



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:36 PM UTC

PDB ID : 4B2Z / pdb_00004b2z
Title : Structure of Osh6 in complex with phosphatidylserine
Authors : Maeda, K.; Anand, K.; Chiapparino, A.; Kumar, A.; Poletto, M.; Kaksonen, M.; Gavin, A.C.
Deposited on : 2012-07-19
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

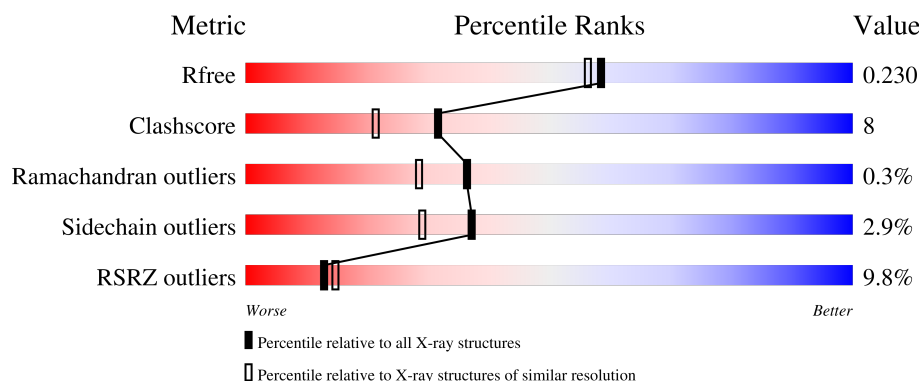
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	448	8% 77% 10% • 11%
1	B	448	9% 77% 11% • 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DTT	B	1437	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7029 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 Oxysterol-binding protein homolog 6.

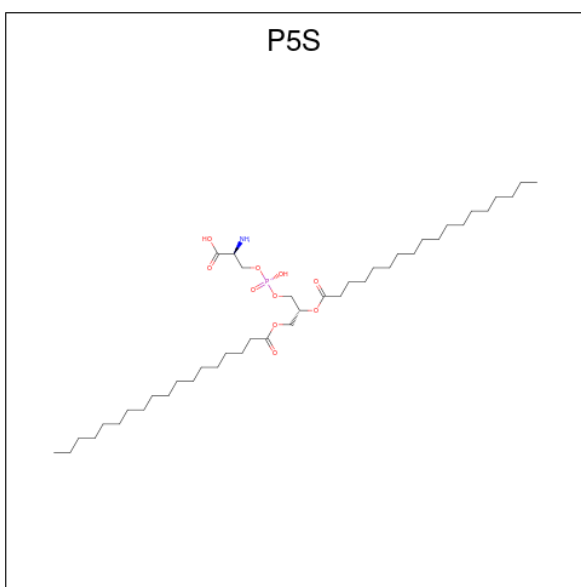
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	15	0	0
			3264	2102	548	603	11			
1	B	400	Total	C	N	O	S	7	0	0
			3269	2105	549	604	11			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



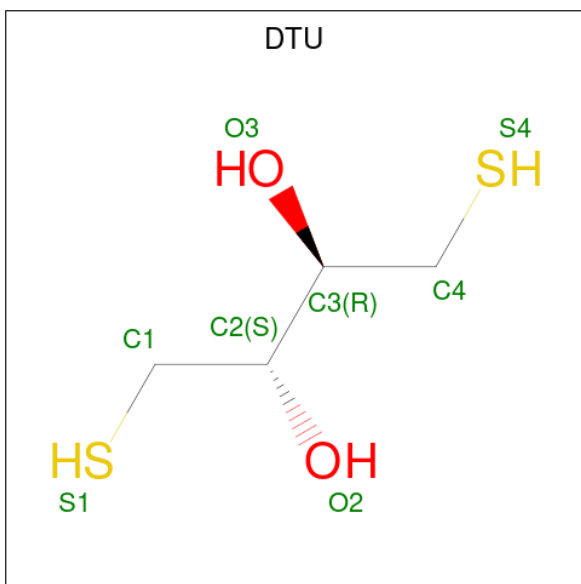
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy} (hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



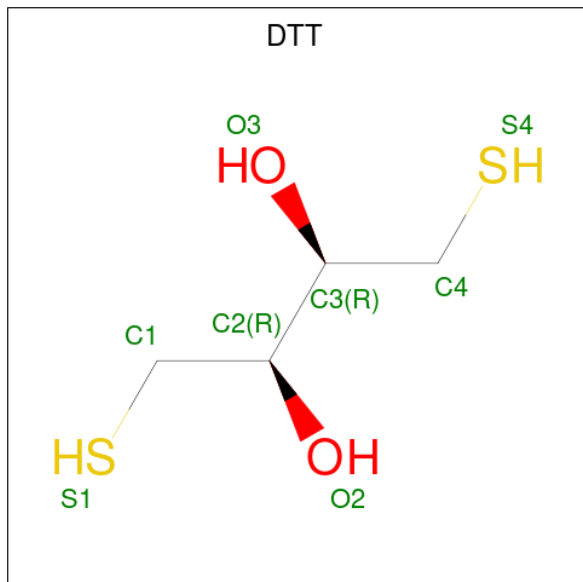
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	41	1	10	1		
3	B	1	Total	C	N	O	P	0	0
			54	42	1	10	1		

