195	VAL	N-CA	-5.54	1.39	1.46
1	C	244	ILE	CA-CB	-5.53	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	GLU	N-CA	5.42	1.53	1.46
1	B	235	ILE	CA-CB	-5.40	1.47	1.54
1	C	55	ALA	CA-C	-5.33	1.45	1.52
1	C	94	LEU	C-O	-5.30	1.17	1.23
1	B	103	HIS	CA-CB	-5.29	1.44	1.53
1	C	101	ALA	N-CA	5.25	1.52	1.46
1	B	161	LYS	CA-C	-5.19	1.45	1.52
1	A	98	ASP	CA-C	-5.18	1.45	1.52
1	C	287	LYS	CA-C	-5.17	1.46	1.52
1	B	226	CYS	CA-C	-5.14	1.46	1.52
1	C	226	CYS	CA-CB	-5.05	1.44	1.53
1	B	117	PRO	C-O	5.04	1.29	1.23
1	A	259	ILE	C-O	-5.04	1.19	1.24
1	A	272	LEU	CA-CB	-5.02	1.45	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	279	THR	N-CA-C	11.28	126.87	112.89
1	B	138	LYS	CA-C-N	8.73	132.84	120.28
1	B	138	LYS	C-N-CA	8.73	132.84	120.28
1	A	109	VAL	CA-C-N	-7.46	111.29	119.19
1	A	109	VAL	C-N-CA	-7.46	111.29	119.19
1	A	279	THR	N-CA-C	7.25	120.23	111.82
1	C	185	ASN	N-CA-C	6.55	120.59	112.47
1	C	139	SER	N-CA-C	6.50	120.47	112.54
1	C	184	GLU	CA-C-N	-6.20	112.94	122.61
1	C	184	GLU	C-N-CA	-6.20	112.94	122.61
1	A	153	ILE	N-CA-C	6.13	116.31	110.42
1	B	261	ILE	CA-C-N	-6.08	113.42	119.56
1	B	261	ILE	C-N-CA	-6.08	113.42	119.56
1	A	134	LEU	N-CA-C	6.05	118.66	111.33
1	A	213	TYR	CA-CB-CG	-5.91	103.25	113.90
1	C	185	ASN	CB-CA-C	-5.73	102.36	111.48
1	A	303	ASN	CB-CA-C	5.73	121.97	109.99
1	B	113	VAL	N-CA-C	-5.68	106.27	111.67
1	B	139	SER	CA-CB-OG	5.67	122.44	111.10
1	A	185	ASN	N-CA-C	5.51	120.89	113.72
1	C	48	SER	N-CA-C	5.49	117.43	108.76
1	C	130	ILE	N-CA-C	-5.33	105.34	110.72
1	B	188	ASN	N-CA-CB	-5.25	104.01	111.84
1	C	213	TYR	CA-CB-CG	-5.21	104.53	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	280	GLY	N-CA-C	5.16	123.28	112.45
1	A	177	GLU	N-CA-CB	-5.13	103.77	111.56
1	B	196	ASP	N-CA-C	-5.05	101.94	109.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2251	0	2260	25	0
1	B	2253	0	2266	27	0
1	C	2257	0	2270	27	0
2	A	8	0	9	0	0
2	B	8	0	9	0	0
2	C	8	0	9	0	0
3	A	24	0	24	2	0
3	B	24	0	24	1	0
3	C	24	0	24	1	0
4	B	6	0	7	0	0
5	C	34	0	48	23	0
6	A	84	0	0	0	0
6	B	147	0	0	4	0
6	C	160	0	0	5	0
All	All	7288	0	6950	88	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 6.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ASN:HD22	5:C:602:1PG:H12	1.26	0.97
5:C:602:1PG:H92	6:C:2140:HOH:O	1.73	0.86
1:B:258:ASN:HD22	5:C:602:1PG:H81	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:602:1PG:H101	5:C:602:1PG:O3	1.79	0.82
1:C:258:ASN:HD22	5:C:602:1PG:C1	1.95	0.80
1:C:311:PRO:HD3	5:C:602:1PG:H21	1.63	0.80
1:B:258:ASN:HD22	5:C:602:1PG:C8	1.97	0.78
6:B:2137:HOH:O	5:C:602:1PG:H52	1.84	0.76
1:A:105[B]:MET:HE3	1:A:298:TYR:CD1	2.22	0.74
1:B:306:ALA:O	5:C:602:1PG:H102	1.88	0.73
1:A:241:LYS:HE3	1:A:317:GLU:O	1.94	0.67
1:A:105[B]:MET:HE3	1:A:298:TYR:HD1	1.59	0.66
1:C:188:ASN:HD21	1:C:222:PRO:HD3	1.60	0.65
5:C:602:1PG:H13	5:C:602:1PG:H62	1.81	0.63
1:A:127:ASP:OD2	3:A:501:S4M:HE2	1.99	0.62
1:B:181:LYS:O	1:B:184:GLU:HG2	2.00	0.61
1:C:188:ASN:ND2	1:C:222:PRO:HD3	2.14	0.60
1:C:258:ASN:ND2	5:C:602:1PG:H12	2.08	0.58
1:C:212:PHE:CE2	1:C:216:ILE:HD11	2.40	0.57
1:A:105[B]:MET:CE	1:A:299:TYR:HA	2.35	0.57
1:C:229:GLN:HE21	1:C:231:GLU:H	1.52	0.56
1:B:310:LEU:HD13	1:B:314:LEU:HD23	1.87	0.56
1:A:243:MET:CE	1:A:246:TYR:CE2	2.88	0.56
1:B:94:LEU:HD12	1:B:94:LEU:C	2.31	0.56
