



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:32 PM BST

PDB ID : 5X8G
Title : Binary complex structure of a double mutant I454RA456K of o-Succinylbenzoate CoA Synthetase (MenE) from Bacillus Subtilis bound with its product analogue OSB-NCoA at 1.90 angstrom
Authors : Chen, Y.; Guo, Z.
Deposited on : 2017-03-02
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

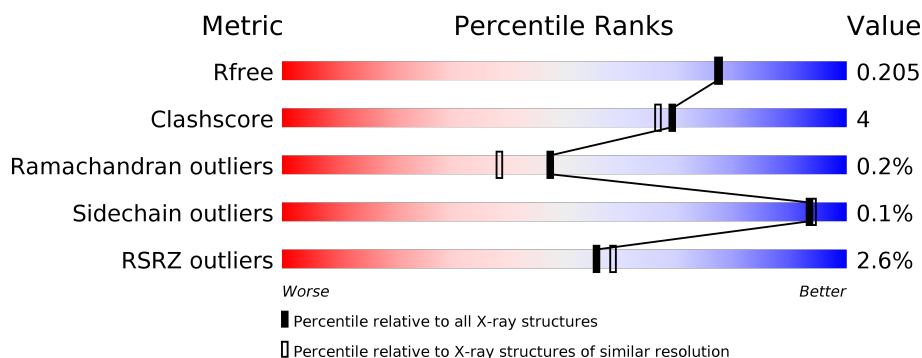
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	485	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	B	485	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	C	485	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	D	485	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16815 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.

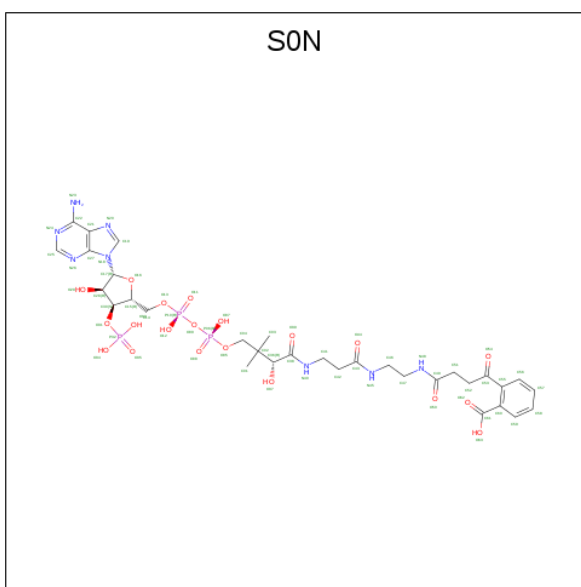
- Molecule 1 is a protein called 2-succinylbenzoate--CoA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	7	1
			3709	2368	614	704	23			
1	B	483	Total	C	N	O	S	0	6	1
			3681	2354	610	695	22			
1	D	483	Total	C	N	O	S	0	8	1
			3698	2359	619	697	23			
1	C	485	Total	C	N	O	S	0	7	1
			3725	2377	616	709	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	ARG	ILE	engineered mutation	UNP P23971
A	456	LYS	ALA	engineered mutation	UNP P23971
B	454	ARG	ILE	engineered mutation	UNP P23971
B	456	LYS	ALA	engineered mutation	UNP P23971
D	454	ARG	ILE	engineered mutation	UNP P23971
D	456	LYS	ALA	engineered mutation	UNP P23971
C	454	ARG	ILE	engineered mutation	UNP P23971
C	456	LYS	ALA	engineered mutation	UNP P23971

- Molecule 2 is o-succinylbenzoyl-N-coenzyme A (three-letter code: S0N) (formula: $C_{32}H_{45}N_8O_{20}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			63	32	8	20	3		
2	B	1	Total	C	N	O	P	0	0
			63	32	8	20	3		
2	D	1	Total	C	N	O	P	0	0
			63	32	8	20	3		
2	C	1	Total	C	N	O	P	0	0
			63	32	8	20	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mg	0	0
			3	3		
3	A	3	Total	Mg	0	0
			3	3		
3	D	2	Total	Mg	0	0
			2	2		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

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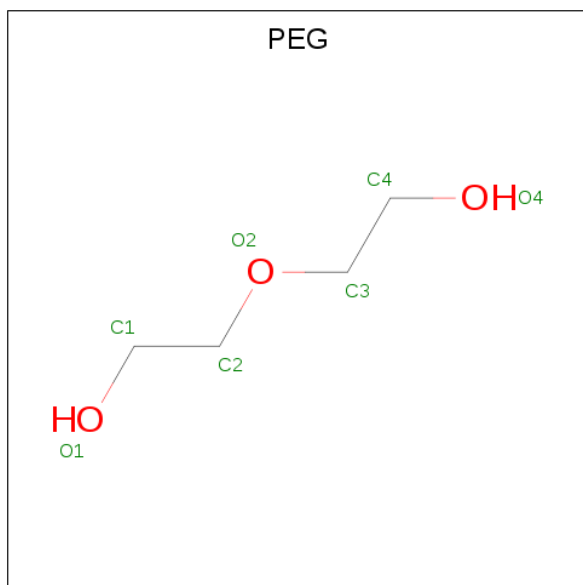
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	D	1	Total	Ca	0	0
			1	1		
4	C	4	Total	Ca	0	0
			4	4		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

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

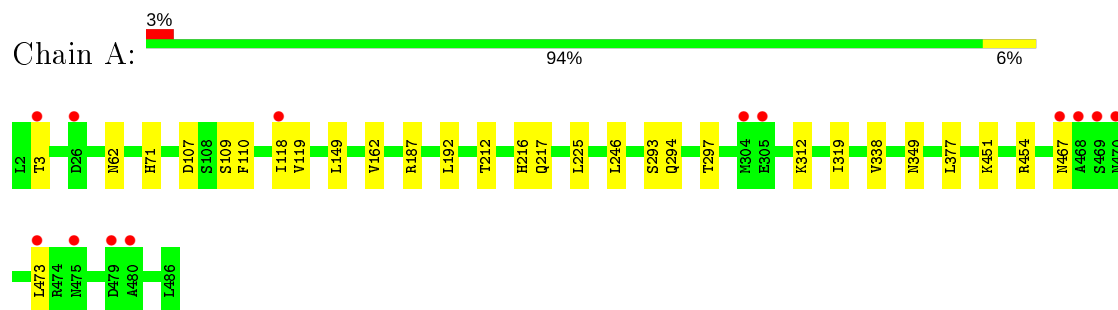
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	441	Total	O	0	0
			441	441		
7	B	424	Total	O	0	0
			424	424		
7	D	372	Total	O	0	0
			372	372		
7	C	442	Total	O	0	0
			442	442		

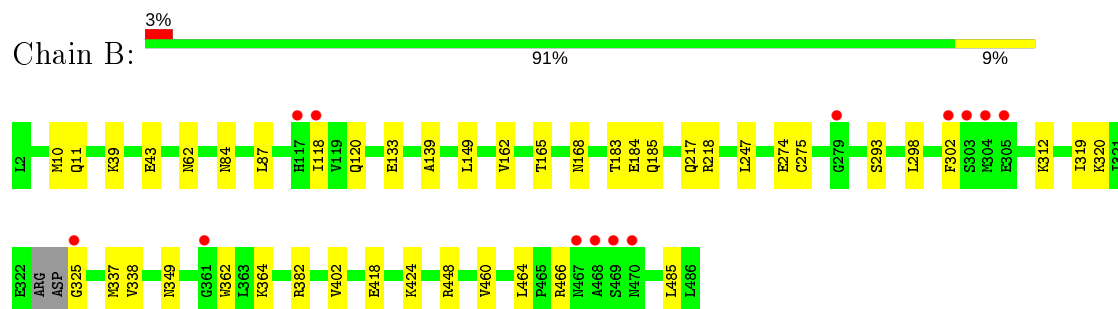
3 Residue-property plots [i](#)

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.

