



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:42 AM UTC

PDB ID : 2BR4 / pdb_00002br4
Title : cmcI-D160 Mg-SAM
Authors : Oster, L.M.; Lester, D.R.; Terwisscha van Scheltinga, A.; Svenda, M.;
Genereux, C.; Andersson, I.
Deposited on : 2005-05-01
Resolution : 2.59 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

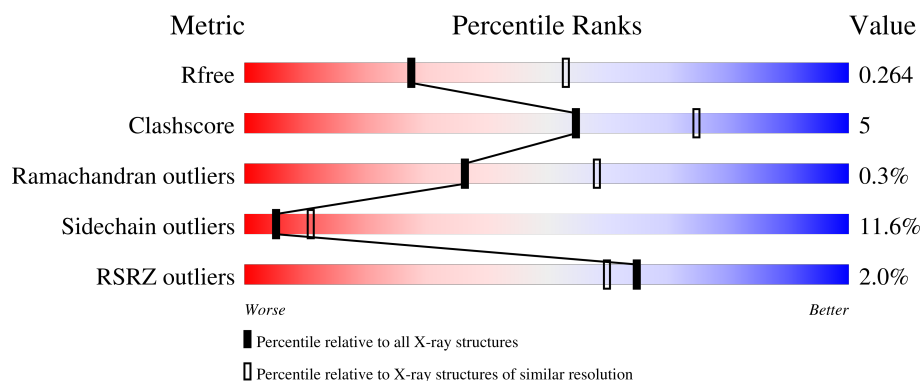
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	236	4% 78% 18% ..
1	B	236	2% 81% 16% ..
1	C	236	82% 14% ..
1	D	236	% 79% 17% ..
1	E	236	2% 82% 15% ..

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Mol	Chain	Length	Quality of chain
1	F	236	2% 84% 12% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12075 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 CEPHALOSPORIN HYDROXYLASE CMCI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	1	0
			1912	1219	330	351	12			
1	B	232	Total	C	N	O	S	0	3	0
			1926	1227	331	356	12			
1	C	232	Total	C	N	O	S	0	2	0
			1923	1225	329	357	12			
1	D	230	Total	C	N	O	S	0	1	0
			1906	1214	327	353	12			
1	E	233	Total	C	N	O	S	0	2	0
			1930	1229	333	356	12			
1	F	231	Total	C	N	O	S	0	0	0
			1909	1217	328	352	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	PHE	LEU	engineered mutation	UNP O85726
B	200	PHE	LEU	engineered mutation	UNP O85726
C	200	PHE	LEU	engineered mutation	UNP O85726
D	200	PHE	LEU	engineered mutation	UNP O85726
E	200	PHE	LEU	engineered mutation	UNP O85726
F	200	PHE	LEU	engineered mutation	UNP O85726

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

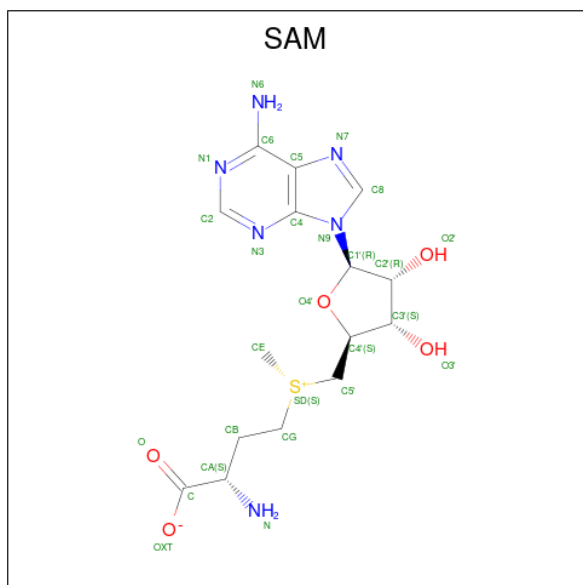
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

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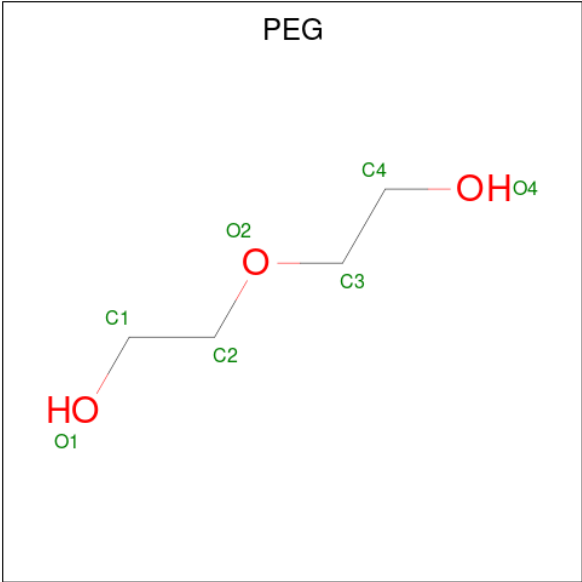
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



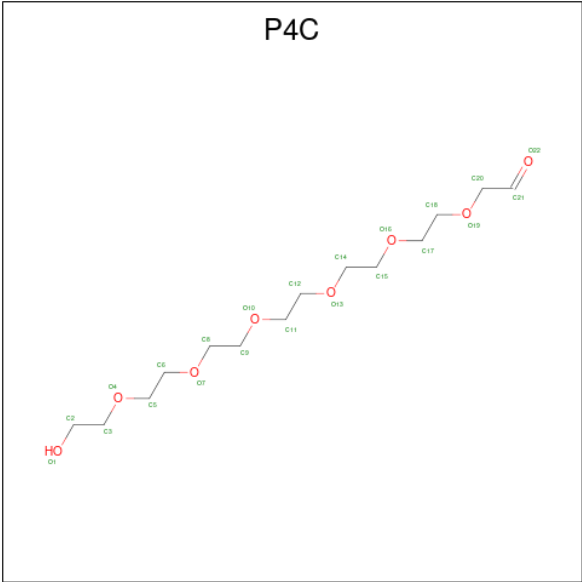
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	15	6	4	1		
3	E	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
3	F	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is O-ACETALDEHYDYL-HEXAETHYLENE GLYCOL (CCD ID: P4C) (formula: C₁₄H₂₈O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			22	14	8		
5	B	1	Total	C	O	0	0
			22	14	8		
5	D	1	Total	C	O	0	0
			22	14	8		

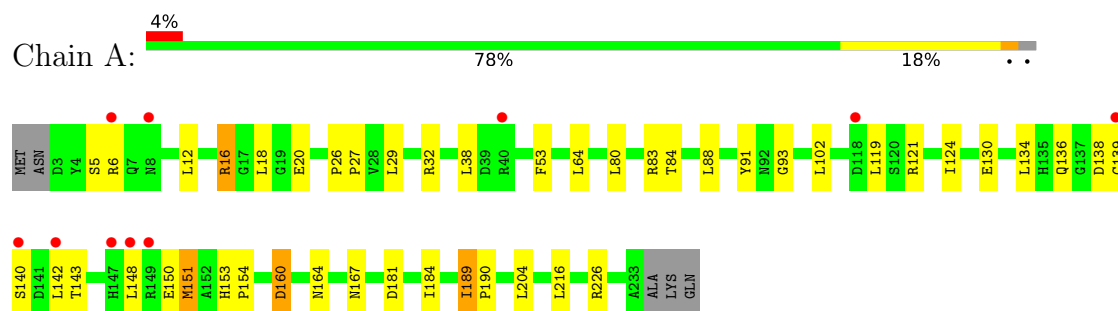
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	53	Total	O	0	0
			53	53		
6	B	87	Total	O	0	0
			87	87		
6	C	67	Total	O	0	0
			67	67		
6	D	44	Total	O	0	0
			44	44		
6	E	34	Total	O	0	0
			34	34		
6	F	30	Total	O	0	0
			30	30		