1:C:94:LEU:C	1:C:94:LEU:HD12	2.31	0.56
1:A:243:MET:HE1	1:A:246:TYR:HE2	1.71	0.55
1:A:259:ILE:HD11	1:A:271:ILE:HD11	1.88	0.55
1:A:105[B]:MET:HE3	1:A:298:TYR:CE1	2.43	0.54
5:C:602:1PG:C9	6:C:2140:HOH:O	2.44	0.54
1:A:243:MET:HE1	1:A:246:TYR:CE2	2.43	0.53
1:B:209:ASN:ND2	1:B:212:PHE:H	2.06	0.53
1:A:290:SER:HB2	1:A:292:GLU:OE1	2.09	0.53
1:B:258:ASN:ND2	5:C:602:1PG:H81	2.17	0.53
5:C:602:1PG:H41	5:C:602:1PG:O6	2.08	0.52
1:B:315:LEU:HD21	6:B:2139:HOH:O	2.10	0.52
5:C:602:1PG:H13	5:C:602:1PG:C6	2.39	0.52
1:B:65:TYR:OH	1:B:67:THR:HG21	2.10	0.52
1:B:41:LYS:CD	1:B:59:LYS:HE2	2.40	0.51
1:C:142:ASN:HD21	1:C:173:ASN:HD22	1.58	0.51
1:B:127:ASP:OD2	3:B:501:S4M:HE2	2.11	0.51
1:C:291:LYS:HD3	6:C:2137:HOH:O	2.11	0.51
1:A:191:ASP:OD1	1:A:221:LYS:HD2	2.11	0.50
1:C:284:PRO:HG2	1:C:301:TYR:CE1	2.47	0.50
1:B:258:ASN:HB3	5:C:602:1PG:H81	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:LYS:CD	6:C:2137:HOH:O	2.61	0.49
1:A:243:MET:HE2	1:A:246:TYR:CE2	2.48	0.49
5:C:602:1PG:H62	5:C:602:1PG:O2	2.13	0.49
1:B:116:GLU:N	1:B:117:PRO:CD	2.77	0.48
1:C:211:ASN:HD21	1:C:215:LYS:NZ	2.12	0.48
1:C:127:ASP:OD1	3:C:503:S4M:HE2	2.14	0.48
6:B:2137:HOH:O	5:C:602:1PG:C5	2.53	0.47
5:C:602:1PG:C8	6:C:2140:HOH:O	2.62	0.47
1:C:47:PHE:HZ	5:C:702:1PG:H72	1.78	0.47
1:B:41:LYS:HD2	1:B:59:LYS:HE2	1.97	0.47
1:B:139:SER:HB3	6:B:2058:HOH:O	2.15	0.47
1:A:68:LYS:O	1:B:161:LYS:NZ	2.49	0.46
1:C:229:GLN:NE2	1:C:231:GLU:H	2.13	0.46
1:A:310:LEU:HD13	1:A:314:LEU:HD23	1.96	0.46
1:C:188:ASN:HD22	1:C:221:LYS:HA	1.80	0.46
1:A:282:THR:HG22	1:A:308:PHE:CG	2.51	0.46
1:A:94:LEU:C	1:A:94:LEU:HD12	2.40	0.45
1:A:304:HIS:CD2	1:A:304:HIS:C	2.94	0.45
1:A:123:VAL:HG13	1:A:179:ALA:CB	2.47	0.44
1:C:310:LEU:HD13	1:C:314:LEU:HD23	2.00	0.44
1:C:258:ASN:HB3	5:C:602:1PG:H31	1.98	0.44
1:B:258:ASN:HD22	5:C:602:1PG:H82	1.79	0.44
1:C:259:ILE:HD11	1:C:271:ILE:HD11	2.00	0.44
1:A:50:MET:HG3	1:A:201:ILE:HD12	1.99	0.44
1:C:284:PRO:HG2	1:C:301:TYR:CD1	2.53	0.43
1:B:304:HIS:CD2	1:B:304:HIS:C	2.96	0.43
1:B:186:VAL:HG22	1:B:219:ALA:CB	2.49	0.43
1:B:199:ASP:OD1	1:B:231:GLU:OE2	2.37	0.43
1:B:234:TRP:CE2	1:C:262:PRO:HD3	2.53	0.43
1:A:284:PRO:HG2	1:A:301:TYR:CE2	2.54	0.42
1:A:105[B]:MET:HE1	1:A:299:TYR:HA	2.00	0.42
1:B:211:ASN:HD21	1:B:215:LYS:NZ	2.17	0.42
1:A:196:ASP:OD1	3:A:501:S4M:HG2	2.19	0.42
1:B:299:TYR:CD1	1:B:299:TYR:C	2.98	0.41
1:C:44:PHE:O	1:C:57:SER:HA	2.21	0.41
1:C:282:THR:HG22	1:C:308:PHE:CG	2.56	0.41
5:C:602:1PG:C1	5:C:602:1PG:H61	2.51	0.41
1:C:41:LYS:HB2	1:C:59:LYS:HE2	2.01	0.41
1:A:75:LEU:HB3	1:A:87:VAL:HB	2.02	0.41
1:A:105[B]:MET:CE	1:A:298:TYR:HD1	2.28	0.41
1:B:209:ASN:HD22	1:B:212:PHE:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:TYR:C	1:C:72:GLN:HG3	2.46	0.40
1:B:95:THR:HG21	1:B:263:THR:HG21	2.03	0.40
1:B:259:ILE:HD11	1:B:271:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/283 (99%)	272 (97%)	9 (3%)	0	100	100
1	B	281/283 (99%)	272 (97%)	9 (3%)	0	100	100
1	C	280/283 (99%)	271 (97%)	9 (3%)	0	100	100
All	All	842/849 (99%)	815 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	252/254 (99%)	245 (97%)	7 (3%)	38	18
1	B	254/254 (100%)	246 (97%)	8 (3%)	35	15
1	C	254/254 (100%)	250 (98%)	4 (2%)	55	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	760/762 (100%)	741 (98%)	19 (2%)	42	22

