



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2025 – 01:15 pm BST

PDB ID : 9H12 / pdb_00009h12
Title : Crystal structure of OXA-48 in complex with nacubactam
Authors : Hoff, J.F.; Goudar, K.E.; Hinchliffe, P.; Spencer, J.
Deposited on : 2024-10-09
Resolution : 1.51 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

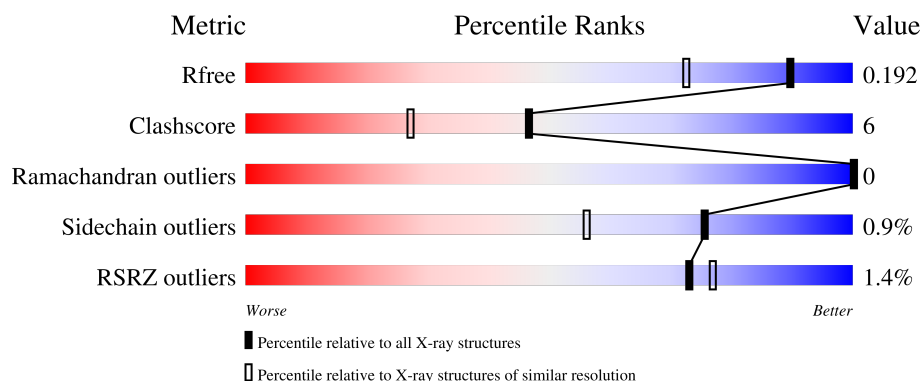
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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}	164625	5293 (1.54-1.50)
Clashscore	180529	5759 (1.54-1.50)
Ramachandran outliers	177936	5653 (1.54-1.50)
Sidechain outliers	177891	5650 (1.54-1.50)
RSRZ outliers	164620	5293 (1.54-1.50)

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	245	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 90% 10% </div> </div>
1	B	245	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 96%);"></div> <div style="display: flex; justify-content: space-between; width: 92%; margin: 0 auto;"> 92% 8% </div> </div>

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
4	PEG	B	306	-	-	X	-
7	DMS	A	316	-	-	X	-
7	DMS	B	309	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4685 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	9	0
			2057	1308	362	379	8			
1	B	245	Total	C	N	O	S	0	8	0
			2059	1308	368	375	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	expression tag	UNP Q6XEC0
A	22	PRO	-	expression tag	UNP Q6XEC0
B	21	GLY	-	expression tag	UNP Q6XEC0
B	22	PRO	-	expression tag	UNP Q6XEC0

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

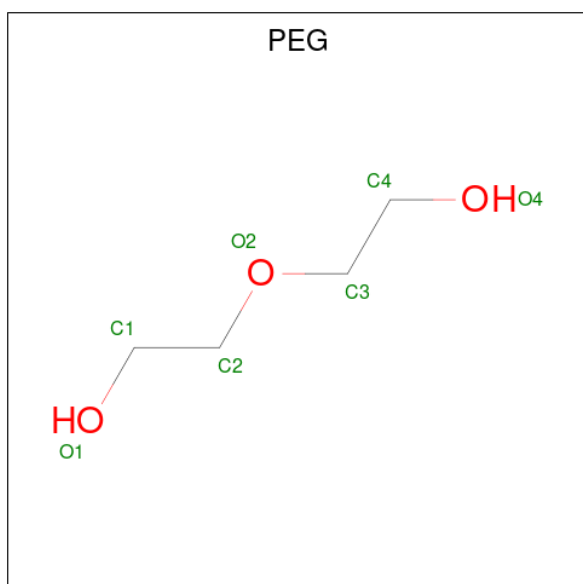
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



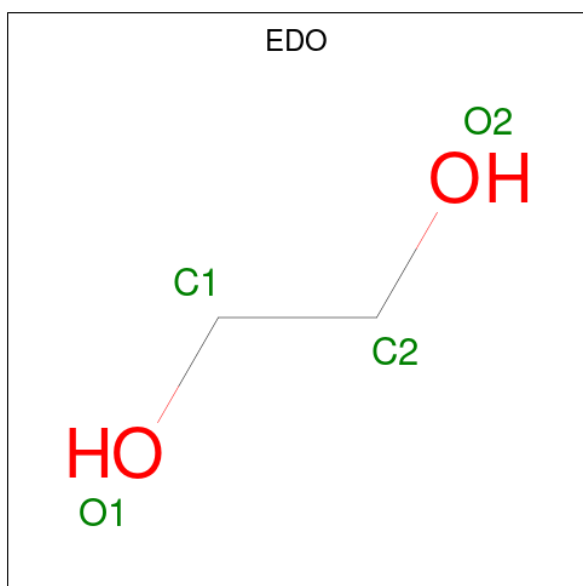
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

