



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:01 am BST

PDB ID : 2XDM
Title : Crystal structure of a complex between Actinomadura R39 DD peptidase and a peptidoglycan mimetic boronate inhibitor
Authors : Rocaboy, M.; Sauvage, E.; Herman, R.; Kerff, F.; Charlier, P.
Deposited on : 2010-05-04
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

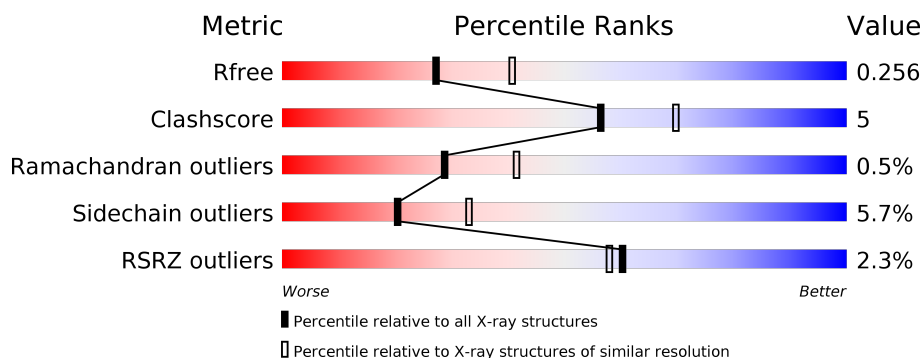
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	466	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>•</div> </div> </div>
1	B	466	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>•</div> </div> </div>
1	C	466	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>•</div> </div> </div>
1	D	466	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>•</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14096 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 D-ALANYL-D-ALANINE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3352	2076	564	706	6			
1	B	466	Total	C	N	O	S	0	0	1
			3344	2071	564	703	6			
1	C	465	Total	C	N	O	S	0	0	0
			3343	2071	563	703	6			
1	D	466	Total	C	N	O	S	0	0	0
			3352	2076	564	706	6			

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

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

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

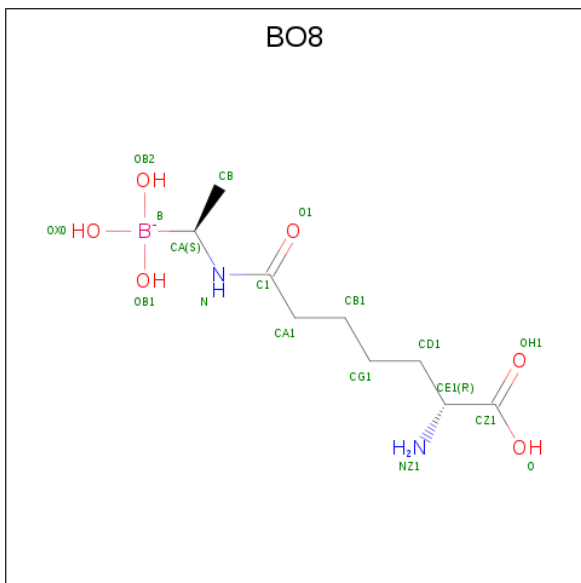
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Co 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Co	0	0
			2	2		

- Molecule 4 is (D-ALPHA-AMINOPIMELYLAMINO)-D-1-ETHYLBORONIC ACID (three-letter code: BO8) (formula: $C_9H_{20}BN_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	B	C	N	O	0	0
			17	1	9	2	5		
4	C	1	Total	B	C	N	O	0	0
			17	1	9	2	5		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

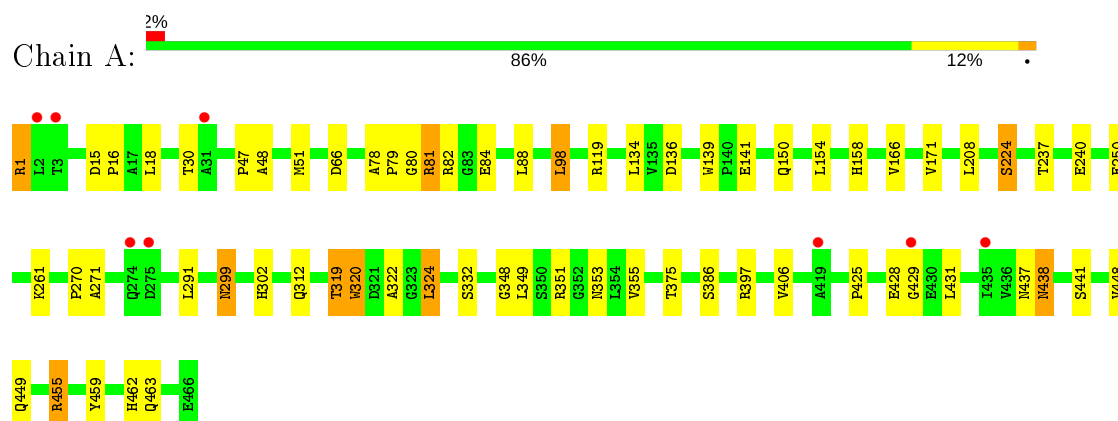
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	181	Total	O	0	0
			181	181		
6	B	119	Total	O	0	0
			119	119		
6	C	142	Total	O	0	0
			142	142		
6	D	113	Total	O	0	0
			113	113		