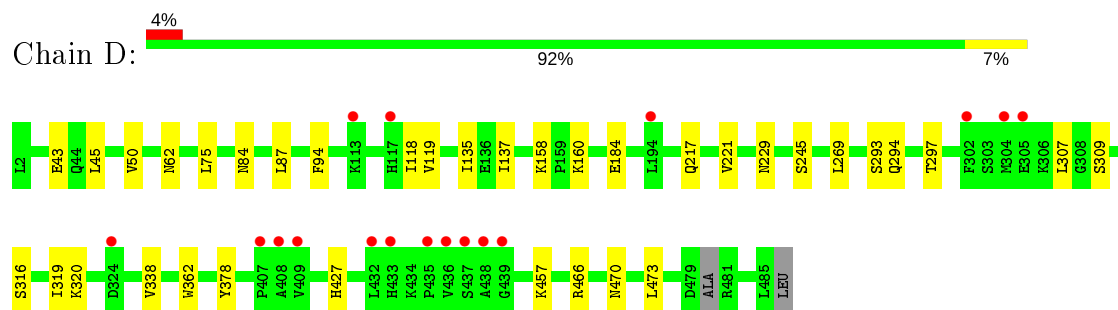
- Molecule 1: 2-succinylbenzoate--CoA ligase



- Molecule 1: 2-succinylbenzoate--CoA ligase

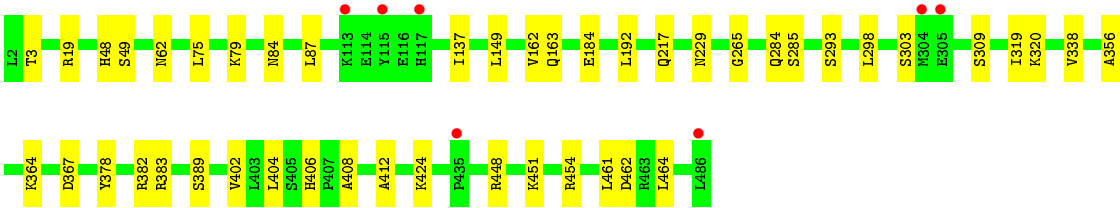


- Molecule 1: 2-succinylbenzoate--CoA ligase



- Molecule 1: 2-succinylbenzoate--CoA ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.95Å 96.48Å 97.66Å 80.14° 77.81° 81.17°	Depositor
Resolution (Å)	31.03 – 1.90 31.03 – 1.90	Depositor EDS
% Data completeness (in resolution range)	91.5 (31.03-1.90) 91.6 (31.03-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.164 , 0.206 0.165 , 0.205	Depositor DCC
R_{free} test set	1989 reflections (1.10%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.059 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16815	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: NA, MG, PEG, CA, S0N

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	0.39	0/3800	0.55	0/5153
1	B	0.44	0/3772	0.55	0/5116
1	C	0.44	0/3814	0.56	0/5170
1	D	0.39	0/3793	0.53	0/5144
All	All	0.42	0/15179	0.55	0/20583

There are no bond length outliers.

There are no bond angle outliers.

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	3709	0	3627	22	0
1	B	3681	0	3599	36	0
1	C	3725	0	3650	33	0
1	D	3698	0	3608	22	0
2	A	63	0	40	1	0
2	B	63	0	40	2	0
2	C	63	0	40	1	0
2	D	63	0	40	0	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	21	0	30	3	0
6	C	14	0	20	0	0
6	D	14	0	20	5	0
7	A	441	0	0	3	2
7	B	424	0	0	8	0
7	C	442	0	0	10	1
7	D	372	0	0	2	1
All	All	16815	0	14714	110	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