- Molecule 4 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (CCD ID: DTU) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			8	4	2	2		

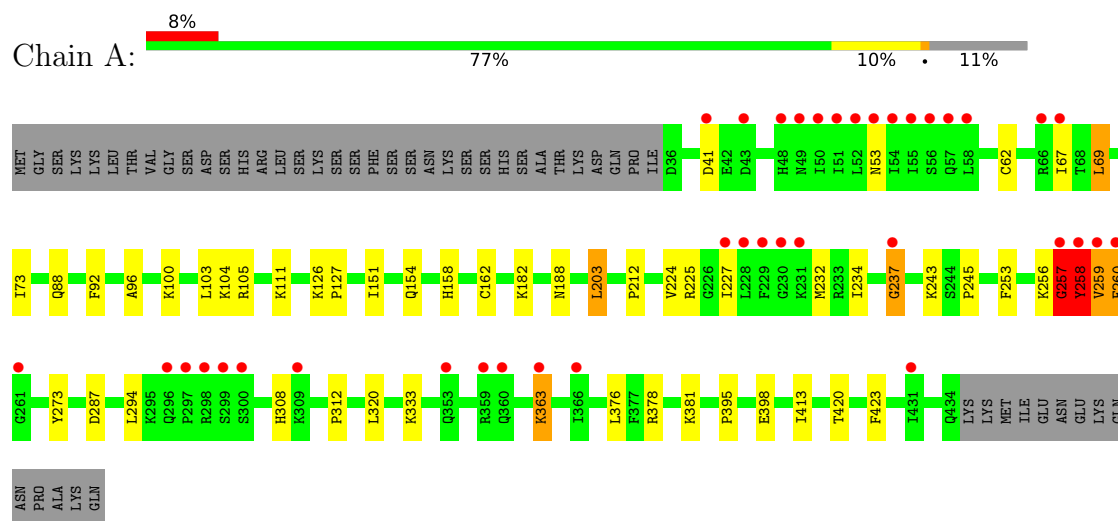
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	167	Total	O	0	0
			167	167		
6	B	196	Total	O	0	0
			196	196		

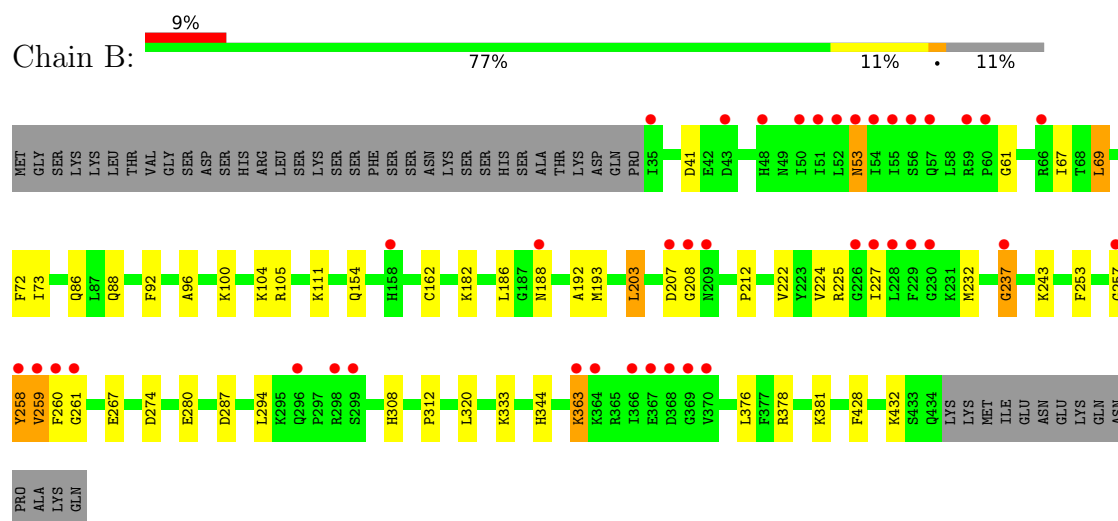
3 Residue-property plots

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: Oxysterol-binding protein homolog 6