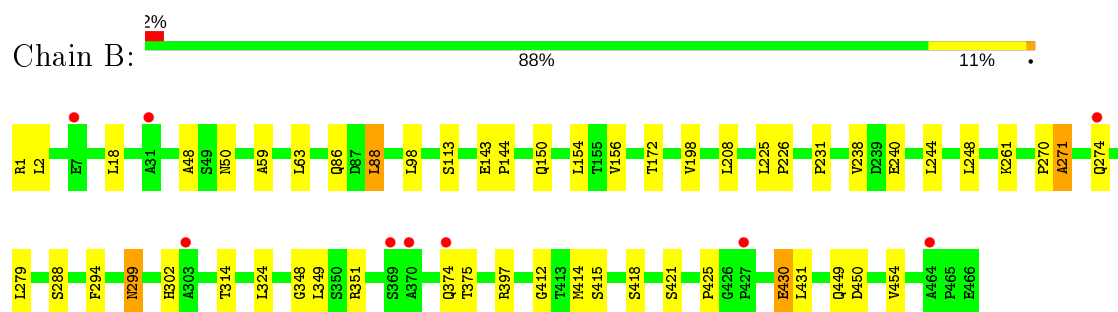
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

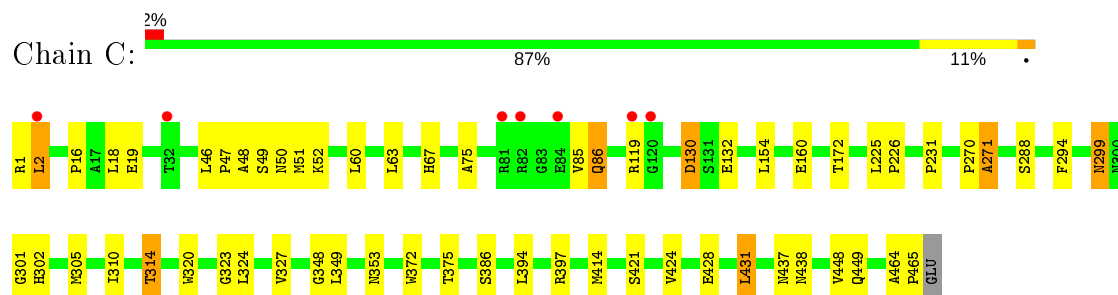
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



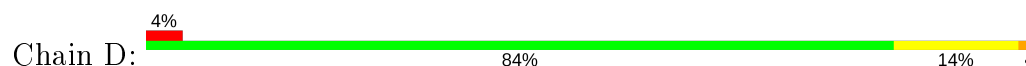
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

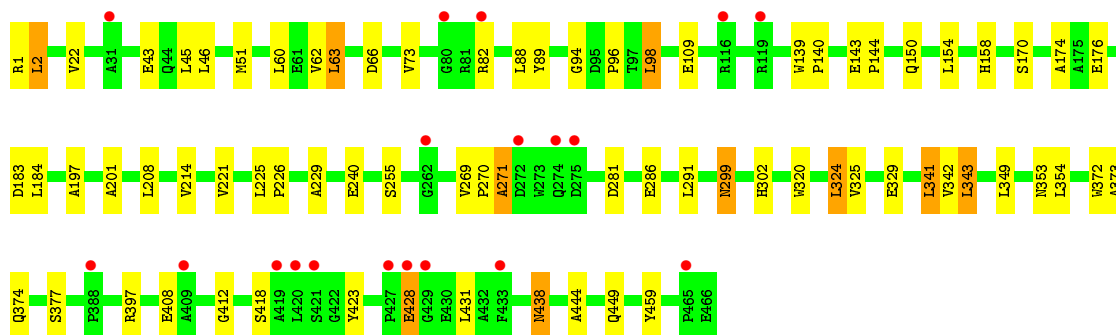


• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.31Å 91.57Å 106.87Å 90.00° 94.37° 90.00°	Depositor
Resolution (Å)	32.43 – 2.40 32.42 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (32.43-2.40) 99.7 (32.42-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.262 0.196 , 0.256	Depositor DCC
R_{free} test set	3901 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14096	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: BO8, CO, SO4, MES