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)
2:A:501:S0N:O16	2:A:501:S0N:C17	1.63	1.21
2:B:501:S0N:C17	2:B:501:S0N:O16	1.64	1.14
1:B:184:GLU:H	6:D:507:PEG:H32	1.44	0.81
1:A:349:ASN:ND2	1:B:349[B]:ASN:HD21	1.81	0.79
1:C:356:ALA:O	1:C:364:LYS:NZ	2.19	0.76
1:B:418:GLU:OE1	1:B:424:LYS:NZ	2.19	0.76
6:A:508:PEG:H32	1:C:184:GLU:H	1.52	0.75
1:B:184:GLU:N	6:D:507:PEG:H32	2.02	0.74
1:B:312:LYS:NZ	7:B:601:HOH:O	2.22	0.72
1:C:229:ASN:OD1	7:C:601:HOH:O	2.07	0.72
1:C:406:HIS:HD2	1:C:408:ALA:H	1.37	0.72
1:A:312:LYS:NZ	7:A:601:HOH:O	2.23	0.71
1:C:319[A]:ILE:HG22	1:C:338:VAL:HG12	1.74	0.68
1:B:319[A]:ILE:HG22	1:B:338:VAL:HG12	1.76	0.67
1:B:118:ILE:HG13	1:B:118:ILE:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:LEU:O	1:D:50:VAL:HG13	1.97	0.64
2:C:508:S0N:O33	7:C:602:HOH:O	2.14	0.64
1:C:406:HIS:CD2	1:C:408:ALA:H	2.16	0.62
1:D:75:LEU:HD22	1:D:137:ILE:HD12	1.81	0.61
1:C:382:ARG:NH2	7:C:612:HOH:O	2.34	0.61
1:B:165:THR:H	1:B:168:ASN:HD22	1.48	0.60
1:A:349:ASN:ND2	1:B:349[B]:ASN:ND2	2.49	0.60
1:A:467:ASN:HB3	1:A:473:LEU:HD21	1.82	0.59
1:A:62:ASN:HB2	1:A:217:GLN:HA	1.84	0.59
1:C:75:LEU:HD22	1:C:137:ILE:HD12	1.85	0.59
1:D:294:GLN:OE1	1:D:297[A]:THR:HG21	2.02	0.59
1:B:165:THR:H	1:B:168:ASN:ND2	2.02	0.57
1:A:118:ILE:HG22	1:A:119:VAL:HG13	1.86	0.57
1:C:62:ASN:HB2	1:C:217:GLN:HA	1.87	0.57
1:B:448[A]:ARG:NH1	7:B:610:HOH:O	2.37	0.57
1:C:149:LEU:HD12	1:C:162:VAL:O	2.05	0.57
1:B:11:GLN:HE22	1:D:316:SER:H	1.52	0.57
1:B:424:LYS:NZ	7:B:609:HOH:O	2.37	0.57
1:D:184:GLU:H	6:D:506:PEG:H41	1.69	0.57
1:D:62:ASN:HB2	1:D:217:GLN:HA	1.87	0.56
1:A:216:HIS:HD2	7:A:675:HOH:O	1.87	0.56
1:B:62:ASN:HB2	1:B:217:GLN:HA	1.86	0.56
1:B:185:GLN:NE2	7:B:613:HOH:O	2.39	0.56
1:D:84:ASN:HB3	1:D:87:LEU:HG	1.87	0.55
1:B:11:GLN:NE2	1:D:316:SER:H	2.05	0.55
1:A:349:ASN:HD21	1:B:349[B]:ASN:HD21	1.55	0.55
1:D:269:LEU:HD22	1:D:307:LEU:HG	1.88	0.54
1:B:464:LEU:O	1:B:466:ARG:HG3	2.07	0.54
1:A:319[A]:ILE:HG22	1:A:338:VAL:HG12	1.89	0.54
1:A:107:ASP:OD1	1:A:109[B]:SER:OG	2.16	0.53
1:A:319[B]:ILE:HD11	1:A:377:LEU:HD13	1.90	0.53
1:D:319[A]:ILE:HG22	1:D:338:VAL:HG12	1.90	0.53
1:C:424:LYS:HD2	7:C:836:HOH:O	2.09	0.53
1:D:229:ASN:ND2	7:D:608:HOH:O	2.41	0.52
1:C:284:GLN:HE21	1:C:285[A]:SER:H	1.57	0.52
1:D:184:GLU:H	6:D:506:PEG:C4	2.23	0.52
1:D:160:LYS:NZ	7:D:610:HOH:O	2.42	0.52
1:C:461:LEU:HD22	1:C:464:LEU:HD23	1.92	0.52
1:C:284:GLN:HE21	1:C:285[B]:SER:H	1.58	0.51
1:A:294:GLN:OE1	1:A:297[A]:THR:HG21	2.10	0.51
1:D:94:PHE:CE1	1:D:158:LYS:HD3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:HD21	1:B:275:CYS:SG	2.51	0.51
1:C:265:GLY:O	7:C:603:HOH:O	2.19	0.50
1:D:466:ARG:HD3	1:D:470:ASN:O	2.11	0.50
6:A:508:PEG:C3	1:C:184:GLU:H	2.22	0.50
1:C:19:ARG:HD3	7:C:642:HOH:O	2.12	0.50
1:C:451:LYS:HG3	1:C:454:ARG:NH1	2.27	0.49
1:B:10:MET:HE1	1:B:139:ALA:O	2.13	0.49
1:B:402:VAL:HG13	1:B:448[A]:ARG:HD2	1.95	0.48
1:B:183:THR:OG1	6:D:507:PEG:H11	2.14	0.48
1:C:84:ASN:HB3	1:C:87:LEU:HG	1.97	0.47
1:D:43:GLU:HG2	1:D:135:ILE:HG12	1.96	0.47
1:B:382:ARG:NH1	7:B:604:HOH:O	2.29	0.47
1:B:84:ASN:HB3	1:B:87:LEU:HG	1.97	0.47
1:C:309:SER:HB2	1:C:378:TYR:CZ	2.50	0.47
1:A:225:LEU:HD21	1:A:246:LEU:HD11	1.97	0.47
1:A:109[B]:SER:OG	1:A:110:PHE:CD1	2.68	0.46
1:C:79:LYS:NZ	7:C:611:HOH:O	2.32	0.46
1:B:320:LYS:HE2	1:B:362:TRP:CD2	2.51	0.46
1:B:133:GLU:HG2	7:B:875:HOH:O	2.16	0.46
6:A:508:PEG:H32	1:C:184:GLU:N	2.25	0.45
1:B:39:LYS:O	1:B:43:GLU:HG3	2.17	0.45
1:B:298:LEU:HD11	1:B:302:PHE:HB2	1.97	0.45
1:D:320:LYS:HE2	1:D:362:TRP:CD2	2.52	0.45
1:D:221:VAL:HG21	1:D:245:SER:HB3	1.99	0.45
1:A:349:ASN:CG	1:B:349[B]:ASN:ND2	2.69	0.45
1:B:460:VAL:HG13	1:B:485:LEU:HB2	2.00	0.44
1:A:71:HIS:HE1	7:A:777:HOH:O	2.01	0.44
1:A:187:ARG:HG2	1:A:212:THR:HB	2.00	0.43
1:D:427:HIS:CE1	1:D:457:LYS:HD2	2.52	0.43
1:C:3:THR:OG1	7:C:605:HOH:O	2.21	0.43
1:C:319[B]:ILE:HG12	1:C:320:LYS:N	2.34	0.43
1:B:325:GLY:CA	7:B:850:HOH:O	2.65	0.43
1:C:389:SER:HB2	1:C:424:LYS:O	2.19	0.43
1:B:149:LEU:HA	1:B:162:VAL:O	2.18	0.43
1:B:337:MET:HG2	1:B:364:LYS:HG2	2.00	0.43
1:C:163:GLN:NE2	7:C:611:HOH:O	2.41	0.43
1:C:462:ASP:OD2	7:C:604:HOH:O	2.21	0.43
1:C:48:HIS:O	1:C:49:SER:OG	2.29	0.43
1:A:3:THR:O	1:A:3:THR:HG22	2.18	0.43
1:C:298:LEU:HD21	1:C:303:SER:HA	2.01	0.43
1:C:149:LEU:HD12	1:C:162:VAL:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LEU:O	1:A:192:LEU:HD12	2.19	0.43
1:A:451:LYS:HD3	1:A:454:ARG:NH1	2.33	0.43
1:D:466:ARG:HA	1:D:473:LEU:HD22	2.01	0.43
1:D:309:SER:HB2	1:D:378:TYR:CZ	2.54	0.41
1:D:118:ILE:HG22	1:D:119:VAL:HG13	2.02	0.41
1:C:367:ASP:OD1	1:C:383:ARG:HD2	2.20	0.41
1:C:402:VAL:HG13	1:C:448[A]:ARG:HD2	2.03	0.41
1:B:218:ARG:NH2	2:B:501:S0N:O07	2.49	0.41
1:C:404:LEU:CD2	1:C:412:ALA:HB3	2.51	0.41
1:A:149:LEU:HA	1:A:162:VAL:O	2.21	0.41
1:B:247:LEU:HD23	1:B:274:GLU:OE1	2.21	0.40
1:A:3:THR:O	1:A:3:THR:CG2	2.70	0.40
1:B:120:GLN:NE2	7:B:615:HOH:O	2.40	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:627:HOH:O	7:C:629:HOH:O[1_455]	2.12	0.08
7:A:616:HOH:O	7:D:849:HOH:O[1_556]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	490/485 (101%)	479 (98%)	10 (2%)	1 (0%)	47	38
1	B	485/485 (100%)	474 (98%)	10 (2%)	1 (0%)	47	38
1	C	489/485 (101%)	477 (98%)	11 (2%)	1 (0%)	47	38
1	D	487/485 (100%)	476 (98%)	10 (2%)	1 (0%)	47	38
All	All	1951/1940 (101%)	1906 (98%)	41 (2%)	4 (0%)	47	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	SER
1	B	293	SER
1	D	293	SER
1	C	293	SER