• Molecule 1: Oxysterol-binding protein homolog 6



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.00Å 72.60Å 122.90Å 90.00° 111.40° 90.00°	Depositor
Resolution (Å)	46.57 – 1.95 46.57 – 1.95	Depositor EDS
% Data completeness (in resolution range)	91.8 (46.57-1.95) 91.8 (46.57-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.198 , 0.236 0.189 , 0.230	Depositor DCC
R_{free} test set	1318 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7029	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, DTT, P5S, DTU

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	0.46	0/3350	0.75	4/4531 (0.1%)
1	B	0.50	0/3355	0.74	2/4538 (0.0%)
All	All	0.48	0/6705	0.74	6/9069 (0.1%)

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
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	TYR	N-CA-C	9.76	127.38	111.37
1	A	237	GLY	N-CA-C	5.43	126.05	113.18
1	B	259	VAL	N-CA-C	5.29	120.34	109.34
1	B	237	GLY	N-CA-C	5.27	125.68	113.18
1	A	260	PHE	N-CA-C	-5.20	104.10	110.65
1	A	259	VAL	CB-CA-C	-5.18	98.80	111.02

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	GLY	Peptide
1	B	257	GLY	Peptide
1	B	260	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3264	0	3247	52	0
1	B	3269	0	3249	51	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	53	0	75	10	0
3	B	54	0	80	13	0
4	A	8	0	10	3	0
5	B	8	0	10	6	0
6	A	167	0	0	3	0
6	B	196	0	0	8	1
All	All	7029	0	6671	108	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 8.