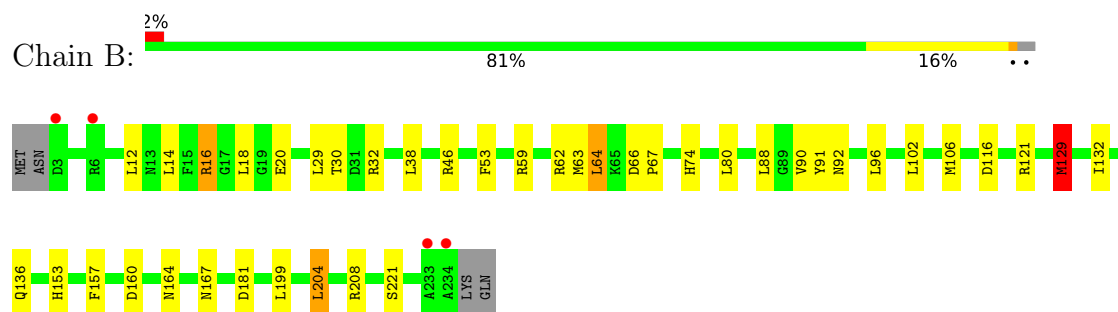
3 Residue-property plots

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

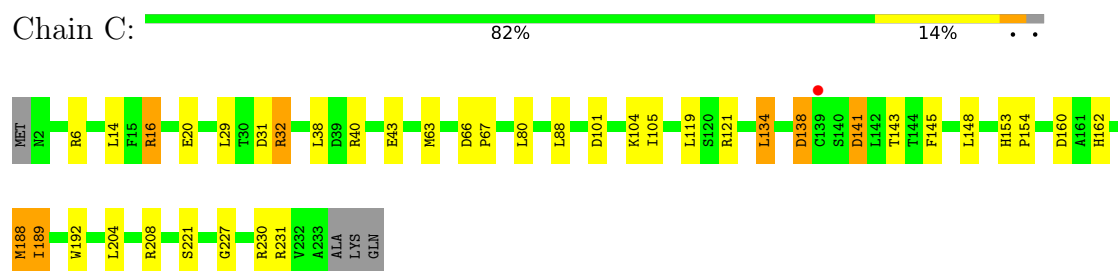
• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI



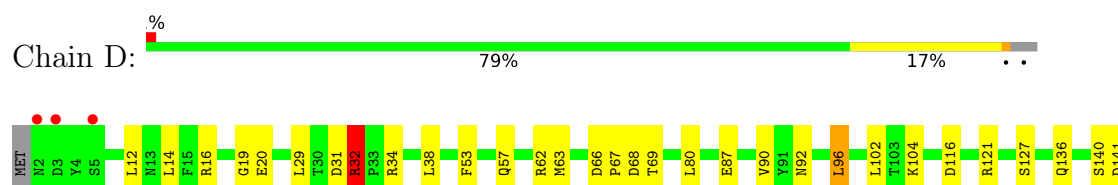
• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI



• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

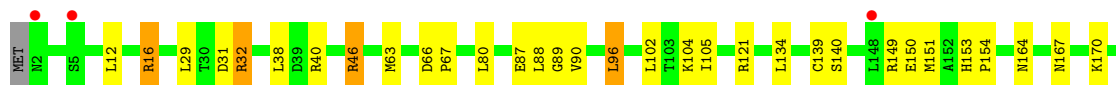
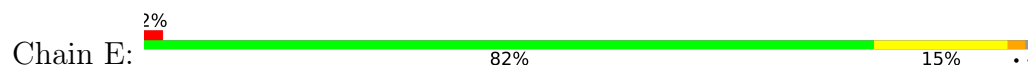


• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

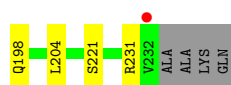
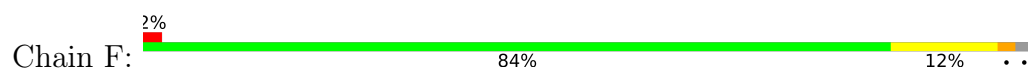




• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI



• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.54Å 102.36Å 181.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.30 – 2.59 51.30 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.6 (51.30-2.59) 99.8 (51.30-2.59)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.199 , 0.261 0.203 , 0.264	Depositor DCC
R_{free} test set	2701 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12075	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P4C, MG, PEG, SAM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	1/1972 (0.1%)	0.80	0/2681
1	B	0.59	1/1993 (0.1%)	0.79	0/2710
1	C	0.56	0/1986	0.78	0/2701
1	D	0.53	0/1965	0.78	1/2672 (0.0%)
1	E	0.55	1/1993 (0.1%)	0.79	0/2710
1	F	0.52	0/1964	0.78	0/2671
All	All	0.55	3/11873 (0.0%)	0.79	1/16145 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	MET	SD-CE	-8.18	1.59	1.79
1	A	189	ILE	CA-CB	6.93	1.57	1.54
1	E	215	MET	SD-CE	-5.96	1.64	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	32	ARG	N-CA-C	5.10	112.81	108.22

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	1912	0	1819	23	0
1	B	1926	0	1825	26	0
1	C	1923	0	1819	23	0
1	D	1906	0	1803	16	0
1	E	1930	0	1831	16	0
1	F	1909	0	1812	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	27	0	22	7	0
3	B	27	0	22	5	0
3	C	27	0	22	0	0
3	D	26	0	22	0	0
3	E	27	0	22	2	0
3	F	27	0	22	1	0
4	A	7	0	10	0	0
4	B	7	0	10	3	0
4	D	7	0	10	0	0
5	A	22	0	25	2	0
5	B	22	0	23	3	0
5	D	22	0	24	0	0
6	A	53	0	0	1	0
6	B	87	0	0	1	0
6	C	67	0	0	0	0
6	D	44	0	0	0	0
6	E	34	0	0	0	0
6	F	30	0	0	0	0
All	All	12075	0	11143	110	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 5.