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	388/414 (94%)	388 (100%)	0	100	100
1	B	384/414 (93%)	384 (100%)	0	100	100
1	C	393/414 (95%)	392 (100%)	1 (0%)	92	93
1	D	387/414 (94%)	387 (100%)	0	100	100
All	All	1552/1656 (94%)	1551 (100%)	1 (0%)	93	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	192	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	164	GLN
1	A	216	HIS
1	A	349	ASN
1	B	11	GLN
1	B	120	GLN
1	B	168	ASN
1	B	393	ASN
1	D	120	GLN
1	D	226	HIS

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Mol	Chain	Res	Type
1	D	251	ASN
1	C	251	ASN
1	C	284	GLN
1	C	406	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 22 are monoatomic - leaving 11 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	$\# Z > 2$
6	PEG	D	506	-	6,6,6	0.52	0	5,5,5	0.30	0
2	S0N	D	501	3	56,66,66	3.90	13 (23%)	70,97,97	1.54	11 (15%)
6	PEG	D	507	-	6,6,6	0.54	0	5,5,5	0.48	0
2	S0N	C	508	3,4	56,66,66	3.95	14 (25%)	70,97,97	1.62	10 (14%)
2	S0N	A	501	3	56,66,66	3.91	13 (23%)	70,97,97	1.62	13 (18%)
6	PEG	A	508	-	6,6,6	0.62	0	5,5,5	0.37	0
6	PEG	C	506	-	6,6,6	0.55	0	5,5,5	0.28	0
6	PEG	C	507	-	6,6,6	0.56	0	5,5,5	0.30	0
6	PEG	A	510	-	6,6,6	0.52	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	S0N	B	501	3	56,66,66	3.99	13 (23%)	70,97,97	1.65	13 (18%)
6	PEG	A	509	-	6,6,6	0.52	0	5,5,5	0.27	0

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
6	PEG	D	506	-	-	2/4/4/4	-
2	S0N	D	501	3	-	8/56/80/80	0/4/4/4
6	PEG	D	507	-	-	3/4/4/4	-
2	S0N	C	508	3,4	-	11/56/80/80	0/4/4/4
2	S0N	A	501	3	-	7/56/80/80	0/4/4/4
6	PEG	A	508	-	-	3/4/4/4	-
6	PEG	C	506	-	-	2/4/4/4	-
6	PEG	C	507	-	-	3/4/4/4	-
6	PEG	A	510	-	-	3/4/4/4	-
2	S0N	B	501	3	-	9/56/80/80	0/4/4/4
6	PEG	A	509	-	-	3/4/4/4	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	508	S0N	C28-C17	-16.91	1.28	1.53
2	D	501	S0N	C28-C17	-16.84	1.28	1.53
2	B	501	S0N	C28-C17	-16.57	1.28	1.53
2	B	501	S0N	O16-C17	16.41	1.64	1.41
2	A	501	S0N	O16-C17	16.39	1.63	1.41
2	C	508	S0N	O16-C17	15.89	1.63	1.41
2	A	501	S0N	C28-C17	-15.80	1.29	1.53
2	D	501	S0N	O16-C17	15.33	1.62	1.41
2	A	501	S0N	C60-C61	9.66	1.56	1.47
2	B	501	S0N	C60-C61	9.58	1.56	1.47
2	C	508	S0N	C60-C61	9.24	1.56	1.47
2	D	501	S0N	C60-C61	8.79	1.55	1.47
2	B	501	S0N	O16-C15	-6.81	1.29	1.45
2	D	501	S0N	O16-C15	-6.80	1.29	1.45
2	C	508	S0N	O16-C15	-6.64	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	S0N	O16-C15	-6.60	1.30	1.45
2	A	501	S0N	C55-C53	5.92	1.60	1.48
2	D	501	S0N	C55-C53	5.79	1.59	1.48
2	D	501	S0N	C38-N40	5.74	1.46	1.33
2	B	501	S0N	C55-C53	5.64	1.59	1.48
2	C	508	S0N	C49-N48	5.56	1.46	1.33
2	B	501	S0N	C38-N40	5.51	1.45	1.33
2	B	501	S0N	C49-N48	5.38	1.45	1.33
2	C	508	S0N	C55-C53	5.27	1.58	1.48
2	A	501	S0N	C38-N40	5.20	1.45	1.33
2	C	508	S0N	C38-N40	5.17	1.44	1.33
2	D	501	S0N	C49-N48	5.15	1.45	1.33
2	C	508	S0N	C43-N45	5.14	1.45	1.33
2	A	501	S0N	C49-N48	5.04	1.44	1.33
2	A	501	S0N	C43-N45	4.76	1.44	1.33
2	D	501	S0N	C43-N45	4.76	1.44	1.33
2	C	508	S0N	C52-C53	4.75	1.58	1.51
2	B	501	S0N	C43-N45	4.62	1.43	1.33
2	D	501	S0N	C52-C53	4.60	1.57	1.51
2	B	501	S0N	C52-C53	4.50	1.57	1.51
2	A	501	S0N	C52-C53	4.29	1.57	1.51
2	A	501	S0N	O29-C28	3.63	1.51	1.43
2	D	501	S0N	O29-C28	3.59	1.51	1.43
2	B	501	S0N	O29-C28	3.57	1.51	1.43
2	C	508	S0N	O29-C28	3.57	1.51	1.43
2	B	501	S0N	C22-N23	2.76	1.44	1.34
2	B	501	S0N	C21-C27	-2.74	1.33	1.40
2	A	501	S0N	C21-C27	-2.73	1.33	1.40
2	D	501	S0N	C21-C27	-2.71	1.33	1.40
2	C	508	S0N	C22-N23	2.69	1.43	1.34
2	D	501	S0N	C22-N23	2.66	1.43	1.34
2	C	508	S0N	C21-C27	-2.61	1.34	1.40
2	D	501	S0N	C25-N26	2.52	1.36	1.32
2	A	501	S0N	C22-N23	2.43	1.42	1.34
2	C	508	S0N	C25-N26	2.32	1.35	1.32
2	A	501	S0N	C25-N26	2.31	1.35	1.32
2	B	501	S0N	C25-N26	2.21	1.35	1.32
2	C	508	S0N	C01-C02	-2.01	1.49	1.53