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	0.50	0/3411	0.66	1/4666 (0.0%)
1	B	0.46	0/3403	0.60	0/4656
1	C	0.47	0/3402	0.62	0/4654
1	D	0.45	0/3411	0.64	2/4666 (0.0%)
All	All	0.47	0/13627	0.63	3/18642 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	LEU	CA-CB-CG	6.45	130.14	115.30
1	D	341	LEU	CA-CB-CG	5.76	128.54	115.30
1	D	98	LEU	CA-CB-CG	5.27	127.41	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3352	0	3201	34	0
1	B	3344	0	3194	26	0
1	C	3343	0	3194	38	0
1	D	3352	0	3201	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	25	0	0	0	0
2	B	25	0	0	0	0
2	C	25	0	0	1	0
2	D	25	0	0	0	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
4	B	17	0	18	1	0
4	C	17	0	18	2	0
5	D	12	0	12	1	0
6	A	181	0	0	5	0
6	B	119	0	0	0	0
6	C	142	0	0	0	0
6	D	113	0	0	1	0
All	All	14096	0	12838	131	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (131) 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:A:319:THR:HG22	1:A:322:ALA:H	1.44	0.83
1:B:351:ARG:NH2	1:B:415:SER:O	2.12	0.83
1:C:75:ALA:HB1	1:C:85:VAL:HG11	1.65	0.79
1:B:288:SER:HB2	1:B:375:THR:HG21	1.64	0.79
1:A:406:VAL:HG12	1:A:425:PRO:HD2	1.67	0.77
1:D:226:PRO:HG2	1:D:229:ALA:HB2	1.72	0.70
1:C:47:PRO:HG3	1:C:51:MET:HE2	1.75	0.68
1:B:150:GLN:HE22	1:B:240:GLU:H	1.41	0.67
1:A:81:ARG:HD3	1:A:82:ARG:HG2	1.78	0.67
1:A:150:GLN:HE22	1:A:240:GLU:H	1.43	0.66
1:C:18:LEU:HD11	1:C:448:VAL:HG11	1.78	0.66
1:B:50:ASN:ND2	1:B:421:SER:OG	2.30	0.65
1:D:299:ASN:ND2	1:D:302:HIS:H	1.96	0.64
1:B:294:PHE:HB2	1:B:302:HIS:HD2	1.63	0.64
1:C:310:ILE:O	1:C:314:THR:HB	1.98	0.63
1:D:158:HIS:HD2	6:D:2060:HOH:O	1.82	0.63
1:C:160:GLU:HG2	2:C:604:SO4:O2	2.01	0.61
1:C:397:ARG:HH12	1:C:449:GLN:HE21	1.49	0.61
1:C:270:PRO:O	1:C:271:ALA:CB	2.50	0.60
1:B:156:VAL:HG21	1:B:248:LEU:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PRO:HD2	6:A:2144:HOH:O	2.00	0.59
1:B:397:ARG:HH12	1:B:449:GLN:HE21	1.48	0.59
1:B:1:ARG:HD2	1:D:2:LEU:HB2	1.84	0.59
1:B:270:PRO:O	1:B:271:ALA:HB3	2.02	0.58
1:C:270:PRO:O	1:C:271:ALA:HB3	2.04	0.58
1:A:397:ARG:HH12	1:A:449:GLN:HE21	1.50	0.58
1:C:47:PRO:HG3	1:C:51:MET:CE	2.34	0.58
1:C:130:ASP:HB3	1:C:132:GLU:H	1.68	0.57
1:A:150:GLN:NE2	1:A:240:GLU:H	2.02	0.57
1:D:270:PRO:O	1:D:271:ALA:HB3	2.04	0.57
1:C:172:THR:HG22	1:C:231:PRO:HB3	1.86	0.57
1:D:377:SER:HB2	1:D:408:GLU:OE1	2.05	0.56
1:D:150:GLN:HE22	1:D:240:GLU:H	1.53	0.55
1:D:66:ASP:HA	1:D:286:GLU:HB3	1.89	0.55
1:C:424:VAL:HB	1:C:431:LEU:HB2	1.89	0.54
1:C:294:PHE:HB2	1:C:302:HIS:HD2	1.72	0.54
1:B:425:PRO:HA	1:B:430:GLU:HB2	1.91	0.53
1:C:323:GLY:O	1:C:327:VAL:HG23	2.08	0.53
1:B:172:THR:HG22	1:B:231:PRO:HB3	1.90	0.53
1:A:47:PRO:HG3	1:A:355:VAL:HG13	1.91	0.53
1:A:84:GLU:CD	1:A:119:ARG:HE	2.12	0.53
1:D:150:GLN:NE2	1:D:240:GLU:H	2.07	0.53
1:D:197:ALA:HB2	1:D:221:VAL:HG12	1.92	0.51
1:D:45:LEU:HD22	1:D:438:ASN:HB2	1.93	0.50
1:A:80:GLY:HA2	1:B:314:THR:O	2.11	0.50
1:B:150:GLN:NE2	1:B:240:GLU:H	2.08	0.49
1:A:299:ASN:ND2	1:A:302:HIS:H	2.10	0.49
1:A:51:MET:HE2	1:A:353:ASN:HB3	1.95	0.49
1:D:51:MET:HE2	1:D:353:ASN:HB3	1.93	0.49
1:A:320:TRP:O	1:A:324:LEU:HB2	2.13	0.49
1:D:299:ASN:HD22	1:D:302:HIS:H	1.61	0.48
1:A:351:ARG:NH2	6:A:2145:HOH:O	2.46	0.48
1:D:1:ARG:HD2	1:D:459:TYR:HD1	1.78	0.48
1:C:85:VAL:HG12	1:C:86:GLN:H	1.79	0.48
1:A:48:ALA:O	1:A:348:GLY:HA3	2.14	0.47
1:A:78:ALA:HB1	1:A:79:PRO:HD2	1.95	0.47
1:B:414:MET:HB2	4:B:500:BO8:OH1	2.13	0.47
1:C:48:ALA:O	1:C:348:GLY:HA3	2.14	0.47
1:C:85:VAL:HG12	1:C:86:GLN:N	2.29	0.47
1:C:75:ALA:CB	1:C:85:VAL:HG11	2.42	0.47