All (108) 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:B:227:ILE:HG22	1:B:232:MET:HE3	1.15	1.14
1:A:227:ILE:HG22	1:A:232:MET:HE3	1.14	1.11
1:A:224:VAL:HG21	1:A:232:MET:HE2	1.42	1.01
1:B:224:VAL:HG21	1:B:232:MET:HE2	1.41	0.98
1:B:61:GLY:HA2	5:B:1437:DTT:S1	2.14	0.88
1:A:245:PRO:HA	5:B:1437:DTT:H12	1.61	0.81
1:A:227:ILE:CG2	1:A:232:MET:HE3	2.06	0.81
1:A:182:LYS:HE2	6:B:2182:HOH:O	1.81	0.80
6:A:2153:HOH:O	1:B:182:LYS:HE2	1.82	0.80
1:B:53:ASN:HB3	6:B:2011:HOH:O	1.82	0.79
1:B:227:ILE:CG2	1:B:232:MET:HE3	2.06	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:VAL:CG2	1:A:232:MET:HE2	2.17	0.74
1:B:224:VAL:CG2	1:B:232:MET:HE2	2.18	0.72
1:B:267:GLU:HG3	6:B:2124:HOH:O	1.90	0.71
1:B:237:GLY:O	6:B:2113:HOH:O	2.08	0.70
1:A:260:PHE:O	1:A:260:PHE:CD1	2.44	0.70
1:A:363:LYS:HE3	1:A:363:LYS:HA	1.75	0.69
1:B:222:VAL:HG12	3:B:1436:P5S:H44	1.77	0.66
1:B:363:LYS:HA	1:B:363:LYS:HE3	1.78	0.65
1:B:92:PHE:CE1	1:B:111:LYS:HE2	2.34	0.63
3:B:1436:P5S:H41	3:B:1436:P5S:H45	1.82	0.62
1:A:127:PRO:HD2	3:A:1436:P5S:O18	1.99	0.61
1:A:258:TYR:H	1:A:258:TYR:HD1	1.45	0.61
1:B:232:MET:HE1	3:B:1436:P5S:H52A	1.81	0.61
1:B:237:GLY:O	1:B:253:PHE:O	2.19	0.61
1:A:188:ASN:O	1:A:227:ILE:HG12	2.01	0.61
1:A:420:THR:HG23	4:A:1437:DTU:H3	1.83	0.60
1:A:423:PHE:HB2	4:A:1437:DTU:O2	2.01	0.60
3:B:1436:P5S:H45	3:B:1436:P5S:C41	2.32	0.59
1:A:154:GLN:NE2	1:A:162:CYS:HB3	2.18	0.59
1:A:62:CYS:HB3	1:B:208:GLY:HA3	1.85	0.58
1:A:92:PHE:CE1	1:A:111:LYS:HE2	2.40	0.57
1:B:232:MET:HE1	3:B:1436:P5S:C52	2.35	0.57
1:A:237:GLY:O	1:A:253:PHE:O	2.22	0.56
1:A:243:LYS:HD3	5:B:1437:DTT:S4	2.48	0.54
1:A:363:LYS:HE3	1:A:363:LYS:CA	2.37	0.53
1:B:188:ASN:O	1:B:227:ILE:HG12	2.08	0.53
1:B:222:VAL:O	3:B:1436:P5S:H43A	2.08	0.53
1:A:225:ARG:NH1	1:B:274:ASP:HA	2.24	0.52
1:B:428:PHE:O	1:B:432:LYS:HG3	2.09	0.52
1:A:256:LYS:C	1:A:257:GLY:O	2.53	0.52
1:A:234:ILE:HD11	3:A:1436:P5S:H45	1.93	0.51
1:B:154:GLN:NE2	1:B:162:CYS:HB3	2.25	0.51
1:A:258:TYR:CD1	1:A:258:TYR:N	2.78	0.51
1:A:287:ASP:OD1	1:A:308:HIS:CE1	2.64	0.51
1:A:420:THR:OG1	4:A:1437:DTU:H2	2.10	0.51
1:A:73:ILE:HB	3:A:1436:P5S:H49A	1.93	0.51
3:B:1436:P5S:O18	3:B:1436:P5S:H22A	2.10	0.50
1:B:258:TYR:CD1	1:B:258:TYR:N	2.75	0.49
1:B:363:LYS:HE3	1:B:363:LYS:CA	2.42	0.49
1:A:287:ASP:OD1	1:A:308:HIS:HE1	1.95	0.49
1:A:88:GLN:HE21	1:A:312:PRO:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLY:HA2	6:B:2106:HOH:O	2.13	0.48
1:A:67:ILE:HD12	1:A:67:ILE:C	2.38	0.48
1:A:320:LEU:HD11	1:A:333:LYS:HE3	1.95	0.48
1:B:192:ALA:HB2	3:B:1436:P5S:H20	1.95	0.48
1:A:73:ILE:HB	3:A:1436:P5S:C49	2.44	0.47
1:A:126:LYS:HB3	3:A:1436:P5S:H48	1.95	0.47
1:A:260:PHE:O	1:A:260:PHE:HD1	1.95	0.47
1:B:287:ASP:OD1	1:B:308:HIS:CE1	2.67	0.47
1:B:320:LEU:HD11	1:B:333:LYS:HE3	1.96	0.47
1:A:273:TYR:OH	5:B:1437:DTT:H41	2.15	0.47
1:A:256:LYS:HG2	1:A:257:GLY:O	2.15	0.47
1:B:192:ALA:CB	3:B:1436:P5S:H20	2.45	0.46
1:B:100:LYS:O	1:B:105:ARG:NH2	2.47	0.46
1:B:203:LEU:HA	1:B:212:PRO:HB3	1.97	0.46
1:B:287:ASP:OD1	1:B:308:HIS:HE1	1.98	0.46
1:A:232:MET:HE1	3:A:1436:P5S:C52	2.46	0.46
1:A:203:LEU:HA	1:A:212:PRO:HB3	1.98	0.46
3:B:1436:P5S:H24	3:B:1436:P5S:H21	1.62	0.46
1:B:86:GLN:NE2	6:B:2028:HOH:O	2.48	0.45
1:B:222:VAL:HG11	3:B:1436:P5S:H21A	1.97	0.45
6:A:2101:HOH:O	1:B:243:LYS:HE2	2.15	0.45
1:B:67:ILE:C	1:B:67:ILE:HD12	2.42	0.45
1:B:88:GLN:HE21	1:B:312:PRO:HB2	1.80	0.45
1:B:104:LYS:HE2	1:B:104:LYS:HB3	1.72	0.45
1:B:222:VAL:CG1	3:B:1436:P5S:H44	2.45	0.45
1:B:378:ARG:HH11	1:B:378:ARG:HG3	1.82	0.45
1:A:395:PRO:HB2	1:A:398:GLU:HB2	1.98	0.45
1:B:193:MET:HE3	5:B:1437:DTT:O2	2.17	0.45
1:B:207:ASP:OD1	1:B:207:ASP:C	2.60	0.45
1:B:280:GLU:HG3	6:B:2121:HOH:O	2.16	0.44
1:B:67:ILE:CD1	1:B:69:LEU:HD13	2.47	0.44
1:A:126:LYS:HG2	3:A:1436:P5S:H49	1.98	0.44
1:A:73:ILE:C	1:A:73:ILE:HD12	2.43	0.44
1:A:225:ARG:O	1:A:232:MET:HA	2.16	0.44
1:A:100:LYS:O	1:A:105:ARG:NH2	2.50	0.44
1:A:158:HIS:HD2	6:A:2071:HOH:O	2.00	0.44
1:A:151:ILE:HD11	1:A:413:ILE:HD11	2.00	0.44
1:A:67:ILE:HD12	1:A:67:ILE:O	2.18	0.43
1:A:232:MET:HE1	3:A:1436:P5S:H52A	1.99	0.43
1:A:67:ILE:CD1	1:A:69:LEU:HD13	2.48	0.43
1:A:363:LYS:HA	1:A:363:LYS:CE	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ILE:C	1:B:73:ILE:HD12	2.44	0.43
3:B:1436:P5S:H50	3:B:1436:P5S:H46A	1.74	0.43
1:A:104:LYS:HE2	1:A:104:LYS:HB3	1.70	0.43
1:B:53:ASN:CG	6:B:2011:HOH:O	2.63	0.42
3:A:1436:P5S:H44A	3:A:1436:P5S:H20A	2.01	0.42
1:A:378:ARG:HH11	1:A:378:ARG:HG3	1.84	0.42
1:B:225:ARG:O	1:B:232:MET:HA	2.19	0.42
3:A:1436:P5S:H46A	3:A:1436:P5S:H50	1.86	0.41
1:B:67:ILE:HD12	1:B:67:ILE:O	2.20	0.41
1:B:96:ALA:O	1:B:105:ARG:HG3	2.19	0.41
1:A:257:GLY:HA3	1:A:260:PHE:H	1.85	0.40
1:A:96:ALA:O	1:A:105:ARG:HG3	2.22	0.40
1:B:92:PHE:CZ	1:B:111:LYS:HE2	2.56	0.40
1:B:186:LEU:CD2	5:B:1437:DTT:S1	3.10	0.40
1:B:72:PHE:HA	1:B:344:HIS:CE1	2.57	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)
6:B:2011:HOH:O	6:B:2195:HOH:O[4_556]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/448 (89%)	377 (95%)	19 (5%)	1 (0%)	36	28
1	B	398/448 (89%)	380 (96%)	17 (4%)	1 (0%)	36	28
All	All	795/896 (89%)	757 (95%)	36 (4%)	2 (0%)	36	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	GLY
1	B	261	GLY