All (47) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	508	S0N	N26-C25-N24	-5.70	119.77	128.68
2	B	501	S0N	N26-C25-N24	-5.60	119.93	128.68
2	A	501	S0N	N26-C25-N24	-5.59	119.94	128.68
2	D	501	S0N	N26-C25-N24	-5.50	120.09	128.68
2	C	508	S0N	C51-C52-C53	-5.42	106.20	112.76
2	C	508	S0N	C41-C42-C43	-5.22	103.67	112.36
2	A	501	S0N	C41-C42-C43	-4.88	104.22	112.36
2	D	501	S0N	C41-C42-C43	-4.86	104.27	112.36
2	D	501	S0N	C51-C52-C53	-4.73	107.04	112.76
2	A	501	S0N	C51-C52-C53	-4.47	107.35	112.76
2	B	501	S0N	C41-C42-C43	-4.27	105.25	112.36
2	B	501	S0N	C51-C52-C53	-4.12	107.77	112.76
2	B	501	S0N	O05-C04-C02	-4.01	104.10	110.55
2	A	501	S0N	C30-C28-C17	3.84	108.40	99.89
2	C	508	S0N	C01-C02-C36	3.67	115.18	108.82
2	B	501	S0N	C21-C22-N23	3.55	125.74	120.35
2	B	501	S0N	C14-C15-C30	-3.35	103.30	114.40
2	B	501	S0N	C30-C28-C17	3.30	107.19	99.89
2	C	508	S0N	C21-C22-N23	3.19	125.20	120.35
2	B	501	S0N	C41-N40-C38	-3.18	116.92	122.59
2	A	501	S0N	C14-C15-C30	-3.09	104.16	114.40
2	A	501	S0N	C21-C22-N23	3.01	124.93	120.35
2	A	501	S0N	C47-N48-C49	-2.97	117.32	122.84
2	D	501	S0N	P10-O09-P06	-2.94	122.75	132.83
2	D	501	S0N	C41-N40-C38	-2.86	117.48	122.59
2	D	501	S0N	C21-C22-N23	2.83	124.66	120.35
2	A	501	S0N	O05-C04-C02	-2.76	106.12	110.55
2	B	501	S0N	C01-C02-C36	2.70	113.50	108.82
2	B	501	S0N	C59-C60-C55	2.68	121.07	118.03
2	C	508	S0N	C52-C51-C49	-2.57	108.05	112.56
2	D	501	S0N	O50-C49-N48	-2.38	118.51	123.01
2	A	501	S0N	O50-C49-N48	-2.35	118.58	123.01
2	C	508	S0N	C51-C49-N48	2.33	120.35	116.42
2	D	501	S0N	C01-C02-C36	2.30	112.81	108.82
2	C	508	S0N	O05-C04-C02	-2.22	106.97	110.55
2	D	501	S0N	O05-C04-C02	-2.20	107.01	110.55
2	A	501	S0N	C59-C60-C55	2.18	120.50	118.03
2	C	508	S0N	C47-N48-C49	-2.15	118.84	122.84
2	C	508	S0N	P10-O09-P06	-2.14	125.47	132.83
2	B	501	S0N	C47-N48-C49	-2.10	118.94	122.84
2	D	501	S0N	C51-C49-N48	2.09	119.94	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	S0N	C51-C49-N48	2.08	119.93	116.42
2	B	501	S0N	O50-C49-N48	-2.08	119.10	123.01
2	D	501	S0N	C59-C60-C55	2.05	120.36	118.03
2	A	501	S0N	C41-N40-C38	-2.04	118.94	122.59
2	A	501	S0N	C01-C02-C36	2.04	112.35	108.82
2	B	501	S0N	C51-C49-N48	2.00	119.80	116.42

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	S0N	C04-O05-P06-O09
2	D	501	S0N	C14-O13-P10-O11
2	A	501	S0N	C04-O05-P06-O08
2	A	501	S0N	C14-O13-P10-O11
2	A	501	S0N	C30-O31-P32-O35
2	B	501	S0N	C04-O05-P06-O08
2	B	501	S0N	O13-C14-C15-C30
2	B	501	S0N	C30-O31-P32-O35
2	C	508	S0N	C04-O05-P06-O08
2	C	508	S0N	C14-O13-P10-O09
2	B	501	S0N	O13-C14-C15-O16
2	A	501	S0N	C51-C52-C53-C55
2	B	501	S0N	C51-C52-C53-C55
2	D	501	S0N	C51-C52-C53-C55
2	C	508	S0N	C51-C52-C53-C55
6	C	507	PEG	O2-C3-C4-O4
6	C	506	PEG	O2-C3-C4-O4
6	D	507	PEG	O1-C1-C2-O2
6	D	506	PEG	O1-C1-C2-O2
6	A	509	PEG	O1-C1-C2-O2
6	A	509	PEG	O2-C3-C4-O4
2	D	501	S0N	C51-C52-C53-O54
2	A	501	S0N	C51-C52-C53-O54
2	B	501	S0N	C51-C52-C53-O54
6	C	507	PEG	O1-C1-C2-O2
6	A	508	PEG	O1-C1-C2-O2
2	C	508	S0N	C51-C52-C53-O54
6	A	510	PEG	O2-C3-C4-O4
6	D	506	PEG	C4-C3-O2-C2
6	A	510	PEG	C1-C2-O2-C3
6	A	509	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
2	D	501	S0N	C14-O13-P10-O09
2	A	501	S0N	C04-O05-P06-O09
2	C	508	S0N	C04-O05-P06-O09
6	C	507	PEG	C1-C2-O2-C3
6	D	507	PEG	C1-C2-O2-C3
2	D	501	S0N	P06-O09-P10-O11
2	C	508	S0N	P06-O09-P10-O12
2	D	501	S0N	C04-O05-P06-O07
2	D	501	S0N	C04-O05-P06-O08
2	C	508	S0N	C14-O13-P10-O12
6	A	508	PEG	C1-C2-O2-C3
6	A	510	PEG	C4-C3-O2-C2
2	B	501	S0N	P06-O09-P10-O11
6	C	506	PEG	C1-C2-O2-C3
6	D	507	PEG	C4-C3-O2-C2
2	C	508	S0N	O37-C36-C38-O39
2	C	508	S0N	O37-C36-C38-N40
2	B	501	S0N	C04-O05-P06-O09
2	B	501	S0N	C30-O31-P32-O34
2	C	508	S0N	P06-O09-P10-O11
6	A	508	PEG	O2-C3-C4-O4
2	A	501	S0N	O50-C49-C51-C52
2	C	508	S0N	O50-C49-C51-C52

