



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:12 AM UTC

PDB ID : 4RDR / pdb_00004rdr
Title : Structure of the bacterial Zn-transporter ZnuD from *Neisseria meningitidis*
(locked conformation bound to zinc and cadmium ions)
Authors : Calmettes, C.; Moraes, T.F.
Deposited on : 2014-09-19
Resolution : 2.47 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

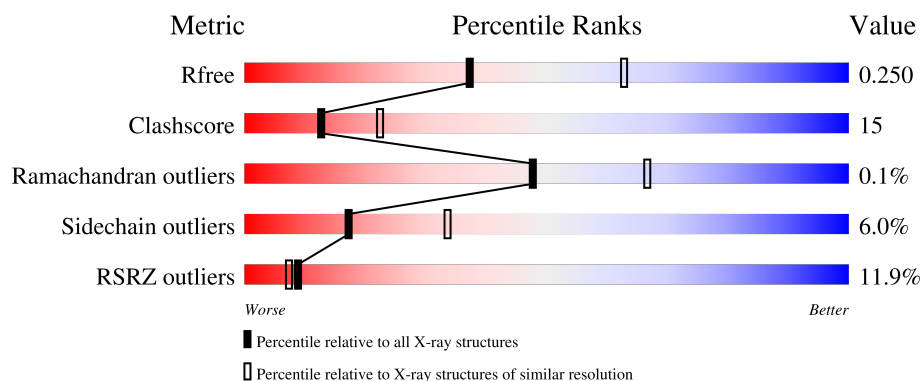
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	748	

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	SO4	A	810	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	812	-	-	X	-
5	SO4	A	820	-	-	X	-
7	EDO	A	838	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5985 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 ZnuD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	Se	0	1	0
			5633	3528	1039	1057	2	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MSE	-	expression tag	UNP Q9JZN9
A	-12	ALA	-	expression tag	UNP Q9JZN9
A	-11	HIS	-	expression tag	UNP Q9JZN9
A	-10	HIS	-	expression tag	UNP Q9JZN9
A	-9	HIS	-	expression tag	UNP Q9JZN9
A	-8	HIS	-	expression tag	UNP Q9JZN9
A	-7	HIS	-	expression tag	UNP Q9JZN9
A	-6	HIS	-	expression tag	UNP Q9JZN9
A	-5	LEU	-	expression tag	UNP Q9JZN9
A	-4	VAL	-	expression tag	UNP Q9JZN9
A	-3	PRO	-	expression tag	UNP Q9JZN9
A	-2	ARG	-	expression tag	UNP Q9JZN9
A	-1	GLY	-	expression tag	UNP Q9JZN9
A	0	SER	-	expression tag	UNP Q9JZN9

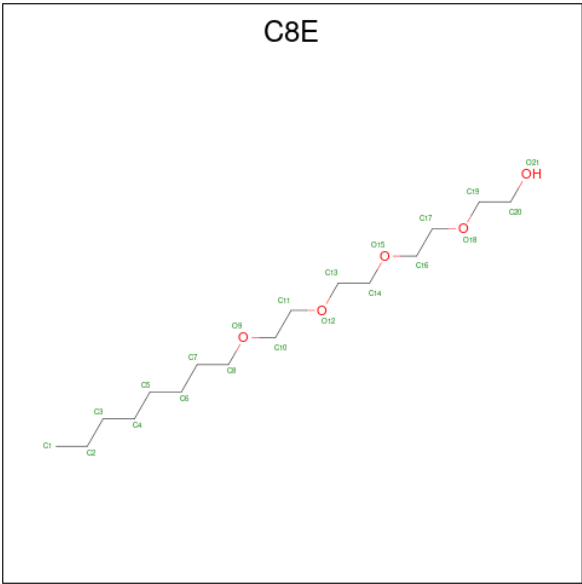
- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cd	0	0
			2	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

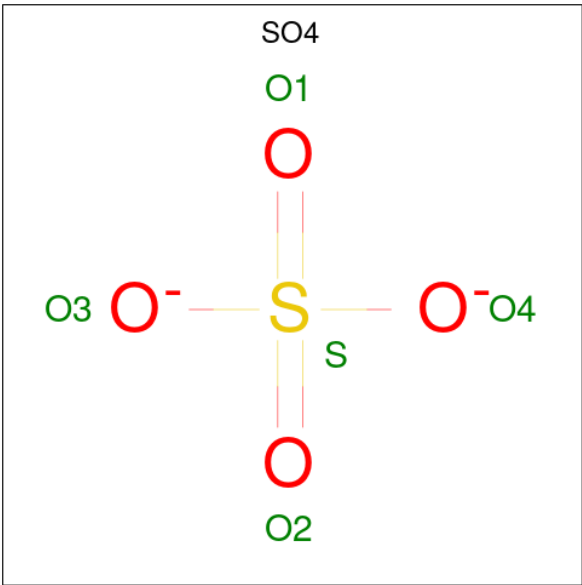
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	16	5		
4	A	1	Total	C	O	0	0
			21	16	5		
4	A	1	Total	C	O	0	0
			21	16	5		
4	A	1	Total	C	O	0	0
			21	16	5		
4	A	1	Total	C	O	0	0
			21	16	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



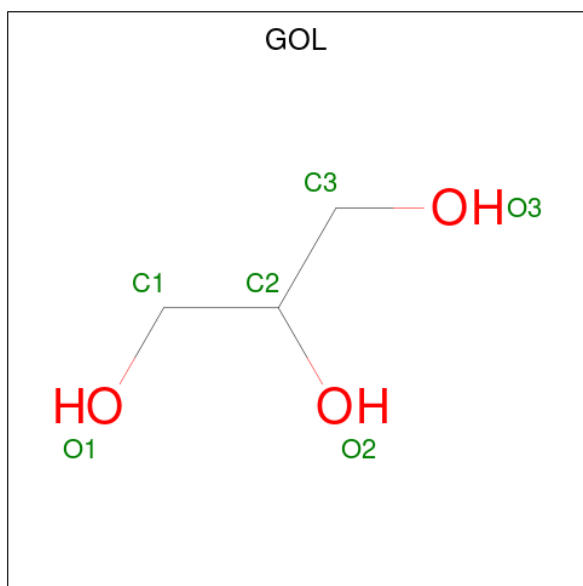
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total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

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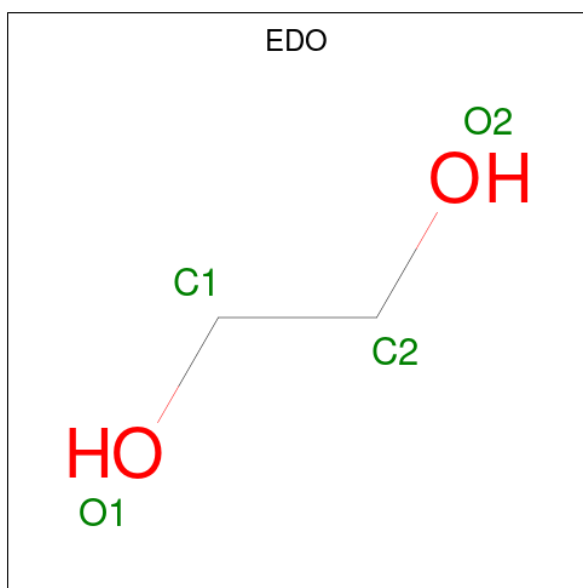
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