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



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



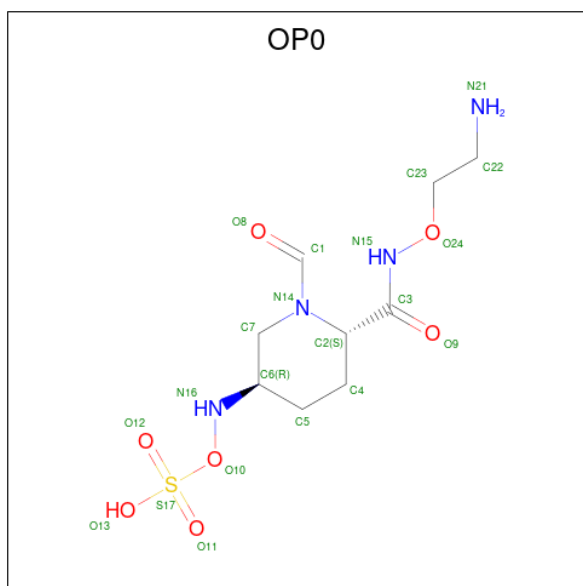
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

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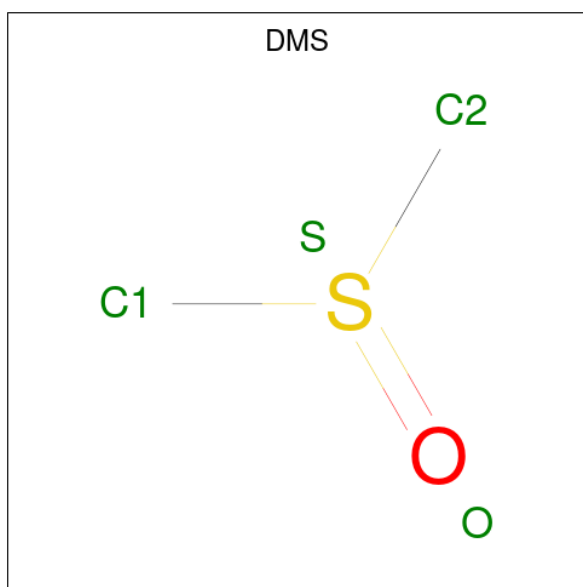
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is (2S,5R)-N-(2-aminoethoxy)-1-formyl-5-[(sulfooxy)amino]piperidine-2-carboxamide (CCD ID: OP0) (formula: C₉H₁₈N₄O₇S) (labeled as "Ligand of Interest" by depositor).



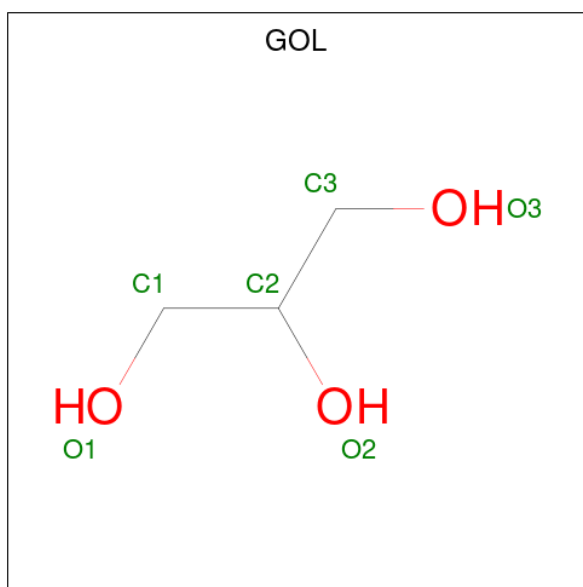
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	1
			42	18	8	14	2		
6	B	1	Total	C	N	O	S	0	0
			21	9	4	7	1		

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



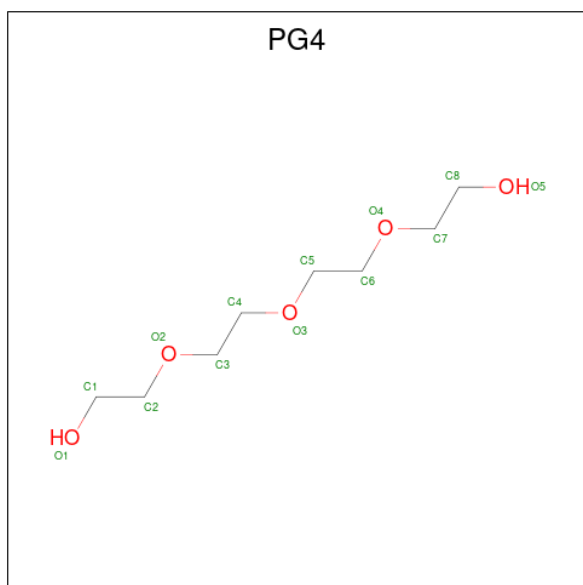
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	1
			6	3	3		

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

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	181	Total	O	0	4
			182	182		
10	B	148	Total	O	0	3
			149	149		

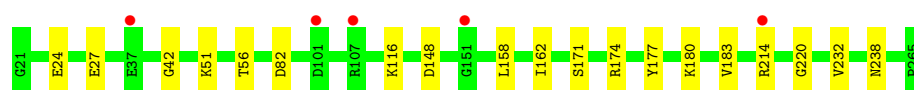
3 Residue-property plots [i](#)