1:D:325:VAL:O	1:D:329:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:ASN:ND2	1:C:302:HIS:H	2.12	0.47
1:D:208:LEU:HD22	1:D:225:LEU:HD13	1.97	0.47
1:D:324:LEU:HG	1:D:343:LEU:HB3	1.97	0.46
1:D:1:ARG:HD2	1:D:459:TYR:CD1	2.50	0.46
1:A:18:LEU:HD11	1:A:448:VAL:HG11	1.98	0.46
1:C:49:SER:CB	4:C:500:BO8:OB1	2.65	0.45
1:D:373:ALA:HB1	5:D:1467:MES:H32	1.98	0.45
1:D:62:VAL:HG12	1:D:63:LEU:HD13	1.98	0.45
1:C:50:ASN:ND2	1:C:421:SER:OG	2.50	0.45
1:B:59:ALA:O	1:B:63:LEU:HB2	2.17	0.45
1:B:88:LEU:HD21	1:B:279:LEU:HD12	1.99	0.45
1:C:63:LEU:O	1:C:67:HIS:HB2	2.16	0.45
1:D:22:VAL:HG11	1:D:43:GLU:HG2	1.99	0.45
1:C:1:ARG:CG	1:C:2:LEU:H	2.30	0.44
1:D:270:PRO:O	1:D:271:ALA:CB	2.64	0.44
1:C:52:LYS:HD3	1:C:294:PHE:CE2	2.52	0.44
1:C:414:MET:HG2	4:C:500:BO8:HB11	1.98	0.44
1:C:437:ASN:C	1:C:438:ASN:HD22	2.20	0.44
1:A:224:SER:HB3	6:A:2093:HOH:O	2.17	0.44
1:B:412:GLY:O	1:B:418:SER:HA	2.18	0.44
1:A:261:LYS:HD2	1:A:261:LYS:HA	1.81	0.43
1:A:270:PRO:O	1:A:271:ALA:HB3	2.18	0.43
1:A:1:ARG:NH2	1:A:459:TYR:HA	2.33	0.43
1:A:51:MET:CE	1:A:353:ASN:HB3	2.48	0.43
1:B:238:VAL:HG21	1:B:244:LEU:HD22	2.00	0.43
1:C:464:ALA:HA	1:C:465:PRO:HD3	1.91	0.43
1:B:270:PRO:O	1:B:271:ALA:CB	2.64	0.43
1:C:60:LEU:HD13	1:C:372:TRP:CE3	2.53	0.43
1:B:208:LEU:HD13	1:B:225:LEU:HB2	2.01	0.43
1:D:176:GLU:HB2	1:D:201:ALA:HA	2.01	0.43
1:A:1:ARG:HD3	6:A:2001:HOH:O	2.18	0.43
1:B:48:ALA:O	1:B:348:GLY:HA3	2.19	0.43
1:D:342:VAL:HB	1:D:354:LEU:HB2	2.01	0.43
1:C:51:MET:CE	1:C:353:ASN:HB3	2.49	0.43
1:A:166:VAL:HG12	1:A:237:THR:HA	2.01	0.43
1:B:299:ASN:ND2	1:B:302:HIS:H	2.17	0.43
1:B:294:PHE:HB2	1:B:302:HIS:CD2	2.48	0.42
1:D:423:TYR:HA	1:D:431:LEU:O	2.19	0.42
1:D:60:LEU:HD13	1:D:372:TRP:CE3	2.54	0.42
1:A:15:ASP:HA	1:A:16:PRO:HD2	1.82	0.42
1:D:397:ARG:HH12	1:D:449:GLN:HE21	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ARG:HG3	1:C:2:LEU:H	1.85	0.42
1:C:16:PRO:O	1:C:19:GLU:HB2	2.19	0.42
1:C:288:SER:HB2	1:C:375:THR:OG1	2.19	0.42
1:A:1:ARG:HH21	1:A:459:TYR:HA	1.85	0.41
1:A:139:TRP:HB3	1:A:141:GLU:OE1	2.20	0.41
1:D:143:GLU:N	1:D:144:PRO:CD	2.83	0.41
1:A:1:ARG:CZ	1:A:455:ARG:HH22	2.33	0.41
1:A:397:ARG:HH12	1:A:449:GLN:NE2	2.17	0.41
1:A:406:VAL:HG11	1:A:462:HIS:NE2	2.35	0.41
1:C:294:PHE:HB2	1:C:302:HIS:CD2	2.52	0.41
1:B:143:GLU:N	1:B:144:PRO:CD	2.83	0.41
1:D:412:GLY:O	1:D:418:SER:HA	2.21	0.41
1:A:437:ASN:C	1:A:438:ASN:HD22	2.24	0.41
1:D:94:GLY:O	1:D:96:PRO:HD3	2.19	0.41
1:D:139:TRP:HA	1:D:140:PRO:HD3	1.94	0.41
1:D:269:VAL:HA	1:D:270:PRO:HD3	1.87	0.41
1:D:73:VAL:HA	1:D:89:TYR:O	2.21	0.41
1:C:301:GLY:O	1:C:305:MET:HG3	2.21	0.41
1:C:397:ARG:HH12	1:C:449:GLN:NE2	2.16	0.41
1:A:299:ASN:HD22	1:A:299:ASN:C	2.24	0.41
1:C:1:ARG:HG3	1:C:2:LEU:N	2.36	0.41
1:C:225:LEU:HD12	1:C:226:PRO:HD2	2.03	0.41
1:B:225:LEU:HA	1:B:226:PRO:HD3	1.93	0.40
1:A:171:VAL:HG21	1:A:208:LEU:HD21	2.03	0.40
1:D:418:SER:HB2	1:D:444:ALA:HB1	2.03	0.40
1:A:158:HIS:HD2	6:A:2073:HOH:O	2.03	0.40
1:B:450:ASP:O	1:B:454:VAL:HG23	2.22	0.40
1:D:170:SER:OG	1:D:183:ASP:HB3	2.21	0.40
1:C:172:THR:HG22	1:C:231:PRO:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/466 (100%)	447 (96%)	16 (3%)	1 (0%)	47	62
1	B	464/466 (100%)	447 (96%)	15 (3%)	2 (0%)	34	48
1	C	463/466 (99%)	444 (96%)	16 (4%)	3 (1%)	25	36
1	D	464/466 (100%)	445 (96%)	16 (3%)	3 (1%)	25	36
All	All	1855/1864 (100%)	1783 (96%)	63 (3%)	9 (0%)	29	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	428	GLU
1	B	271	ALA
1	C	271	ALA
1	C	130	ASP
1	D	271	ALA
1	A	429	GLY
1	B	86	GLN
1	D	174	ALA
1	C	86	GLN