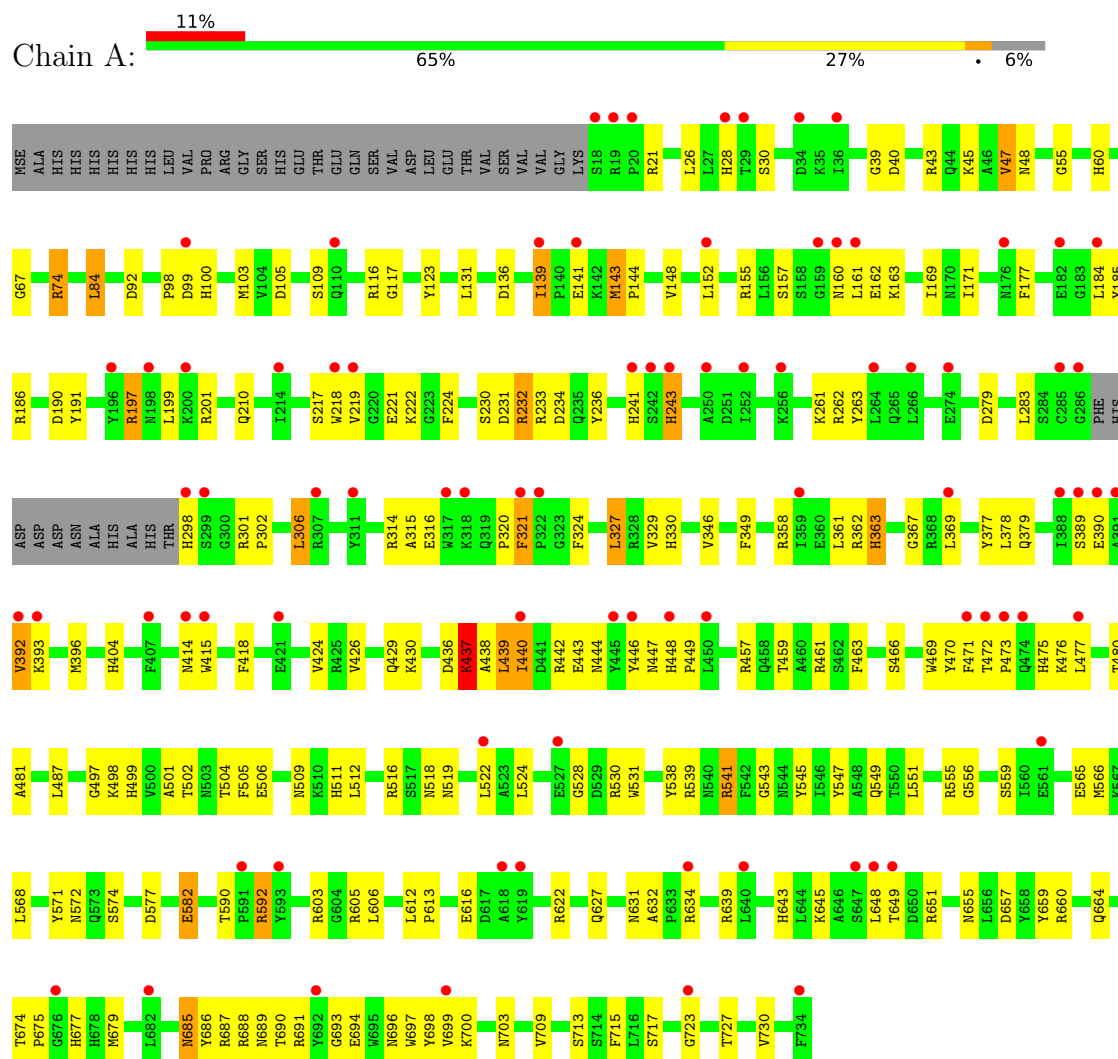
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	95	Total	O	0	0
			95	95		

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: ZnuD



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.07Å 155.82Å 159.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.98 – 2.47 39.98 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.98-2.47) 92.9 (39.98-2.47)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.218 , 0.248 0.220 , 0.250	Depositor DCC
R_{free} test set	2005 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5985	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: ZN, C8E, SO4, GOL, CD, EDO

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	0.43	0/5767	0.85	10/7793 (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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ILE	CA-C-N	9.56	131.79	119.84
1	A	139	ILE	C-N-CA	9.56	131.79	119.84
1	A	693	GLY	N-CA-C	7.00	121.56	111.12
1	A	437	LYS	N-CA-C	5.42	116.99	111.14
1	A	556	GLY	CA-C-N	5.33	125.15	119.28
1	A	556	GLY	C-N-CA	5.33	125.15	119.28
1	A	47	VAL	N-CA-C	5.32	115.53	110.53
1	A	197	ARG	N-CA-C	5.09	121.63	110.80
1	A	117	GLY	CA-C-N	5.07	124.73	119.56
1	A	117	GLY	C-N-CA	5.07	124.73	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	LYS	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	5633	0	5433	173	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	105	0	170	11	0
5	A	105	0	0	10	0
6	A	24	0	32	1	0
7	A	20	0	30	10	0
8	A	95	0	0	16	0
All	All	5985	0	5665	176	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 15.