All (110) 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:16:ARG:HG2	1:C:16:ARG:HH11	1.29	0.96
1:A:91:TYR:HB2	3:A:301:SAM:HE2	1.47	0.94
1:A:18:LEU:CD2	3:A:301:SAM:HE1	2.04	0.87
1:A:164:ASN:HD21	1:A:167:ASN:HD22	1.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:CD2	3:B:301:SAM:HE1	2.09	0.82
1:B:91:TYR:HB2	3:B:301:SAM:HE2	1.64	0.78
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.51	0.76
1:B:16[B]:ARG:HG2	1:B:16[B]:ARG:HH11	1.49	0.76
1:A:18:LEU:HD22	3:A:301:SAM:HE1	1.68	0.76
1:F:16:ARG:HG2	1:F:16:ARG:HH11	1.50	0.76
1:E:213:MET:HE3	1:E:215:MET:HE1	1.69	0.75
1:C:16:ARG:HH11	1:C:16:ARG:CG	2.00	0.75
1:C:16:ARG:HG2	1:C:16:ARG:NH1	2.04	0.69
1:B:18:LEU:HD22	3:B:301:SAM:HE1	1.76	0.68
1:E:88:LEU:HD22	1:E:139:CYS:SG	2.34	0.67
1:D:143:THR:HG22	1:D:147:HIS:CE1	2.32	0.65
5:B:500:P4C:H171	6:B:2086:HOH:O	1.95	0.65
1:E:164:ASN:HD21	1:E:167:ASN:ND2	1.95	0.64
1:B:164:ASN:HD21	1:B:167:ASN:HD22	1.44	0.64
1:B:16[A]:ARG:HB3	1:B:16[A]:ARG:NH1	2.13	0.63
1:A:64:LEU:CD1	3:A:301:SAM:HE3	2.29	0.61
5:A:500:P4C:H32	6:A:2043:HOH:O	2.00	0.60
1:E:139:CYS:SG	3:E:301:SAM:C2	2.91	0.58
1:D:188:MET:HG2	1:D:192:TRP:CZ2	2.38	0.58
1:E:164:ASN:HD21	1:E:167:ASN:HD22	1.49	0.58
1:A:153:HIS:HD2	1:A:181:ASP:OD2	1.87	0.57
1:B:16[A]:ARG:HD3	4:B:401:PEG:C3	2.35	0.56
1:C:31:ASP:C	1:C:32:ARG:HG3	2.31	0.55
1:B:64:LEU:HD23	1:B:64:LEU:N	2.22	0.55
1:D:62:ARG:O	1:D:92:ASN:ND2	2.40	0.54
1:F:139:CYS:SG	3:F:301:SAM:C2	2.96	0.54
1:B:91:TYR:CB	3:B:301:SAM:HE2	2.37	0.54
1:D:19:GLY:HA2	1:F:195:TYR:O	2.09	0.53
1:A:91:TYR:HB2	3:A:301:SAM:CE	2.29	0.53
1:B:16[A]:ARG:HH22	5:B:500:P4C:H151	1.73	0.53
1:B:16[B]:ARG:HH11	1:B:16[B]:ARG:CG	2.22	0.52
1:B:153:HIS:HD2	1:B:181:ASP:OD2	1.93	0.52
1:C:162:HIS:CE1	1:C:188:MET:HE3	2.45	0.52
1:F:16:ARG:HH11	1:F:16:ARG:CG	2.23	0.52
1:B:16[A]:ARG:HD3	4:B:401:PEG:H31	1.92	0.51
5:B:500:P4C:H152	1:C:16:ARG:NH2	2.26	0.51
1:D:192:TRP:HE1	1:F:13:ASN:ND2	2.09	0.51
1:C:138:ASP:HB3	1:C:141:ASP:OD2	2.11	0.50
1:A:88:LEU:HD22	1:A:139:CYS:SG	2.51	0.50
1:D:162:HIS:CG	1:D:188:MET:HE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:HIS:HA	1:C:154:PRO:C	2.37	0.49
1:C:101:ASP:O	1:C:105:ILE:HG12	2.13	0.49
1:E:90:VAL:HG13	1:E:96:LEU:HD22	1.95	0.48
1:C:16:ARG:CG	1:C:16:ARG:NH1	2.66	0.48
1:C:204:LEU:HD22	1:F:38:LEU:HG	1.96	0.47
1:B:74:HIS:CE1	1:B:106:MET:HE2	2.50	0.47
1:E:16[B]:ARG:HH11	1:E:16[B]:ARG:HG2	1.80	0.47
1:A:226:ARG:HD3	1:B:46:ARG:HD2	1.96	0.46
1:E:153:HIS:HA	1:E:154:PRO:C	2.41	0.46
1:C:162:HIS:CG	1:C:188:MET:HE3	2.50	0.46
1:A:153:HIS:HA	1:A:154:PRO:C	2.41	0.46
1:D:90:VAL:HG13	1:D:96:LEU:HD22	1.98	0.46
1:B:129:MET:HE2	1:B:132:ILE:HD12	1.97	0.46
1:C:88:LEU:HD21	1:C:145:PHE:CE2	2.51	0.46
1:A:119:LEU:H	1:A:136:GLN:HE21	1.62	0.46
1:D:66:ASP:HB2	1:D:67:PRO:CD	2.46	0.46
1:D:162:HIS:CE1	1:D:188:MET:HE3	2.51	0.45
1:A:148:LEU:HB3	1:A:151:MET:HE1	1.98	0.45
5:A:500:P4C:O22	3:E:301:SAM:HE1	2.16	0.45
1:B:90:VAL:HG13	1:B:96:LEU:HD22	1.99	0.45
1:E:213:MET:HG2	1:E:215:MET:CE	2.46	0.45
1:E:153:HIS:HE1	1:E:176:LEU:O	2.00	0.45
1:D:31:ASP:C	1:D:32:ARG:HG3	2.41	0.45
1:A:53:PHE:CD2	1:A:53:PHE:C	2.96	0.44
1:F:65:LYS:HZ2	1:F:186:GLU:CD	2.26	0.44
1:A:189:ILE:HB	1:A:190:PRO:HD3	2.00	0.43
1:C:188:MET:HG2	1:C:192:TRP:CZ2	2.53	0.43
1:E:66:ASP:HB2	1:E:67:PRO:CD	2.49	0.43
1:E:213:MET:HE3	1:E:215:MET:CE	2.45	0.43
1:D:167:ASN:HD22	1:D:167:ASN:HA	1.66	0.43
1:F:189:ILE:HB	1:F:190:PRO:HD3	2.01	0.43
1:A:160:ASP:HB3	3:A:301:SAM:HG1	2.01	0.43
1:D:68[A]:ASP:OD1	1:D:69:THR:N	2.52	0.43
1:E:153:HIS:HB3	1:E:154:PRO:HA	2.00	0.42
1:B:116:ASP:O	1:B:136:GLN:HA	2.20	0.42
1:D:143:THR:CG2	1:D:147:HIS:CE1	3.00	0.42
1:C:66:ASP:HB2	1:C:67:PRO:HD2	2.01	0.42
1:E:16[A]:ARG:HB3	1:E:16[A]:ARG:HH11	1.84	0.42
1:A:38:LEU:HD13	1:B:204:LEU:HD22	2.02	0.42
1:C:88:LEU:HD21	1:C:145:PHE:HE2	1.83	0.42
1:B:88:LEU:HD11	1:B:157:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:THR:HG21	1:A:151:MET:HG3	2.01	0.41
1:F:53:PHE:CD2	1:F:53:PHE:C	2.98	0.41
1:C:189:ILE:HD12	1:C:227:GLY:HA2	2.01	0.41
1:E:31:ASP:C	1:E:32:ARG:HG3	2.45	0.41
1:B:66:ASP:HB2	1:B:67:PRO:CD	2.51	0.41
1:A:93:GLY:O	1:A:124:ILE:HD11	2.20	0.41
1:F:16:ARG:CG	1:F:16:ARG:NH1	2.83	0.41
1:A:16:ARG:HG2	1:A:16:ARG:NH1	2.23	0.41
1:C:105:ILE:HD11	1:F:105:ILE:HG21	2.03	0.41
1:D:116:ASP:O	1:D:136:GLN:HA	2.20	0.41
1:A:164:ASN:ND2	1:A:167:ASN:HD22	2.03	0.41
1:C:188:MET:HE2	1:C:188:MET:CA	2.51	0.41
1:B:18:LEU:HD21	3:B:301:SAM:HE1	1.96	0.41
1:B:62:ARG:O	1:B:92:ASN:ND2	2.46	0.41
1:D:162:HIS:ND1	1:D:188:MET:HE3	2.36	0.41
1:B:199:LEU:HB2	1:C:20[A]:GLU:OE1	2.20	0.40
1:C:119:LEU:HD22	1:C:134:LEU:HG	2.03	0.40
1:B:16[A]:ARG:HB3	1:B:16[A]:ARG:CZ	2.51	0.40
1:B:16[A]:ARG:HD3	4:B:401:PEG:H32	2.02	0.40
1:A:26:PRO:HA	1:A:27:PRO:HD3	2.00	0.40
1:C:188:MET:HG3	1:C:192:TRP:CE2	2.56	0.40
1:A:64:LEU:HD12	3:A:301:SAM:HE3	2.02	0.40
1:C:162:HIS:CD2	1:C:188:MET:HE3	2.57	0.40
1:D:226:ARG:HD3	1:E:46:ARG:HD3	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	230/236 (98%)	218 (95%)	11 (5%)	1 (0%)	30 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	233/236 (99%)	225 (97%)	7 (3%)	1 (0%)	30	51
1	C	232/236 (98%)	226 (97%)	6 (3%)	0	100	100
1	D	229/236 (97%)	218 (95%)	10 (4%)	1 (0%)	30	51
1	E	233/236 (99%)	226 (97%)	6 (3%)	1 (0%)	30	51
1	F	229/236 (97%)	217 (95%)	12 (5%)	0	100	100
All	All	1386/1416 (98%)	1330 (96%)	52 (4%)	4 (0%)	36	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	SER
1	E	89	GLY
1	D	53	PHE
1	B	53	PHE

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	204/207 (99%)	182 (89%)	22 (11%)	6	13
1	B	206/207 (100%)	186 (90%)	20 (10%)	8	17
1	C	206/207 (100%)	182 (88%)	24 (12%)	5	11
1	D	204/207 (99%)	179 (88%)	25 (12%)	4	9
1	E	206/207 (100%)	179 (87%)	27 (13%)	4	8
1	F	204/207 (99%)	178 (87%)	26 (13%)	4	9
All	All	1230/1242 (99%)	1086 (88%)	144 (12%)	5	11

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	6	ARG

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Mol	Chain	Res	Type
1	A	12	LEU
1	A	16	ARG
1	A	20	GLU
1	A	29	LEU
1	A	32	ARG
1	A	80	LEU
1	A	83	ARG
1	A	102	LEU
1	A	121	ARG
1	A	130	GLU
1	A	134	LEU
1	A	138	ASP
1	A	142	LEU
1	A	143	THR
1	A	150	GLU
1	A	151	MET
1	A	160	ASP
1	A	184	ILE
1	A	204	LEU
1	A	216	LEU
1	B	12	LEU
1	B	14	LEU
1	B	16[A]	ARG
1	B	16[B]	ARG
1	B	20	GLU
1	B	29	LEU
1	B	30	THR
1	B	32	ARG
1	B	38	LEU
1	B	59	ARG
1	B	63	MET
1	B	64	LEU
1	B	80	LEU
1	B	102	LEU
1	B	121	ARG
1	B	129	MET
1	B	160	ASP
1	B	204	LEU
1	B	208	ARG
1	B	221	SER
1	C	6	ARG
1	C	14	LEU

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Mol	Chain	Res	Type
1	C	16	ARG
1	C	29	LEU
1	C	32	ARG
1	C	38	LEU
1	C	40	ARG
1	C	43	GLU
1	C	63	MET
1	C	80	LEU
1	C	104	LYS
1	C	121	ARG
1	C	134	LEU
1	C	138	ASP
1	C	141	ASP
1	C	143	THR
1	C	148	LEU
1	C	160	ASP
1	C	188	MET
1	C	189	ILE
1	C	208	ARG
1	C	221	SER
1	C	230	ARG
1	C	231	ARG
1	D	12	LEU
1	D	14	LEU
1	D	16	ARG
1	D	20	GLU
1	D	29	LEU
1	D	32	ARG
1	D	34	ARG
1	D	38	LEU
1	D	57	GLN
1	D	63	MET
1	D	80	LEU
1	D	87	GLU
1	D	96	LEU
1	D	102	LEU
1	D	104	LYS
1	D	121	ARG
1	D	127	SER
1	D	140	SER
1	D	141	ASP
1	D	160	ASP