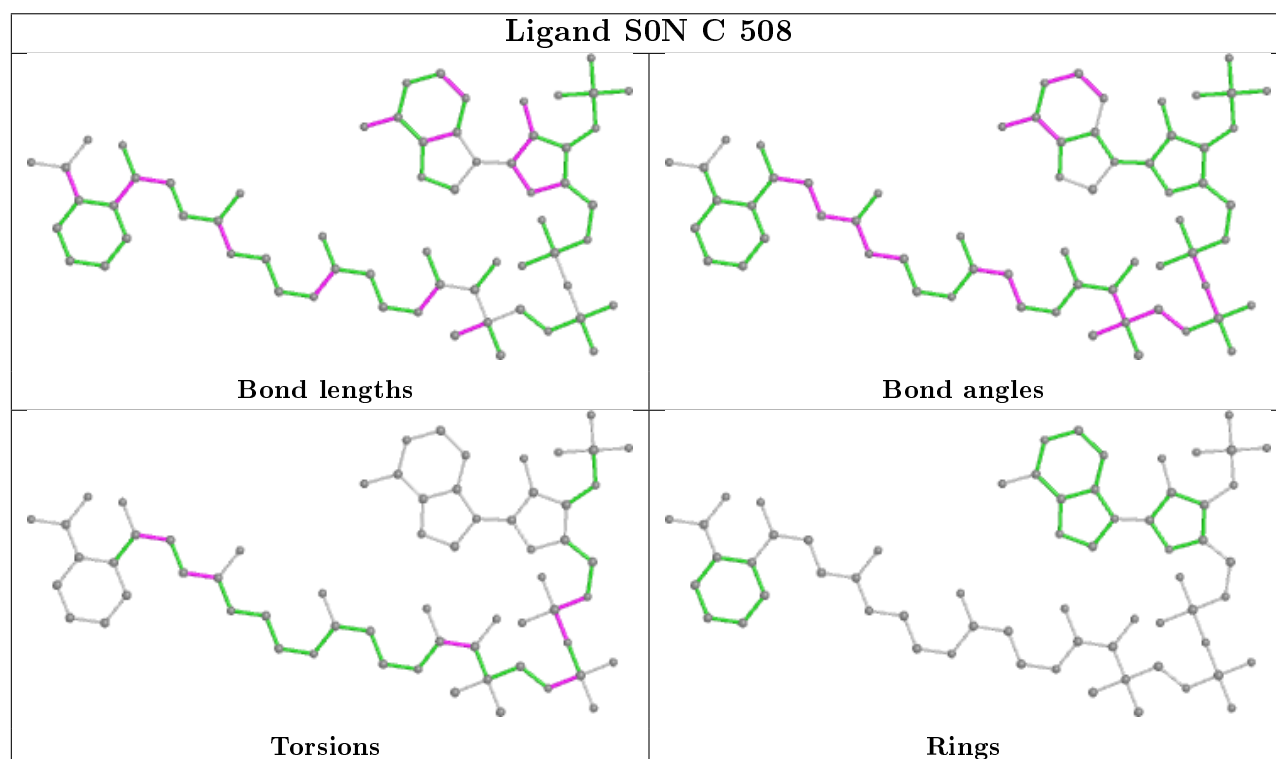
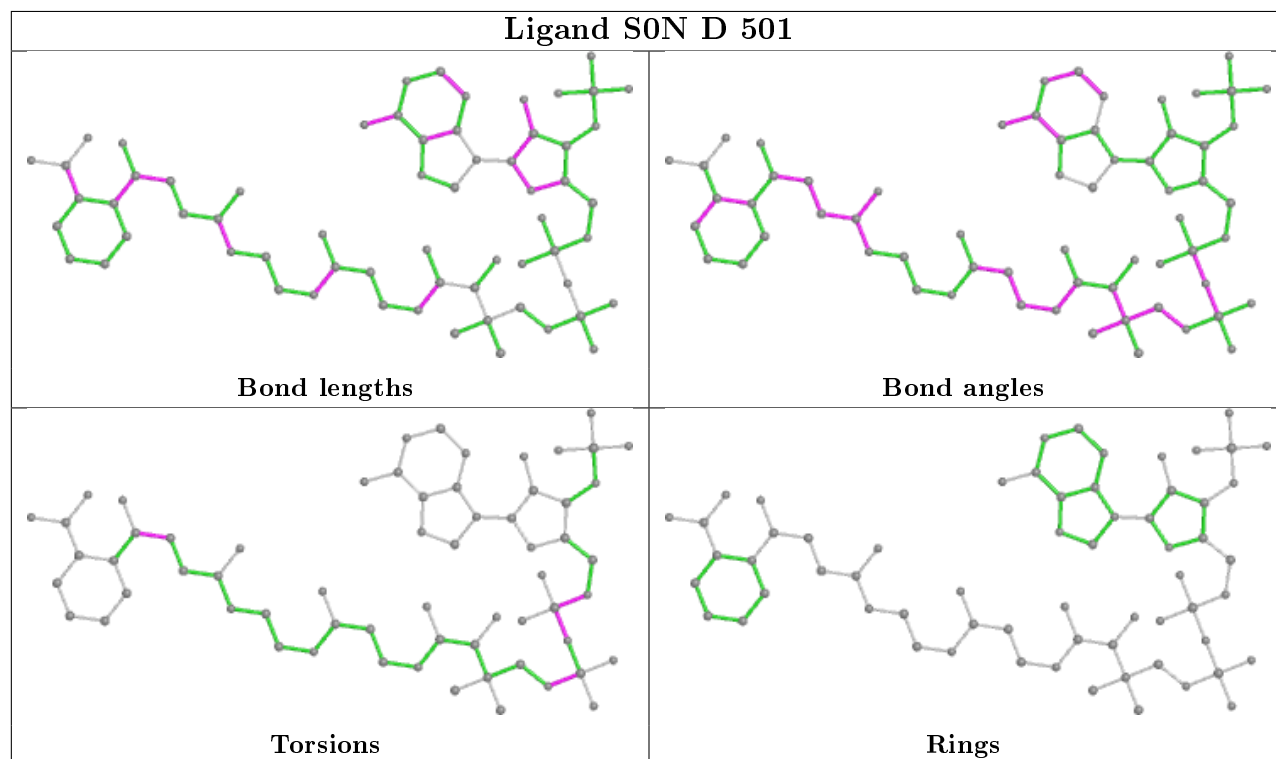
There are no ring outliers.

