Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 12:54 PM JST

PDB ID	:	5X8F
Title	:	Ternary complex structure of a double mutant I454RA456K of o-Succinylbenzoate CoA Synthetase (MenE) from Bacillus Subtilis bound with AMP and its product analogue OSB-NCoA at 1.76 angstrom
Authors	:	Chen, Y.; Guo, Z.
Deposited on	:	2017-03-02
Resolution	:	1.76 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

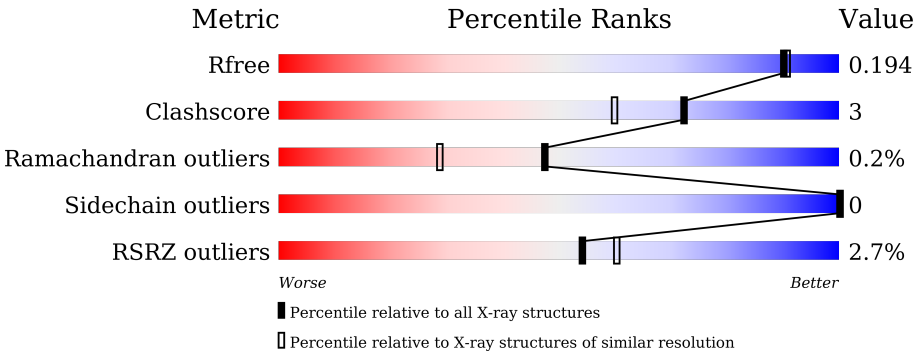
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (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 <=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	3% 92% 8%
1	B	485	4% 94% 6%
1	C	485	2% 94% 6%
1	D	485	3% 91% 9%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17221 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.

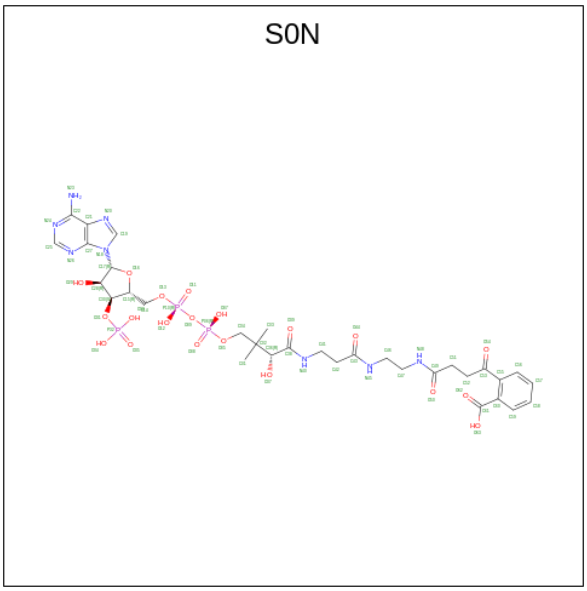
- Molecule 1 is a protein called 2-succinylbenzoate--CoA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	7	1
			3702	2363	615	701	23			
1	B	485	Total	C	N	O	S	0	4	0
			3678	2351	612	692	23			
1	C	485	Total	C	N	O	S	0	3	1
			3707	2365	626	693	23			
1	D	484	Total	C	N	O	S	0	6	0
			3692	2362	617	690	23			

There are 8 discrepancies between the modelled and reference sequences:

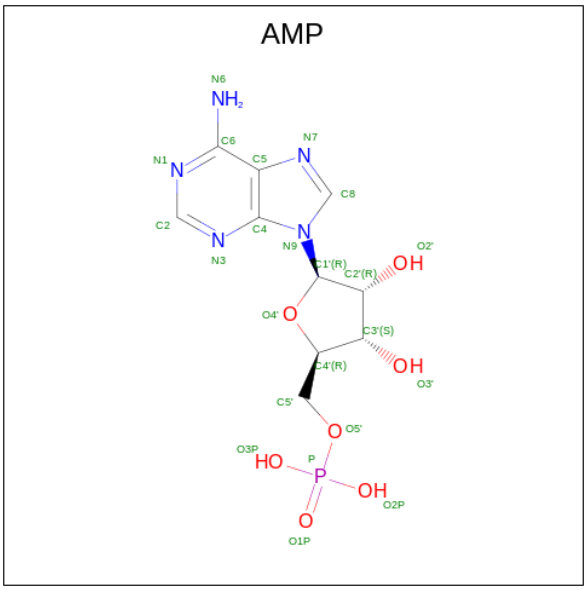
Chain	Residue	Modelled	Actual	Comment	Reference
A	454	ARG	ILE	engineered mutation	UNP P23971
A	456	LYS	ALA	engineered mutation	UNP P23971
B	454	ARG	ILE	engineered mutation	UNP P23971
B	456	LYS	ALA	engineered mutation	UNP P23971
C	454	ARG	ILE	engineered mutation	UNP P23971
C	456	LYS	ALA	engineered mutation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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

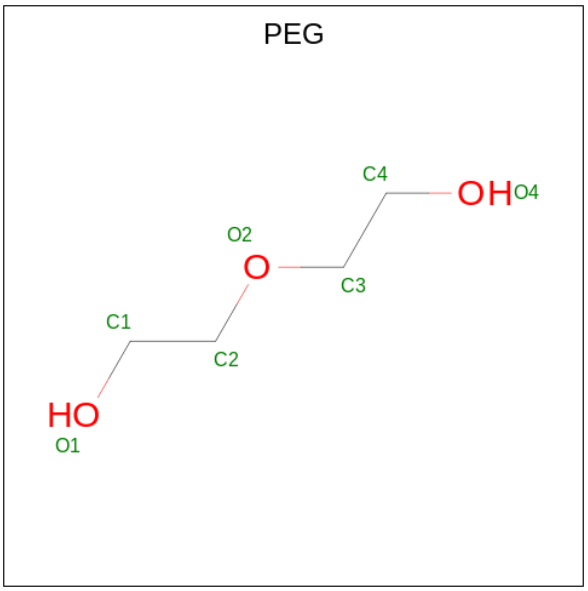
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	Mg	0	0
			8	8		
4	B	8	Total	Mg	0	0
			8	8		
4	C	4	Total	Mg	0	0
			4	4		
4	D	7	Total	Mg	0	0
			7	7		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	Na	0	0
			5	5		
5	B	9	Total	Na	0	0
			9	9		
5	C	8	Total	Na	0	0
			8	8		
5	D	11	Total	Na	0	0
			11	11		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is water.

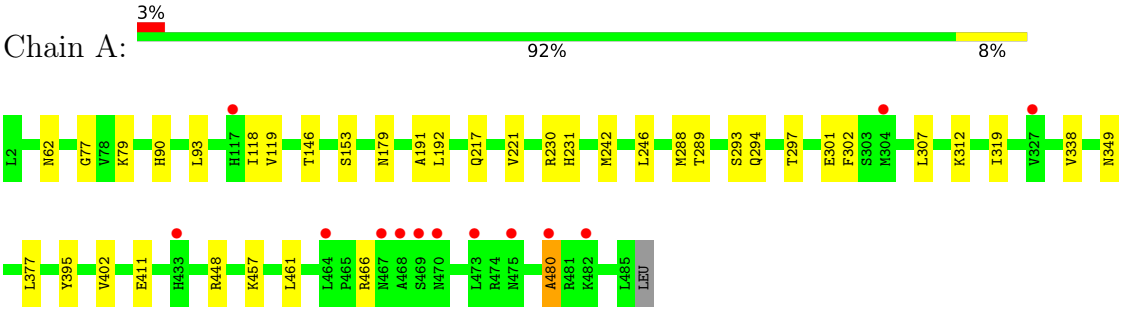
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	509	Total O 509 509	0	0
8	B	496	Total O 496 496	0	0
8	C	528	Total O 528 528	0	0
8	D	499	Total O 499 499	0	0

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.

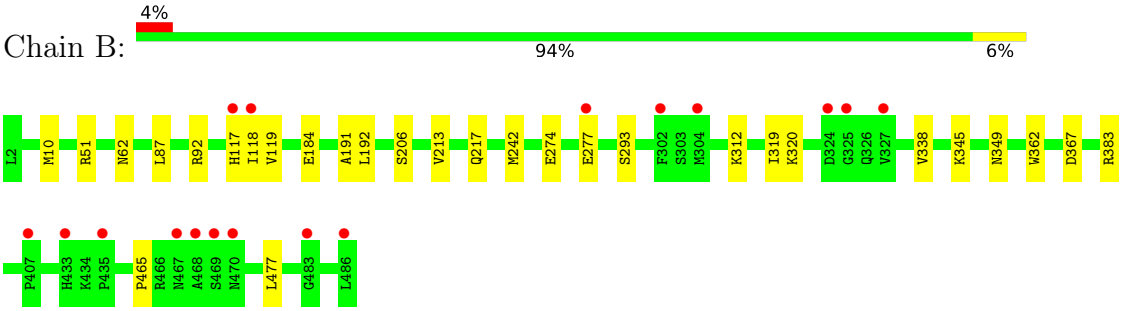
• Molecule 1: 2-succinylbenzoate--CoA ligase

Chain A:



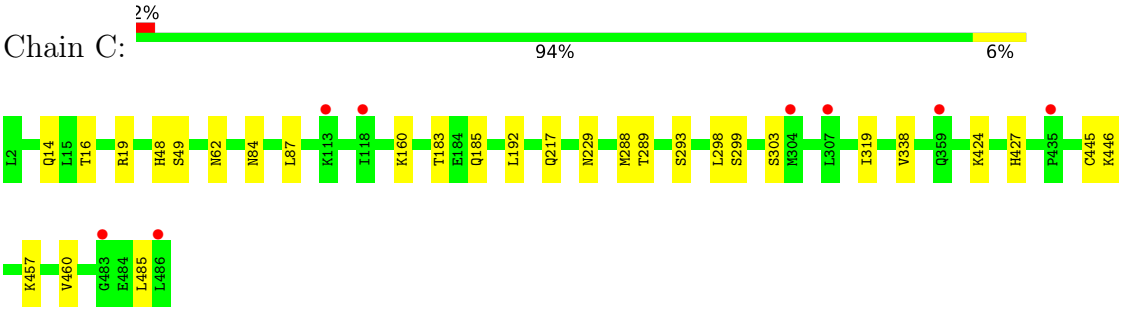
• Molecule 1: 2-succinylbenzoate--CoA ligase