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	360/405 (89%)	349 (97%)	11 (3%)	35	26
1	B	360/405 (89%)	350 (97%)	10 (3%)	38	30
All	All	720/810 (89%)	699 (97%)	21 (3%)	37	29

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	A	53	ASN
1	A	69	LEU
1	A	103	LEU
1	A	203	LEU
1	A	258	TYR
1	A	259	VAL
1	A	294	LEU
1	A	363	LYS
1	A	376	LEU
1	A	381	LYS
1	B	41	ASP
1	B	53	ASN
1	B	69	LEU
1	B	203	LEU
1	B	258	TYR
1	B	259	VAL
1	B	294	LEU
1	B	363	LYS
1	B	376	LEU
1	B	381	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	88	GLN
1	A	95	GLN
1	A	146	GLN
1	A	147	GLN
1	A	154	GLN
1	A	188	ASN
1	A	308	HIS
1	A	357	HIS
1	A	358	GLN
1	B	57	GLN
1	B	86	GLN
1	B	88	GLN
1	B	95	GLN
1	B	146	GLN
1	B	147	GLN
1	B	154	GLN
1	B	308	HIS
1	B	357	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DTT	B	1437	-	7,7,7	1.46	1 (14%)	4,8,8	1.74	1 (25%)
3	P5S	A	1436	-	51,52,53	1.78	10 (19%)	53,59,60	1.52	8 (15%)
2	SO4	B	1435	-	4,4,4	0.24	0	6,6,6	0.24	0
4	DTU	A	1437	-	7,7,7	1.49	2 (28%)	4,8,8	1.71	1 (25%)
2	SO4	A	1435	-	4,4,4	0.30	0	6,6,6	0.24	0
3	P5S	B	1436	-	52,53,53	1.63	8 (15%)	54,60,60	1.66	8 (14%)