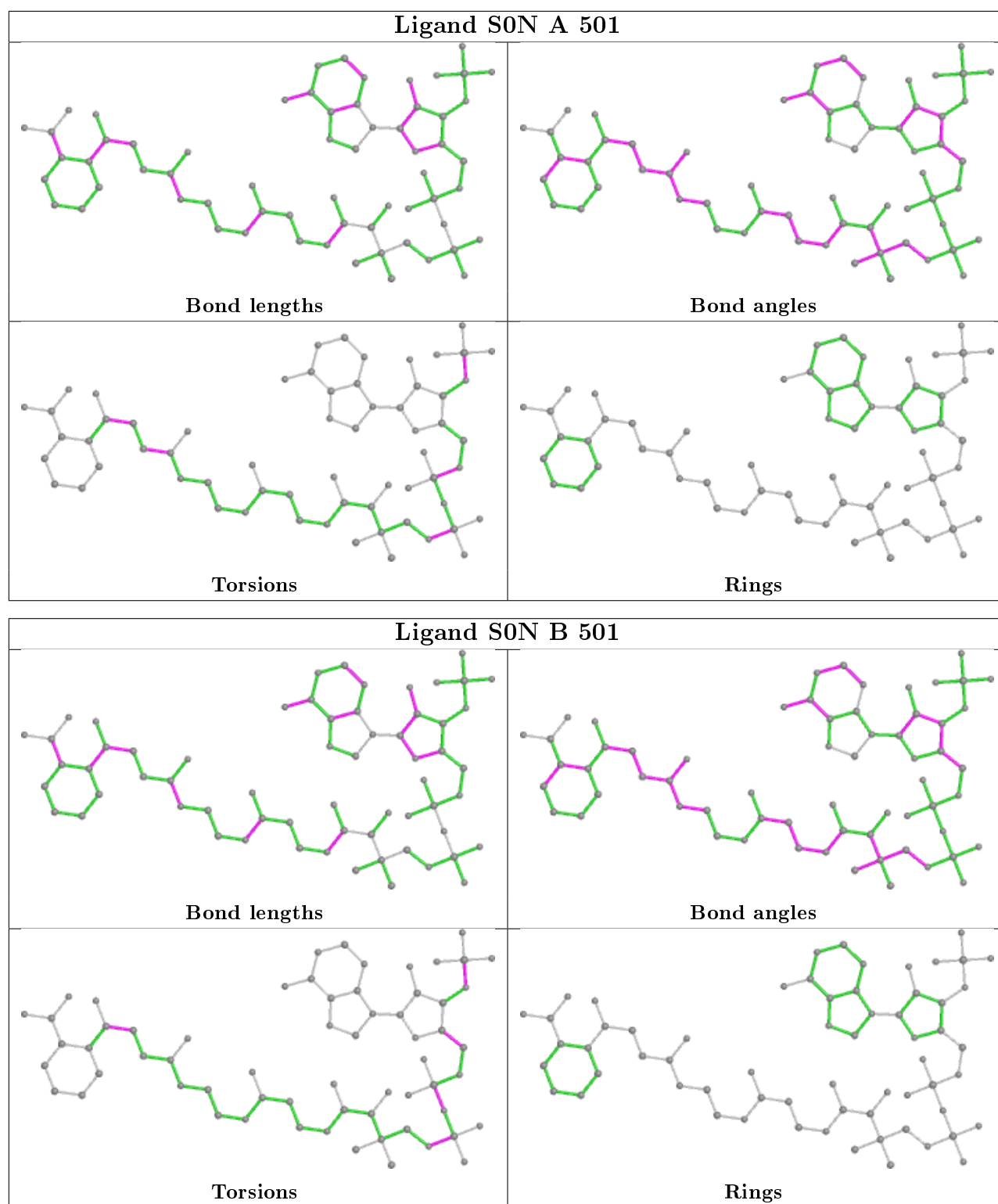
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	506	PEG	2	0
6	D	507	PEG	3	0
2	C	508	S0N	1	0
2	A	501	S0N	1	0
6	A	508	PEG	3	0
2	B	501	S0N	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	485/485 (100%)	-0.22	13 (2%) 54 57	13, 26, 55, 97	0
1	B	483/485 (99%)	-0.13	13 (2%) 54 57	13, 27, 57, 92	0
1	C	485/485 (100%)	-0.27	7 (1%) 75 77	13, 28, 51, 69	0
1	D	483/485 (99%)	-0.10	17 (3%) 44 47	14, 31, 62, 88	0
All	All	1936/1940 (99%)	-0.18	50 (2%) 56 58	13, 28, 57, 97	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	304	MET	6.2
1	A	468	ALA	4.9
1	B	303	SER	4.4
1	B	468	ALA	4.3
1	B	118	ILE	4.0
1	D	324	ASP	3.7
1	D	433	HIS	3.7
1	B	469	SER	3.6
1	B	305	GLU	3.6
1	B	117	HIS	3.6
1	A	469	SER	3.6
1	D	436	VAL	3.5
1	A	467	ASN	3.4
1	D	113	LYS	3.4
1	A	470	ASN	3.3
1	B	302	PHE	3.2
1	A	3	THR	3.2
1	B	467	ASN	3.2
1	A	118	ILE	3.1
1	D	438	ALA	3.1
1	D	437	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	435	PRO	2.9
1	A	480	ALA	2.9
1	C	486	LEU	2.8
1	A	304	MET	2.8
1	D	117	HIS	2.7
1	B	470	ASN	2.7
1	D	407	PRO	2.6
1	C	305[A]	GLU	2.5
1	A	26	ASP	2.4
1	C	113	LYS	2.3
1	D	304	MET	2.3
1	D	194	LEU	2.3
1	C	435	PRO	2.2
1	D	305[A]	GLU	2.2
1	B	279	GLY	2.2
1	B	325	GLY	2.2
1	A	473	LEU	2.2
1	B	361	GLY	2.1
1	A	479	ASP	2.1
1	C	115	TYR	2.1
1	D	408	ALA	2.1
1	D	409	VAL	2.1
1	A	475	ASN	2.1
1	D	302	PHE	2.1
1	C	117	HIS	2.1
1	D	432	LEU	2.1
1	C	304	MET	2.0
1	D	439	GLY	2.0
1	A	305[A]	GLU	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 monosaccharides 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.

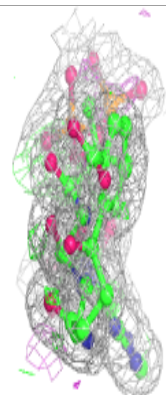
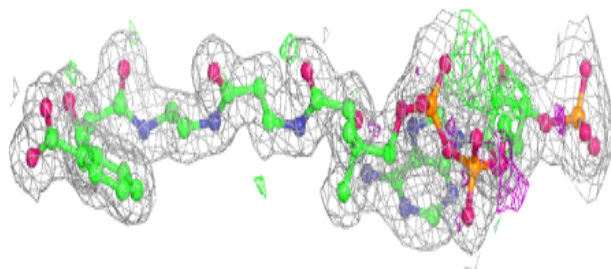
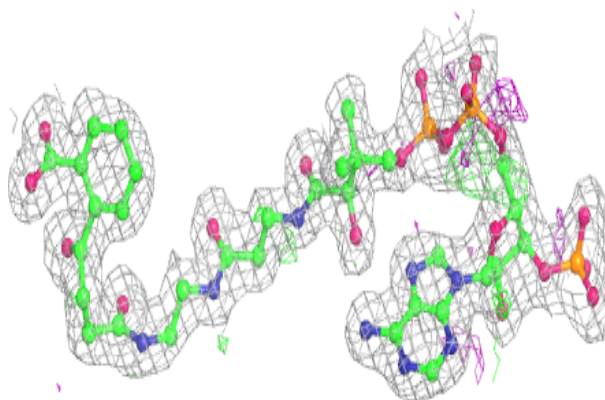
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	D	504	1/1	0.78	0.14	83,83,83,83	0
5	NA	D	505	1/1	0.79	0.10	58,58,58,58	0
6	PEG	D	507	7/7	0.80	0.17	39,40,48,49	0
6	PEG	A	508	7/7	0.83	0.20	33,48,51,51	0
3	MG	A	504	1/1	0.87	0.07	64,64,64,64	0
6	PEG	D	506	7/7	0.89	0.14	34,41,46,49	0
3	MG	B	504	1/1	0.89	0.10	54,54,54,54	0
2	S0N	C	508	63/63	0.90	0.11	13,25,58,65	0
4	CA	C	503	1/1	0.91	0.08	55,55,55,55	0
6	PEG	C	506	7/7	0.91	0.10	44,46,48,52	0
5	NA	C	505	1/1	0.91	0.15	52,52,52,52	0
2	S0N	D	501	63/63	0.92	0.11	13,24,61,72	0
5	NA	B	506	1/1	0.92	0.20	51,51,51,51	0
4	CA	C	504	1/1	0.92	0.31	30,30,30,30	0
5	NA	A	507	1/1	0.92	0.11	48,48,48,48	0
4	CA	A	506	1/1	0.93	0.10	69,69,69,69	0
5	NA	B	507	1/1	0.93	0.13	55,55,55,55	0
2	S0N	B	501	63/63	0.94	0.09	14,21,46,49	0
6	PEG	A	509	7/7	0.94	0.09	39,46,50,51	0
3	MG	B	503	1/1	0.94	0.11	55,55,55,55	0
6	PEG	C	507	7/7	0.95	0.10	53,58,59,64	0
6	PEG	A	510	7/7	0.96	0.10	35,43,47,51	0
2	S0N	A	501	63/63	0.96	0.10	13,21,33,42	0
4	CA	C	502	1/1	0.96	0.04	72,72,72,72	0
3	MG	D	503	1/1	0.96	0.29	45,45,45,45	0
3	MG	C	509	1/1	0.98	0.07	24,24,24,24	0
3	MG	A	502	1/1	0.99	0.08	19,19,19,19	0
3	MG	B	502	1/1	0.99	0.03	24,24,24,24	0
3	MG	D	502	1/1	0.99	0.06	19,19,19,19	0
4	CA	C	501	1/1	0.99	0.06	40,40,40,40	0
4	CA	A	505	1/1	0.99	0.07	27,27,27,27	0
4	CA	B	505	1/1	0.99	0.08	27,27,27,27	0
3	MG	A	503	1/1	0.99	0.05	28,28,28,28	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.