Chain B:



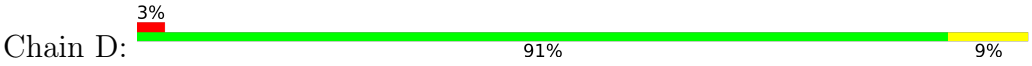
• Molecule 1: 2-succinylbenzoate--CoA ligase

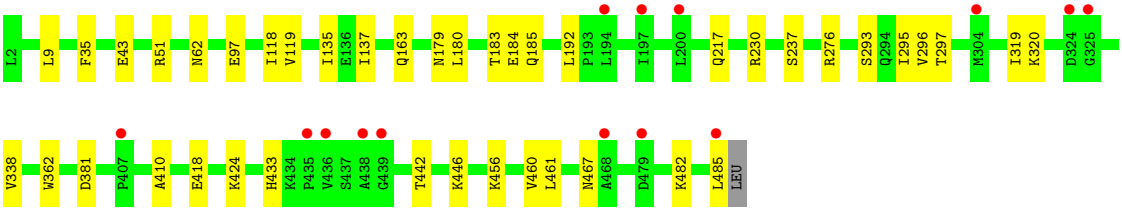
Chain C:



• Molecule 1: 2-succinylbenzoate--CoA ligase

Chain D:




L2
L9
F35
E43
R51
N62
E97
I118
V119
I135
E136
I137
Q163
N179
L180
T183
E184
Q185
L192
P193
L194
I197
L200
Q217
R230
S237
R276
S293
Q294
I295
V296
T297
M304
I319
K320
D324
G325
V338
W362
D381
P407
A410
E418
K424
H433
K434
P435
V436
S437
A438
G439
T442
K446
K456
V460
L461
N467
A468
D479
K482
L485
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.87Å 96.36Å 98.07Å 80.44° 77.96° 81.11°	Depositor
Resolution (Å)	29.96 – 1.76 29.96 – 1.76	Depositor EDS
% Data completeness (in resolution range)	92.9 (29.96-1.76) 92.9 (29.96-1.76)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.163 , 0.194 0.163 , 0.194	Depositor DCC
R_{free} test set	1995 reflections (0.86%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.049 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17221	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 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AMP, CA, NA, PEG, 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	0.36	0/3794	0.57	1/5146 (0.0%)
1	B	0.37	0/3762	0.56	1/5106 (0.0%)
1	C	0.36	0/3785	0.53	0/5131
1	D	0.36	0/3785	0.57	1/5134 (0.0%)
All	All	0.36	0/15126	0.56	3/20517 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	51	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	B	191	ALA	C-N-CA	7.08	139.40	121.70
1	A	191	ALA	C-N-CA	6.46	137.84	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3702	0	3608	29	0
1	B	3678	0	3588	19	0
1	C	3707	0	3635	21	0
1	D	3692	0	3628	28	0
2	A	63	0	40	2	0
2	B	63	0	40	2	0
2	C	63	0	40	0	0
2	D	63	0	40	0	0
3	A	23	0	12	4	0
3	C	23	0	12	2	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
4	C	4	0	0	0	0
4	D	7	0	0	0	0
5	A	5	0	0	0	0
5	B	9	0	0	0	0
5	C	8	0	0	0	0
5	D	11	0	0	0	0
6	A	14	0	20	0	0
6	B	14	0	20	4	0
6	C	14	0	20	1	0
6	D	7	0	10	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	509	0	0	9	1
8	B	496	0	0	4	0
8	C	528	0	0	6	0
8	D	499	0	0	10	1
All	All	17221	0	14713	100	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (100) 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:445:CYS:SG	8:C:974:HOH:O	2.39	0.81
1:D:460:VAL:HG23	1:D:485:LEU:HD11	1.61	0.80
1:A:312:LYS:NZ	8:A:602:HOH:O	2.16	0.78
1:B:312:LYS:NZ	8:B:601:HOH:O	2.18	0.76
1:D:418:GLU:OE2	8:D:601:HOH:O	2.05	0.72
1:C:16:THR:HB	1:C:19:ARG:HG3	1.72	0.71
1:A:221:VAL:HG13	1:A:246:LEU:HD23	1.74	0.70
1:D:118:ILE:HG22	1:D:119:VAL:HG13	1.76	0.68
1:A:349[B]:ASN:OD1	1:B:349:ASN:ND2	2.26	0.68
1:C:319:ILE:HG22	1:C:338:VAL:HG12	1.76	0.68
1:B:319:ILE:HG22	1:B:338:VAL:HG12	1.76	0.67
1:A:77:GLY:O	8:A:601:HOH:O	2.12	0.67
1:D:163:GLN:NE2	8:D:608:HOH:O	2.28	0.66
1:D:456:LYS:NZ	8:D:605:HOH:O	2.24	0.66
1:C:229[B]:ASN:OD1	8:C:601:HOH:O	2.12	0.65
1:C:62:ASN:HB2	1:C:217:GLN:HA	1.82	0.62
3:A:502:AMP:N3	8:A:608:HOH:O	2.31	0.61
1:A:319[A]:ILE:HG22	1:A:338:VAL:HG12	1.82	0.61
1:A:79:LYS:NZ	8:A:610:HOH:O	2.33	0.60
1:A:457:LYS:NZ	8:A:611:HOH:O	2.34	0.60
1:D:184:GLU:O	8:D:602:HOH:O	2.17	0.59
6:B:520:PEG:H12	8:B:638:HOH:O	2.03	0.58
1:A:62:ASN:HB2	1:A:217:GLN:HA	1.87	0.57
1:C:424:LYS:NZ	8:C:619:HOH:O	2.38	0.56
1:A:230:ARG:HD3	1:A:231:HIS:CE1	2.41	0.56
1:A:79:LYS:HD2	1:A:146:THR:O	2.05	0.56
1:B:62:ASN:HB2	1:B:217:GLN:HA	1.88	0.55
1:C:14:GLN:HA	6:C:515:PEG:H12	1.89	0.55
1:A:179:ASN:OD1	1:A:297[B]:THR:HG21	2.08	0.54
1:C:192:LEU:HD12	1:C:192:LEU:O	2.09	0.52
1:D:424:LYS:NZ	8:D:617:HOH:O	2.41	0.52
1:D:442:THR:HG22	1:D:446:LYS:HE3	1.90	0.52
1:D:456:LYS:NZ	8:D:603:HOH:O	2.20	0.52
1:A:289:THR:N	3:A:502:AMP:O2P	2.40	0.52
1:D:62:ASN:HB2	1:D:217:GLN:HA	1.91	0.52
1:A:307:LEU:HD13	8:A:960:HOH:O	2.10	0.52
1:C:288:MET:HA	3:C:502:AMP:O3P	2.10	0.51
1:D:192:LEU:HD11	1:D:237:SER:O	2.11	0.51
1:B:345:LYS:HB2	6:B:520:PEG:H11	1.92	0.51
1:C:84:ASN:HB3	1:C:87:LEU:HG	1.92	0.51
1:D:179:ASN:OD1	1:D:297[B]:THR:HG21	2.11	0.51
1:B:51:ARG:NH1	8:B:610:HOH:O	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:GLU:OE1	1:D:118:ILE:HG23	2.11	0.50
1:D:43:GLU:HG2	1:D:135:ILE:HG12	1.93	0.50
3:A:502:AMP:O3'	8:A:603:HOH:O	2.20	0.50
1:A:192:LEU:CD2	2:A:501:S0N:H41	2.43	0.49
1:B:184:GLU:HG2	6:B:519:PEG:O2	2.13	0.49
1:C:48:HIS:O	1:C:49:SER:OG	2.25	0.48
1:A:192:LEU:HD21	1:A:242:MET:SD	2.53	0.47
1:A:294:GLN:OE1	1:A:297[A]:THR:HG21	2.15	0.47
1:D:381:ASP:OD2	8:D:604:HOH:O	2.20	0.47
1:C:192:LEU:HD12	1:C:192:LEU:C	2.35	0.47
1:C:460:VAL:HG23	1:C:485:LEU:HB2	1.97	0.47
1:D:276:ARG:NE	8:D:633:HOH:O	2.48	0.47
1:B:192:LEU:CD2	2:B:501:S0N:H41	2.46	0.47
1:D:410:ALA:HB2	1:D:433:HIS:CD2	2.50	0.46
1:A:402:VAL:HG13	1:A:448[A]:ARG:HD2	1.98	0.46
1:A:192:LEU:HD22	2:A:501:S0N:H41	1.96	0.46
6:B:519:PEG:H41	1:D:180:LEU:O	2.14	0.46
1:D:319[A]:ILE:HG22	1:D:338:VAL:HG12	1.97	0.46
1:A:301:GLU:HG3	1:A:302:PHE:CD2	2.51	0.45
1:C:427:HIS:CE1	1:C:457:LYS:HD2	2.51	0.45
1:C:289:THR:N	3:C:502:AMP:O3P	2.44	0.45
1:D:9:LEU:HD21	1:D:35:PHE:HA	1.97	0.45
1:A:118:ILE:HG22	1:A:119:VAL:HG13	1.99	0.45
1:D:320:LYS:HE2	1:D:362:TRP:CD2	2.52	0.45
1:A:288:MET:HA	3:A:502:AMP:O2P	2.17	0.44
1:A:461:LEU:HD21	1:A:480:ALA:O	2.16	0.44
1:B:274:GLU:HA	1:B:277:GLU:HG2	1.99	0.44
1:B:320:LYS:HE2	1:B:362:TRP:CD2	2.52	0.44
1:D:461:LEU:HG	1:D:482:LYS:HB3	1.99	0.44
1:B:117:HIS:CD2	1:B:118:ILE:HG12	2.53	0.44
1:C:183:THR:HG23	1:C:185:GLN:H	1.82	0.44
1:B:87:LEU:O	1:B:92:ARG:NH2	2.50	0.43
1:B:367:ASP:OD1	1:B:383:ARG:HD2	2.19	0.43
1:C:298:LEU:HD21	1:C:303:SER:HA	2.00	0.43
1:D:276:ARG:NE	8:D:634:HOH:O	2.51	0.43
1:D:295:ILE:HG23	1:D:296:VAL:HG23	2.01	0.43
1:A:192:LEU:HD23	1:A:192:LEU:HA	1.81	0.43
1:B:118:ILE:HG22	1:B:119:VAL:HG13	1.99	0.43
1:A:153[B]:SER:HA	1:A:395:TYR:CZ	2.55	0.42
1:C:446:LYS:HE3	1:C:446:LYS:HB2	1.77	0.42
1:A:217:GLN:NE2	8:A:622:HOH:O	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:ASN:HB2	8:D:709:HOH:O	2.19	0.42
1:C:160:LYS:NZ	8:C:653:HOH:O	2.53	0.42
1:A:93:LEU:HD22	1:A:118:ILE:HD12	2.02	0.42
1:B:10:MET:HE1	8:B:852:HOH:O	2.19	0.41
1:C:229[B]:ASN:OD1	8:C:603:HOH:O	2.22	0.41
1:B:192:LEU:HD22	2:B:501:S0N:H41	2.02	0.41
1:D:230:ARG:HE	1:D:230:ARG:HB2	1.69	0.41
6:D:520:PEG:H32	6:D:520:PEG:H12	1.90	0.41
1:B:192:LEU:HD21	1:B:242:MET:SD	2.60	0.41
1:B:206:SER:HB2	1:B:213:VAL:HG23	2.02	0.41
1:D:183:THR:HG23	1:D:185:GLN:H	1.85	0.41
1:A:319[B]:ILE:CD1	1:A:377:LEU:HD22	2.50	0.41
1:A:411:GLU:OE1	1:A:466:ARG:NH2	2.50	0.41
1:A:90:HIS:HD2	8:A:643:HOH:O	2.02	0.41
1:B:465:PRO:HD2	1:B:477:LEU:HD23	2.02	0.41
1:D:137:ILE:H	1:D:137:ILE:HG13	1.63	0.41
1:C:299:SER:OG	8:C:602:HOH:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:622:HOH:O	8:D:683:HOH:O[1_556]	2.03	0.17