All (176) 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:516:ARG:HH21	7:A:838:EDO:H11	0.97	1.07
1:A:516:ARG:NH2	7:A:838:EDO:H11	1.71	1.06
1:A:516:ARG:HH21	7:A:838:EDO:C1	1.70	1.04
1:A:263:TYR:HB3	1:A:440:ILE:HD11	1.53	0.89
1:A:143:MSE:HE3	1:A:144:PRO:HD2	1.59	0.82
1:A:664:GLN:NE2	5:A:814:SO4:O2	2.22	0.73
1:A:362:ARG:NH2	5:A:820:SO4:O3	2.21	0.73
1:A:243:HIS:CE1	1:A:298:HIS:O	2.42	0.72
1:A:234:ASP:HB2	1:A:306:LEU:HG	1.72	0.72
1:A:414:ASN:ND2	8:A:935:HOH:O	2.23	0.71
1:A:590:THR:HG22	1:A:592:ARG:H	1.56	0.71
1:A:241:HIS:ND1	8:A:994:HOH:O	2.24	0.71
1:A:687:ARG:NH2	1:A:694:GLU:OE1	2.23	0.71
1:A:457:ARG:NH1	5:A:812:SO4:S	2.63	0.70
1:A:603:ARG:NH2	5:A:810:SO4:O4	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:OE2	1:A:186:ARG:NH2	2.25	0.70
1:A:518:ASN:ND2	7:A:838:EDO:O2	2.24	0.70
1:A:530:ARG:HG3	1:A:531:TRP:CD1	2.27	0.70
1:A:645:LYS:NZ	8:A:968:HOH:O	2.24	0.69
1:A:315:ALA:HB3	1:A:329:VAL:HG22	1.74	0.69
1:A:457:ARG:NH1	5:A:812:SO4:O1	2.26	0.69
1:A:84:LEU:HD22	1:A:131:LEU:HD11	1.75	0.68
1:A:160:ASN:HB3	1:A:162:GLU:H	1.58	0.68
1:A:45:LYS:O	1:A:155:ARG:NH2	2.26	0.67
1:A:592:ARG:NH1	8:A:971:HOH:O	2.26	0.67
1:A:516:ARG:O	1:A:543:GLY:HA3	1.97	0.65
1:A:320:PRO:HB2	1:A:321:PHE:HD1	1.61	0.65
1:A:457:ARG:NH1	5:A:812:SO4:O2	2.22	0.65
1:A:116:ARG:NH2	8:A:905:HOH:O	2.25	0.64
1:A:185:TYR:HD1	1:A:210:GLN:HB3	1.61	0.63
1:A:516:ARG:HH21	7:A:838:EDO:C2	2.11	0.63
1:A:43:ARG:NH2	1:A:109:SER:O	2.32	0.62
1:A:262:ARG:NH1	1:A:443:GLU:OE2	2.33	0.62
1:A:415:TRP:HD1	1:A:418:PHE:HD2	1.47	0.61
1:A:463:PHE:HB2	4:A:808:C8E:H11	1.82	0.61
1:A:555:ARG:NH2	1:A:613:PRO:O	2.33	0.61
1:A:613:PRO:HB2	1:A:622:ARG:HD3	1.81	0.61
1:A:518:ASN:HD22	4:A:808:C8E:H201	1.65	0.61
1:A:686:TYR:HB3	1:A:697[B]:TRP:HB2	1.83	0.60
1:A:459:THR:HB	6:A:830:GOL:H2	1.83	0.60
1:A:233:ARG:HD3	4:A:804:C8E:H202	1.82	0.60
1:A:471:PHE:O	1:A:475:HIS:HB3	2.02	0.60
1:A:389:SER:N	1:A:390:GLU:HA	2.17	0.59
1:A:279:ASP:OD1	1:A:622:ARG:NH2	2.27	0.59
1:A:685:ASN:N	1:A:685:ASN:OD1	2.35	0.59
1:A:634:ARG:HB2	1:A:713:SER:HA	1.85	0.58
1:A:424:VAL:HG12	1:A:463:PHE:HD1	1.68	0.58
1:A:136:ASP:OD1	1:A:314:ARG:NH1	2.34	0.58
1:A:105:ASP:OD2	7:A:836:EDO:O1	2.22	0.57
1:A:603:ARG:HH12	1:A:631:ASN:ND2	2.01	0.57
1:A:232:ARG:NH1	1:A:234:ASP:OD2	2.37	0.57
1:A:690:THR:OG1	1:A:691:ARG:N	2.39	0.56
1:A:221:GLU:HB3	1:A:222:LYS:HA	1.87	0.56
1:A:136:ASP:CG	1:A:314:ARG:HH22	2.14	0.56
1:A:330:HIS:HB3	1:A:358:ARG:HG3	1.87	0.56
1:A:139:ILE:HG23	1:A:217:SER:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ARG:NH1	8:A:972:HOH:O	2.38	0.55
1:A:48:ASN:ND2	8:A:907:HOH:O	2.37	0.55
1:A:98:PRO:HG3	1:A:715:PHE:CD1	2.41	0.55
1:A:686:TYR:HB3	1:A:697[A]:TRP:HB2	1.88	0.55
1:A:547:TYR:OH	1:A:549:GLN:NE2	2.40	0.55
1:A:530:ARG:HG3	1:A:531:TRP:HD1	1.70	0.55
1:A:163:LYS:HD2	4:A:807:C8E:H112	1.89	0.54
1:A:530:ARG:NH1	8:A:977:HOH:O	2.40	0.54
1:A:659:TYR:HB2	1:A:679:MSE:HB3	1.89	0.54
1:A:160:ASN:HB3	1:A:162:GLU:N	2.22	0.54
1:A:74:ARG:HB3	1:A:538:TYR:CZ	2.43	0.53
1:A:418:PHE:CE1	4:A:806:C8E:H72	2.43	0.53
1:A:418:PHE:HE1	4:A:806:C8E:H31	1.73	0.53
1:A:378:LEU:HB3	1:A:404:HIS:HB2	1.89	0.53
1:A:509:ASN:HB3	1:A:512:LEU:HG	1.89	0.53
1:A:677:HIS:CE1	1:A:709:VAL:HG13	2.43	0.53
1:A:157:SER:HB2	1:A:162:GLU:HB3	1.89	0.53
1:A:469:TRP:CE3	4:A:806:C8E:H52	2.44	0.53
1:A:505:PHE:HB3	1:A:568:LEU:HD13	1.92	0.52
1:A:141:GLU:HG2	1:A:224:PHE:CE1	2.44	0.52
1:A:155:ARG:NH1	8:A:939:HOH:O	2.43	0.52
1:A:367:GLY:H	1:A:369:LEU:HD23	1.75	0.51
1:A:703:ASN:ND2	1:A:723:GLY:O	2.44	0.51
1:A:446:TYR:HB3	1:A:447:ASN:OD1	2.11	0.50
1:A:549:GLN:HE22	1:A:627:GLN:HE22	1.59	0.50
1:A:55:GLY:HA2	1:A:639:ARG:HH12	1.75	0.50
1:A:74:ARG:HD2	1:A:538:TYR:CE1	2.46	0.50
1:A:43:ARG:HB3	7:A:834:EDO:H12	1.92	0.50
1:A:84:LEU:HD21	1:A:123:TYR:CD1	2.47	0.49
1:A:549:GLN:CD	1:A:612:LEU:HD11	2.37	0.49
1:A:505:PHE:HB2	1:A:566:MSE:HE3	1.93	0.49