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	78	GLU
1	A	139	SER
1	A	249	LYS
1	A	278	ASP
1	A	279	THR
1	A	316	LYS
1	B	115	LYS
1	B	139	SER
1	B	155	VAL
1	B	185	ASN
1	B	186	VAL
1	B	209	ASN
1	B	283	LYS
1	B	318	ILE
1	C	155	VAL
1	C	185	ASN
1	C	252	LYS
1	C	291	LYS

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

Mol	Chain	Res	Type
1	A	73	ASN
1	A	218	ASN
1	A	320	ASN
1	B	54	GLN
1	B	93	GLN
1	B	142	ASN
1	B	162	ASN
1	B	188	ASN
1	B	209	ASN
1	B	210	GLN
1	B	211	ASN
1	B	258	ASN
1	B	285	ASN

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Mol	Chain	Res	Type
1	C	54	GLN
1	C	93	GLN
1	C	173	ASN
1	C	188	ASN
1	C	211	ASN
1	C	229	GLN
1	C	258	ASN
1	C	320	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](#)

9 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	$\# Z > 2$
5	1PG	C	602	-	16,16,16	1.12	0	15,15,15	1.65	4 (26%)
5	1PG	C	702	-	16,16,16	0.51	0	15,15,15	0.86	0
3	S4M	C	503	-	25,26,26	1.05	2 (8%)	33,37,37	2.37	12 (36%)
3	S4M	B	501	-	25,26,26	1.39	2 (8%)	33,37,37	2.07	11 (33%)
2	4MN	B	401	-	8,8,8	0.92	1 (12%)	10,10,10	1.24	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	601	-	5,5,5	1.34	1 (20%)	5,5,5	0.97	0
2	4MN	A	401	-	8,8,8	1.09	1 (12%)	10,10,10	0.90	0
3	S4M	A	501	-	25,26,26	1.17	1 (4%)	33,37,37	2.04	12 (36%)
2	4MN	C	401	-	8,8,8	0.99	0	10,10,10	2.15	5 (50%)