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: Beta-lactamase



- Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.76Å 121.76Å 159.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.88 – 1.51 60.88 – 1.51	Depositor EDS
% Data completeness (in resolution range)	100.0 (60.88-1.51) 99.9 (60.88-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.51Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.173 , 0.192 0.173 , 0.192	Depositor DCC
R_{free} test set	5517 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4685	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: PEG, GOL, DMS, PGE, OP0, EDO, CL, PG4

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	0.28	0/2111	0.48	0/2855
1	B	0.26	0/2110	0.48	0/2851
All	All	0.27	0/4221	0.48	0/5706

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	2057	0	2003	23	0
1	B	2059	0	2008	22	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	40	0	56	7	0
3	B	10	0	14	1	0
4	A	28	0	40	5	0
4	B	7	0	10	5	0
5	A	28	0	42	2	0
5	B	16	0	24	2	0
6	A	42	0	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	21	0	16	2	0
7	A	8	0	12	7	0
7	B	4	0	6	6	0
8	A	6	0	8	0	0
8	B	12	0	16	0	0
9	B	13	0	18	0	0
10	A	182	0	0	2	1
10	B	149	0	0	1	1
All	All	4685	0	4305	49	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 6.

All (49) 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:42:GLY:H	5:B:310:EDO:H11	1.38	0.86
1:B:174:ARG:HH11	7:B:309:DMS:H12	1.41	0.85
1:B:24:GLU:OE1	10:B:401:HOH:O	1.99	0.80
1:B:174:ARG:HD3	7:B:309:DMS:H13	1.64	0.79
1:B:171:SER:HA	7:B:309:DMS:H11	1.68	0.75
1:B:158[A]:LEU:HD22	6:B:308:OP0:H16	1.71	0.72
1:A:174:ARG:HH11	7:A:316:DMS:H12	1.54	0.71
1:A:92:VAL:HG22	7:A:318:DMS:H23	1.74	0.70
1:A:174:ARG:HD3	7:A:316:DMS:H13	1.74	0.69
3:A:320:PGE:H1	3:B:311:PGE:H42	1.76	0.67
1:A:59:LEU:HB2	3:A:319:PGE:H3	1.81	0.61
1:B:180:LYS:HZ2	4:B:306:PEG:H41	1.66	0.61
1:A:107:ARG:NH1	4:A:307:PEG:O4	2.39	0.56
1:A:21:GLY:N	10:A:405:HOH:O	2.39	0.55
1:A:137:LYS:NZ	4:A:306:PEG:H32	2.23	0.54
5:A:314:EDO:H21	10:A:417:HOH:O	2.07	0.54
1:B:174:ARG:HD3	7:B:309:DMS:C1	2.35	0.52
1:A:174:ARG:HH11	7:A:316:DMS:C1	2.21	0.52
1:A:134:ARG:HG2	4:A:306:PEG:H31	1.91	0.51
1:A:174:ARG:NH1	7:A:316:DMS:H12	2.26	0.49
1:A:65:ALA:HB1	1:A:163:ARG:HB3	1.95	0.49
1:B:174:ARG:NH1	7:B:309:DMS:H12	2.18	0.48
1:A:201:GLY:HA2	3:A:320:PGE:H3	1.97	0.47
1:A:137:LYS:HZ2	4:A:306:PEG:H32	1.79	0.46
1:B:42:GLY:N	5:B:310:EDO:H11	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LYS:HZ3	4:B:306:PEG:H22	1.80	0.46
1:A:59:LEU:CB	3:A:319:PGE:H3	2.46	0.46
1:A:171:SER:HA	7:A:316:DMS:H11	1.98	0.45
1:A:200:ASN:O	3:A:320:PGE:H3	2.17	0.44
1:A:106:ASN:C	1:A:107:ARG:HG2	2.43	0.44
1:B:180:LYS:NZ	4:B:306:PEG:H41	2.31	0.44
4:A:308:PEG:H21	4:A:308:PEG:H41	1.59	0.44
1:B:174:ARG:HH11	7:B:309:DMS:C1	2.21	0.44
1:B:214[A]:ARG:HE	6:B:308:OP0:H18	1.83	0.43
1:A:180:LYS:NZ	5:A:313:EDO:H12	2.34	0.43
1:B:27:GLU:HA	1:B:56:THR:O	2.19	0.43
1:A:31:TRP:HB2	1:A:57:ASN:HB3	2.01	0.42
1:B:180:LYS:NZ	4:B:306:PEG:H22	2.34	0.42
3:A:320:PGE:H32	1:B:116:LYS:CE	2.50	0.42
1:B:177:TYR:CZ	1:B:232[A]:VAL:HG21	2.55	0.42
1:A:220:GLY:O	1:A:238:ASN:HA	2.19	0.41
1:B:148:ASP:O	1:B:162:ILE:HB	2.20	0.41
1:A:171:SER:HA	7:A:316:DMS:C1	2.51	0.41
1:B:220:GLY:O	1:B:238:ASN:HA	2.21	0.41
4:B:306:PEG:H41	4:B:306:PEG:H22	1.82	0.41
1:B:51:LYS:HA	1:B:51:LYS:HD3	1.97	0.40
1:A:70:SER:HB2	1:A:210:GLY:HA2	2.04	0.40
1:A:177:TYR:CZ	1:A:232[A]:VAL:HG21	2.56	0.40
3:A:320:PGE:H32	1:B:116:LYS:NZ	2.36	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)
10:A:559:HOH:O	10:B:406:HOH:O[3_545]	2.18	0.02