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	339/339 (100%)	312 (92%)	27 (8%)	12	18
1	B	338/339 (100%)	323 (96%)	15 (4%)	28	45
1	C	338/339 (100%)	325 (96%)	13 (4%)	33	51
1	D	339/339 (100%)	317 (94%)	22 (6%)	17	27
All	All	1354/1356 (100%)	1277 (94%)	77 (6%)	20	33

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	30	THR

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Mol	Chain	Res	Type
1	A	66	ASP
1	A	81	ARG
1	A	88	LEU
1	A	98	LEU
1	A	134	LEU
1	A	136	ASP
1	A	154	LEU
1	A	224	SER
1	A	250	GLU
1	A	291	LEU
1	A	299	ASN
1	A	312	GLN
1	A	319	THR
1	A	320	TRP
1	A	324	LEU
1	A	332	SER
1	A	349	LEU
1	A	375	THR
1	A	386	SER
1	A	428	GLU
1	A	431	LEU
1	A	438	ASN
1	A	441	SER
1	A	455	ARG
1	A	463	GLN
1	B	2	LEU
1	B	18	LEU
1	B	88	LEU
1	B	98	LEU
1	B	113	SER
1	B	154	LEU
1	B	198	VAL
1	B	261	LYS
1	B	274	GLN
1	B	299	ASN
1	B	324	LEU
1	B	349	LEU
1	B	374	GLN
1	B	430	GLU
1	B	431	LEU
1	C	2	LEU
1	C	46	LEU

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Mol	Chain	Res	Type
1	C	119	ARG
1	C	154	LEU
1	C	299	ASN
1	C	314	THR
1	C	320	TRP
1	C	324	LEU
1	C	349	LEU
1	C	386	SER
1	C	394	LEU
1	C	428	GLU
1	C	431	LEU
1	D	2	LEU
1	D	46	LEU
1	D	63	LEU
1	D	82	ARG
1	D	88	LEU
1	D	98	LEU
1	D	109	GLU
1	D	154	LEU
1	D	184	LEU
1	D	214	VAL
1	D	255	SER
1	D	281	ASP
1	D	291	LEU
1	D	299	ASN
1	D	320	TRP
1	D	324	LEU
1	D	341	LEU
1	D	343	LEU
1	D	349	LEU
1	D	374	GLN
1	D	428	GLU
1	D	438	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	50	ASN
1	A	150	GLN
1	A	158	HIS
1	A	299	ASN