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	1PG	C	602	-	-	7/14/14/14	-
5	1PG	C	702	-	-	10/14/14/14	-
3	S4M	C	503	-	-	4/12/28/28	0/3/3/3
3	S4M	B	501	-	-	5/12/28/28	0/3/3/3
2	4MN	B	401	-	-	-	0/1/1/1
4	GOL	B	601	-	-	4/4/4/4	-
2	4MN	A	401	-	-	-	0/1/1/1
3	S4M	A	501	-	-	5/12/28/28	0/3/3/3
2	4MN	C	401	-	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	S4M	C4-N9	-5.58	1.26	1.37
3	C	503	S4M	C8-N7	3.23	1.37	1.31
4	B	601	GOL	O2-C2	-2.98	1.34	1.43
3	A	501	S4M	C5-C4	-2.84	1.34	1.39
3	C	503	S4M	C4-N9	-2.47	1.32	1.37
2	B	401	4MN	C6-C5	-2.22	1.35	1.40
2	A	401	4MN	C3-C4	2.05	1.42	1.38
3	B	501	S4M	C8-N7	2.04	1.35	1.31

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	S4M	N1-C2-N3	-6.62	118.56	128.58
3	C	503	S4M	C5-C4-N3	-6.45	117.84	126.72
3	B	501	S4M	N1-C2-N3	-5.44	120.35	128.58
3	C	503	S4M	N1-C2-N3	-4.67	121.51	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	S4M	N9-C8-N7	-4.48	107.58	113.94
3	C	503	S4M	N3-C4-N9	4.18	134.28	127.17
3	B	501	S4M	C4-N9-C8	3.75	109.68	105.74
3	C	503	S4M	C2-N3-C4	3.68	120.82	111.83
3	C	503	S4M	C4-N9-C8	3.62	109.54	105.74
3	B	501	S4M	O2'-C2'-C1'	3.52	122.21	110.10
3	B	501	S4M	O4'-C1'-C2'	-3.36	99.42	106.62
3	A	501	S4M	C2-N3-C4	3.36	120.04	111.83
2	C	401	4MN	C6-C5-N1	3.36	127.09	120.90
3	B	501	S4M	C3'-C2'-C1'	3.11	107.34	101.46
2	C	401	4MN	C4-C5-C6	-3.09	113.51	118.16
5	C	602	1PG	O5-C10-C11	3.01	123.37	110.11
3	B	501	S4M	N9-C8-N7	-2.97	109.73	113.94
3	A	501	S4M	N9-C8-N7	-2.96	109.74	113.94
3	C	503	S4M	CE-SD-C5'	2.85	122.94	100.54
3	C	503	S4M	O4'-C1'-C2'	-2.84	100.54	106.62
3	A	501	S4M	O4'-C1'-C2'	-2.80	100.63	106.62
3	B	501	S4M	O4'-C4'-C5'	2.78	115.91	108.88
2	C	401	4MN	C1-C2-C3	2.78	128.01	120.96
3	A	501	S4M	C5-C4-N3	-2.57	123.17	126.72
5	C	602	1PG	O4-C8-C9	2.50	121.77	110.35
3	A	501	S4M	CE-SD-C5'	2.41	119.51	100.54
3	A	501	S4M	C5-C6-N6	-2.39	117.37	123.29
3	A	501	S4M	C4-N9-C8	2.36	108.21	105.74
3	B	501	S4M	C2-N1-C6	2.29	122.49	118.73
3	C	503	S4M	C4-C5-N7	-2.27	107.99	110.58
3	C	503	S4M	C5-N7-C8	2.26	107.00	103.45
2	B	401	4MN	C1-C2-C3	-2.26	115.24	120.96
3	B	501	S4M	CE-SD-C5'	2.24	118.18	100.54
3	A	501	S4M	N6-C6-N1	2.22	123.33	118.38
3	A	501	S4M	C4'-O4'-C1'	-2.20	104.62	109.47
3	C	503	S4M	C6-C5-C4	2.20	120.18	117.18
5	C	602	1PG	O3-C6-C7	2.17	120.25	110.35
3	A	501	S4M	C2-N1-C6	2.16	122.27	118.73
3	B	501	S4M	C4'-O4'-C1'	-2.14	104.75	109.47
3	B	501	S4M	C2-N3-C4	2.14	117.05	111.83
3	A	501	S4M	O4'-C4'-C5'	2.10	114.19	108.88
2	C	401	4MN	C3-C4-C5	2.07	123.19	120.66
2	C	401	4MN	C7-C6-C5	2.06	123.18	120.66
5	C	602	1PG	O3-C5-C4	2.04	119.64	110.35
2	B	401	4MN	C4-C3-C2	-2.03	119.03	121.37
3	C	503	S4M	C4'-O4'-C1'	-2.03	104.99	109.47

There are no chirality outliers.