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	489/485 (101%)	478 (98%)	10 (2%)	1 (0%)	47	29
1	B	487/485 (100%)	477 (98%)	9 (2%)	1 (0%)	47	29
1	C	486/485 (100%)	478 (98%)	7 (1%)	1 (0%)	47	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	489/485 (101%)	479 (98%)	9 (2%)	1 (0%)	47 29
All	All	1951/1940 (101%)	1912 (98%)	35 (2%)	4 (0%)	47 29

All (4) Ramachandran outliers are listed below:

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

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	385/414 (93%)	385 (100%)	0	100 100
1	B	383/414 (92%)	383 (100%)	0	100 100
1	C	387/414 (94%)	387 (100%)	0	100 100
1	D	386/414 (93%)	386 (100%)	0	100 100
All	All	1541/1656 (93%)	1541 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	393	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 76 ligands modelled in this entry, 63 are monoatomic - leaving 13 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	520	5	6,6,6	0.57	0	5,5,5	0.30	0
2	S0N	D	501	4	58,66,66	3.66	14 (24%)	74,97,97	1.61	10 (13%)
6	PEG	B	519	-	6,6,6	0.52	0	5,5,5	0.24	0
6	PEG	C	515	-	6,6,6	0.55	0	5,5,5	0.17	0
2	S0N	C	501	4	58,66,66	3.72	14 (24%)	74,97,97	1.48	9 (12%)
6	PEG	A	517	-	6,6,6	0.54	0	5,5,5	0.23	0
2	S0N	B	501	4	58,66,66	3.69	14 (24%)	74,97,97	1.59	10 (13%)
3	AMP	A	502	-	22,25,25	0.93	1 (4%)	25,38,38	1.34	2 (8%)
3	AMP	C	502	-	22,25,25	0.85	1 (4%)	25,38,38	1.35	5 (20%)
6	PEG	C	516	-	6,6,6	0.55	0	5,5,5	0.39	0
6	PEG	B	520	-	6,6,6	0.54	0	5,5,5	0.21	0
2	S0N	A	501	4	58,66,66	3.60	13 (22%)	74,97,97	1.54	11 (14%)
6	PEG	A	516	-	6,6,6	0.55	0	5,5,5	0.30	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	520	5	-	2/4/4/4	-
2	S0N	D	501	4	-	13/60/80/80	0/4/4/4
6	PEG	B	519	-	-	2/4/4/4	-
6	PEG	C	515	-	-	0/4/4/4	-
2	S0N	C	501	4	-	11/60/80/80	0/4/4/4
6	PEG	A	517	-	-	1/4/4/4	-
2	S0N	B	501	4	-	11/60/80/80	0/4/4/4
3	AMP	A	502	-	-	2/6/26/26	0/3/3/3
3	AMP	C	502	-	-	5/6/26/26	0/3/3/3
6	PEG	C	516	-	-	2/4/4/4	-
6	PEG	B	520	-	-	2/4/4/4	-
2	S0N	A	501	4	-	12/60/80/80	0/4/4/4
6	PEG	A	516	-	-	2/4/4/4	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	S0N	C28-C17	-17.09	1.27	1.53
2	B	501	S0N	C28-C17	-17.00	1.28	1.53
2	D	501	S0N	C28-C17	-16.81	1.28	1.53
2	A	501	S0N	C28-C17	-16.16	1.29	1.53
2	C	501	S0N	O16-C17	15.93	1.63	1.41
2	D	501	S0N	O16-C17	15.74	1.63	1.41
2	B	501	S0N	O16-C17	15.60	1.62	1.41
2	A	501	S0N	O16-C17	15.43	1.62	1.41
2	B	501	S0N	O16-C15	-7.21	1.28	1.45
2	A	501	S0N	O16-C15	-6.81	1.29	1.45
2	D	501	S0N	O16-C15	-6.74	1.29	1.45
2	C	501	S0N	O16-C15	-6.66	1.30	1.45
2	C	501	S0N	C55-C53	5.97	1.60	1.48
2	A	501	S0N	C38-N40	5.60	1.45	1.33
2	A	501	S0N	C55-C53	5.58	1.59	1.48
2	D	501	S0N	C55-C53	5.42	1.59	1.48
2	B	501	S0N	C55-C53	5.37	1.59	1.48
2	B	501	S0N	C38-N40	5.25	1.45	1.33
2	C	501	S0N	C38-N40	5.21	1.45	1.33
2	D	501	S0N	C38-N40	5.10	1.44	1.33
2	C	501	S0N	C52-C53	5.09	1.58	1.51
2	B	501	S0N	C49-N48	5.07	1.44	1.33
2	C	501	S0N	C49-N48	4.87	1.44	1.33
2	D	501	S0N	C49-N48	4.83	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	S0N	C49-N48	4.71	1.44	1.33
2	D	501	S0N	C52-C53	4.42	1.57	1.51
2	C	501	S0N	C43-N45	4.39	1.43	1.33
2	B	501	S0N	C52-C53	4.36	1.57	1.51
2	D	501	S0N	C43-N45	4.33	1.43	1.33
2	A	501	S0N	C52-C53	4.31	1.57	1.51
2	B	501	S0N	C43-N45	4.27	1.43	1.33
2	A	501	S0N	C43-N45	4.06	1.42	1.33
2	B	501	S0N	O29-C28	3.53	1.51	1.43
2	D	501	S0N	O29-C28	3.52	1.51	1.43
2	A	501	S0N	O29-C28	3.46	1.51	1.43
2	C	501	S0N	O29-C28	3.43	1.51	1.43
2	B	501	S0N	C21-C27	-3.04	1.32	1.40
2	C	501	S0N	C60-C61	3.01	1.56	1.49
2	A	501	S0N	C60-C61	2.96	1.56	1.49
2	B	501	S0N	C60-C61	2.94	1.55	1.49
2	A	501	S0N	C21-C27	-2.88	1.33	1.40
2	D	501	S0N	C22-N23	2.81	1.44	1.34
2	D	501	S0N	C21-C27	-2.81	1.33	1.40
2	D	501	S0N	C60-C61	2.70	1.55	1.49
2	C	501	S0N	C22-N23	2.67	1.43	1.34
2	B	501	S0N	C22-N23	2.62	1.43	1.34
2	C	501	S0N	C21-C27	-2.57	1.34	1.40
3	A	502	AMP	C5-C4	2.55	1.47	1.40
2	D	501	S0N	C25-N26	2.55	1.36	1.32
2	A	501	S0N	C25-N26	2.49	1.36	1.32
2	C	501	S0N	C25-N26	2.49	1.36	1.32
3	C	502	AMP	C5-C4	2.44	1.47	1.40
2	B	501	S0N	C25-N26	2.40	1.36	1.32
2	A	501	S0N	C22-N23	2.33	1.42	1.34
2	C	501	S0N	C01-C02	-2.16	1.49	1.53
2	B	501	S0N	C01-C02	-2.08	1.49	1.53
2	D	501	S0N	C59-C60	-2.06	1.36	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	S0N	C41-C42-C43	-5.76	102.77	112.36
2	D	501	S0N	N26-C25-N24	-5.63	119.88	128.68
2	B	501	S0N	C51-C52-C53	-5.61	105.98	112.76
2	D	501	S0N	C41-C42-C43	-5.59	103.04	112.36
2	D	501	S0N	C51-C52-C53	-5.53	106.06	112.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	S0N	N26-C25-N24	-5.49	120.10	128.68
2	B	501	S0N	C41-C42-C43	-5.42	103.33	112.36
2	A	501	S0N	N26-C25-N24	-5.42	120.21	128.68
2	C	501	S0N	N26-C25-N24	-5.21	120.54	128.68
2	C	501	S0N	C51-C52-C53	-5.01	106.70	112.76
2	A	501	S0N	C51-C52-C53	-4.70	107.08	112.76
2	A	501	S0N	C30-C28-C17	4.05	108.86	99.89
2	A	501	S0N	C41-C42-C43	-3.89	105.88	112.36
2	A	501	S0N	O05-C04-C02	-3.76	104.50	110.55
2	B	501	S0N	C30-C28-C17	3.52	107.68	99.89
3	A	502	AMP	C4-C5-N7	-3.44	105.81	109.40
3	C	502	AMP	N3-C2-N1	-3.44	123.31	128.68
2	D	501	S0N	C01-C02-C36	3.39	114.70	108.82
2	B	501	S0N	C21-C22-N23	3.24	125.28	120.35
3	A	502	AMP	N3-C2-N1	-3.11	123.82	128.68
2	D	501	S0N	O05-C04-C02	-3.00	105.72	110.55
2	C	501	S0N	C21-C22-N23	2.93	124.81	120.35
2	D	501	S0N	C21-C22-N23	2.87	124.72	120.35
2	A	501	S0N	C01-C02-C36	2.85	113.77	108.82
2	C	501	S0N	C01-C02-C36	2.64	113.41	108.82
2	B	501	S0N	O05-C04-C02	-2.59	106.39	110.55
2	B	501	S0N	O50-C49-N48	-2.54	118.22	123.01
2	A	501	S0N	P10-O09-P06	-2.52	124.17	132.83
2	C	501	S0N	C47-N48-C49	-2.52	118.17	122.84
3	C	502	AMP	C4-C5-N7	-2.49	106.81	109.40
2	A	501	S0N	O50-C49-N48	-2.45	118.40	123.01
2	B	501	S0N	C47-N48-C49	-2.44	118.31	122.84
2	A	501	S0N	C21-C22-N23	2.42	124.03	120.35
2	D	501	S0N	P10-O09-P06	-2.40	124.59	132.83
2	C	501	S0N	O50-C49-N48	-2.37	118.53	123.01
2	D	501	S0N	C47-N48-C49	-2.34	118.49	122.84
2	B	501	S0N	C41-N40-C38	-2.31	118.47	122.59
3	C	502	AMP	O2P-P-O5'	-2.28	100.66	106.73
2	A	501	S0N	C46-N45-C43	-2.27	118.62	122.84
2	D	501	S0N	O50-C49-N48	-2.16	118.94	123.01
3	C	502	AMP	C2-N1-C6	2.14	122.41	118.75
2	C	501	S0N	P10-O09-P06	-2.12	125.56	132.83
2	D	501	S0N	C52-C51-C49	-2.06	108.94	112.56
3	C	502	AMP	O3P-P-O2P	2.06	115.51	107.64
2	C	501	S0N	C41-N40-C38	-2.02	118.98	122.59
2	A	501	S0N	O54-C53-C55	-2.00	117.29	120.83
2	B	501	S0N	P10-O09-P06	-2.00	125.96	132.83