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Mol	Chain	Res	Type
1	A	312	GLN
1	A	437	ASN
1	A	449	GLN
1	A	463	GLN
1	B	44	GLN
1	B	50	ASN
1	B	150	GLN
1	B	158	HIS
1	B	299	ASN
1	B	302	HIS
1	B	396	ASN
1	B	437	ASN
1	B	449	GLN
1	B	463	GLN
1	C	44	GLN
1	C	50	ASN
1	C	158	HIS
1	C	299	ASN
1	C	302	HIS
1	C	437	ASN
1	C	449	GLN
1	D	44	GLN
1	D	50	ASN
1	D	150	GLN
1	D	158	HIS
1	D	299	ASN
1	D	302	HIS
1	D	437	ASN
1	D	449	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 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	$\# Z > 2$
2	SO4	D	600	-	4,4,4	0.18	0	6,6,6	0.44	0
2	SO4	A	602	-	4,4,4	0.20	0	6,6,6	0.16	0
2	SO4	A	601	-	4,4,4	0.17	0	6,6,6	0.19	0
2	SO4	B	601	-	4,4,4	0.16	0	6,6,6	0.35	0
2	SO4	C	604	-	4,4,4	0.19	0	6,6,6	0.35	0
5	MES	D	1467	-	12,12,12	2.18	1 (8%)	14,16,16	2.41	6 (42%)
2	SO4	C	602	-	4,4,4	0.14	0	6,6,6	0.21	0
2	SO4	C	601	-	4,4,4	0.13	0	6,6,6	0.30	0
2	SO4	A	600	-	4,4,4	0.21	0	6,6,6	0.25	0
2	SO4	C	600	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	B	603	-	4,4,4	0.21	0	6,6,6	0.43	0
2	SO4	C	603	-	4,4,4	0.17	0	6,6,6	0.32	0
2	SO4	B	604	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	D	604	-	4,4,4	0.18	0	6,6,6	0.18	0
2	SO4	D	601	-	4,4,4	0.18	0	6,6,6	0.22	0
2	SO4	B	602	-	4,4,4	0.12	0	6,6,6	0.42	0
4	BO8	C	500	1	9,16,17	2.12	1 (11%)	9,20,23	1.21	1 (11%)
4	BO8	B	500	1	9,16,17	2.18	1 (11%)	9,20,23	1.09	1 (11%)
2	SO4	B	600	-	4,4,4	0.16	0	6,6,6	0.20	0
2	SO4	D	602	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	D	603	-	4,4,4	0.12	0	6,6,6	0.28	0
2	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.33	0
2	SO4	A	604	-	4,4,4	0.15	0	6,6,6	0.33	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	BO8	C	500	1	-	0/10/19/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MES	D	1467	-	-	4/6/14/14	0/1/1/1
4	BO8	B	500	1	-	2/10/19/21	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1467	MES	C8-S	-7.19	1.67	1.77
4	B	500	BO8	CA-N	-6.42	1.34	1.46
4	C	500	BO8	CA-N	-6.30	1.34	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1467	MES	C5-N4-C3	5.30	120.76	108.83
5	D	1467	MES	C7-N4-C5	3.60	120.43	111.23
5	D	1467	MES	C6-C5-N4	-3.16	105.32	110.10
5	D	1467	MES	C7-N4-C3	2.96	118.81	111.23
5	D	1467	MES	O1S-S-C8	2.89	110.40	106.92
4	B	500	BO8	CB1-CA1-C1	-2.55	106.11	113.26
4	C	500	BO8	O1-C1-CA1	-2.21	117.98	122.02
5	D	1467	MES	C2-C3-N4	-2.20	106.77	110.10

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1467	MES	C7-C8-S-O2S
5	D	1467	MES	C7-C8-S-O3S
5	D	1467	MES	C8-C7-N4-C3
5	D	1467	MES	C7-C8-S-O1S
4	B	500	BO8	O1-C1-CA1-CB1
4	B	500	BO8	N-C1-CA1-CB1

There are no ring outliers.

4 monomers are involved in 5 short contacts:

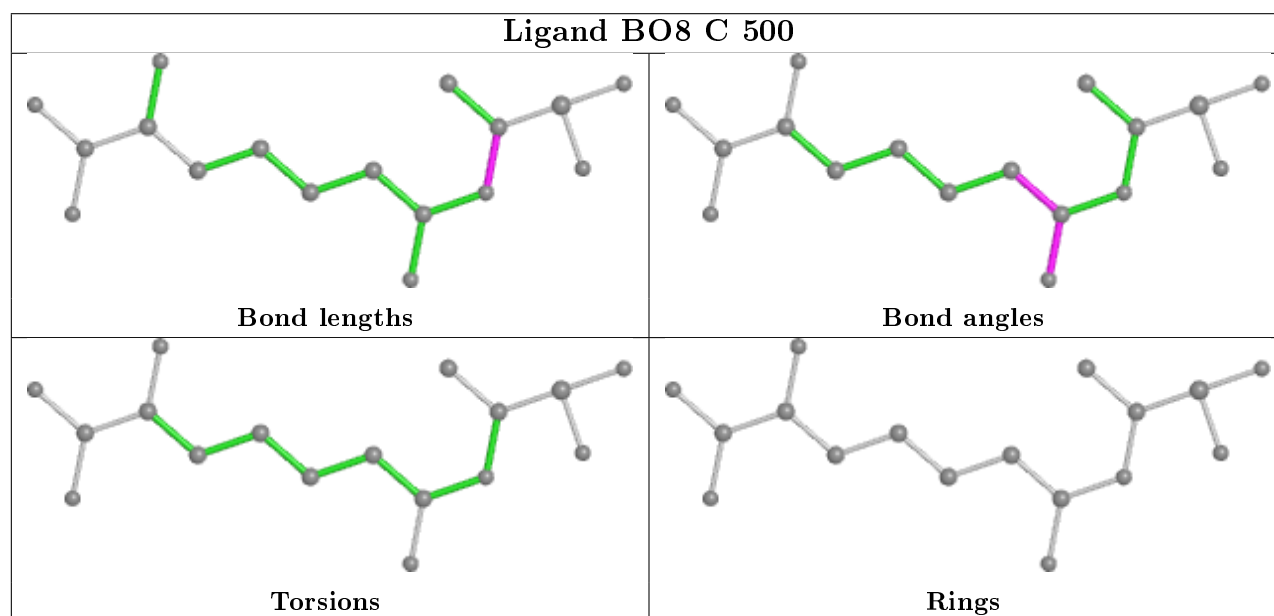
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	604	SO4	1	0
5	D	1467	MES	1	0
4	C	500	BO8	2	0