All (35) torsion outliers are listed below:

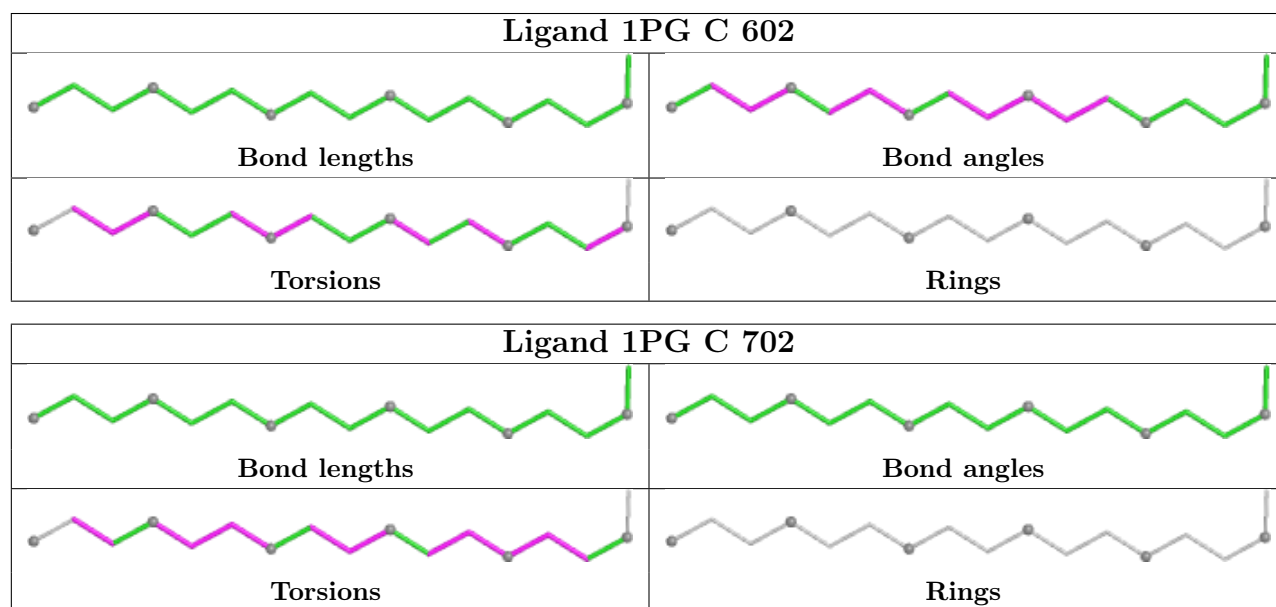
Mol	Chain	Res	Type	Atoms
3	A	501	S4M	CA-CB-CG-SD
3	A	501	S4M	CB-CG-SD-CE
3	A	501	S4M	O4'-C4'-C5'-SD
3	A	501	S4M	C3'-C4'-C5'-SD
3	B	501	S4M	CA-CB-CG-SD
3	B	501	S4M	O4'-C4'-C5'-SD
3	C	503	S4M	CA-CB-CG-SD
4	B	601	GOL	C1-C2-C3-O3
5	C	702	1PG	O4-C8-C9-O5
5	C	602	1PG	C11-C10-O5-C9
5	C	602	1PG	C3-C2-O1-C1
5	C	602	1PG	O5-C10-C11-O6
4	B	601	GOL	O1-C1-C2-C3
4	B	601	GOL	O2-C2-C3-O3
5	C	702	1PG	O5-C10-C11-O6
5	C	702	1PG	O2-C4-C5-O3
5	C	702	1PG	O1-C2-C3-O2
5	C	602	1PG	C4-C5-O3-C6
5	C	702	1PG	C9-C8-O4-C7
5	C	602	1PG	C9-C8-O4-C7
5	C	602	1PG	C6-C7-O4-C8
5	C	702	1PG	C5-C4-O2-C3
5	C	702	1PG	C8-C9-O5-C10
3	C	503	S4M	O4'-C4'-C5'-SD
3	A	501	S4M	CB-CG-SD-C5'
3	B	501	S4M	C3'-C4'-C5'-SD
3	C	503	S4M	C3'-C4'-C5'-SD
5	C	702	1PG	O3-C6-C7-O4
5	C	702	1PG	C2-C3-O2-C4
5	C	702	1PG	C7-C6-O3-C5
5	C	602	1PG	C5-C4-O2-C3
3	B	501	S4M	CB-CG-SD-CE
3	C	503	S4M	CB-CG-SD-CE
4	B	601	GOL	O1-C1-C2-O2
3	B	501	S4M	N-CA-CB-CG