1:A:649:THR:C	1:A:651:ARG:H	2.21	0.49
1:A:697[B]:TRP:CD1	1:A:730:VAL:HG13	2.48	0.49
1:A:67:GLY:HA3	1:A:236:TYR:CD2	2.48	0.48
1:A:197:ARG:C	1:A:199:LEU:H	2.21	0.48
1:A:39:GLY:O	1:A:43:ARG:HG2	2.13	0.48
1:A:436:ASP:OD2	1:A:439:LEU:HB3	2.14	0.48
1:A:55:GLY:HA2	1:A:639:ARG:NH1	2.29	0.48
1:A:60:HIS:ND1	5:A:827:SO4:O4	2.40	0.48
1:A:505:PHE:HB2	1:A:566:MSE:CE	2.43	0.48
1:A:426:VAL:HG22	1:A:461:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:NH2	5:A:820:SO4:O2	2.38	0.47
1:A:436:ASP:C	1:A:438:ALA:HB3	2.39	0.47
1:A:616:GLU:HB2	1:A:622:ARG:NH2	2.28	0.47
1:A:316:GLU:HA	1:A:327:LEU:O	2.14	0.47
1:A:687:ARG:HD3	1:A:696:ASN:OD1	2.15	0.47
1:A:99:ASP:HB3	1:A:100:HIS:CD2	2.49	0.47
1:A:603:ARG:NH2	5:A:810:SO4:S	2.87	0.47
1:A:498:LYS:HG3	1:A:566:MSE:HE1	1.96	0.46
1:A:549:GLN:NE2	1:A:627:GLN:HE22	2.14	0.46
1:A:477:LEU:HD12	1:A:524:LEU:HD13	1.97	0.46
1:A:698:TYR:OH	7:A:834:EDO:O2	2.32	0.46
1:A:539:ARG:HD2	1:A:541:ARG:CZ	2.45	0.46
1:A:148:VAL:HG12	1:A:171:ILE:HG12	1.98	0.45
1:A:60:HIS:CE1	1:A:639:ARG:HE	2.35	0.45
1:A:559:SER:OG	8:A:906:HOH:O	2.20	0.45
1:A:261:LYS:HB3	1:A:263:TYR:CZ	2.52	0.45
1:A:472:THR:O	1:A:475:HIS:HB2	2.16	0.45
1:A:473:PRO:HA	1:A:475:HIS:N	2.32	0.45
1:A:643:HIS:ND1	1:A:657:ASP:OD1	2.37	0.45
1:A:92:ASP:HB3	1:A:103:MSE:HG2	1.99	0.45
1:A:528:GLY:O	1:A:530:ARG:N	2.45	0.44
1:A:470:TYR:CE2	1:A:476:LYS:HE2	2.52	0.44
1:A:538:TYR:OH	8:A:918:HOH:O	2.21	0.44
1:A:243:HIS:HE1	1:A:298:HIS:O	1.94	0.44
1:A:466:SER:HB2	1:A:480:THR:HG23	1.99	0.44
1:A:461:ARG:NE	8:A:942:HOH:O	2.48	0.44
1:A:232:ARG:HD3	1:A:234:ASP:OD1	2.17	0.44
1:A:700:LYS:HB3	1:A:727:THR:HB	2.00	0.44
1:A:448:HIS:HA	1:A:449:PRO:HD3	1.88	0.43
1:A:424:VAL:HG12	1:A:463:PHE:CD1	2.52	0.43
1:A:396:MSE:HA	1:A:497:GLY:HA3	2.01	0.43
1:A:473:PRO:HA	1:A:475:HIS:H	1.83	0.43
1:A:674:THR:HG22	1:A:675:PRO:O	2.18	0.43
1:A:697[B]:TRP:HD1	1:A:730:VAL:HG13	1.83	0.43
4:A:806:C8E:H71	4:A:806:C8E:H102	1.75	0.43
1:A:92:ASP:HB2	8:A:958:HOH:O	2.19	0.43
1:A:283:LEU:HD21	1:A:566:MSE:HE2	2.00	0.43
1:A:516:ARG:HH21	7:A:838:EDO:H22	1.83	0.43
1:A:565:GLU:OE1	8:A:908:HOH:O	2.21	0.43
1:A:551:LEU:O	1:A:555:ARG:HD2	2.19	0.43
1:A:47:VAL:HG21	1:A:186:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:VAL:HG11	1:A:349:PHE:CE1	2.54	0.42
1:A:74:ARG:NH2	1:A:582:GLU:OE2	2.40	0.42
1:A:415:TRP:CD1	1:A:418:PHE:HD2	2.33	0.42
1:A:377:TYR:OH	1:A:379:GLN:NE2	2.51	0.42
1:A:390:GLU:HG3	1:A:392:VAL:N	2.34	0.42
1:A:603:ARG:HH12	1:A:631:ASN:HD21	1.67	0.42
1:A:686:TYR:CE1	1:A:688:ARG:HB2	2.53	0.42
1:A:190:ASP:O	1:A:201:ARG:HD3	2.20	0.42
1:A:530:ARG:CZ	8:A:977:HOH:O	2.67	0.42
1:A:437:LYS:HA	1:A:440:ILE:HG22	2.01	0.42
1:A:649:THR:O	1:A:651:ARG:N	2.50	0.42
1:A:28:HIS:CE1	1:A:30:SER:HB2	2.55	0.42
1:A:301:ARG:HA	1:A:302:PRO:HD3	1.82	0.42
1:A:430:LYS:HE2	5:A:812:SO4:O2	2.20	0.42
4:A:808:C8E:H142	4:A:808:C8E:H111	1.84	0.42
1:A:40:ASP:OD1	1:A:40:ASP:N	2.53	0.42
1:A:437:LYS:O	1:A:440:ILE:HG22	2.19	0.41
4:A:808:C8E:H52	4:A:808:C8E:H81	1.62	0.41
1:A:143:MSE:HG2	1:A:219:VAL:HG21	2.02	0.41
1:A:606:LEU:HD23	1:A:632:ALA:HA	2.03	0.41
1:A:499:HIS:CE1	1:A:501:ALA:HB3	2.56	0.41
1:A:545:TYR:N	1:A:574:SER:O	2.52	0.41
1:A:60:HIS:CE1	1:A:639:ARG:HH21	2.39	0.41
1:A:191:TYR:OH	7:A:835:EDO:O2	2.34	0.41
1:A:324:PHE:HA	1:A:363:HIS:HA	2.03	0.41
1:A:506:GLU:OE2	1:A:571:TYR:OH	2.31	0.41
1:A:429:GLN:HB2	1:A:487:LEU:HD13	2.02	0.41
1:A:502:THR:O	1:A:504:THR:HG23	2.21	0.41
1:A:541:ARG:HD2	1:A:577:ASP:OD1	2.21	0.41
1:A:687:ARG:CZ	1:A:696:ASN:HD21	2.33	0.41
1:A:160:ASN:H	1:A:161:LEU:HA	1.87	0.40
1:A:231:ASP:OD2	8:A:945:HOH:O	2.21	0.40
1:A:162:GLU:OE2	1:A:186:ARG:HD2	2.21	0.40
1:A:197:ARG:HD3	1:A:197:ARG:HA	1.90	0.40
1:A:143:MSE:HA	1:A:144:PRO:HD3	1.98	0.40
1:A:655:ASN:HD21	1:A:700:LYS:NZ	2.20	0.40
1:A:481:ALA:HA	1:A:519:ASN:O	2.22	0.40
1:A:518:ASN:HD22	4:A:808:C8E:C20	2.33	0.40