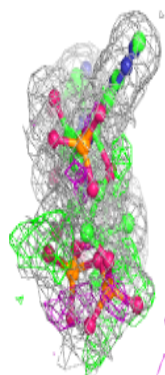
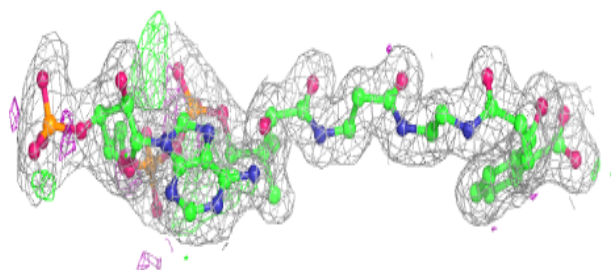
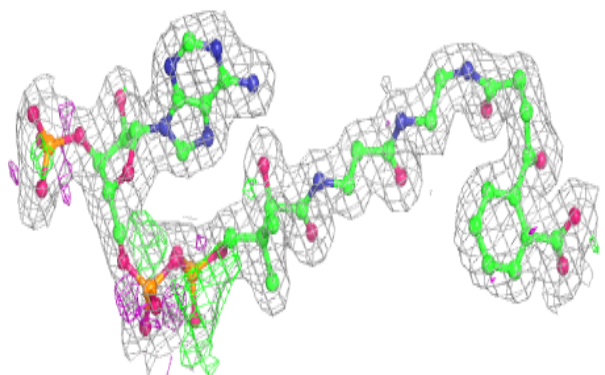
Electron density around S0N C 508:

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



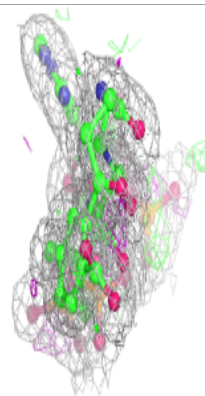
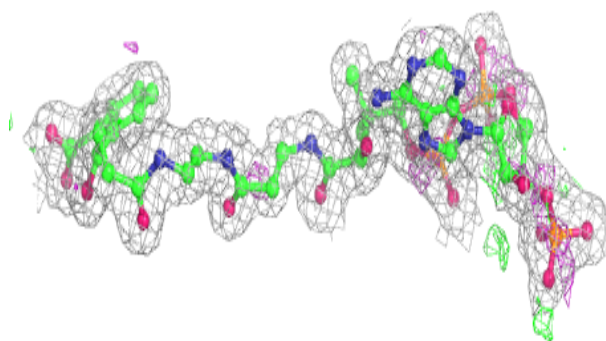
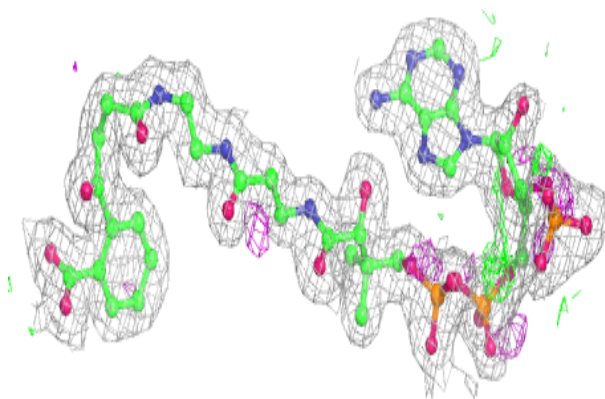
Electron density around S0N D 501:

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

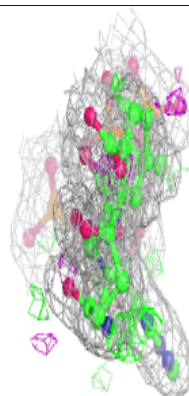
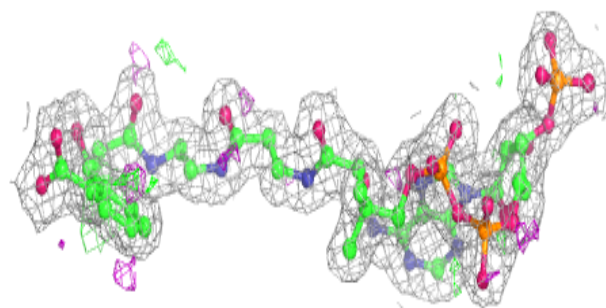
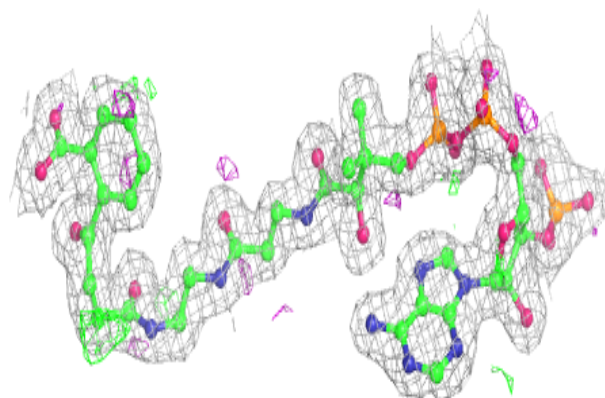


Electron density around S0N B 501:

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

**Electron density around S0N 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)



6.5 Other polymers

There are no such residues in this entry.