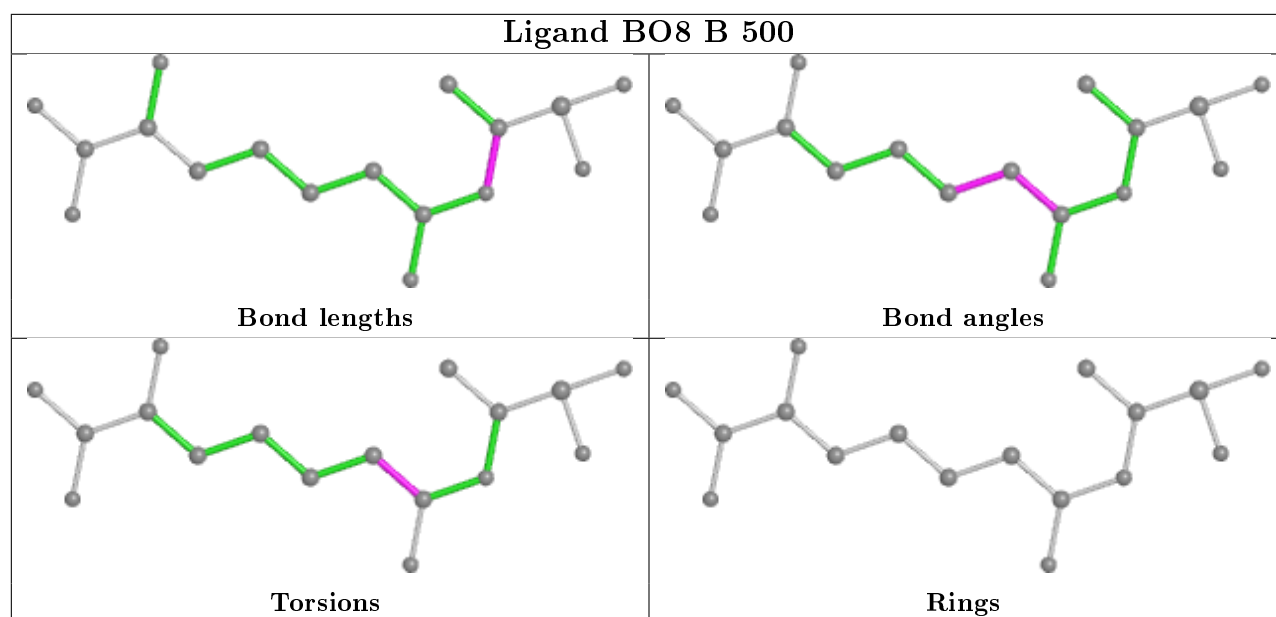
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	500	BO8	1	0

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 ⓘ

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	466/466 (100%)	-0.22	8 (1%) 70 68	17, 29, 50, 78	0
1	B	466/466 (100%)	-0.20	9 (1%) 66 64	20, 35, 56, 72	0
1	C	465/466 (99%)	-0.29	7 (1%) 73 72	23, 34, 53, 141	0
1	D	466/466 (100%)	-0.12	19 (4%) 37 36	20, 38, 63, 83	0
All	All	1863/1864 (99%)	-0.21	43 (2%) 60 58	17, 34, 57, 141	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	427	PRO	3.9
1	C	82	ARG	3.7
1	B	370	ALA	3.5
1	D	419	ALA	3.4
1	D	429	GLY	3.3
1	A	31	ALA	3.2
1	D	275	ASP	3.1
1	B	369	SER	3.0
1	B	31	ALA	3.0
1	C	81	ARG	2.9
1	A	3	THR	2.7
1	A	419	ALA	2.7
1	D	274	GLN	2.7
1	D	80	GLY	2.7
1	D	388	PRO	2.7
1	A	2	LEU	2.6
1	C	119	ARG	2.6
1	D	421	SER	2.5
1	A	274	GLN	2.5
1	D	465	PRO	2.4
1	D	82	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	303	ALA	2.4
1	C	32	THR	2.3
1	A	275	ASP	2.3
1	D	409	ALA	2.3
1	A	429	GLY	2.3
1	D	420	LEU	2.3
1	D	119	ARG	2.3
1	B	7	GLU	2.2
1	D	262	GLY	2.2
1	B	464	ALA	2.2
1	D	433	PHE	2.1
1	C	2	LEU	2.1
1	C	120	GLY	2.1
1	D	31	ALA	2.1
1	D	428	GLU	2.1
1	B	274	GLN	2.1
1	B	374	GLN	2.1
1	C	84	GLU	2.1
1	D	116	ARG	2.1
1	B	427	PRO	2.0
1	D	272	ASP	2.0
1	A	435	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 carbohydrates 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
2	SO4	D	604	5/5	0.86	0.22	87,87,87,87	0