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	P5S	B	1436	-	-	21/59/59/59	-
4	DTU	A	1437	-	-	6/8/8/8	-
5	DTT	B	1437	-	-	3/8/8/8	-
3	P5S	A	1436	-	-	15/58/58/59	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1436	P5S	O37-C38	5.41	1.49	1.34
3	B	1436	P5S	O37-C38	5.40	1.49	1.34
3	A	1436	P5S	P12-O15	-4.28	1.35	1.55
3	B	1436	P5S	P12-O15	-4.24	1.35	1.55
3	A	1436	P5S	C48-C46	-3.51	1.34	1.51
3	A	1436	P5S	O19-C17	3.51	1.43	1.33
3	B	1436	P5S	C48-C46	-3.48	1.34	1.51
3	A	1436	P5S	C3-C2	3.34	1.61	1.50
3	B	1436	P5S	O19-C17	3.22	1.42	1.33
3	B	1436	P5S	C3-C2	3.00	1.60	1.50
3	A	1436	P5S	C1-C2	2.96	1.60	1.50
3	A	1436	P5S	P12-OG	-2.48	1.49	1.59
3	A	1436	P5S	O37-C2	2.38	1.52	1.46
3	B	1436	P5S	O37-C2	2.29	1.52	1.46
3	A	1436	P5S	C20-C17	2.26	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1437	DTU	O3-C3	-2.22	1.38	1.43
3	B	1436	P5S	C1-C2	2.19	1.57	1.50
4	A	1437	DTU	C4-S4	-2.17	1.77	1.81
3	B	1436	P5S	P12-OG	-2.16	1.50	1.59
5	B	1437	DTT	O2-C2	-2.13	1.38	1.43
3	A	1436	P5S	C21-C20	2.00	1.59	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1436	P5S	O37-C38-C39	6.69	125.95	111.48
3	A	1436	P5S	O37-C38-C39	6.03	124.52	111.48
3	B	1436	P5S	O37-C38-O47	-4.08	114.18	123.70
3	B	1436	P5S	C22-C21-C20	-3.74	99.39	113.13
3	B	1436	P5S	O19-C1-C2	-3.73	97.65	108.40
3	A	1436	P5S	O37-C38-O47	-3.71	115.03	123.70
3	A	1436	P5S	O19-C17-C20	3.06	121.16	111.83
3	B	1436	P5S	C2-O37-C38	2.86	124.64	117.80
3	A	1436	P5S	O19-C17-O18	-2.82	116.56	123.63
3	A	1436	P5S	C2-O37-C38	2.49	123.75	117.80
5	B	1437	DTT	O2-C2-C3	2.46	114.73	109.57
3	A	1436	P5S	CB-CA-C	2.43	119.11	108.68
3	B	1436	P5S	CB-CA-C	2.36	118.81	108.68
4	A	1437	DTU	O3-C3-C2	2.35	114.52	109.57
3	B	1436	P5S	C25-C24-C23	-2.31	102.72	114.37
3	A	1436	P5S	C3-C2-C1	2.19	116.88	111.78
3	A	1436	P5S	OG-P12-O13	-2.15	100.41	108.94
3	B	1436	P5S	P12-O16-C3	-2.11	109.27	121.35

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1436	P5S	O-C-CA-CB
3	A	1436	P5S	OXT-C-CA-CB
3	B	1436	P5S	O-C-CA-CB
4	A	1437	DTU	S1-C1-C2-O2
4	A	1437	DTU	S1-C1-C2-C3
4	A	1437	DTU	C1-C2-C3-O3
4	A	1437	DTU	C1-C2-C3-C4
4	A	1437	DTU	C2-C3-C4-S4
4	A	1437	DTU	O3-C3-C4-S4

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Mol	Chain	Res	Type	Atoms
5	B	1437	DTT	S1-C1-C2-O2
5	B	1437	DTT	O3-C3-C4-S4
3	A	1436	P5S	C46-C48-C49-C50
3	B	1436	P5S	C46-C48-C49-C50
3	B	1436	P5S	C21-C22-C23-C24
3	A	1436	P5S	C17-C20-C21-C22
3	A	1436	P5S	C44-C45-C46-C48
3	B	1436	P5S	C43-C44-C45-C46
3	B	1436	P5S	C45-C46-C48-C49
3	B	1436	P5S	C27-C28-C29-C30
3	B	1436	P5S	C41-C42-C43-C44
3	A	1436	P5S	C43-C44-C45-C46
3	B	1436	P5S	C20-C21-C22-C23
3	B	1436	P5S	C26-C27-C28-C29
5	B	1437	DTT	O2-C2-C3-O3
3	B	1436	P5S	C28-C29-C30-C31
3	A	1436	P5S	C48-C49-C50-C51
3	A	1436	P5S	C28-C29-C30-C31
3	A	1436	P5S	C49-C50-C51-C52
3	B	1436	P5S	C42-C43-C44-C45
3	B	1436	P5S	C44-C45-C46-C48
3	B	1436	P5S	OXT-C-CA-CB
3	B	1436	P5S	CB-OG-P12-O13
3	B	1436	P5S	C40-C41-C42-C43
3	A	1436	P5S	C20-C21-C22-C23
3	B	1436	P5S	C33-C34-C35-C36
3	A	1436	P5S	C50-C51-C52-C53
3	A	1436	P5S	C42-C43-C44-C45
3	B	1436	P5S	C48-C49-C50-C51
3	A	1436	P5S	C26-C27-C28-C29
3	A	1436	P5S	C24-C25-C26-C27
3	B	1436	P5S	C29-C30-C31-C32
3	B	1436	P5S	O18-C17-C20-C21
3	B	1436	P5S	O-C-CA-N
3	B	1436	P5S	O19-C17-C20-C21
3	A	1436	P5S	C32-C33-C34-C35

There are no ring outliers.