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	251/245 (102%)	247 (98%)	4 (2%)	0	100	100
1	B	250/245 (102%)	247 (99%)	3 (1%)	0	100	100
All	All	501/490 (102%)	494 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	221/213 (104%)	219 (99%)	2 (1%)	75	56
1	B	220/213 (103%)	218 (99%)	2 (1%)	75	56
All	All	441/426 (104%)	437 (99%)	4 (1%)	75	56

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	A	243	THR
1	B	82	ASP
1	B	183	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	124	GLN
1	A	152	ASN
1	B	152	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 3 are monoatomic - leaving 31 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	$\# Z > 2$
4	PEG	A	307	-	6,6,6	0.11	0	5,5,5	0.11	0
5	EDO	B	312	-	3,3,3	0.46	0	2,2,2	0.27	0
7	DMS	A	316	-	3,3,3	0.54	0	3,3,3	0.71	0
5	EDO	A	312	-	3,3,3	0.46	0	2,2,2	0.37	0
6	OP0	B	308	1	17,21,21	0.48	0	18,28,28	1.36	1 (5%)
7	DMS	B	309	-	3,3,3	0.51	0	3,3,3	0.62	0
5	EDO	A	313	-	3,3,3	0.47	0	2,2,2	0.34	0
8	GOL	B	304	-	5,5,5	0.91	0	5,5,5	1.20	1 (20%)
5	EDO	B	310	-	3,3,3	0.50	0	2,2,2	0.33	0
8	GOL	A	321[B]	-	5,5,5	0.98	0	5,5,5	0.89	0
3	PGE	A	320	-	9,9,9	0.29	0	8,8,8	0.58	0
3	PGE	A	305	-	9,9,9	0.36	0	8,8,8	0.32	0
6	OP0	A	315[A]	1	17,21,21	0.47	0	18,28,28	1.32	3 (16%)
6	OP0	A	315[B]	1	17,21,21	0.40	0	18,28,28	1.13	1 (5%)
4	PEG	A	308	-	6,6,6	0.12	0	5,5,5	0.09	0
3	PGE	B	311	-	9,9,9	0.30	0	8,8,8	0.38	0
5	EDO	A	309	-	3,3,3	0.51	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	DMS	A	318	-	3,3,3	0.58	0	3,3,3	0.50	0
3	PGE	A	303	-	9,9,9	0.31	0	8,8,8	0.54	0
5	EDO	A	314	-	3,3,3	0.43	0	2,2,2	0.29	0
4	PEG	B	306	-	6,6,6	0.12	0	5,5,5	0.06	0
5	EDO	B	305	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	A	310	-	3,3,3	0.41	0	2,2,2	0.44	0
5	EDO	B	307	-	3,3,3	0.46	0	2,2,2	0.33	0
3	PGE	A	319	-	9,9,9	0.28	0	8,8,8	0.54	0
8	GOL	B	302[A]	-	5,5,5	0.93	0	5,5,5	0.80	0
5	EDO	A	311	-	3,3,3	0.37	0	2,2,2	0.52	0
4	PEG	A	306	-	6,6,6	0.12	0	5,5,5	0.08	0
5	EDO	A	317	-	3,3,3	0.45	0	2,2,2	0.43	0
4	PEG	A	304	-	6,6,6	0.11	0	5,5,5	0.11	0
9	PG4	B	303	-	12,12,12	0.12	0	11,11,11	0.62	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
4	PEG	A	307	-	-	1/4/4/4	-
5	EDO	B	312	-	-	0/1/1/1	-
5	EDO	A	312	-	-	0/1/1/1	-
6	OP0	B	308	1	-	4/11/30/30	0/1/1/1
5	EDO	A	313	-	-	0/1/1/1	-
8	GOL	B	304	-	-	0/4/4/4	-
5	EDO	B	310	-	-	1/1/1/1	-
8	GOL	A	321[B]	-	-	4/4/4/4	-
3	PGE	A	320	-	-	5/7/7/7	-
3	PGE	A	305	-	-	2/7/7/7	-
6	OP0	A	315[A]	1	-	2/11/30/30	0/1/1/1
6	OP0	A	315[B]	1	-	3/11/30/30	0/1/1/1
4	PEG	A	308	-	-	3/4/4/4	-
3	PGE	B	311	-	-	1/7/7/7	-
5	EDO	A	309	-	-	1/1/1/1	-
3	PGE	A	303	-	-	4/7/7/7	-
5	EDO	A	314	-	-	0/1/1/1	-
4	PEG	B	306	-	-	1/4/4/4	-
5	EDO	B	305	-	-	0/1/1/1	-
5	EDO	A	310	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	307	-	-	0/1/1/1	-
3	PGE	A	319	-	-	1/7/7/7	-
8	GOL	B	302[A]	-	-	2/4/4/4	-
5	EDO	A	311	-	-	0/1/1/1	-
4	PEG	A	306	-	-	2/4/4/4	-
5	EDO	A	317	-	-	0/1/1/1	-
4	PEG	A	304	-	-	1/4/4/4	-
9	PG4	B	303	-	-	2/10/10/10	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	308	OP0	O13-S17-O12	4.40	123.78	108.49
6	A	315[B]	OP0	O13-S17-O12	3.55	120.84	108.49
6	A	315[A]	OP0	O13-S17-O12	3.44	120.45	108.49
6	A	315[A]	OP0	O24-N15-C3	-2.28	115.48	118.52
8	B	304	GOL	C3-C2-C1	-2.20	103.14	111.70
6	A	315[A]	OP0	C5-C4-C2	2.06	114.63	110.30