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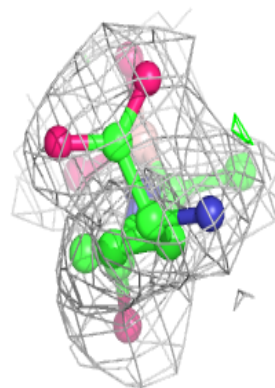
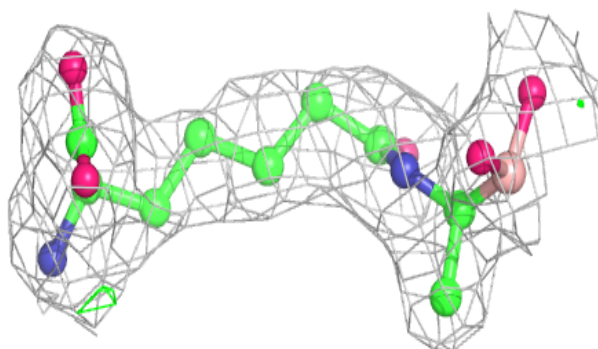
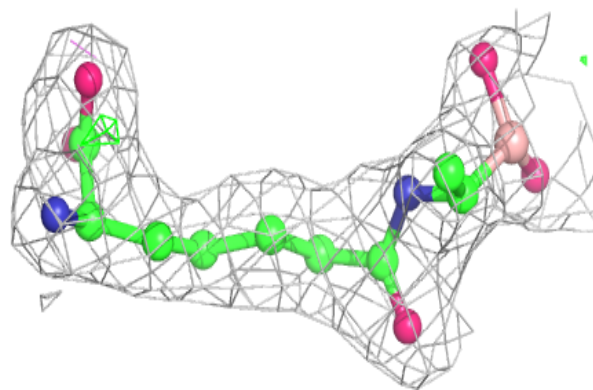
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	A	604	5/5	0.86	0.20	70,71,72,73	0
3	CO	A	611	1/1	0.91	0.19	97,97,97,97	0
5	MES	D	1467	12/12	0.91	0.21	50,52,54,54	0
3	CO	D	611	1/1	0.91	0.41	46,46,46,46	0
2	SO4	D	601	5/5	0.92	0.13	55,55,56,56	0
2	SO4	C	604	5/5	0.93	0.14	55,56,57,57	0
2	SO4	B	604	5/5	0.94	0.24	75,75,75,76	0
3	CO	D	610	1/1	0.94	0.23	45,45,45,45	0
4	BO8	B	500	17/18	0.95	0.11	24,26,38,38	0
2	SO4	D	602	5/5	0.95	0.12	71,72,72,72	0
4	BO8	C	500	17/18	0.95	0.12	23,25,30,31	0
2	SO4	A	602	5/5	0.96	0.12	53,54,55,55	0
2	SO4	B	600	5/5	0.96	0.13	69,69,70,70	0
2	SO4	B	602	5/5	0.96	0.11	58,59,60,60	0
2	SO4	C	600	5/5	0.96	0.14	68,69,69,69	0
2	SO4	C	603	5/5	0.97	0.12	33,33,35,36	0
3	CO	A	610	1/1	0.97	0.09	64,64,64,64	0
2	SO4	D	600	5/5	0.97	0.12	35,37,38,39	0
2	SO4	A	603	5/5	0.97	0.21	48,49,50,51	0
2	SO4	C	602	5/5	0.97	0.08	51,52,52,52	0
2	SO4	B	601	5/5	0.98	0.13	45,45,45,46	0
2	SO4	C	601	5/5	0.98	0.08	45,46,46,46	0
2	SO4	B	603	5/5	0.99	0.17	39,41,41,43	0
2	SO4	D	603	5/5	0.99	0.12	33,33,34,35	0
2	SO4	A	601	5/5	0.99	0.08	32,32,33,34	0
2	SO4	A	600	5/5	0.99	0.09	38,38,39,39	0

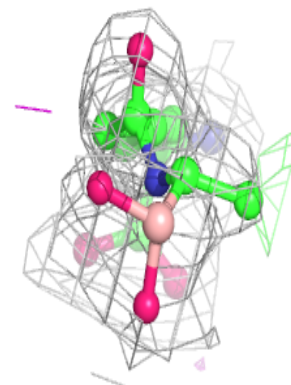
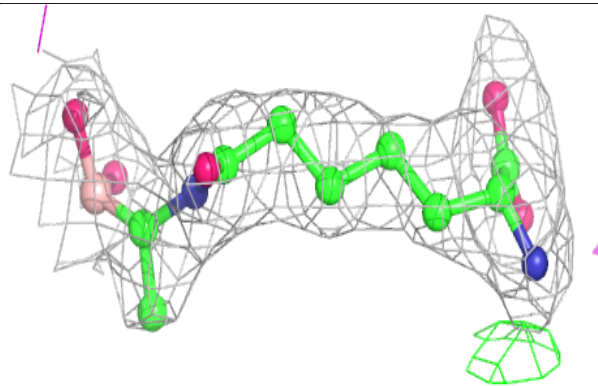
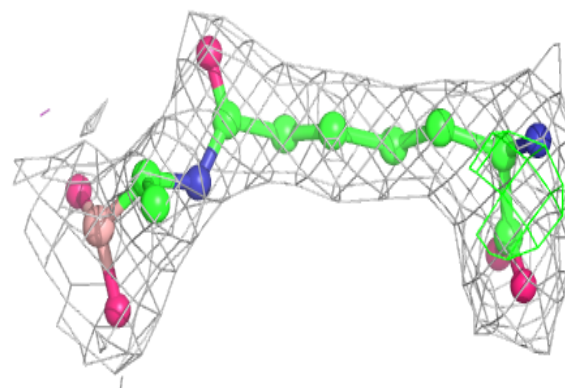
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BO8 B 500:

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

**Electron density around BO8 C 500:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.