There are no symmetry-related clashes.

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	703/748 (94%)	655 (93%)	47 (7%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	392	VAL

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	589/617 (96%)	554 (94%)	35 (6%)	18	34

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	74	ARG
1	A	84	LEU
1	A	143	MSE
1	A	152	LEU
1	A	169	ILE
1	A	177	PHE
1	A	184	LEU
1	A	218	TRP
1	A	230	SER

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Mol	Chain	Res	Type
1	A	232	ARG
1	A	243	HIS
1	A	306	LEU
1	A	321	PHE
1	A	327	LEU
1	A	361	LEU
1	A	363	HIS
1	A	393	LYS
1	A	437	LYS
1	A	439	LEU
1	A	440	ILE
1	A	442	ARG
1	A	444	ASN
1	A	511	HIS
1	A	522	LEU
1	A	541	ARG
1	A	572	ASN
1	A	582	GLU
1	A	592	ARG
1	A	605	ARG
1	A	648	LEU
1	A	685	ASN
1	A	689	ASN
1	A	699	VAL
1	A	717	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	210	GLN
1	A	241	HIS
1	A	243	HIS
1	A	308	ASN
1	A	334	ASN
1	A	379	GLN
1	A	400	ASN
1	A	403	GLN
1	A	404	HIS
1	A	412	GLN
1	A	429	GLN
1	A	456	HIS

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Mol	Chain	Res	Type
1	A	483	HIS
1	A	496	HIS
1	A	518	ASN
1	A	549	GLN
1	A	621	ASN
1	A	630	GLN
1	A	631	ASN
1	A	655	ASN
1	A	677	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](#)

Of 38 ligands modelled in this entry, 3 are monoatomic - leaving 35 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	$\# Z > 2$
7	EDO	A	835	-	3,3,3	0.30	0	2,2,2	0.57	0
5	SO4	A	827	-	4,4,4	0.26	0	6,6,6	0.15	0
5	SO4	A	813	-	4,4,4	0.24	0	6,6,6	0.17	0
5	SO4	A	818	-	4,4,4	0.24	0	6,6,6	0.20	0
7	EDO	A	834	-	3,3,3	0.34	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	838	-	3,3,3	0.34	0	2,2,2	0.34	0
5	SO4	A	809	-	4,4,4	0.33	0	6,6,6	0.17	0
5	SO4	A	823	-	4,4,4	0.21	0	6,6,6	0.12	0
7	EDO	A	836	-	3,3,3	0.29	0	2,2,2	0.54	0
5	SO4	A	819	-	4,4,4	0.25	0	6,6,6	0.27	0
6	GOL	A	831	-	5,5,5	0.56	0	5,5,5	0.54	0
5	SO4	A	829	-	4,4,4	0.26	0	6,6,6	0.15	0
6	GOL	A	833	-	5,5,5	0.49	0	5,5,5	0.34	0
5	SO4	A	815	-	4,4,4	0.25	0	6,6,6	0.30	0
5	SO4	A	824	-	4,4,4	0.24	0	6,6,6	0.19	0
5	SO4	A	810	-	4,4,4	0.29	0	6,6,6	0.14	0
5	SO4	A	814	-	4,4,4	0.26	0	6,6,6	0.24	0
5	SO4	A	820	-	4,4,4	0.26	0	6,6,6	0.25	0
4	C8E	A	806	-	20,20,20	0.86	0	19,19,19	0.81	0
5	SO4	A	812	-	4,4,4	0.26	0	6,6,6	0.13	0
5	SO4	A	817	-	4,4,4	0.22	0	6,6,6	0.19	0
6	GOL	A	832	-	5,5,5	0.14	0	5,5,5	0.36	0
4	C8E	A	804	-	20,20,20	0.94	0	19,19,19	0.87	0
5	SO4	A	822	-	4,4,4	0.22	0	6,6,6	0.12	0
6	GOL	A	830	-	5,5,5	0.43	0	5,5,5	0.37	0
5	SO4	A	821	-	4,4,4	0.22	0	6,6,6	0.14	0
5	SO4	A	811	-	4,4,4	0.24	0	6,6,6	0.16	0
5	SO4	A	826	-	4,4,4	0.22	0	6,6,6	0.13	0
4	C8E	A	805	-	20,20,20	0.80	0	19,19,19	0.90	0
5	SO4	A	825	-	4,4,4	0.23	0	6,6,6	0.17	0
5	SO4	A	828	-	4,4,4	0.21	0	6,6,6	0.13	0
7	EDO	A	837	-	3,3,3	0.35	0	2,2,2	0.33	0
4	C8E	A	808	-	20,20,20	0.78	0	19,19,19	0.86	0
4	C8E	A	807	-	20,20,20	0.67	0	19,19,19	0.79	0
5	SO4	A	816	-	4,4,4	0.24	0	6,6,6	0.15	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	GOL	A	831	-	-	2/4/4/4	-
7	EDO	A	835	-	-	1/1/1/1	-
6	GOL	A	832	-	-	0/4/4/4	-
6	GOL	A	833	-	-	1/4/4/4	-
4	C8E	A	804	-	-	11/18/18/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	C8E	A	805	-	-	13/18/18/18	-
7	EDO	A	834	-	-	0/1/1/1	-
7	EDO	A	838	-	-	1/1/1/1	-
7	EDO	A	837	-	-	1/1/1/1	-
4	C8E	A	806	-	-	11/18/18/18	-
4	C8E	A	808	-	-	10/18/18/18	-
6	GOL	A	830	-	-	0/4/4/4	-
7	EDO	A	836	-	-	0/1/1/1	-
4	C8E	A	807	-	-	14/18/18/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	831	GOL	O1-C1-C2-C3
4	A	807	C8E	C10-C11-O12-C13
4	A	805	C8E	O15-C16-C17-O18
4	A	805	C8E	C6-C7-C8-O9
4	A	807	C8E	O18-C19-C20-O21
4	A	806	C8E	C6-C7-C8-O9
4	A	805	C8E	C17-C16-O15-C14
4	A	808	C8E	C14-C13-O12-C11
4	A	807	C8E	O12-C13-C14-O15
4	A	805	C8E	O18-C19-C20-O21
4	A	804	C8E	C6-C7-C8-O9
4	A	806	C8E	C16-C17-O18-C19
4	A	807	C8E	C6-C7-C8-O9
4	A	804	C8E	C3-C4-C5-C6
4	A	806	C8E	C3-C4-C5-C6
4	A	807	C8E	O9-C10-C11-O12
4	A	808	C8E	C6-C7-C8-O9
4	A	804	C8E	C16-C17-O18-C19
4	A	804	C8E	C4-C5-C6-C7
4	A	805	C8E	O12-C13-C14-O15
4	A	805	C8E	C5-C6-C7-C8
4	A	806	C8E	O9-C10-C11-O12
4	A	807	C8E	C5-C6-C7-C8
4	A	806	C8E	O18-C19-C20-O21