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	S0N	C04-O05-P06-O08
2	A	501	S0N	C14-O13-P10-O11
2	A	501	S0N	C14-O13-P10-O12
2	B	501	S0N	C14-O13-P10-O11
2	B	501	S0N	C14-O13-P10-O12
2	B	501	S0N	C30-O31-P32-O35
2	C	501	S0N	C04-O05-P06-O08
2	C	501	S0N	C04-O05-P06-O09
2	C	501	S0N	C14-O13-P10-O11
2	C	501	S0N	C30-O31-P32-O33
2	D	501	S0N	C04-O05-P06-O08
2	D	501	S0N	C04-O05-P06-O09
2	D	501	S0N	C14-O13-P10-O11
3	C	502	AMP	C5'-O5'-P-O2P
3	C	502	AMP	C5'-O5'-P-O3P
3	A	502	AMP	C3'-C4'-C5'-O5'
3	C	502	AMP	O4'-C4'-C5'-O5'
3	C	502	AMP	C3'-C4'-C5'-O5'
2	A	501	S0N	C51-C52-C53-C55
2	B	501	S0N	C51-C52-C53-C55
2	C	501	S0N	C51-C52-C53-C55
2	D	501	S0N	C51-C52-C53-C55
6	B	519	PEG	O2-C3-C4-O4
6	C	516	PEG	O2-C3-C4-O4
2	C	501	S0N	C51-C52-C53-O54
6	B	519	PEG	O1-C1-C2-O2
6	C	516	PEG	O1-C1-C2-O2
2	B	501	S0N	C51-C52-C53-O54
2	A	501	S0N	C51-C52-C53-O54
3	A	502	AMP	O4'-C4'-C5'-O5'
6	A	516	PEG	O2-C3-C4-O4
6	D	520	PEG	O2-C3-C4-O4
2	D	501	S0N	C51-C52-C53-O54
3	C	502	AMP	C5'-O5'-P-O1P
2	A	501	S0N	C30-O31-P32-O35
2	A	501	S0N	C04-O05-P06-O09
2	D	501	S0N	C30-O31-P32-O34
2	C	501	S0N	C04-O05-P06-O07
6	A	517	PEG	C4-C3-O2-C2
6	A	516	PEG	C4-C3-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	520	PEG	O1-C1-C2-O2
6	B	520	PEG	C1-C2-O2-C3
2	A	501	S0N	N45-C46-C47-N48
6	D	520	PEG	C1-C2-O2-C3
2	D	501	S0N	P06-O09-P10-O11
2	C	501	S0N	C59-C60-C61-O63
2	B	501	S0N	C59-C60-C61-O63
2	D	501	S0N	C59-C60-C61-O63
2	A	501	S0N	C59-C60-C61-O63
2	B	501	S0N	N45-C46-C47-N48
2	A	501	S0N	C59-C60-C61-O62
2	B	501	S0N	C59-C60-C61-O62
2	D	501	S0N	O50-C49-C51-C52
2	D	501	S0N	C59-C60-C61-O62
2	A	501	S0N	C14-O13-P10-O09
2	B	501	S0N	C14-O13-P10-O09
2	D	501	S0N	C52-C53-C55-C56
2	C	501	S0N	C59-C60-C61-O62
2	C	501	S0N	N45-C46-C47-N48
2	C	501	S0N	P06-O09-P10-O12
2	B	501	S0N	C04-O05-P06-O08
2	D	501	S0N	C04-O05-P06-O07
2	D	501	S0N	N48-C49-C51-C52
2	B	501	S0N	O50-C49-C51-C52
2	A	501	S0N	O50-C49-C51-C52

There are no ring outliers.

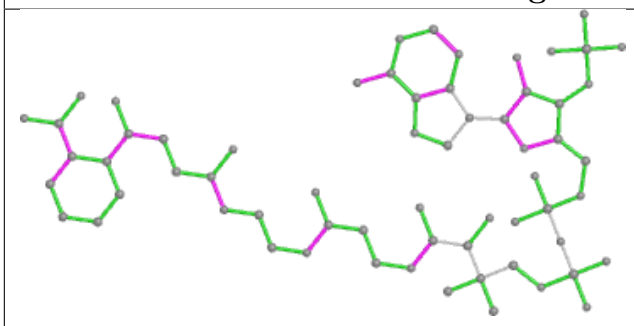
8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	520	PEG	1	0
6	B	519	PEG	2	0
6	C	515	PEG	1	0
2	B	501	S0N	2	0
3	A	502	AMP	4	0
3	C	502	AMP	2	0
6	B	520	PEG	2	0
2	A	501	S0N	2	0

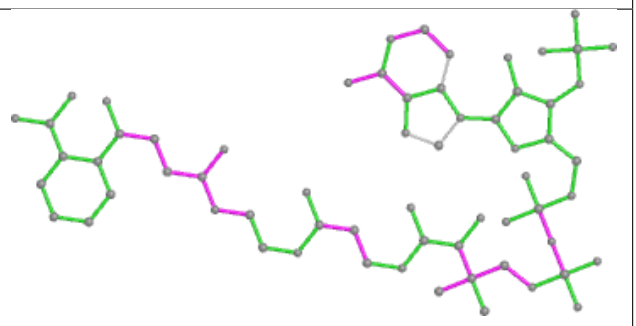
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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