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Mol	Chain	Res	Type
1	D	179	GLU
1	D	188	MET
1	D	189	ILE
1	D	204	LEU
1	D	208	ARG
1	E	12	LEU
1	E	16[A]	ARG
1	E	16[B]	ARG
1	E	29	LEU
1	E	32	ARG
1	E	38	LEU
1	E	40	ARG
1	E	46	ARG
1	E	63	MET
1	E	80	LEU
1	E	87	GLU
1	E	96	LEU
1	E	102	LEU
1	E	104	LYS
1	E	105	ILE
1	E	121	ARG
1	E	134	LEU
1	E	140	SER
1	E	149	ARG
1	E	150	GLU
1	E	151	MET
1	E	170	LYS
1	E	173	VAL
1	E	189	ILE
1	E	199	LEU
1	E	204	LEU
1	E	221	SER
1	F	7	GLN
1	F	12	LEU
1	F	16	ARG
1	F	29	LEU
1	F	38	LEU
1	F	46	ARG
1	F	57	GLN
1	F	63	MET
1	F	64	LEU
1	F	77	LEU

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Mol	Chain	Res	Type
1	F	80	LEU
1	F	102	LEU
1	F	104	LYS
1	F	105	ILE
1	F	121	ARG
1	F	134	LEU
1	F	146	GLU
1	F	150	GLU
1	F	165	THR
1	F	170	LYS
1	F	179	GLU
1	F	189	ILE
1	F	198	GLN
1	F	204	LEU
1	F	221	SER
1	F	231	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	136	GLN
1	A	153	HIS
1	A	162	HIS
1	A	164	ASN
1	A	198	GLN
1	B	7	GLN
1	B	8	ASN
1	B	111	GLN
1	B	153	HIS
1	B	164	ASN
1	C	25	HIS
1	C	74	HIS
1	C	162	HIS
1	D	8	ASN
1	D	136	GLN
1	D	147	HIS
1	D	167	ASN
1	D	175	HIS
1	E	7	GLN
1	E	111	GLN
1	E	131	ASN

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Mol	Chain	Res	Type
1	E	136	GLN
1	E	153	HIS
1	E	164	ASN
1	E	175	HIS
1	E	219	ASN
1	F	13	ASN
1	F	70	GLN
1	F	131	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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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
3	SAM	D	301	-	26,28,29	1.04	3 (11%)	32,40,42	2.07	9 (28%)
3	SAM	C	301	-	27,29,29	1.11	4 (14%)	34,42,42	2.02	9 (26%)
4	PEG	A	401	-	6,6,6	0.44	0	5,5,5	0.19	0
5	P4C	D	500	-	21,21,21	1.55	3 (14%)	20,20,20	4.49	6 (30%)
3	SAM	E	301	-	27,29,29	1.09	4 (14%)	34,42,42	2.05	9 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SAM	F	301	-	27,29,29	1.15	4 (14%)	34,42,42	2.00	9 (26%)
4	PEG	B	401	-	6,6,6	0.40	0	5,5,5	0.37	0
5	P4C	A	500	-	21,21,21	1.54	3 (14%)	20,20,20	4.19	5 (25%)
3	SAM	A	301	-	27,29,29	1.09	4 (14%)	34,42,42	2.06	11 (32%)
3	SAM	B	301	-	27,29,29	1.09	3 (11%)	34,42,42	2.20	11 (32%)
4	PEG	D	401	-	6,6,6	0.43	0	5,5,5	0.23	0
5	P4C	B	500	2	21,21,21	1.57	3 (14%)	20,20,20	4.45	4 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAM	D	301	-	-	6/14/31/33	0/3/3/3
3	SAM	C	301	-	-	4/17/33/33	0/3/3/3
4	PEG	A	401	-	-	2/4/4/4	-
5	P4C	D	500	-	-	13/18/19/19	-
3	SAM	E	301	-	-	8/17/33/33	0/3/3/3
3	SAM	F	301	-	-	3/17/33/33	0/3/3/3
4	PEG	B	401	-	-	2/4/4/4	-
5	P4C	A	500	-	-	9/18/19/19	-
3	SAM	A	301	-	-	6/17/33/33	0/3/3/3
3	SAM	B	301	-	-	6/17/33/33	0/3/3/3
4	PEG	D	401	-	-	1/4/4/4	-
5	P4C	B	500	2	-	8/18/19/19	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	500	P4C	C20-C21	-5.38	1.19	1.48
5	A	500	P4C	C20-C21	-5.38	1.19	1.48
5	B	500	P4C	C20-C21	-5.37	1.19	1.48
5	A	500	P4C	C3-C2	-3.17	1.32	1.49
5	B	500	P4C	C3-C2	-3.10	1.32	1.49
5	D	500	P4C	C3-C2	-2.98	1.33	1.49
3	F	301	SAM	C2-N1	2.68	1.38	1.33
3	F	301	SAM	C2-N3	2.62	1.38	1.33
3	E	301	SAM	C2-N1	2.50	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	SAM	C2-N1	2.46	1.38	1.33
3	C	301	SAM	C2-N1	2.46	1.38	1.33
3	E	301	SAM	C2-N3	2.45	1.38	1.33
3	C	301	SAM	C2-N3	2.40	1.38	1.33
3	B	301	SAM	C2-N1	2.40	1.38	1.33
3	D	301	SAM	C2-N3	2.39	1.38	1.33
3	A	301	SAM	C2-N3	2.38	1.38	1.33
3	B	301	SAM	C2-N3	2.37	1.38	1.33
3	D	301	SAM	C2-N1	2.30	1.38	1.33
3	A	301	SAM	C8-N7	2.29	1.36	1.31
5	B	500	P4C	O19-C20	-2.29	1.33	1.42
3	C	301	SAM	C8-N7	2.27	1.36	1.31
3	C	301	SAM	OXT-C	-2.23	1.23	1.30
3	B	301	SAM	C8-N7	2.23	1.36	1.31
5	D	500	P4C	O19-C20	-2.23	1.33	1.42
3	F	301	SAM	C8-N7	2.19	1.35	1.31
3	A	301	SAM	OXT-C	-2.16	1.23	1.30
3	E	301	SAM	C8-N7	2.15	1.35	1.31
5	A	500	P4C	O19-C20	-2.14	1.34	1.42
3	D	301	SAM	C8-N7	2.13	1.35	1.31
3	F	301	SAM	OXT-C	-2.12	1.23	1.30
3	E	301	SAM	OXT-C	-2.11	1.23	1.30