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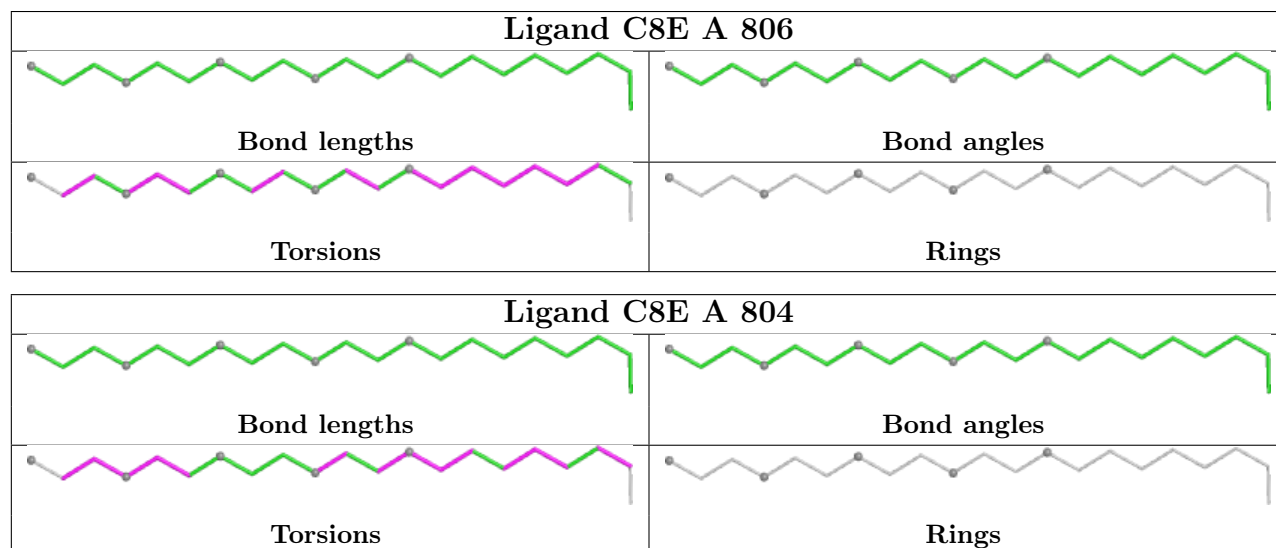
Mol	Chain	Res	Type	Atoms
4	A	808	C8E	C3-C4-C5-C6
4	A	808	C8E	O15-C16-C17-O18
4	A	806	C8E	C4-C5-C6-C7
4	A	807	C8E	C3-C4-C5-C6
4	A	805	C8E	C2-C3-C4-C5
6	A	831	GOL	O1-C1-C2-O2
4	A	807	C8E	C13-C14-O15-C16
4	A	807	C8E	O15-C16-C17-O18
4	A	807	C8E	C1-C2-C3-C4
4	A	806	C8E	C2-C3-C4-C5
4	A	804	C8E	O15-C16-C17-O18
4	A	805	C8E	C1-C2-C3-C4
6	A	833	GOL	O1-C1-C2-O2
7	A	838	EDO	O1-C1-C2-O2
4	A	806	C8E	C7-C8-O9-C10
4	A	808	C8E	C2-C3-C4-C5
4	A	808	C8E	C17-C16-O15-C14
4	A	807	C8E	C16-C17-O18-C19
4	A	805	C8E	C14-C13-O12-C11
4	A	805	C8E	C13-C14-O15-C16
4	A	808	C8E	C10-C11-O12-C13
4	A	807	C8E	C7-C8-O9-C10
4	A	805	C8E	C11-C10-O9-C8
4	A	804	C8E	C10-C11-O12-C13
4	A	804	C8E	C11-C10-O9-C8
4	A	804	C8E	C1-C2-C3-C4
4	A	808	C8E	O18-C19-C20-O21
7	A	837	EDO	O1-C1-C2-O2
4	A	805	C8E	C20-C19-O18-C17
4	A	804	C8E	O18-C19-C20-O21
4	A	804	C8E	C20-C19-O18-C17
7	A	835	EDO	O1-C1-C2-O2
4	A	807	C8E	C20-C19-O18-C17
4	A	807	C8E	C2-C3-C4-C5
4	A	804	C8E	C7-C8-O9-C10
4	A	808	C8E	C7-C8-O9-C10
4	A	806	C8E	O12-C13-C14-O15
4	A	808	C8E	O12-C13-C14-O15
4	A	805	C8E	O9-C10-C11-O12
4	A	806	C8E	C5-C6-C7-C8
4	A	806	C8E	O15-C16-C17-O18

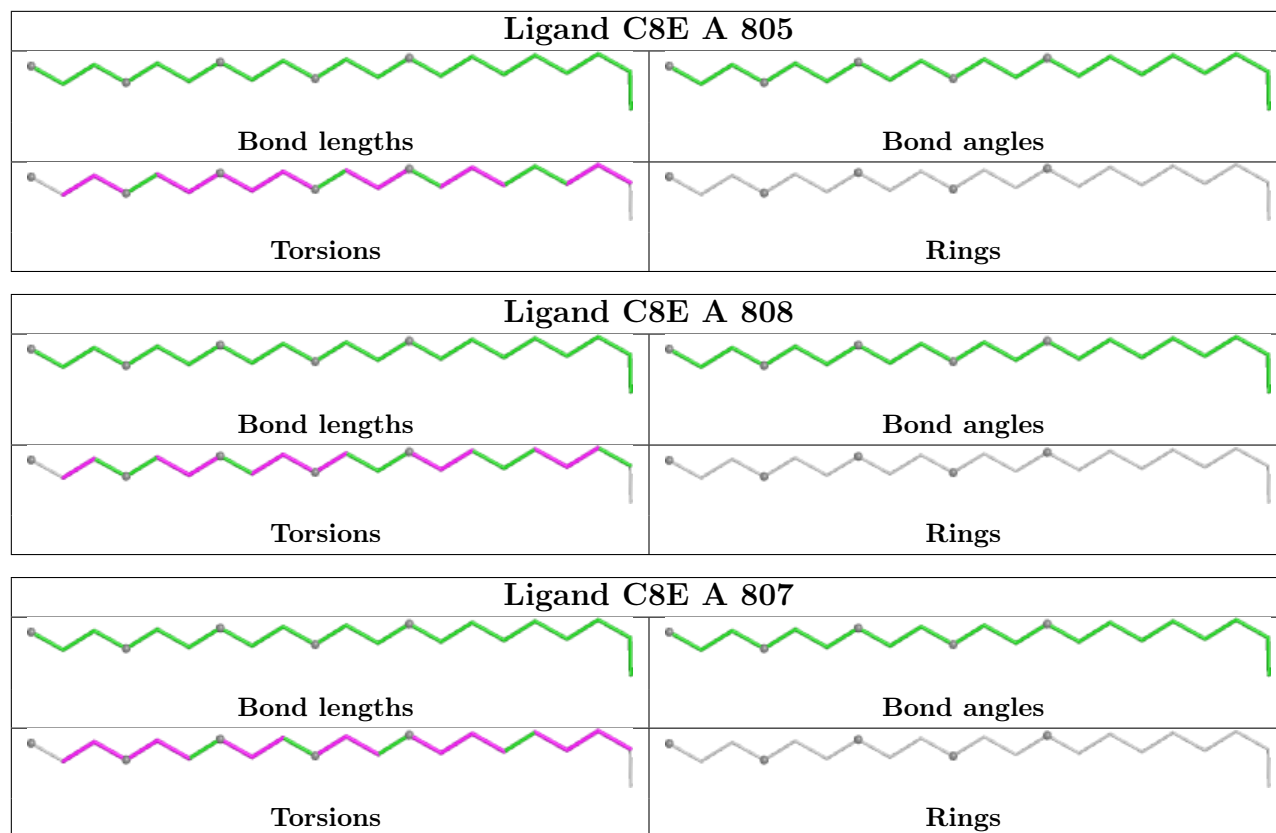
There are no ring outliers.