4 monomers are involved in 32 short contacts:

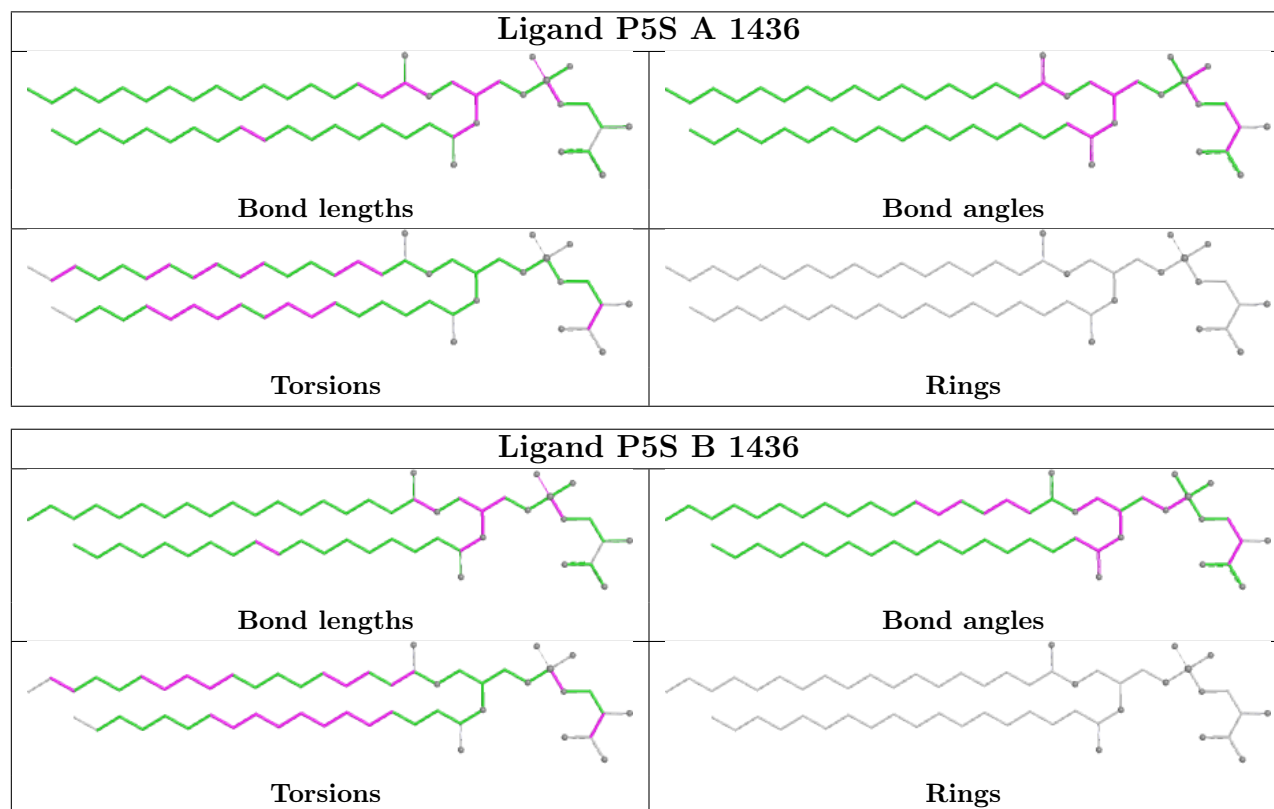
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1437	DTT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1436	P5S	10	0
4	A	1437	DTU	3	0
3	B	1436	P5S	13	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	399/448 (89%)	0.27	38 (9%) 14 15	15, 30, 62, 222	3 (0%)
1	B	400/448 (89%)	0.22	40 (10%) 12 14	15, 28, 60, 222	1 (0%)
All	All	799/896 (89%)	0.24	78 (9%) 13 15	15, 28, 60, 222	4 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	TYR	10.1
1	B	259	VAL	9.5
1	A	51	ILE	8.2
1	A	52	LEU	7.8
1	A	258	TYR	7.6
1	A	259	VAL	7.5
1	A	230	GLY	6.7
1	B	260	PHE	6.5
1	A	54	ILE	6.3
1	A	55	ILE	6.2
1	B	56	SER	6.1
1	B	229	PHE	6.0
1	B	257	GLY	5.6
1	B	208	GLY	5.6
1	B	366	ILE	5.1
1	B	35	ILE	5.0
1	B	48	HIS	5.0
1	A	57	GLN	4.9
1	B	230	GLY	4.8
1	A	48	HIS	4.7
1	B	363	LYS	4.3
1	A	260	PHE	4.3
1	B	228	LEU	4.2
1	B	261	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	52	LEU	4.2
1	A	257	GLY	4.1
1	B	369	GLY	4.1
1	A	229	PHE	4.1
1	A	56	SER	4.0
1	A	298	ARG	4.0
1	B	237	GLY	4.0
1	A	237	GLY	4.0
1	A	53	ASN	3.9
1	A	50	ILE	3.9
1	B	298	ARG	3.8
1	B	370	VAL	3.8
1	B	207	ASP	3.7
1	A	228	LEU	3.7
1	B	43	ASP	3.6
1	A	58	LEU	3.6
1	A	363	LYS	3.4
1	B	57	GLN	3.4
1	A	66	ARG	3.3
1	A	299	SER	3.2
1	A	359	ARG	3.1
1	B	66	ARG	3.1
1	B	53	ASN	3.1
1	A	300	SER	3.1
1	A	49	ASN	3.0
1	A	41	ASP	2.9
1	A	297	PRO	2.9
1	B	188	ASN	2.9
1	A	366	ILE	2.8
1	A	431	ILE	2.8
1	B	54	ILE	2.7
1	B	299	SER	2.7
1	B	364	LYS	2.6
1	B	158	HIS	2.6
1	B	209	ASN	2.6
1	B	59	ARG	2.5
1	A	353	GLN	2.5
1	A	296	GLN	2.5
1	B	296	GLN	2.5
1	A	43	ASP	2.5
1	B	226	GLY	2.4
1	A	67	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	55	ILE	2.3
1	A	360	GLN	2.3
1	A	227	ILE	2.3
1	A	309	LYS	2.3
1	B	367	GLU	2.2
1	B	368	ASP	2.2
1	A	261	GLY	2.2
1	B	50	ILE	2.1
1	B	51	ILE	2.1
1	A	231	LYS	2.1
1	B	60	PRO	2.0
1	B	227	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