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	500	P4C	O22-C21-C20	15.13	170.85	126.10
5	B	500	P4C	O22-C21-C20	15.11	170.80	126.10
5	A	500	P4C	O22-C21-C20	14.42	168.74	126.10
5	D	500	P4C	O19-C20-C21	12.16	173.96	110.90
5	B	500	P4C	O19-C20-C21	12.02	173.24	110.90
5	A	500	P4C	O19-C20-C21	11.07	168.30	110.90
3	D	301	SAM	N3-C2-N1	-6.15	119.27	128.58
3	C	301	SAM	N3-C2-N1	-6.11	119.34	128.58
3	B	301	SAM	N3-C2-N1	-6.07	119.40	128.58
3	A	301	SAM	N3-C2-N1	-6.03	119.45	128.58
3	E	301	SAM	N3-C2-N1	-5.86	119.71	128.58
3	F	301	SAM	N3-C2-N1	-5.84	119.74	128.58
3	B	301	SAM	CG-SD-C5'	4.98	115.61	103.43
3	D	301	SAM	C5-C4-N3	-4.45	120.58	126.72
3	F	301	SAM	C5-C4-N3	-4.30	120.80	126.72
3	C	301	SAM	N9-C8-N7	-4.27	107.88	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	301	SAM	C5-C4-N3	-4.22	120.90	126.72
3	B	301	SAM	C5-C4-N3	-4.22	120.91	126.72
3	A	301	SAM	N9-C8-N7	-4.06	108.17	113.94
3	C	301	SAM	C5-C4-N3	-4.02	121.19	126.72
3	D	301	SAM	N9-C8-N7	-4.01	108.24	113.94
3	E	301	SAM	N9-C8-N7	-4.00	108.26	113.94
3	F	301	SAM	N9-C8-N7	-3.96	108.32	113.94
3	A	301	SAM	C5-C4-N3	-3.94	121.29	126.72
3	B	301	SAM	N9-C8-N7	-3.91	108.39	113.94
3	D	301	SAM	C2-N3-C4	3.63	120.69	111.83
3	C	301	SAM	C5-N7-C8	3.55	109.02	103.45
3	E	301	SAM	C5-N7-C8	3.54	109.02	103.45
3	B	301	SAM	C2-N3-C4	3.52	120.42	111.83
3	C	301	SAM	C2-N3-C4	3.48	120.32	111.83
3	E	301	SAM	C2-N3-C4	3.47	120.31	111.83
3	A	301	SAM	C2-N3-C4	3.43	120.22	111.83
3	F	301	SAM	C2-N3-C4	3.42	120.19	111.83
3	A	301	SAM	C5-N7-C8	3.40	108.79	103.45
3	D	301	SAM	C5-N7-C8	3.38	108.76	103.45
3	F	301	SAM	C5-N7-C8	3.33	108.69	103.45
3	B	301	SAM	C5-N7-C8	3.29	108.62	103.45
5	B	500	P4C	O1-C2-C3	3.27	131.08	111.82
3	D	301	SAM	N3-C4-N9	3.15	132.53	127.17
3	E	301	SAM	OXT-C-O	-3.12	117.01	124.08
3	A	301	SAM	CG-SD-C5'	3.11	111.05	103.43
3	F	301	SAM	N3-C4-N9	3.05	132.36	127.17
3	E	301	SAM	O4'-C1'-N9	2.96	113.78	108.09
3	B	301	SAM	N3-C4-N9	2.89	132.08	127.17
3	B	301	SAM	OXT-C-O	-2.87	117.57	124.08
5	D	500	P4C	O4-C3-C2	2.86	122.72	110.11
3	E	301	SAM	N3-C4-N9	2.78	131.89	127.17
5	B	500	P4C	C20-O19-C18	2.72	123.47	112.40
5	A	500	P4C	O1-C2-C3	2.69	127.67	111.82
5	D	500	P4C	O1-C2-C3	2.61	127.19	111.82
3	C	301	SAM	N3-C4-N9	2.59	131.57	127.17
3	A	301	SAM	N3-C4-N9	2.57	131.54	127.17
3	C	301	SAM	C4-C5-N7	-2.53	107.69	110.58
3	E	301	SAM	C4-C5-N7	-2.52	107.70	110.58
3	F	301	SAM	OXT-C-O	-2.51	118.39	124.08
5	D	500	P4C	C20-O19-C18	2.44	122.31	112.40
5	A	500	P4C	C5-O4-C3	2.35	123.54	113.26
3	A	301	SAM	C4-C5-N7	-2.35	107.90	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	SAM	OXT-C-O	-2.33	118.80	124.08
3	C	301	SAM	C4-N9-C8	2.30	108.16	105.74
3	C	301	SAM	OXT-C-O	-2.29	118.88	124.08
3	B	301	SAM	C4-C5-N7	-2.23	108.03	110.58
3	A	301	SAM	O4'-C1'-N9	2.23	112.36	108.09
3	B	301	SAM	O4'-C1'-N9	2.22	112.36	108.09
3	D	301	SAM	O4'-C1'-N9	2.22	112.35	108.09
3	D	301	SAM	C4-C5-N7	-2.17	108.10	110.58
3	D	301	SAM	C4-N9-C8	2.16	108.01	105.74
3	F	301	SAM	C4-N9-C8	2.16	108.00	105.74
3	F	301	SAM	C4-C5-N7	-2.13	108.15	110.58
3	A	301	SAM	C4-N9-C8	2.13	107.97	105.74
3	B	301	SAM	C4-N9-C8	2.11	107.96	105.74
5	D	500	P4C	C5-O4-C3	2.10	122.44	113.26
5	A	500	P4C	C20-O19-C18	2.05	120.76	112.40

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	SAM	O-C-CA-N
3	A	301	SAM	CA-CB-CG-SD
3	A	301	SAM	O4'-C4'-C5'-SD
3	A	301	SAM	C3'-C4'-C5'-SD
3	B	301	SAM	CA-CB-CG-SD
3	B	301	SAM	C4'-C5'-SD-CG
3	B	301	SAM	O4'-C4'-C5'-SD
3	B	301	SAM	C3'-C4'-C5'-SD
3	C	301	SAM	CA-CB-CG-SD
3	D	301	SAM	O-C-CA-CB
3	D	301	SAM	N-CA-CB-CG
3	D	301	SAM	C-CA-CB-CG
3	D	301	SAM	CA-CB-CG-SD
3	D	301	SAM	CB-CG-SD-CE
3	E	301	SAM	O4'-C4'-C5'-SD
3	E	301	SAM	C3'-C4'-C5'-SD
3	F	301	SAM	N-CA-CB-CG
5	D	500	P4C	C2-C3-O4-C5
5	A	500	P4C	C6-C5-O4-C3
5	D	500	P4C	O16-C17-C18-O19
3	A	301	SAM	OXT-C-CA-N
3	E	301	SAM	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
5	D	500	P4C	O4-C5-C6-O7
4	D	401	PEG	O2-C3-C4-O4
5	A	500	P4C	O16-C17-C18-O19
5	D	500	P4C	O13-C14-C15-O16
3	B	301	SAM	OXT-C-CA-N
4	B	401	PEG	O2-C3-C4-O4
5	D	500	P4C	O1-C2-C3-O4
5	A	500	P4C	O13-C14-C15-O16
5	D	500	P4C	O7-C8-C9-O10
4	A	401	PEG	O1-C1-C2-O2
5	A	500	P4C	C17-C18-O19-C20
5	A	500	P4C	O10-C11-C12-O13
5	A	500	P4C	C21-C20-O19-C18
5	B	500	P4C	O4-C5-C6-O7
4	B	401	PEG	O1-C1-C2-O2
5	D	500	P4C	C21-C20-O19-C18
3	B	301	SAM	O-C-CA-N
3	E	301	SAM	O-C-CA-N
5	D	500	P4C	C12-C11-O10-C9
5	D	500	P4C	C8-C9-O10-C11
5	B	500	P4C	C18-C17-O16-C15
5	B	500	P4C	C11-C12-O13-C14
3	E	301	SAM	CA-CB-CG-SD
5	B	500	P4C	O7-C8-C9-O10
3	C	301	SAM	O4'-C4'-C5'-SD
3	A	301	SAM	C4'-C5'-SD-CG
3	C	301	SAM	C3'-C4'-C5'-SD
5	D	500	P4C	O10-C11-C12-O13
3	F	301	SAM	C-CA-CB-CG
5	B	500	P4C	O16-C17-C18-O19
5	B	500	P4C	O13-C14-C15-O16
5	D	500	P4C	C14-C15-O16-C17
5	A	500	P4C	C9-C8-O7-C6
3	E	301	SAM	O-C-CA-CB
3	E	301	SAM	OXT-C-CA-CB
5	D	500	P4C	C17-C18-O19-C20
5	D	500	P4C	C6-C5-O4-C3
5	B	500	P4C	C8-C9-O10-C11
5	A	500	P4C	O4-C5-C6-O7
4	A	401	PEG	O2-C3-C4-O4
5	A	500	P4C	C18-C17-O16-C15
5	B	500	P4C	O10-C11-C12-O13

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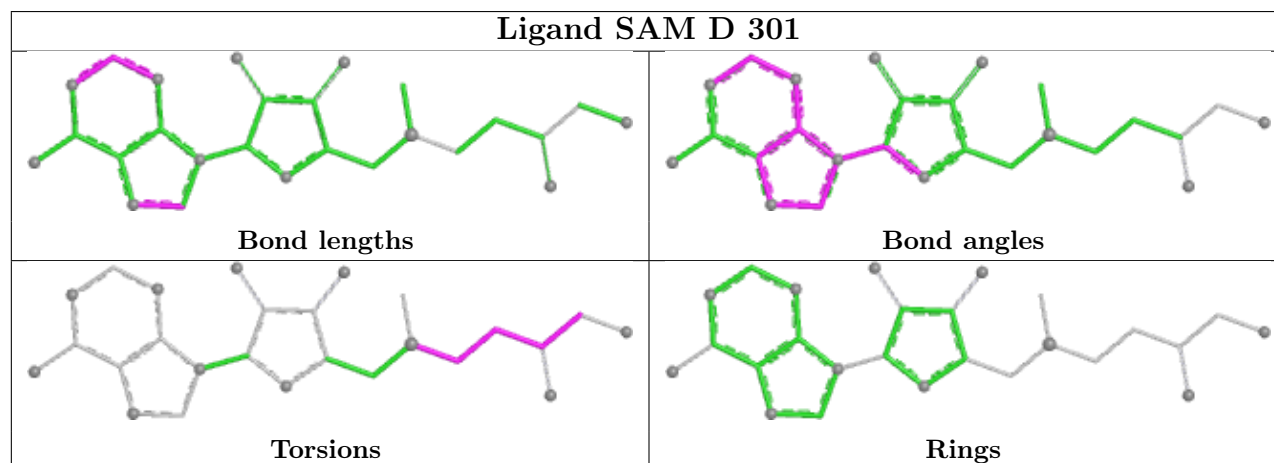
Mol	Chain	Res	Type	Atoms
3	F	301	SAM	OXT-C-CA-N
3	C	301	SAM	CB-CG-SD-C5'
3	D	301	SAM	CB-CG-SD-C5'
3	E	301	SAM	CB-CG-SD-C5'