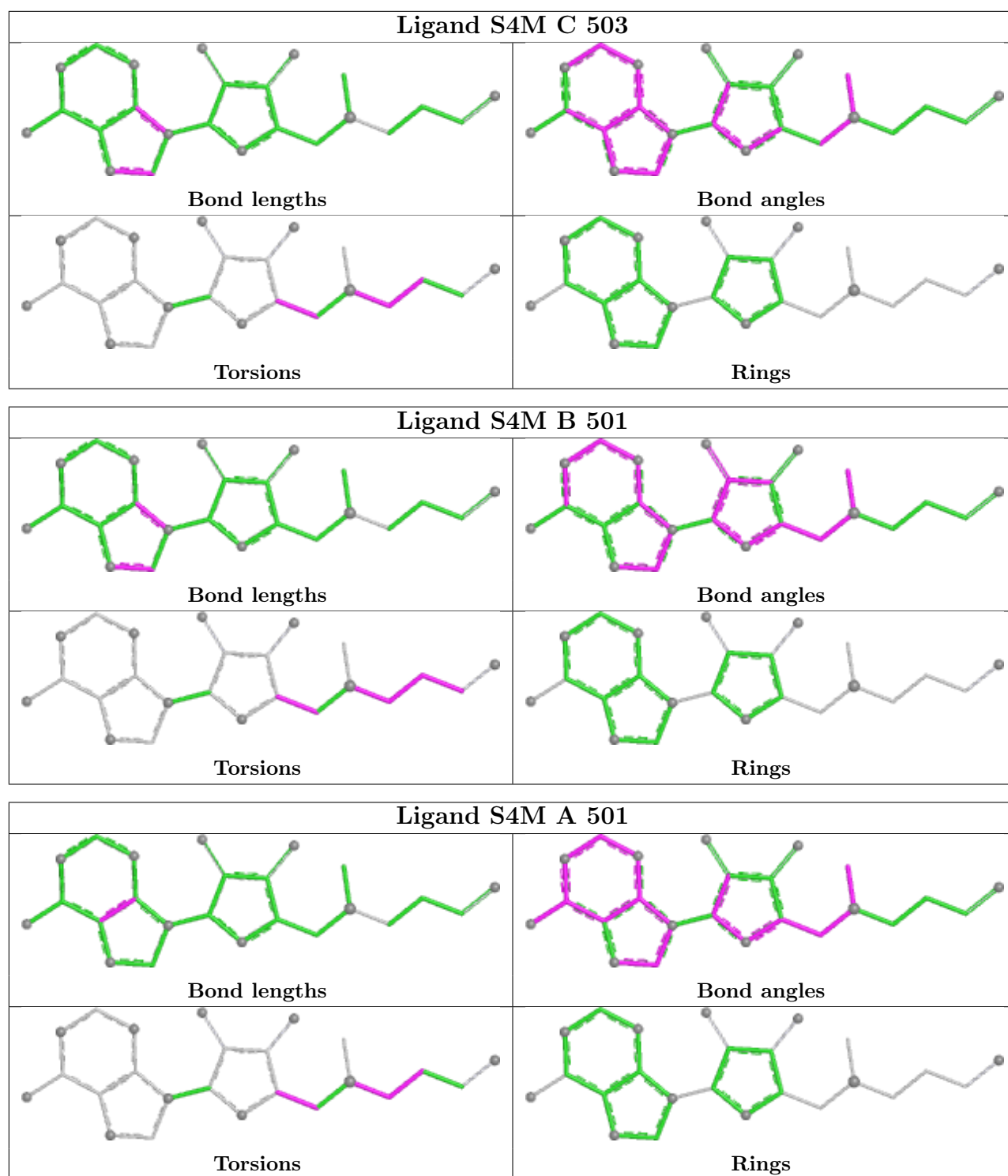
There are no ring outliers.

5 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	602	1PG	22	0
5	C	702	1PG	1	0
3	C	503	S4M	1	0
3	B	501	S4M	1	0
3	A	501	S4M	2	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 ⓘ

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	281/283 (99%)	0.30	10 (3%) 46 52	13, 25, 42, 60	2 (0%)
1	B	280/283 (98%)	-0.13	11 (3%) 43 49	9, 19, 39, 78	3 (1%)
1	C	281/283 (99%)	-0.34	2 (0%) 84 88	10, 17, 33, 52	1 (0%)
All	All	842/849 (99%)	-0.06	23 (2%) 56 62	9, 21, 40, 78	6 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	185	ASN	4.8
1	B	319	GLU	3.5
1	B	318	ILE	3.4
1	B	186	VAL	3.2
1	A	278	ASP	3.0
1	B	320	ASN	2.8
1	A	318	ILE	2.7
1	A	321	ILE	2.7
1	B	295	ASP	2.7
1	B	41	LYS	2.3
1	A	138	LYS	2.3
1	C	185	ASN	2.2
1	A	252	LYS	2.2
1	A	253	LYS	2.2
1	C	65	TYR	2.2
1	B	294	ALA	2.1
1	A	249	LYS	2.1
1	B	277	THR	2.1
1	A	41	LYS	2.1
1	A	277	THR	2.1
1	A	285	ASN	2.0
1	B	285	ASN	2.0
1	B	65	TYR	2.0