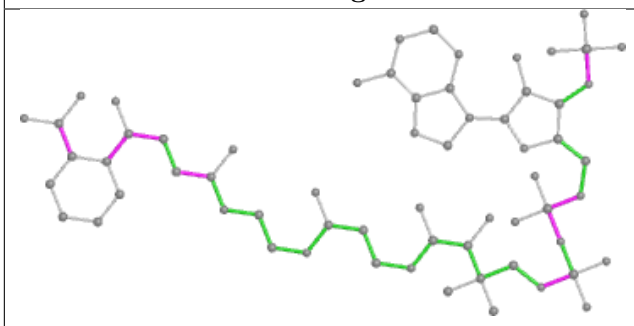
Ligand S0N D 501



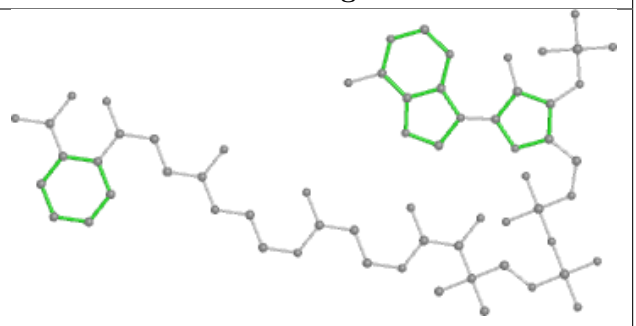
Bond lengths



Bond angles

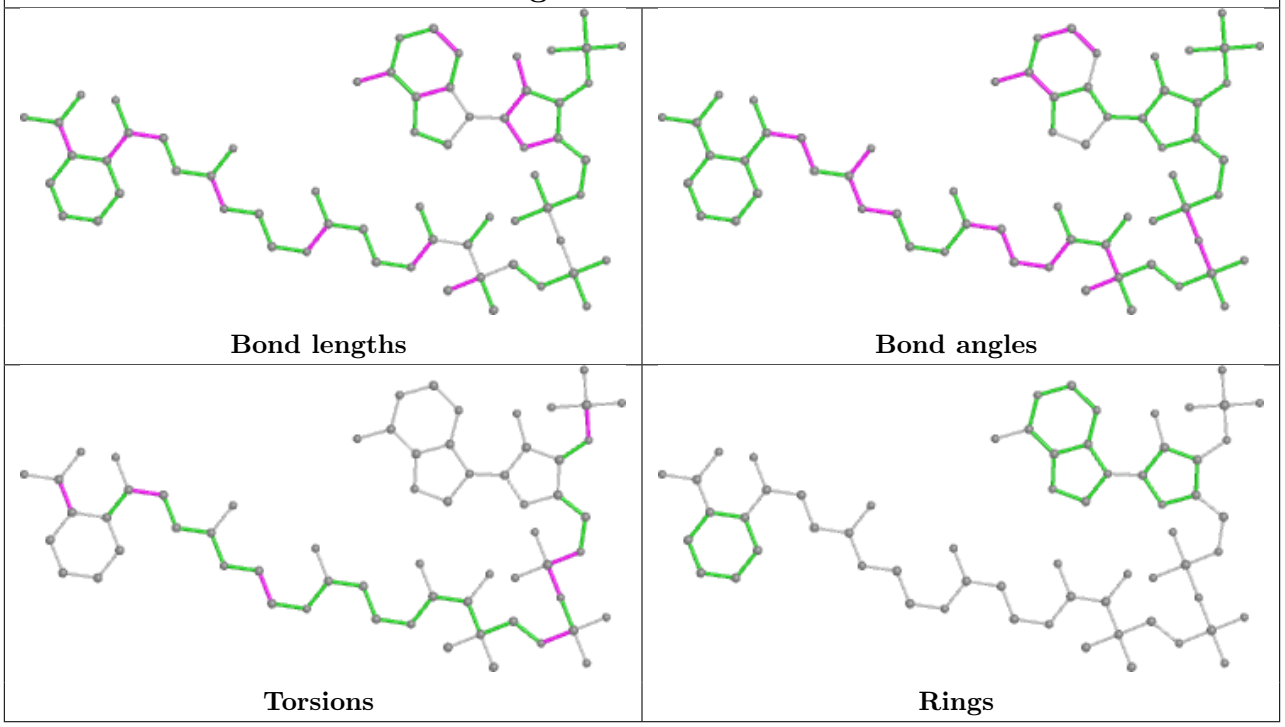


Torsions

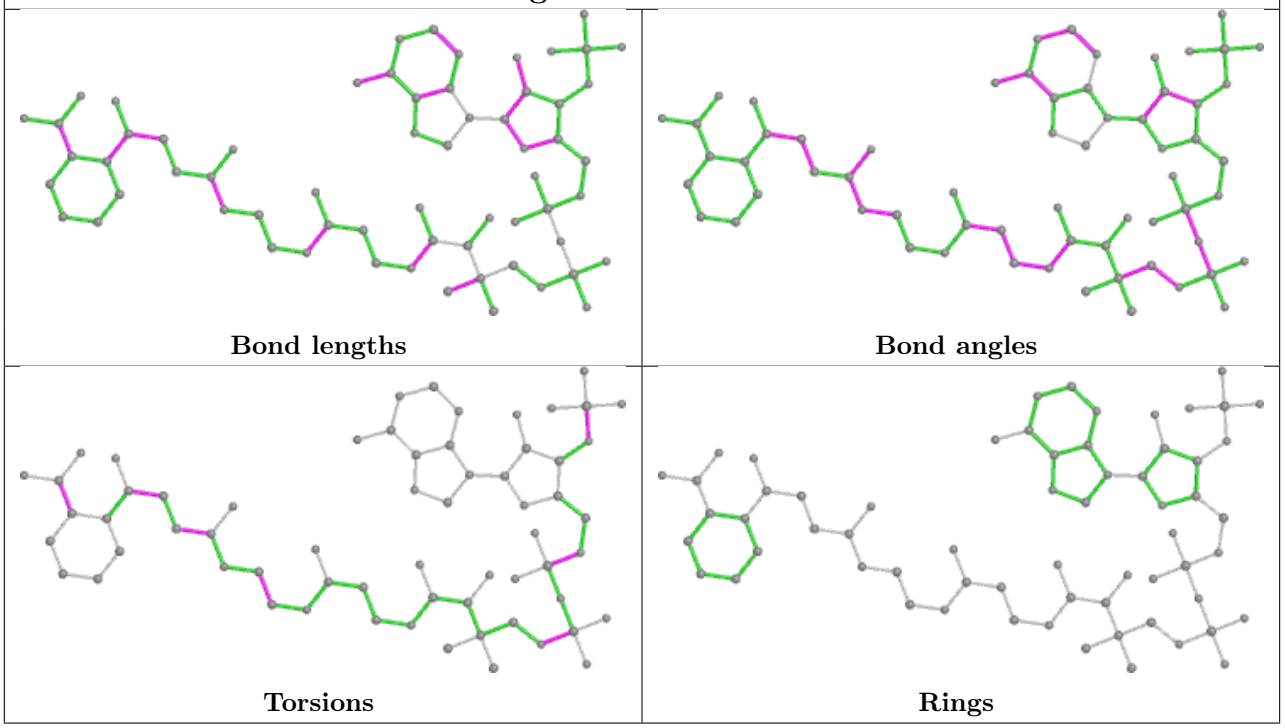


Rings

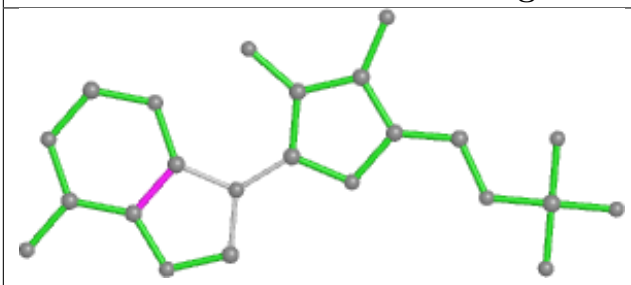
Ligand S0N C 501



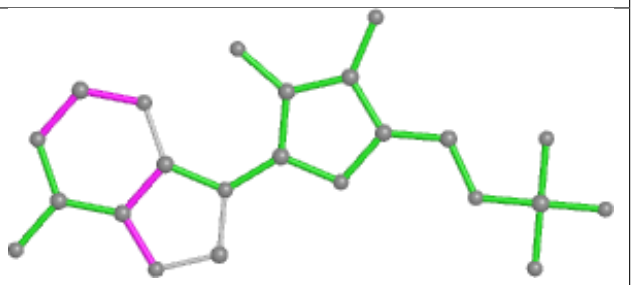
Ligand S0N B 501



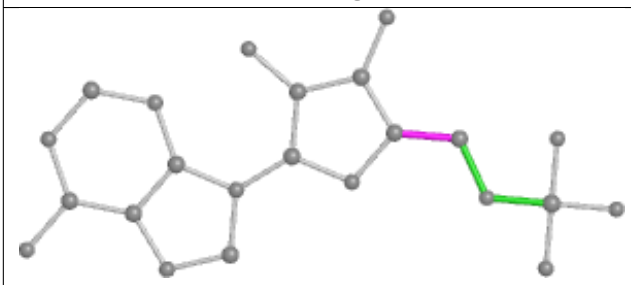
Ligand AMP A 502



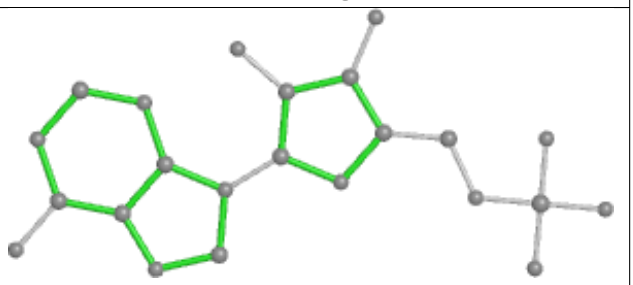
Bond lengths



Bond angles

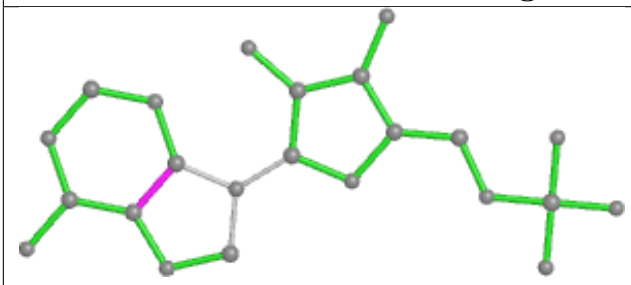


Torsions

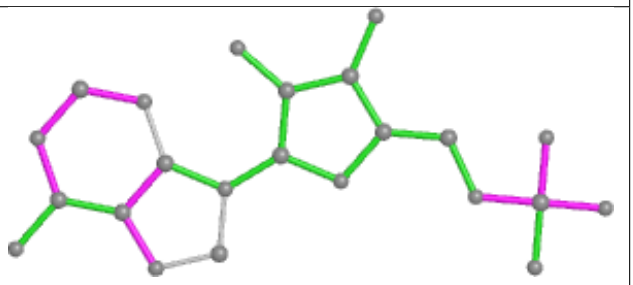


Rings

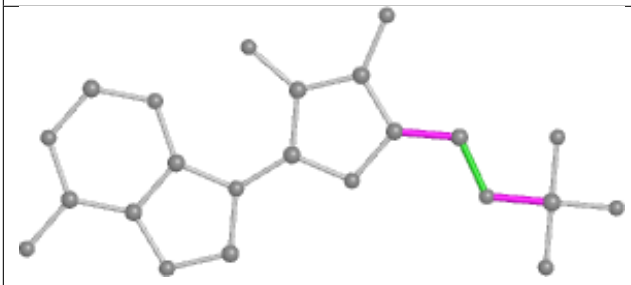
Ligand AMP C 502



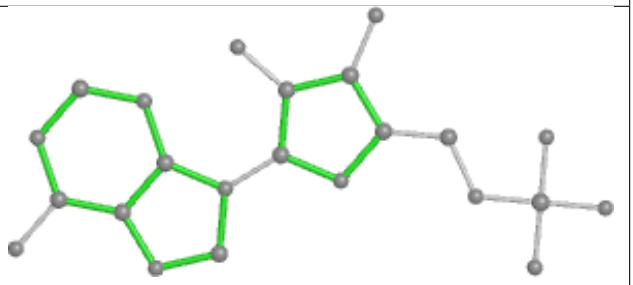
Bond lengths



Bond angles

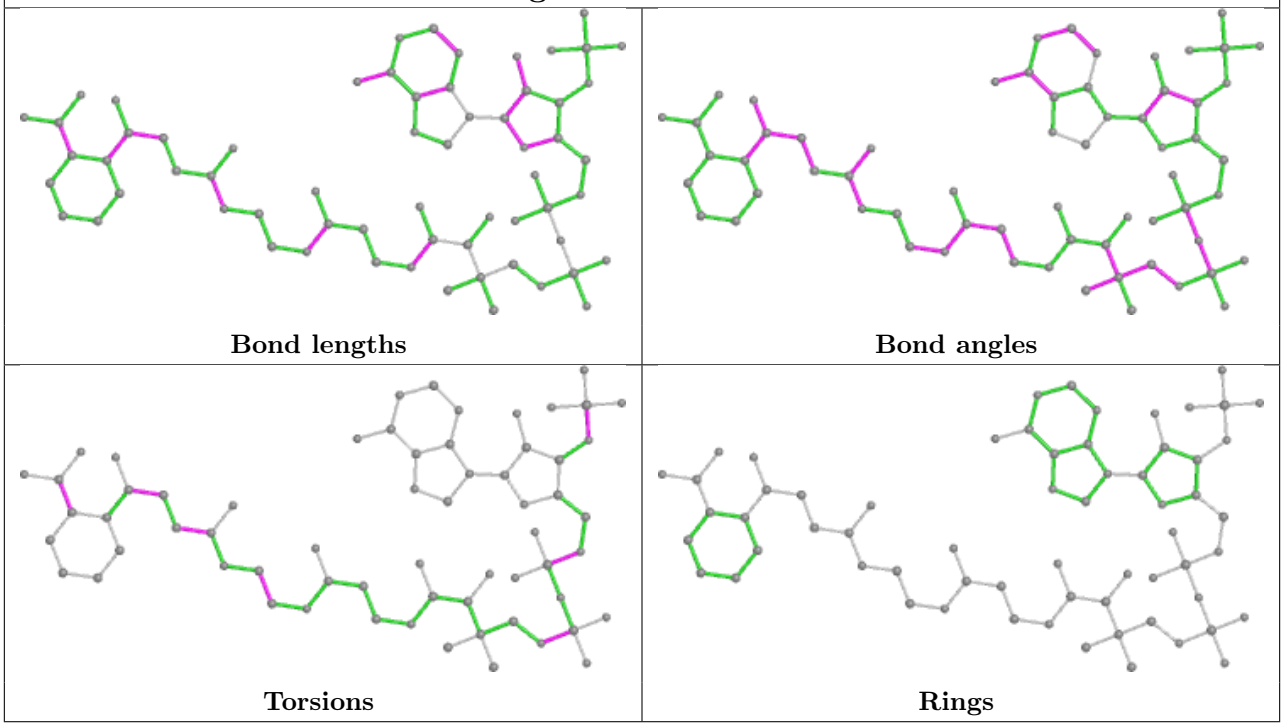


Torsions



Rings

Ligand S0N A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	484/485 (99%)	-0.04	13 (2%) 54 60	12, 24, 50, 85	0
1	B	485/485 (100%)	-0.02	17 (3%) 44 50	11, 23, 51, 69	0
1	C	485/485 (100%)	-0.19	8 (1%) 72 79	12, 25, 45, 64	0
1	D	484/485 (99%)	-0.09	14 (2%) 51 57	13, 26, 54, 87	0
All	All	1938/1940 (99%)	-0.08	52 (2%) 54 60	11, 25, 51, 87	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	468	ALA	7.2
1	C	486	LEU	5.0
1	B	468	ALA	4.9
1	A	469	SER	4.6
1	B	304	MET	4.5
1	D	435	PRO	3.9
1	B	325	GLY	3.9
1	B	435	PRO	3.8
1	A	467	ASN	3.5
1	A	470	ASN	3.4
1	D	324	ASP	3.4
1	B	118	ILE	3.3
1	D	436	VAL	3.2
1	C	118	ILE	3.1
1	D	438	ALA	3.1
1	D	485	LEU	3.1
1	B	470	ASN	3.0
1	B	327	VAL	3.0
1	A	327	VAL	3.0
1	B	117	HIS	2.9
1	A	482	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	480	ALA	2.8
1	D	468	ALA	2.8
1	B	467	ASN	2.8
1	A	473	LEU	2.7
1	B	486	LEU	2.7
1	A	433	HIS	2.7
1	D	407	PRO	2.7
1	C	307	LEU	2.6
1	B	324	ASP	2.6
1	D	304	MET	2.6
1	B	469	SER	2.5
1	B	277	GLU	2.5
1	A	475	ASN	2.5
1	B	302	PHE	2.5
1	C	304	MET	2.4
1	A	117	HIS	2.4