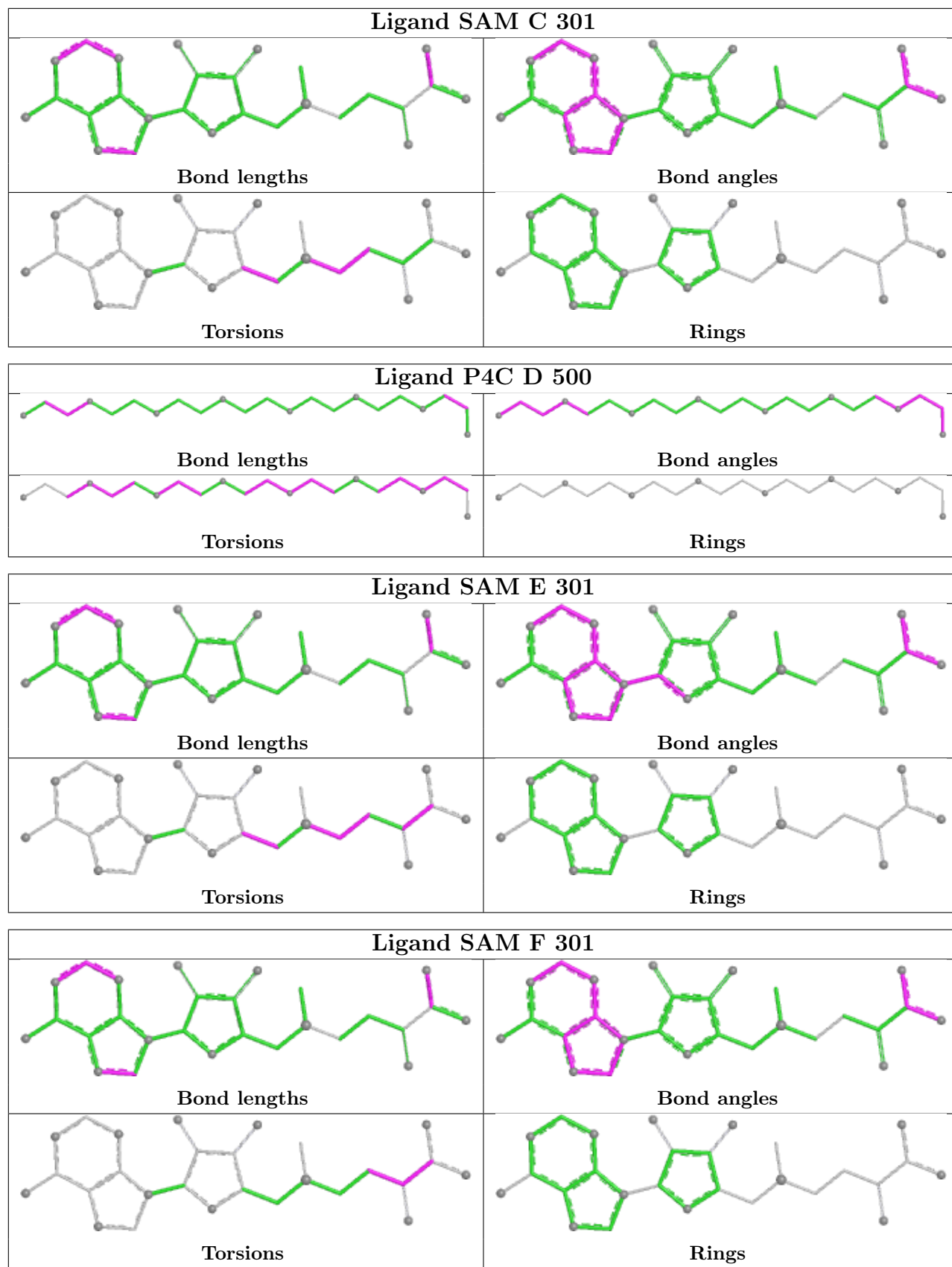
There are no ring outliers.

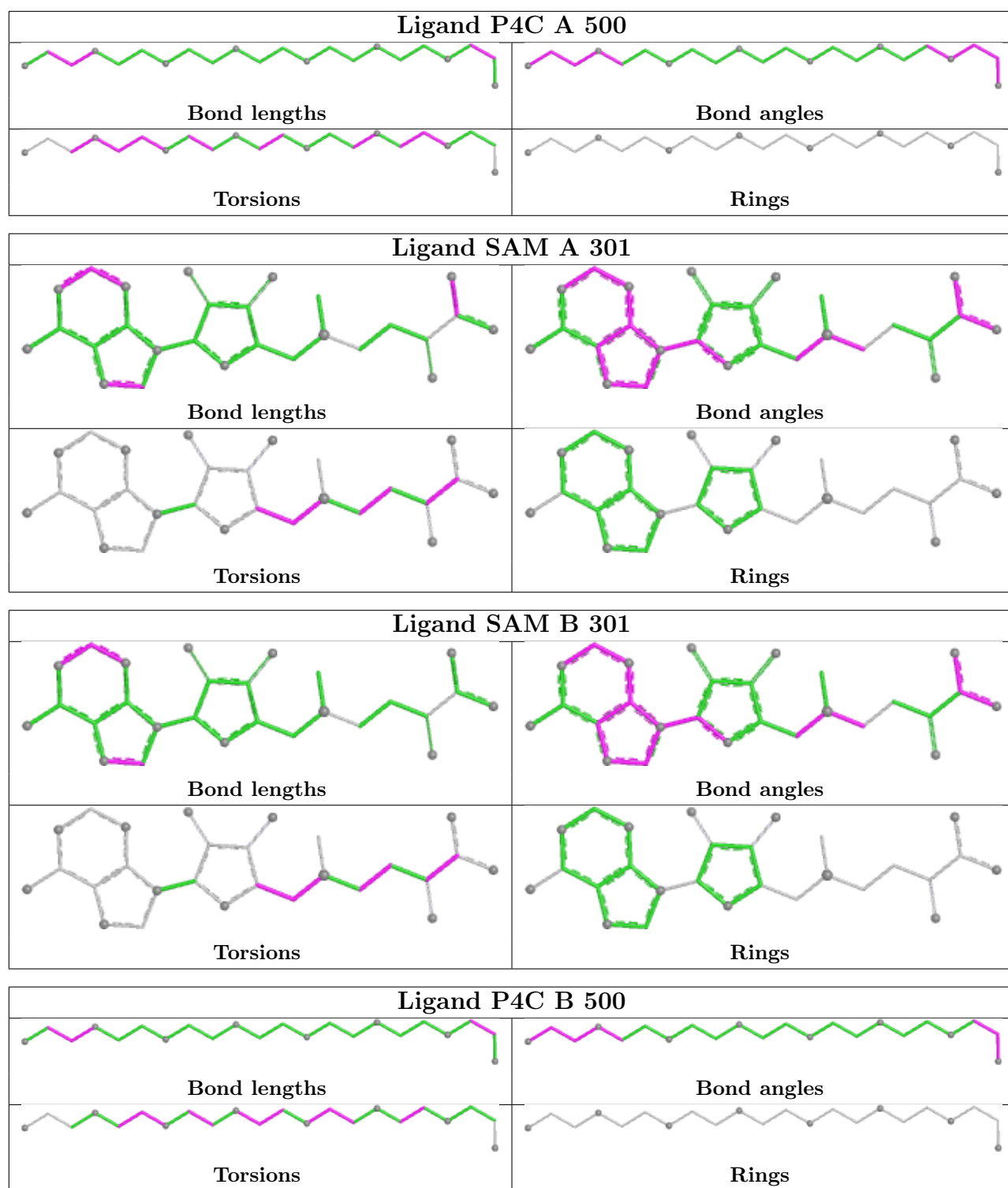
7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	301	SAM	2	0
3	F	301	SAM	1	0
4	B	401	PEG	3	0
5	A	500	P4C	2	0
3	A	301	SAM	7	0
3	B	301	SAM	5	0
5	B	500	P4C	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 ⓘ