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	315[A]	OP0	O8-C1-N14-C2
6	A	315[A]	OP0	O8-C1-N14-C7
6	A	315[B]	OP0	O8-C1-N14-C7
6	A	315[B]	OP0	N21-C22-C23-O24
6	B	308	OP0	O8-C1-N14-C2
6	B	308	OP0	O8-C1-N14-C7
6	B	308	OP0	N21-C22-C23-O24
6	B	308	OP0	C22-C23-O24-N15
3	A	320	PGE	O2-C3-C4-O3
3	A	303	PGE	O3-C5-C6-O4
4	A	308	PEG	C4-C3-O2-C2
4	A	308	PEG	O2-C3-C4-O4
3	A	303	PGE	O2-C3-C4-O3
8	A	321[B]	GOL	O1-C1-C2-C3
8	A	321[B]	GOL	C1-C2-C3-O3
8	B	302[A]	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	A	321[B]	GOL	O2-C2-C3-O3
4	A	306	PEG	O1-C1-C2-O2
8	A	321[B]	GOL	O1-C1-C2-O2
3	A	320	PGE	O1-C1-C2-O2
3	A	319	PGE	C1-C2-O2-C3
3	A	320	PGE	C4-C3-O2-C2
4	B	306	PEG	C4-C3-O2-C2
8	B	302[A]	GOL	O1-C1-C2-O2
5	A	309	EDO	O1-C1-C2-O2
3	B	311	PGE	C1-C2-O2-C3
3	A	303	PGE	C1-C2-O2-C3
3	A	320	PGE	C6-C5-O3-C4
9	B	303	PG4	C8-C7-O4-C6
3	A	303	PGE	O1-C1-C2-O2
4	A	308	PEG	O1-C1-C2-O2
9	B	303	PG4	C1-C2-O2-C3
4	A	304	PEG	O1-C1-C2-O2
3	A	305	PGE	C1-C2-O2-C3
3	A	305	PGE	O1-C1-C2-O2
5	B	310	EDO	O1-C1-C2-O2
6	A	315[B]	OP0	N14-C2-C3-O9
4	A	306	PEG	C1-C2-O2-C3
3	A	320	PGE	C1-C2-O2-C3
4	A	307	PEG	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 36 short contacts:

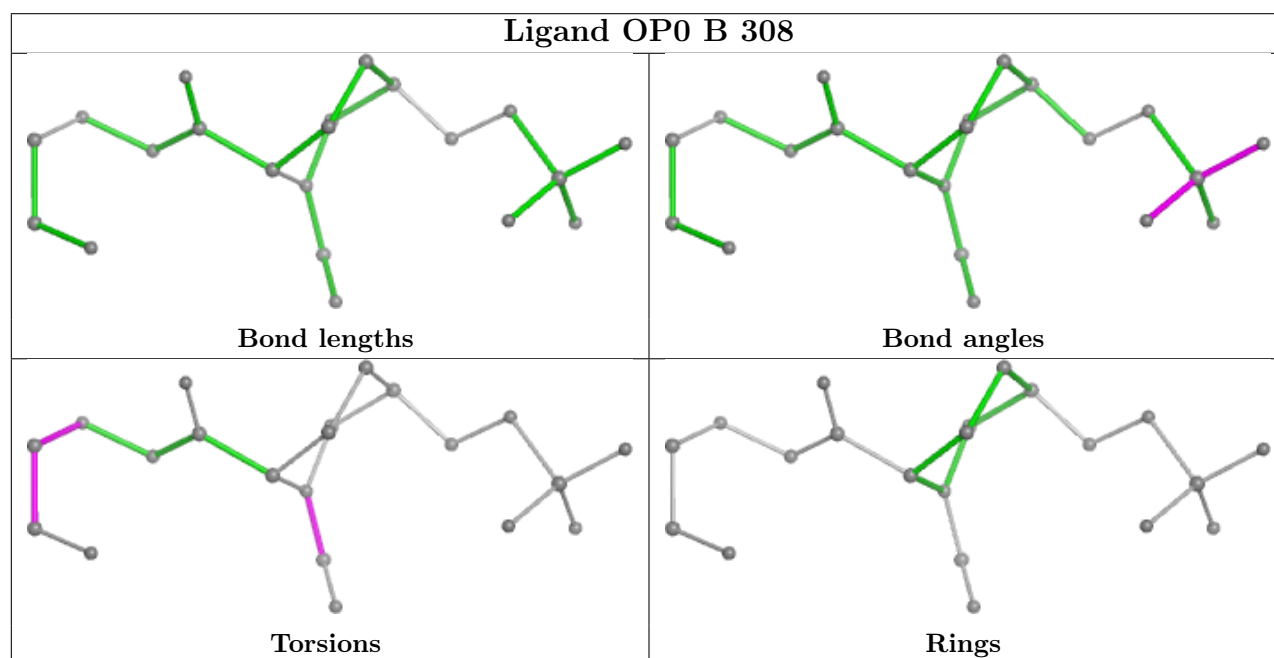
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	307	PEG	1	0
7	A	316	DMS	6	0
6	B	308	OP0	2	0
7	B	309	DMS	6	0
5	A	313	EDO	1	0
5	B	310	EDO	2	0
3	A	320	PGE	5	0
4	A	308	PEG	1	0
3	B	311	PGE	1	0
7	A	318	DMS	1	0
5	A	314	EDO	1	0
4	B	306	PEG	5	0
3	A	319	PGE	2	0

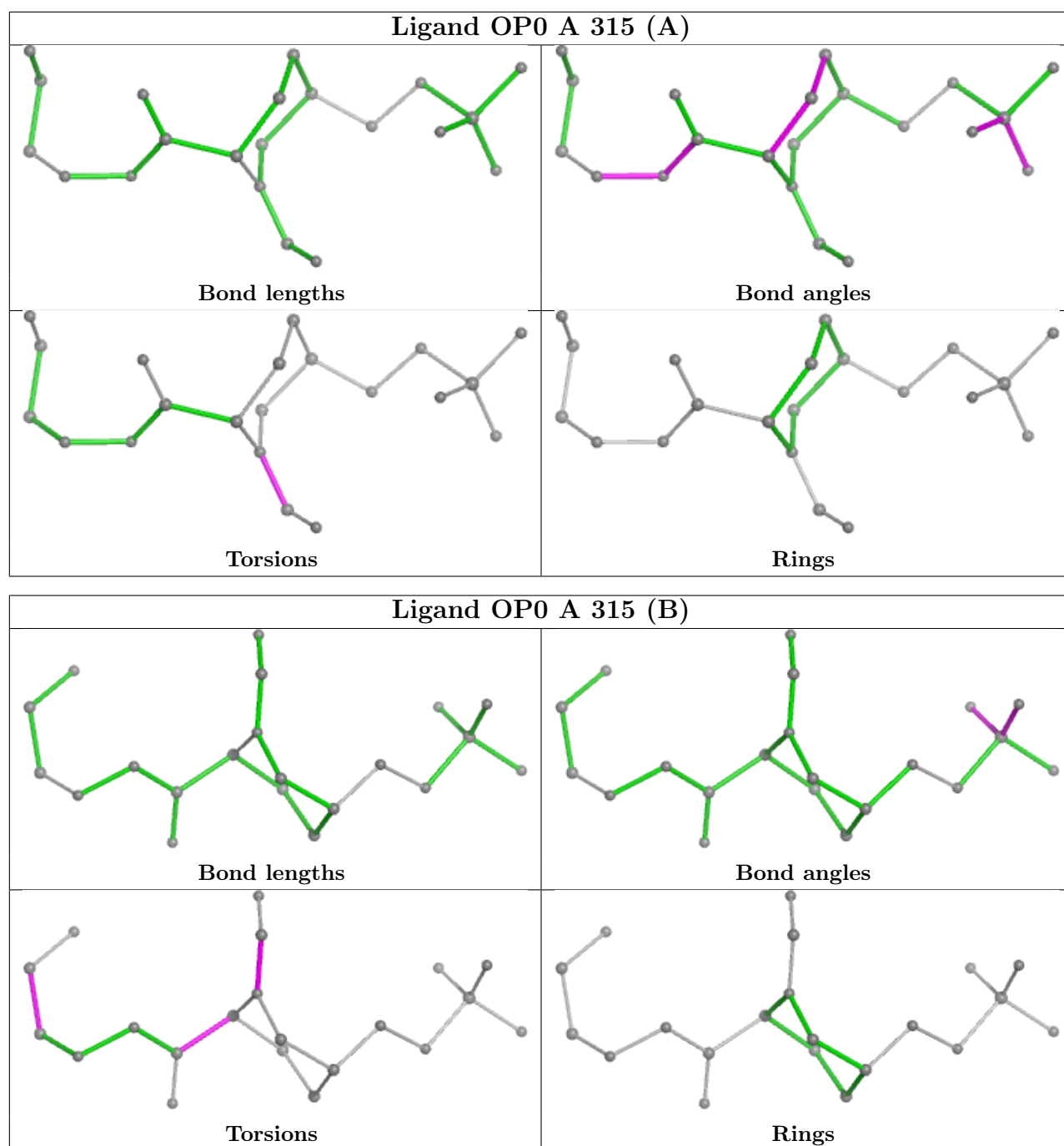
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	306	PEG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	245/245 (100%)	-0.24	2 (0%) 82 86	6, 17, 36, 51	9 (3%)
1	B	245/245 (100%)	-0.17	5 (2%) 64 69	7, 18, 34, 52	7 (2%)
All	All	490/490 (100%)	-0.21	7 (1%) 73 77	6, 18, 35, 52	16 (3%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	GLY	4.0
1	B	214[A]	ARG	3.1
1	B	107[A]	ARG	2.9
1	B	151	GLY	2.7
1	B	37	GLU	2.2
1	A	93	PHE	2.1
1	B	101	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