1	C	359	GLN	2.4
1	C	113	LYS	2.3
1	C	483	GLY	2.3
1	B	433	HIS	2.2
1	A	304	MET	2.2
1	B	407	PRO	2.2
1	A	464	LEU	2.1
1	D	197	ILE	2.1
1	B	483	GLY	2.1
1	D	194	LEU	2.1
1	D	200	LEU	2.1
1	C	435	PRO	2.0
1	D	439	GLY	2.0
1	D	325	GLY	2.0
1	D	479	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	C	513	1/1	0.46	0.24	73,73,73,73	0
3	AMP	A	502	23/23	0.65	0.35	25,37,58,62	23
5	NA	B	513	1/1	0.67	0.17	58,58,58,58	0
3	AMP	C	502	23/23	0.67	0.35	24,34,54,66	23
5	NA	D	510	1/1	0.73	0.29	61,61,61,61	0
5	NA	D	518	1/1	0.77	0.17	61,61,61,61	0
4	MG	B	506	1/1	0.79	0.09	59,59,59,59	0
4	MG	B	507	1/1	0.79	0.14	71,71,71,71	0
5	NA	C	512	1/1	0.80	0.19	62,62,62,62	0
5	NA	D	517	1/1	0.82	0.11	67,67,67,67	0
5	NA	B	514	1/1	0.82	0.25	70,70,70,70	0
6	PEG	C	515	7/7	0.83	0.18	38,53,66,67	0
5	NA	C	508	1/1	0.84	0.21	76,76,76,76	0
4	MG	C	504	1/1	0.84	0.05	65,65,65,65	0
5	NA	D	516	1/1	0.84	0.13	69,69,69,69	0
5	NA	D	519	1/1	0.85	0.08	60,60,60,60	0
5	NA	D	512	1/1	0.85	0.09	50,50,50,50	0
5	NA	C	509	1/1	0.86	0.10	53,53,53,53	0
6	PEG	B	520	7/7	0.86	0.20	31,40,65,68	0
4	MG	B	508	1/1	0.86	0.12	57,57,57,57	0
5	NA	C	511	1/1	0.87	0.06	59,59,59,59	0
6	PEG	B	519	7/7	0.87	0.12	30,37,44,47	0
5	NA	B	515	1/1	0.88	0.13	52,52,52,52	0
5	NA	C	510	1/1	0.88	0.10	50,50,50,50	0
7	CA	B	521	1/1	0.88	0.09	64,64,64,64	0
5	NA	D	509	1/1	0.89	0.11	69,69,69,69	0
5	NA	B	511	1/1	0.89	0.23	64,64,64,64	0
5	NA	D	511	1/1	0.89	0.10	62,62,62,62	0
5	NA	A	514	1/1	0.89	0.13	48,48,48,48	0
5	NA	B	517	1/1	0.90	0.16	40,40,40,40	0
5	NA	C	507	1/1	0.90	0.09	54,54,54,54	0
4	MG	A	505	1/1	0.90	0.10	43,43,43,43	0
2	S0N	C	501	63/63	0.90	0.10	13,22,51,55	0
5	NA	A	513	1/1	0.91	0.08	46,46,46,46	0
2	S0N	D	501	63/63	0.91	0.11	10,21,46,51	0
5	NA	A	515	1/1	0.92	0.09	60,60,60,60	0
4	MG	D	504	1/1	0.93	0.05	36,36,36,36	0

Continued on next page...

Continued from previous page...