14 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	835	EDO	1	0
5	A	827	SO4	1	0
7	A	834	EDO	2	0
7	A	838	EDO	6	0
7	A	836	EDO	1	0
5	A	810	SO4	2	0
5	A	814	SO4	1	0
5	A	820	SO4	2	0
4	A	806	C8E	4	0
5	A	812	SO4	4	0
4	A	804	C8E	1	0
6	A	830	GOL	1	0
4	A	808	C8E	5	0
4	A	807	C8E	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	699/748 (93%)	0.86	83 (11%) 9 7	55, 84, 136, 189	1 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	ALA	5.8
1	A	317	TRP	4.7
1	A	392	VAL	4.5
1	A	218	TRP	4.5
1	A	29	THR	4.4
1	A	298	HIS	4.3
1	A	415	TRP	3.9
1	A	18	SER	3.8
1	A	19	ARG	3.7
1	A	200	LYS	3.6
1	A	421	GLU	3.5
1	A	388	ILE	3.5
1	A	692	TYR	3.4
1	A	472	THR	3.4
1	A	445	TYR	3.2
1	A	219	VAL	3.2
1	A	256	LYS	3.1
1	A	159	GLY	3.1
1	A	182	GLU	3.1
1	A	473	PRO	3.1
1	A	471	PHE	3.0
1	A	593	TYR	3.0
1	A	28	HIS	3.0
1	A	474	GLN	3.0
1	A	196	TYR	2.9
1	A	198	ASN	2.8
1	A	266	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	242	SER	2.8
1	A	649	THR	2.8
1	A	723	GLY	2.7
1	A	414	ASN	2.7
1	A	359	ILE	2.7
1	A	734	PHE	2.7
1	A	393	LYS	2.7
1	A	110	GLN	2.6
1	A	160	ASN	2.6
1	A	676	GLY	2.5
1	A	311	TYR	2.5
1	A	446	TYR	2.5
1	A	440	ILE	2.5
1	A	243	HIS	2.4
1	A	299	SER	2.4
1	A	318	LYS	2.4
1	A	252	ILE	2.4
1	A	285	CYS	2.4
1	A	274	GLU	2.4
1	A	389	SER	2.3
1	A	648	LEU	2.3
1	A	322	PRO	2.3
1	A	448	HIS	2.3
1	A	619	TYR	2.3
1	A	286	GLY	2.3
1	A	369	LEU	2.3
1	A	321	PHE	2.3
1	A	407	PHE	2.3
1	A	561	GLU	2.3
1	A	390	GLU	2.2
1	A	527	GLU	2.2
1	A	591	PRO	2.2
1	A	699	VAL	2.2
1	A	618	ALA	2.2
1	A	264	LEU	2.2
1	A	214	ILE	2.2
1	A	477	LEU	2.2
1	A	522	LEU	2.1
1	A	640	LEU	2.1
1	A	682	LEU	2.1
1	A	307	ARG	2.1
1	A	176	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	20	PRO	2.1
1	A	241	HIS	2.1
1	A	250	ALA	2.1
1	A	450	LEU	2.1
1	A	634	ARG	2.1
1	A	99	ASP	2.1
1	A	141	GLU	2.1
1	A	34	ASP	2.1
1	A	152	LEU	2.0
1	A	161	LEU	2.0
1	A	36	ILE	2.0
1	A	139	ILE	2.0
1	A	184	LEU	2.0
1	A	647	SER	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(Å ²)	Q<0.9
5	SO4	A	821	5/5	0.45	0.20	148,152,153,158	5
6	GOL	A	832	6/6	0.56	0.27	99,111,119,123	0
5	SO4	A	825	5/5	0.58	0.24	137,139,141,145	5
5	SO4	A	826	5/5	0.64	0.16	129,130,134,138	5
5	SO4	A	823	5/5	0.64	0.18	158,160,160,161	5
6	GOL	A	833	6/6	0.68	0.23	107,117,122,128	0
5	SO4	A	822	5/5	0.74	0.26	141,143,148,149	5
5	SO4	A	818	5/5	0.74	0.17	98,116,119,125	5
5	SO4	A	814	5/5	0.75	0.27	74,85,101,104	5