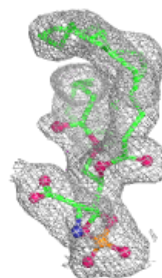
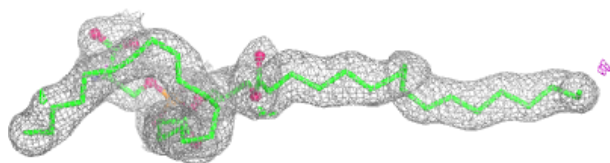
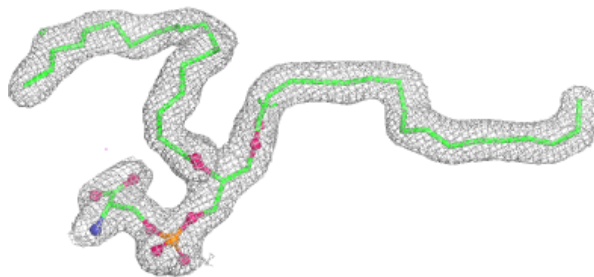
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DTT	B	1437	8/8	0.81	0.29	42,55,177,242	0
2	SO4	B	1435	5/5	0.83	0.22	42,76,85,94	0
2	SO4	A	1435	5/5	0.84	0.15	32,36,78,84	0
4	DTU	A	1437	8/8	0.86	0.16	48,68,84,96	0
3	P5S	A	1436	53/54	0.95	0.08	16,28,37,43	0
3	P5S	B	1436	54/54	0.96	0.08	13,21,36,74	0

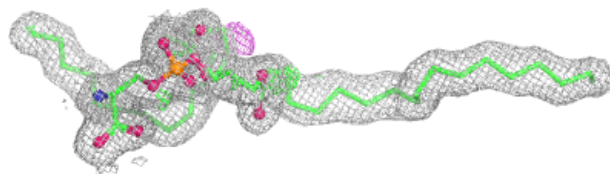
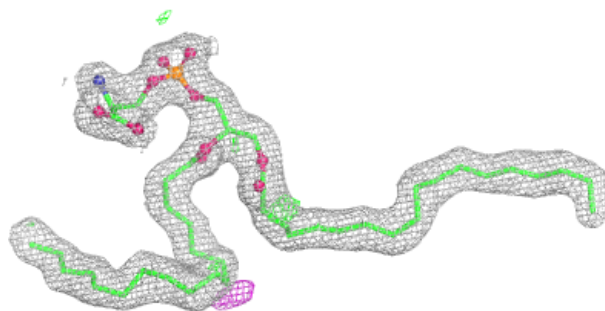
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P5S A 1436:

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

**Electron density around P5S B 1436:**

$2mF_o-DF_c$ (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.