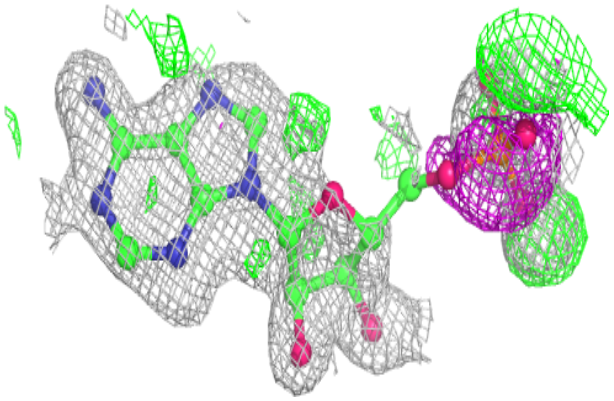
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PEG	D	520	7/7	0.93	0.11	27,37,40,47	0
4	MG	A	510	1/1	0.93	0.20	50,50,50,50	0
6	PEG	A	517	7/7	0.94	0.09	33,39,48,54	0
2	S0N	B	501	63/63	0.94	0.09	14,21,43,48	0
4	MG	C	506	1/1	0.94	0.12	37,37,37,37	0
5	NA	D	513	1/1	0.94	0.23	47,47,47,47	0
6	PEG	C	516	7/7	0.94	0.11	36,43,49,57	0
5	NA	D	515	1/1	0.94	0.21	48,48,48,48	0
6	PEG	A	516	7/7	0.94	0.09	40,43,47,50	0
4	MG	A	507	1/1	0.95	0.11	46,46,46,46	0
2	S0N	A	501	63/63	0.95	0.08	13,20,32,36	0
5	NA	A	511	1/1	0.95	0.12	52,52,52,52	0
5	NA	A	512	1/1	0.95	0.06	46,46,46,46	0
5	NA	B	518	1/1	0.95	0.10	52,52,52,52	0
4	MG	A	504	1/1	0.96	0.17	39,39,39,39	0
4	MG	B	502	1/1	0.96	0.07	27,27,27,27	0
4	MG	B	509	1/1	0.96	0.11	42,42,42,42	0
4	MG	C	503	1/1	0.96	0.05	22,22,22,22	0
4	MG	A	509	1/1	0.96	0.07	40,40,40,40	0
5	NA	C	514	1/1	0.96	0.14	48,48,48,48	0
4	MG	D	508	1/1	0.97	0.06	33,33,33,33	0
5	NA	B	516	1/1	0.97	0.10	39,39,39,39	0
5	NA	D	514	1/1	0.97	0.07	49,49,49,49	0
5	NA	B	512	1/1	0.97	0.10	38,38,38,38	0
7	CA	C	517	1/1	0.97	0.07	62,62,62,62	0
4	MG	D	506	1/1	0.98	0.12	38,38,38,38	0
4	MG	D	507	1/1	0.98	0.05	37,37,37,37	0
4	MG	B	503	1/1	0.98	0.06	32,32,32,32	0
4	MG	B	505	1/1	0.98	0.09	37,37,37,37	0
4	MG	D	503	1/1	0.99	0.04	30,30,30,30	0
4	MG	A	506	1/1	0.99	0.11	37,37,37,37	0
4	MG	D	505	1/1	0.99	0.04	23,23,23,23	0
4	MG	A	503	1/1	0.99	0.05	22,22,22,22	0
4	MG	A	508	1/1	0.99	0.08	36,36,36,36	0
5	NA	B	510	1/1	0.99	0.06	33,33,33,33	0
4	MG	D	502	1/1	0.99	0.06	18,18,18,18	0
7	CA	A	518	1/1	1.00	0.09	34,34,34,34	0
4	MG	B	504	1/1	1.00	0.05	23,23,23,23	0
4	MG	C	505	1/1	1.00	0.07	22,22,22,22	0

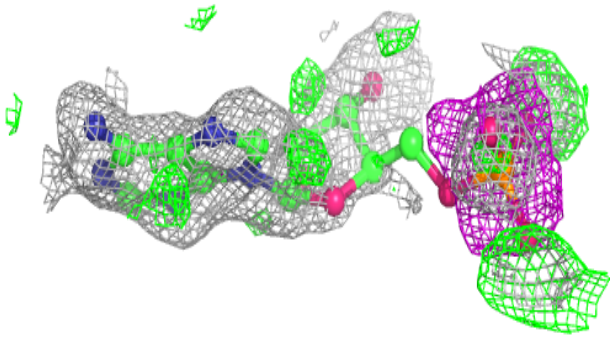
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

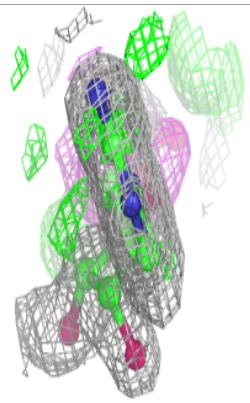
orientation to approximate a three-dimensional view.

Electron density around AMP A 502:

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

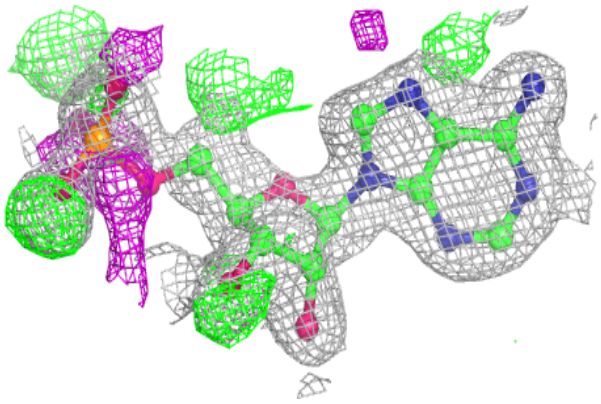


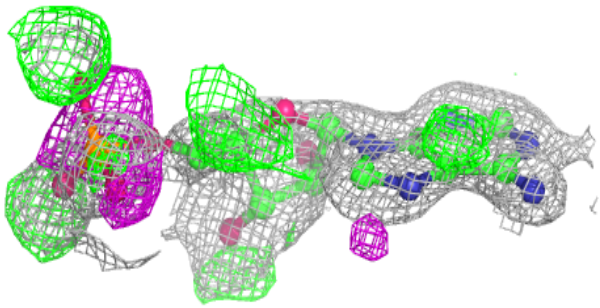


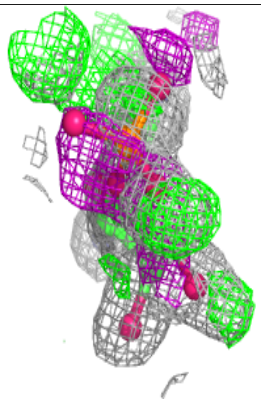


Electron density around AMP C 502:

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

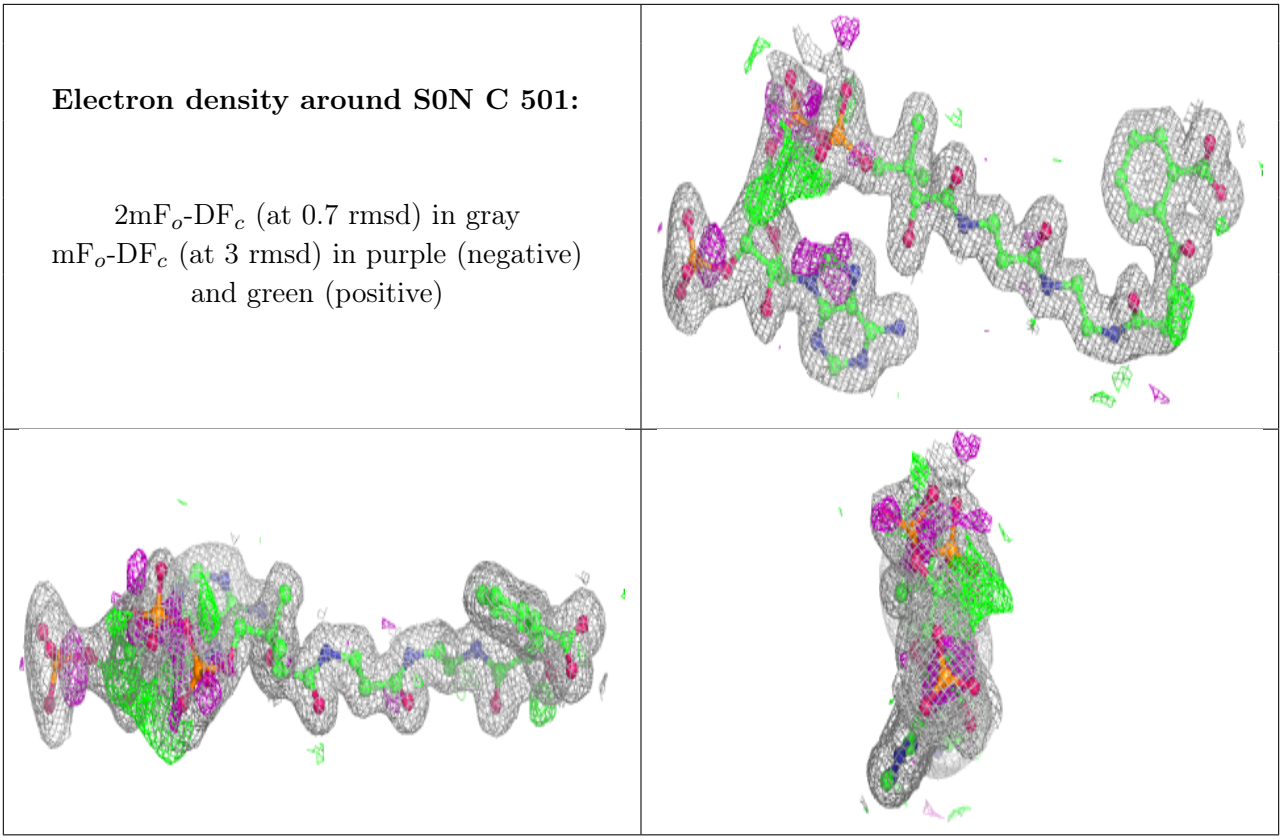






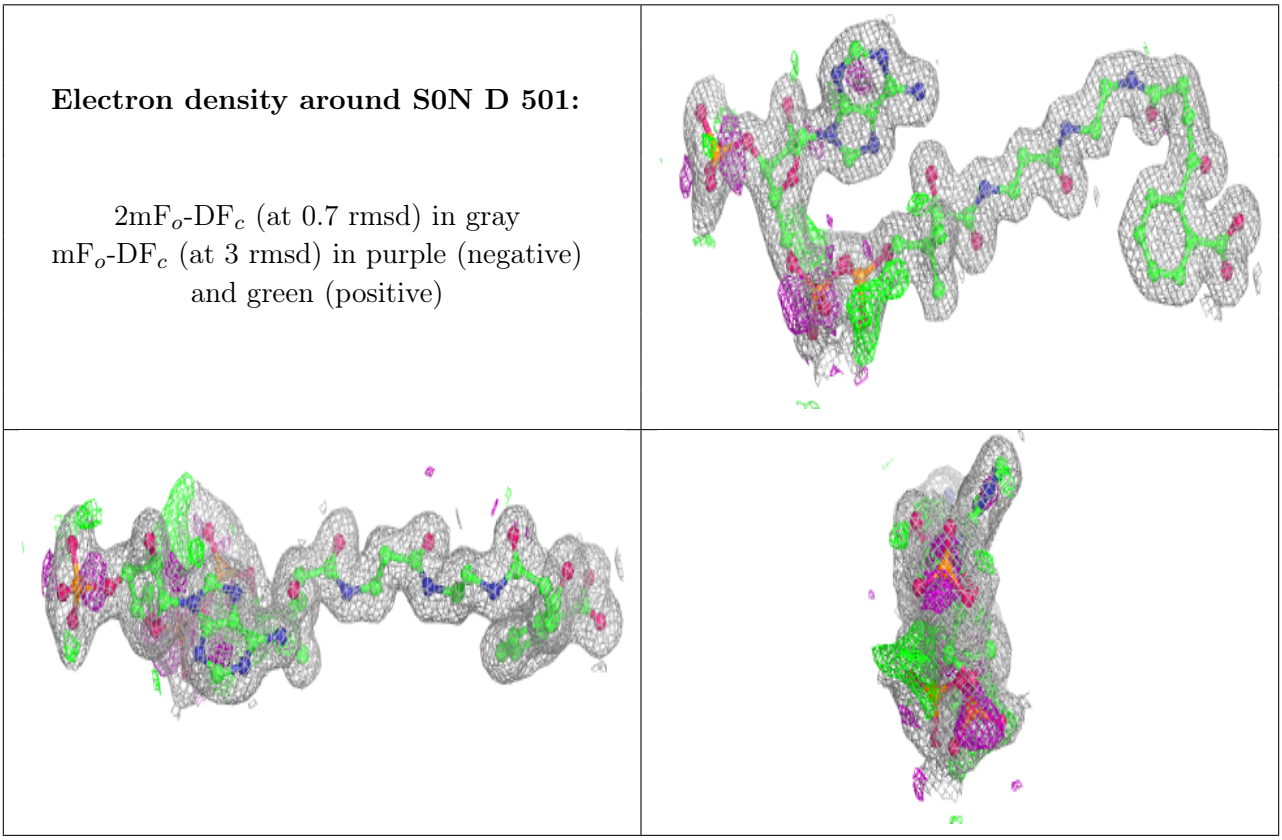
Electron density around S0N C 501:

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



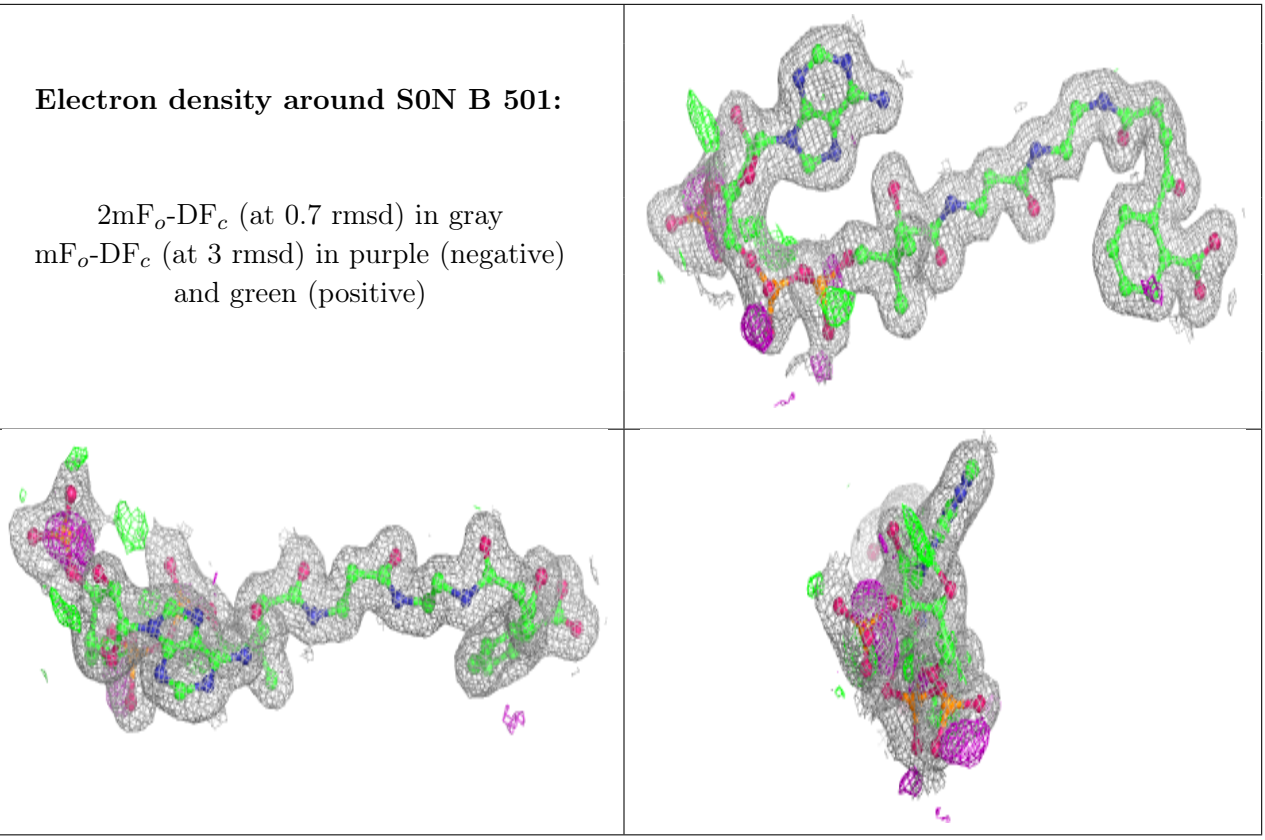
Electron density around S0N D 501:

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



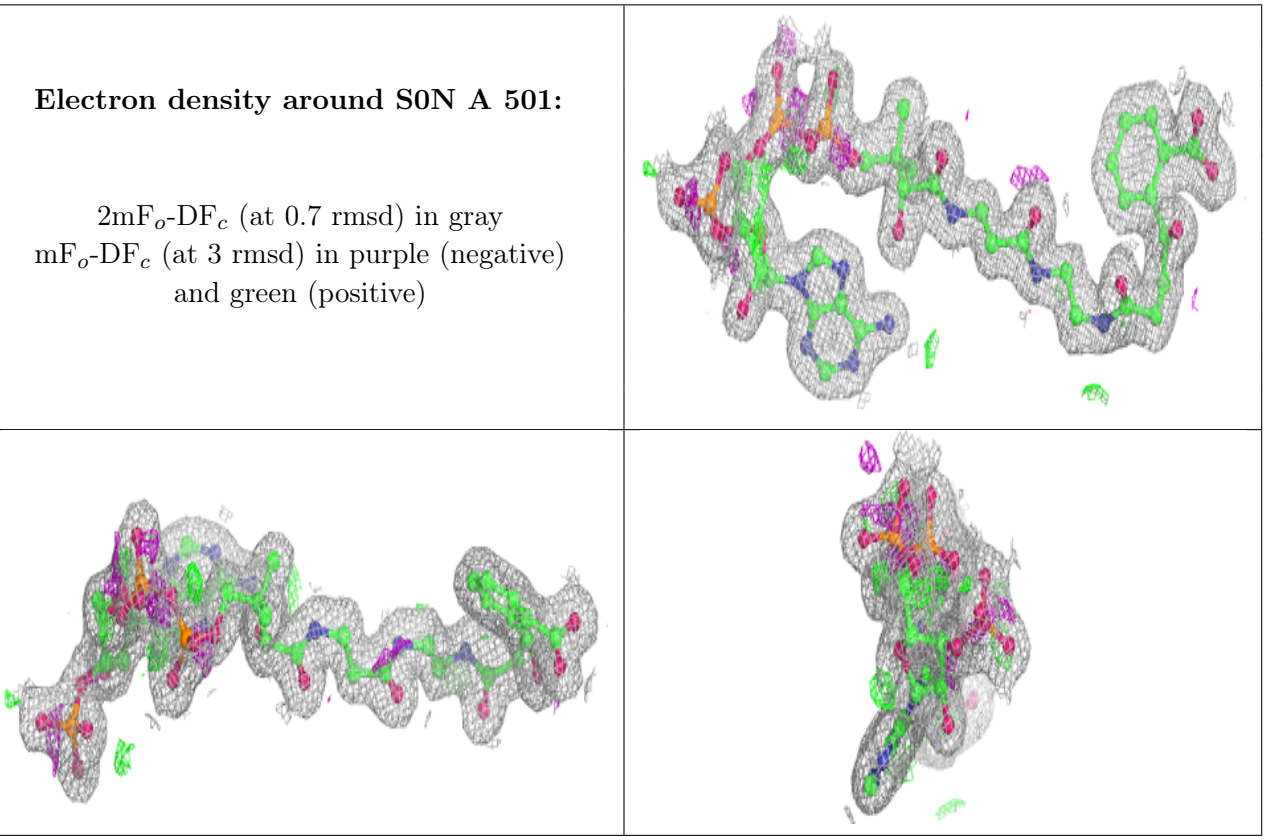
Electron density around S0N B 501:

$2mF_o$-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 (i)

There are no such residues in this entry.