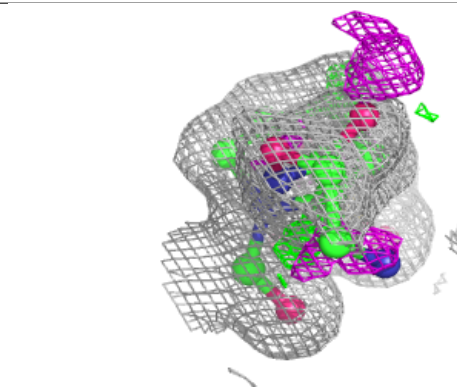
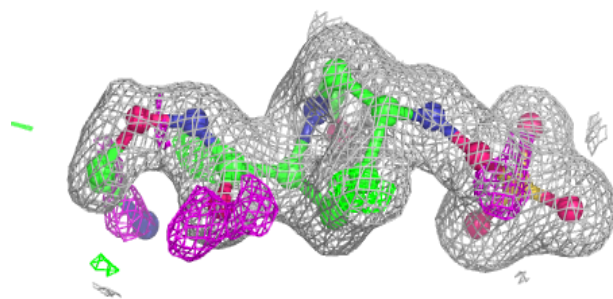
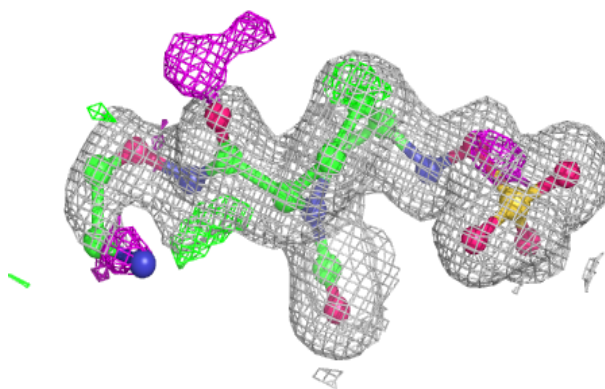
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PEG	A	308	7/7	0.74	0.19	34,44,50,52	0
5	EDO	A	314	4/4	0.79	0.16	32,34,47,47	0
8	GOL	B	304	6/6	0.79	0.21	29,36,46,47	0
4	PEG	A	306	7/7	0.82	0.15	33,38,49,53	0
5	EDO	A	317	4/4	0.82	0.20	30,39,40,45	0
3	PGE	A	319	10/10	0.82	0.19	23,33,41,45	10
4	PEG	A	307	7/7	0.83	0.15	36,38,46,47	0
4	PEG	B	306	7/7	0.83	0.15	38,39,49,52	0
5	EDO	A	310	4/4	0.83	0.17	32,33,37,45	0
9	PG4	B	303	13/13	0.83	0.17	39,45,49,56	0
5	EDO	B	310	4/4	0.84	0.15	28,38,38,40	0
3	PGE	A	320	10/10	0.84	0.20	25,30,34,43	10
5	EDO	A	311	4/4	0.84	0.23	21,33,42,48	0
5	EDO	B	312	4/4	0.85	0.14	35,40,45,47	0
5	EDO	A	313	4/4	0.85	0.14	35,43,49,51	0
4	PEG	A	304	7/7	0.85	0.18	30,33,43,54	7
5	EDO	A	312	4/4	0.86	0.14	35,36,41,50	0
5	EDO	B	305	4/4	0.86	0.14	31,34,35,37	4
5	EDO	A	309	4/4	0.87	0.15	24,32,39,46	0
8	GOL	B	302[A]	6/6	0.87	0.16	26,32,34,35	6
8	GOL	A	321[B]	6/6	0.88	0.17	19,26,29,39	6
7	DMS	A	318	4/4	0.88	0.21	27,35,44,46	4
3	PGE	A	303	10/10	0.90	0.14	26,35,40,42	0
5	EDO	B	307	4/4	0.91	0.13	24,32,33,40	0
7	DMS	B	309	4/4	0.91	0.14	24,29,40,42	0
3	PGE	B	311	10/10	0.93	0.11	18,23,30,46	10
7	DMS	A	316	4/4	0.93	0.13	22,26,31,39	0
3	PGE	A	305	10/10	0.95	0.09	18,22,32,43	0
6	OP0	B	308	21/21	0.96	0.09	15,21,39,42	0
6	OP0	A	315[A]	21/21	0.97	0.07	12,16,27,33	21
6	OP0	A	315[B]	21/21	0.97	0.07	12,17,23,26	21
2	CL	B	301	1/1	0.98	0.08	23,23,23,23	0
2	CL	A	302	1/1	0.98	0.04	17,17,17,17	0
2	CL	A	301	1/1	0.99	0.11	21,21,21,21	0