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

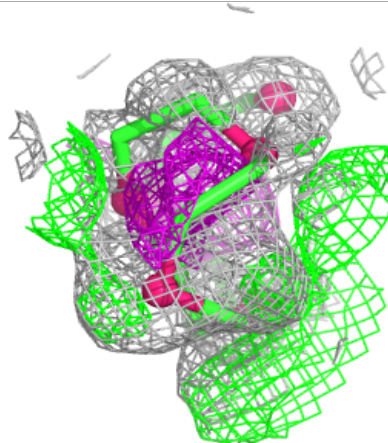
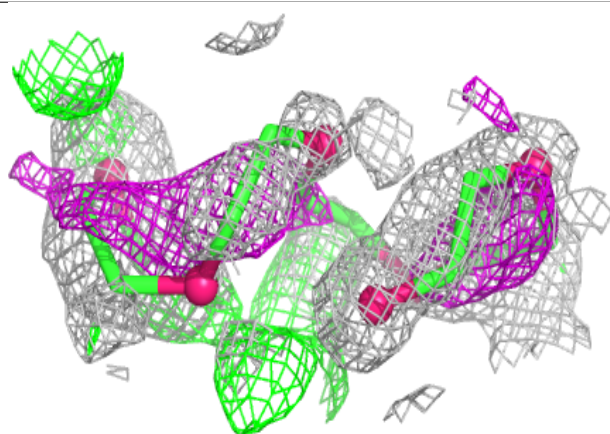
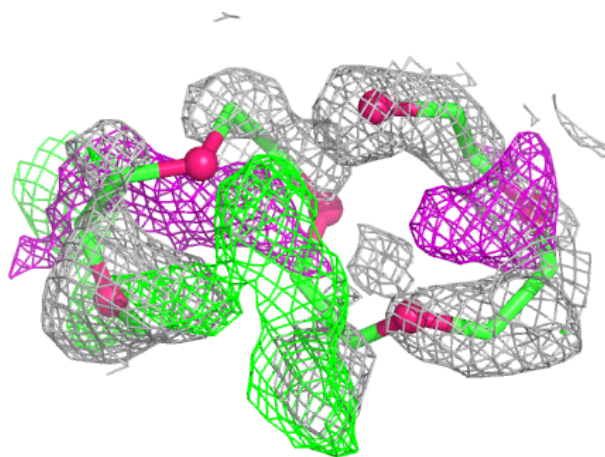
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	1PG	C	602	17/17	0.63	0.31	39,54,78,87	0
4	GOL	B	601	6/6	0.88	0.13	22,31,35,40	0
5	1PG	C	702	17/17	0.88	0.17	31,43,74,75	0
3	S4M	C	503	24/24	0.91	0.09	13,16,29,35	0
3	S4M	A	501	24/24	0.93	0.08	16,20,39,44	0
3	S4M	B	501	24/24	0.93	0.09	16,18,33,37	0
2	4MN	A	401	8/8	0.95	0.08	24,25,26,30	0
2	4MN	C	401	8/8	0.96	0.06	13,14,16,17	0
2	4MN	B	401	8/8	0.97	0.05	15,18,18,19	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.

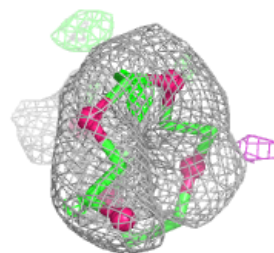
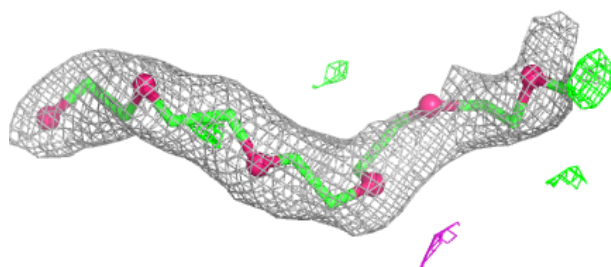
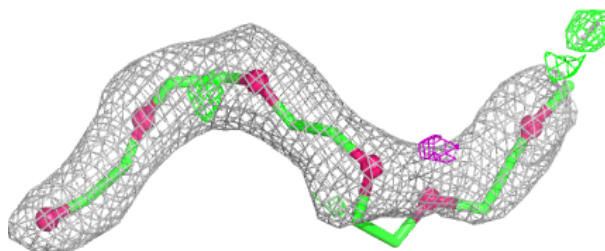
Electron density around 1PG C 602:

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

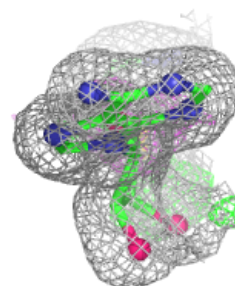
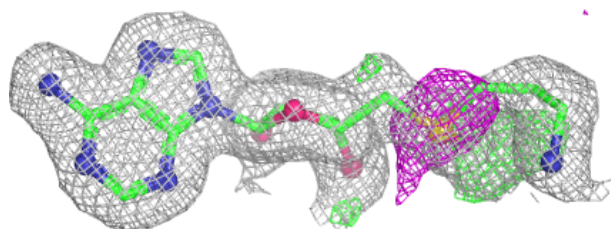
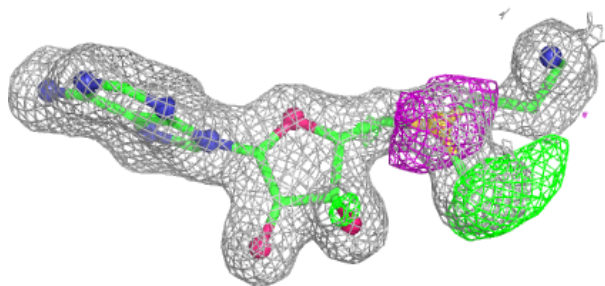


Electron density around 1PG C 702:

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

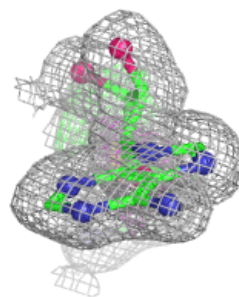
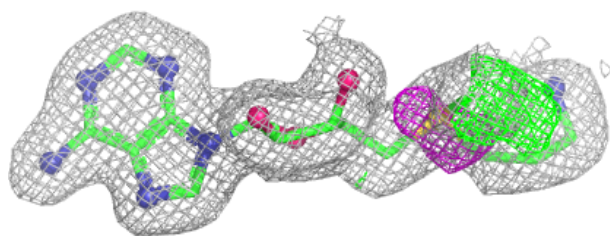
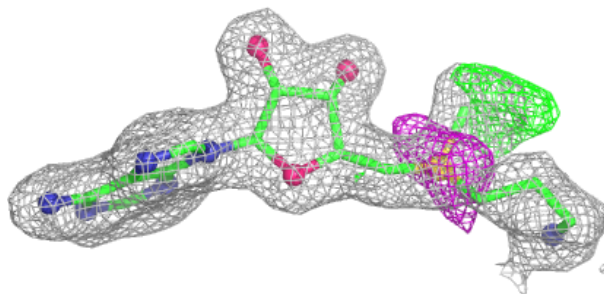
**Electron density around S4M C 503:**

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

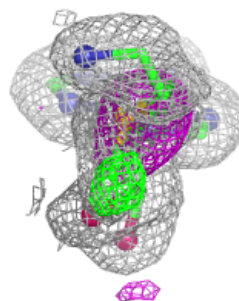
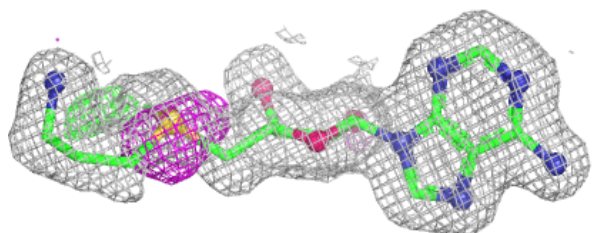
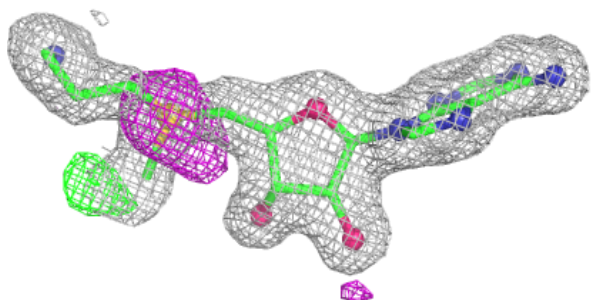


Electron density around S4M A 501:

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

**Electron density around S4M B 501:**

$2mF_o-DF_c$ (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.