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(Å²)	Q<0.9
1	A	231/236 (97%)	0.12	10 (4%)	40	34	12, 25, 54, 64	1 (0%)
1	B	232/236 (98%)	-0.17	4 (1%)	69	64	13, 23, 42, 70	3 (1%)
1	C	232/236 (98%)	-0.14	1 (0%)	88	86	14, 25, 44, 49	2 (0%)
1	D	230/236 (97%)	-0.05	3 (1%)	75	71	15, 26, 39, 82	1 (0%)
1	E	233/236 (98%)	0.09	5 (2%)	63	58	11, 27, 55, 68	2 (0%)
1	F	231/236 (97%)	0.21	5 (2%)	62	57	19, 27, 50, 59	0
All	All	1389/1416 (98%)	0.01	28 (2%)	65	60	11, 26, 48, 82	9 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	232	VAL	4.1
1	F	148	LEU	3.5
1	B	234	ALA	3.2
1	A	140	SER	3.1
1	A	40[A]	ARG	3.1
1	B	3	ASP	2.8
1	E	2	ASN	2.8
1	D	3	ASP	2.8
1	E	234	ALA	2.7
1	A	149	ARG	2.7
1	A	139	CYS	2.5
1	D	2	ASN	2.4
1	A	118	ASP	2.4
1	F	149	ARG	2.4
1	A	6	ARG	2.3
1	E	5	SER	2.3
1	B	233	ALA	2.3
1	E	148	LEU	2.3
1	A	142	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	148	LEU	2.2
1	E	233	ALA	2.2
1	F	147	HIS	2.2
1	C	139	CYS	2.1
1	B	6	ARG	2.1
1	A	147	HIS	2.1
1	A	8	ASN	2.1
1	D	5	SER	2.1
1	F	44	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

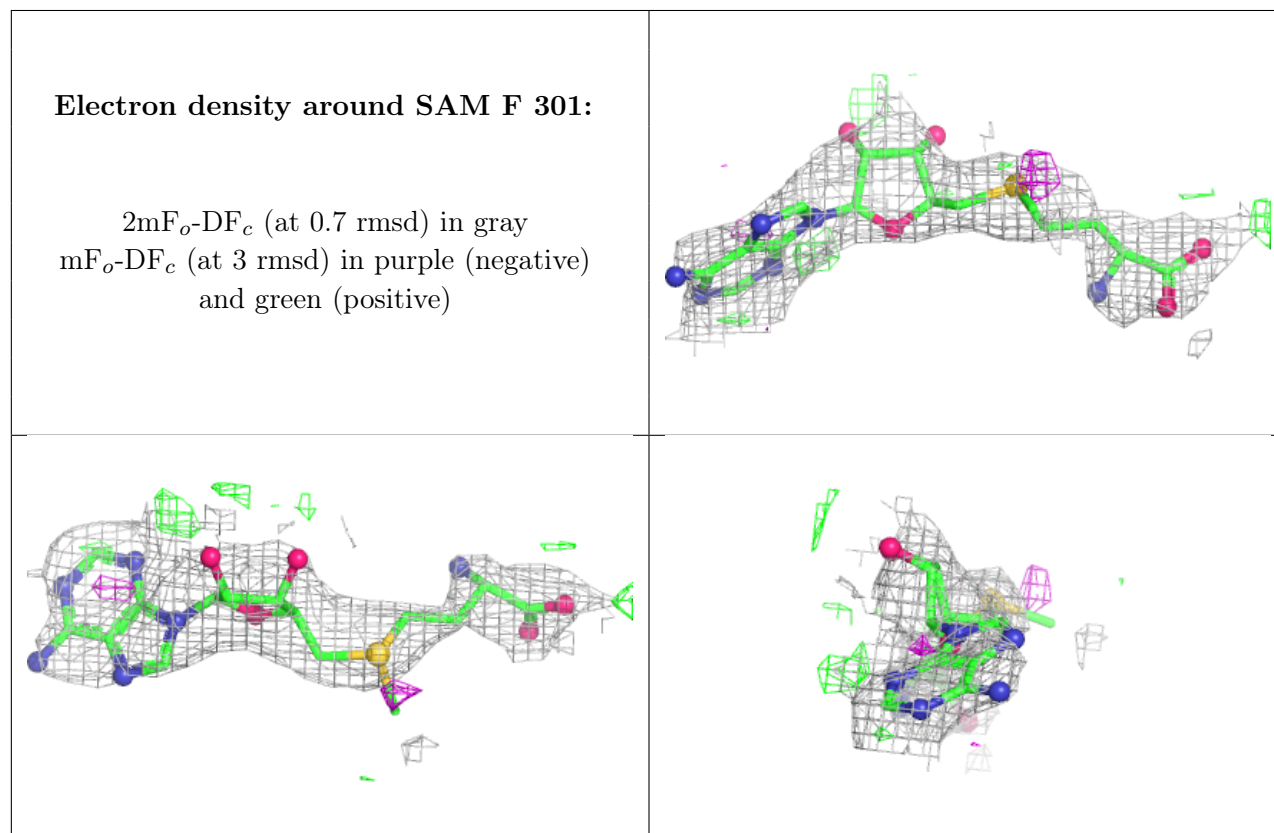
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	D	300	1/1	0.45	0.40	79,79,79,79	0
2	MG	E	300	1/1	0.46	0.32	93,93,93,93	0
2	MG	A	300	1/1	0.70	0.27	95,95,95,95	0
3	SAM	F	301	27/27	0.74	0.20	90,92,92,93	0
2	MG	F	300	1/1	0.75	0.29	91,91,91,91	0
3	SAM	E	301	27/27	0.76	0.20	89,91,91,91	0
3	SAM	A	301	27/27	0.77	0.23	87,90,91,91	0
2	MG	B	300	1/1	0.81	0.19	53,53,53,53	0
2	MG	C	300	1/1	0.82	0.17	50,50,50,50	0
3	SAM	C	301	27/27	0.83	0.20	74,78,81,82	0
3	SAM	B	301	27/27	0.85	0.17	60,63,67,68	0
3	SAM	D	301	26/27	0.85	0.19	68,73,77,77	0
5	P4C	D	500	22/22	0.86	0.20	72,73,77,78	0
4	PEG	A	401	7/7	0.87	0.19	55,55,56,56	0

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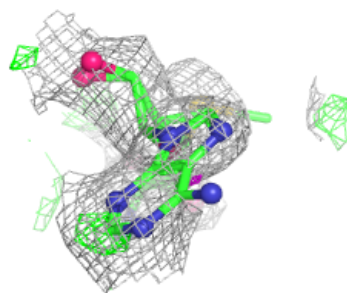
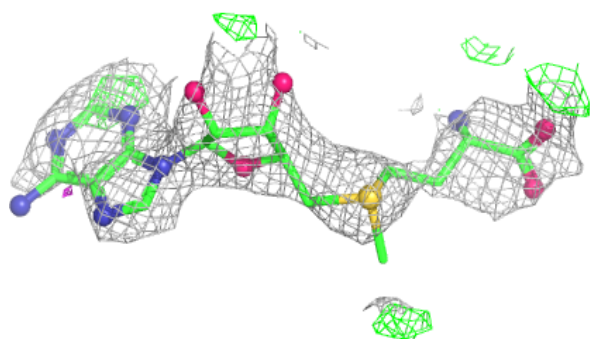
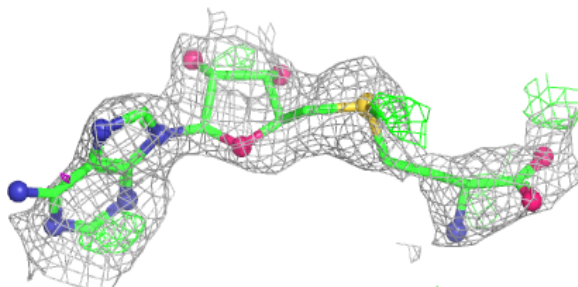
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	P4C	B	500	22/22	0.88	0.19	59,61,67,69	0
4	PEG	B	401	7/7	0.88	0.22	50,51,51,52	0
5	P4C	A	500	22/22	0.90	0.17	68,71,72,72	0
4	PEG	D	401	7/7	0.91	0.21	74,74,75,75	0