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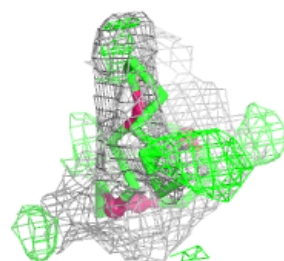
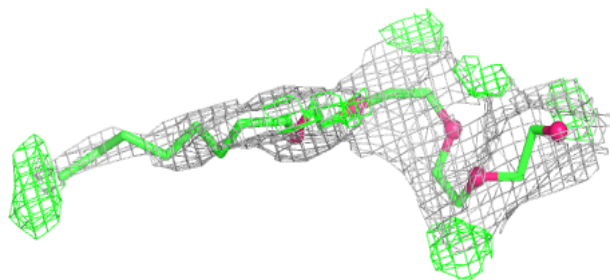
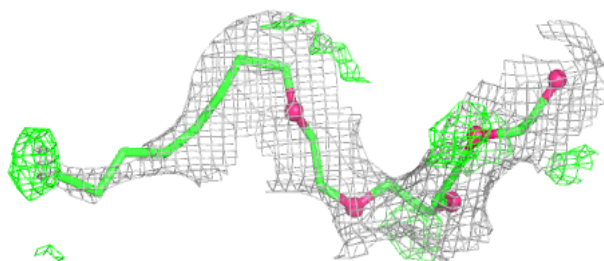
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	A	830	6/6	0.78	0.20	117,124,127,130	0
5	SO4	A	824	5/5	0.79	0.19	133,134,136,136	5
4	C8E	A	807	21/21	0.79	0.28	127,140,146,147	0
5	SO4	A	817	5/5	0.79	0.18	115,118,123,127	5
5	SO4	A	813	5/5	0.80	0.21	82,97,107,109	5
5	SO4	A	828	5/5	0.82	0.35	148,151,153,156	5
4	C8E	A	805	21/21	0.84	0.25	90,103,114,119	0
5	SO4	A	812	5/5	0.84	0.15	99,100,102,103	5
4	C8E	A	808	21/21	0.85	0.25	97,111,141,143	0
5	SO4	A	810	5/5	0.86	0.13	78,79,84,97	5
4	C8E	A	806	21/21	0.86	0.23	73,98,116,122	0
7	EDO	A	838	4/4	0.86	0.18	109,109,111,113	0
5	SO4	A	816	5/5	0.87	0.27	117,118,118,118	5
5	SO4	A	829	5/5	0.87	0.19	137,137,139,140	5
6	GOL	A	831	6/6	0.88	0.14	106,112,119,122	0
7	EDO	A	834	4/4	0.88	0.27	101,106,107,115	0
5	SO4	A	827	5/5	0.88	0.30	145,146,148,150	5
7	EDO	A	837	4/4	0.89	0.19	103,105,109,112	0
7	EDO	A	835	4/4	0.89	0.25	101,109,114,118	0
7	EDO	A	836	4/4	0.90	0.31	127,128,132,132	0
5	SO4	A	820	5/5	0.90	0.10	132,132,133,134	5
5	SO4	A	811	5/5	0.90	0.13	92,96,99,99	5
5	SO4	A	815	5/5	0.91	0.18	95,102,108,116	5
5	SO4	A	819	5/5	0.92	0.28	75,82,87,89	5
4	C8E	A	804	21/21	0.92	0.17	68,92,109,119	0
5	SO4	A	809	5/5	0.93	0.10	79,85,91,92	5
2	CD	A	802	1/1	0.95	0.07	113,113,113,113	0
2	CD	A	801	1/1	0.97	0.08	92,92,92,92	0
3	ZN	A	803	1/1	0.99	0.06	58,58,58,58	0

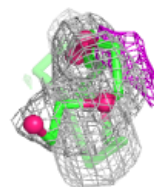
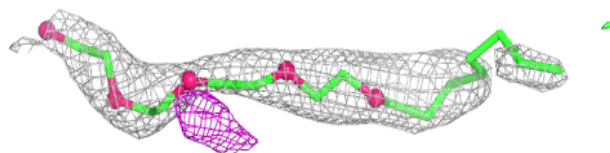
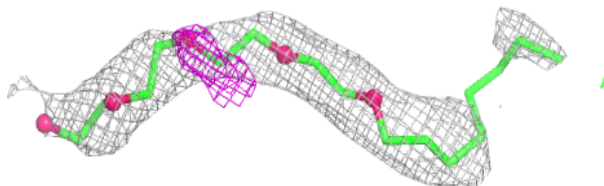
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E A 807:

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

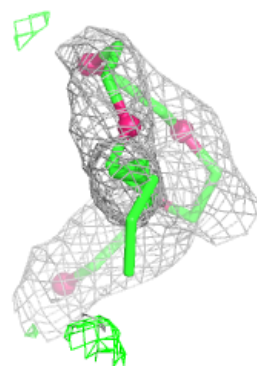
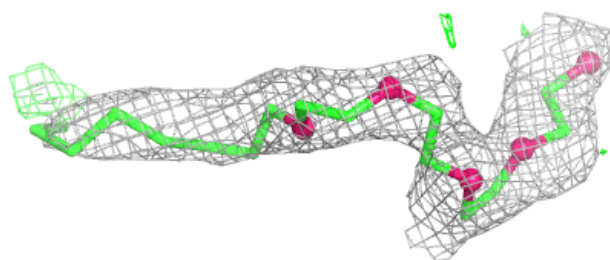
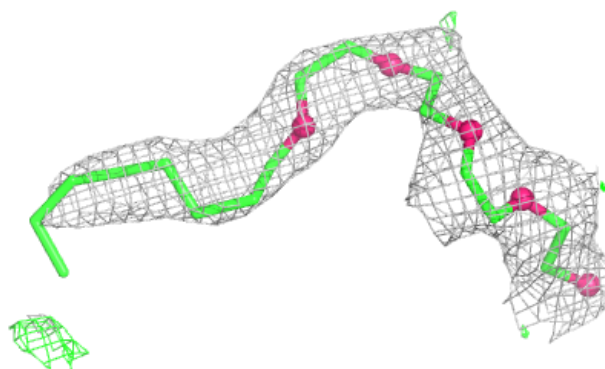
**Electron density around C8E A 805:**

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

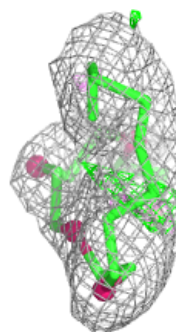
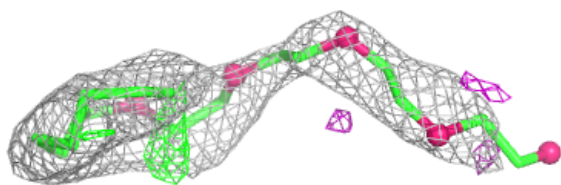
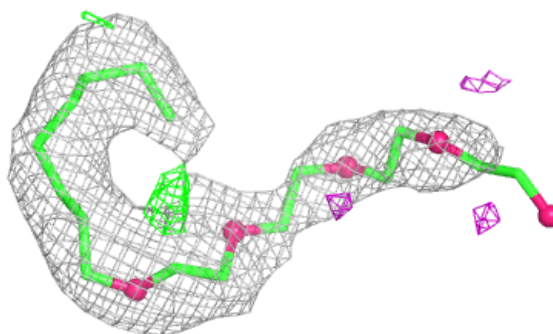


Electron density around C8E A 808:

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

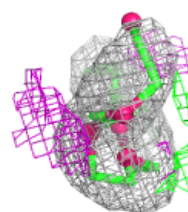
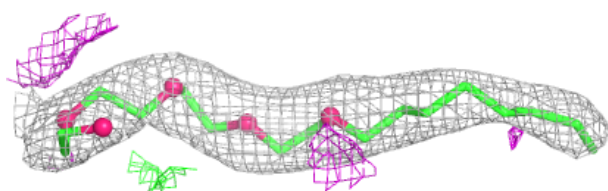
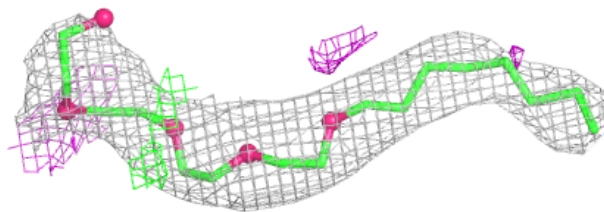
**Electron density around C8E A 806:**

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



Electron density around C8E A 804:

$2mF_o-DF_c$ (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.