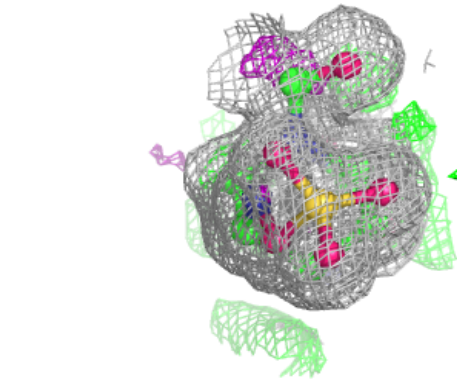
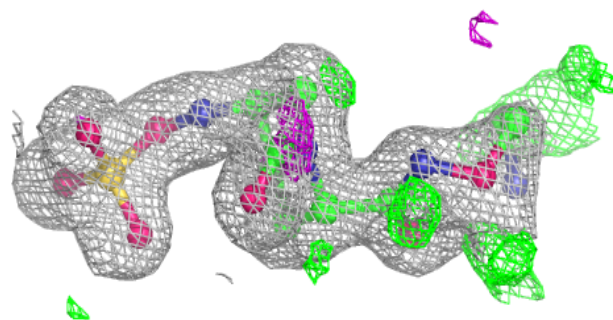
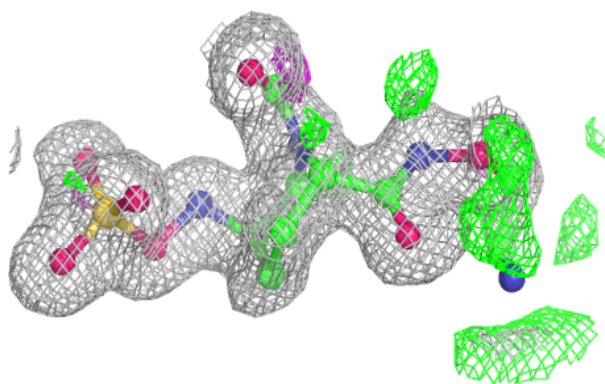
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OP0 B 308:

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

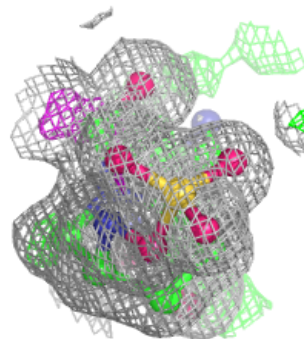
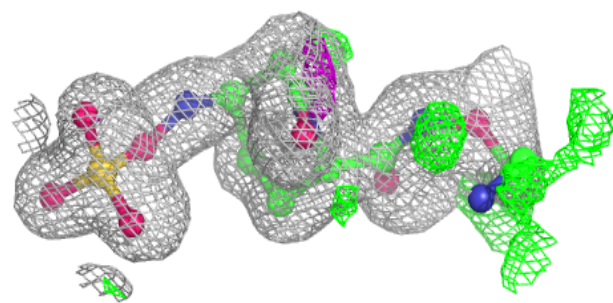
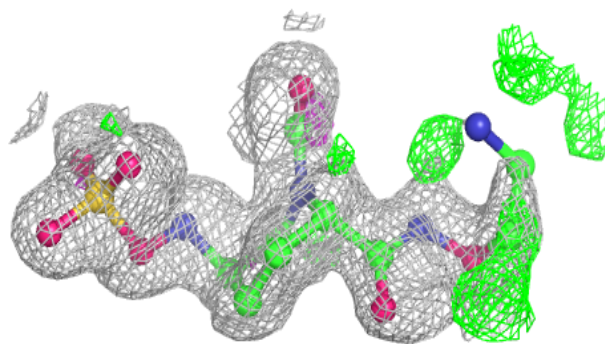
**Electron density around OP0 A 315 (A):**

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



Electron density around OP0 A 315 (B):

$2mF_o-DF_c$ (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.