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

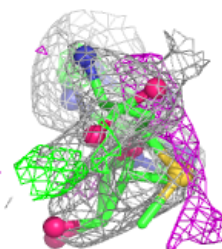
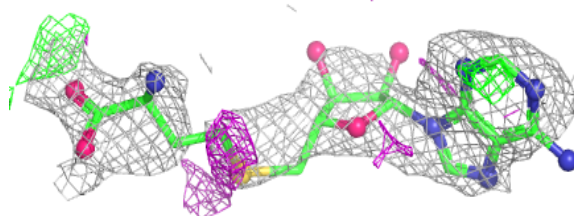
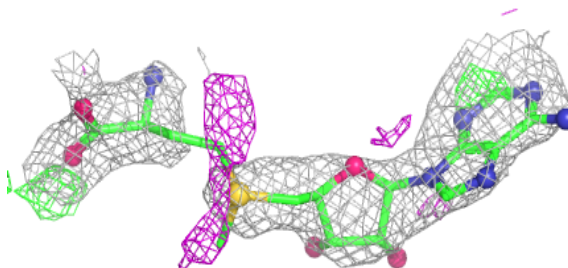


Electron density around SAM E 301:

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

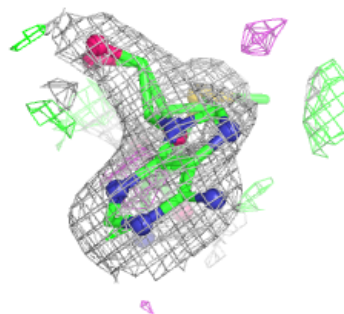
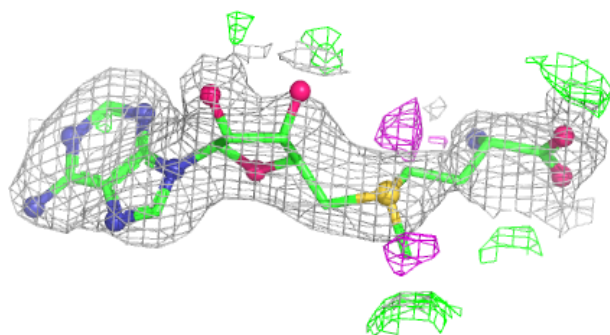
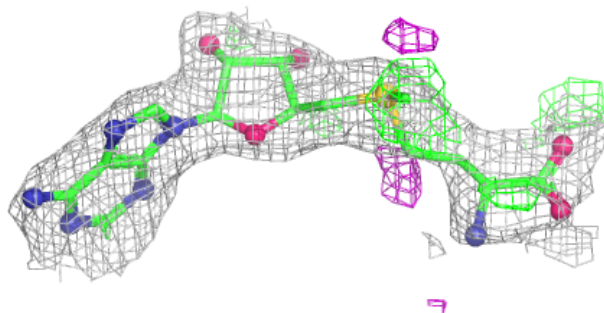
**Electron density around SAM A 301:**

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

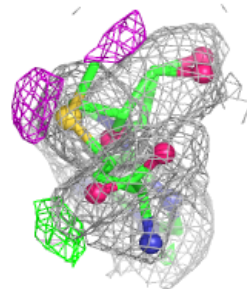
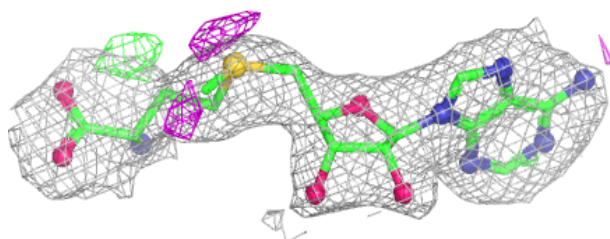
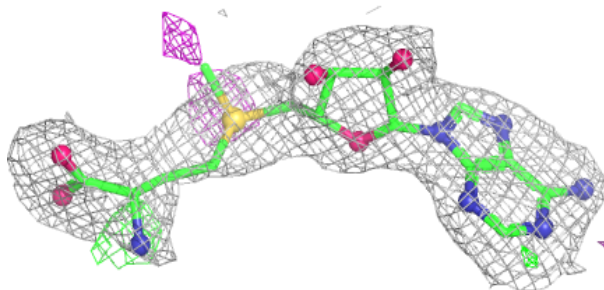


Electron density around SAM C 301:

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

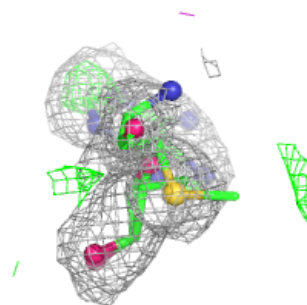
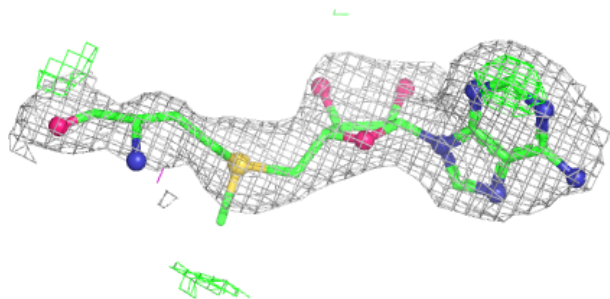
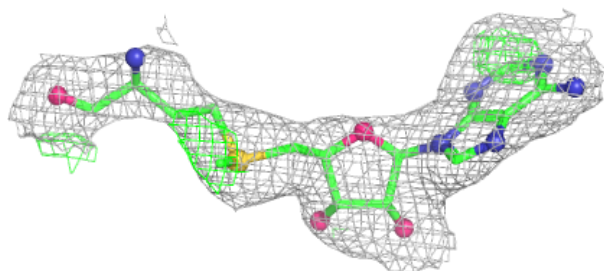
**Electron density around SAM B 301:**

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

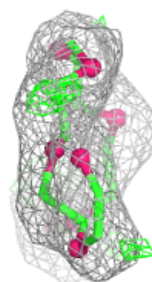
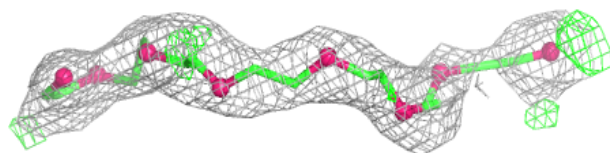
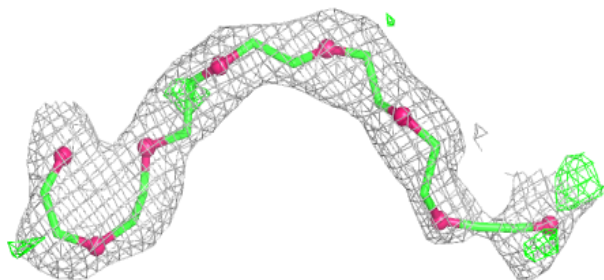


Electron density around SAM D 301:

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

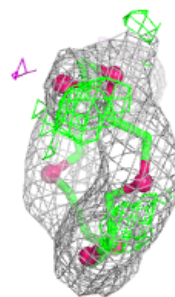
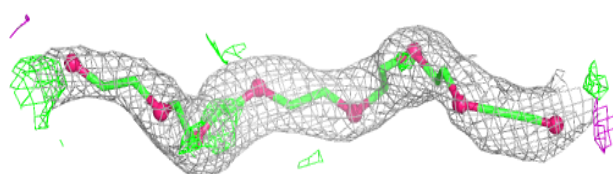
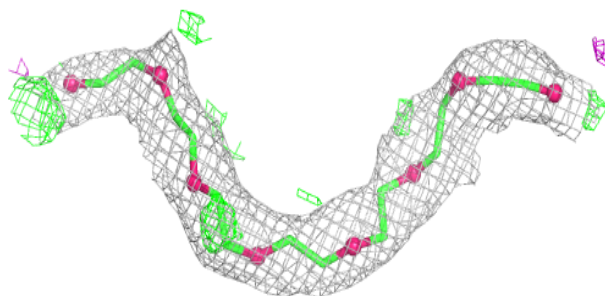
**Electron density around P4C D 500:**

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

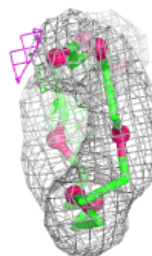
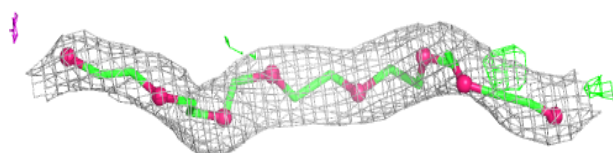
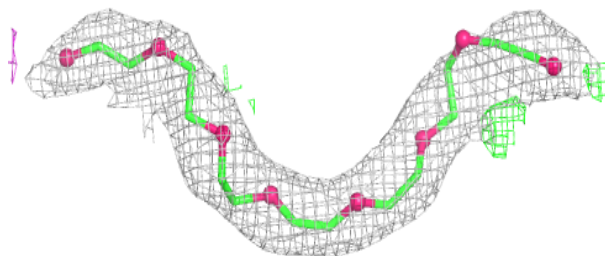


Electron density around P4C B 500:

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

**Electron density around P4C A 500:**

$2mF_o-DF_c$ (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.