



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:48 AM UTC

PDB ID : 8A18 / pdb_00008a18
Title : 1.63 Å resolution hydroquinone inhibited *Sporosarcina pasteurii* urease
Authors : Mazzei, L.; Ciurli, S.; Cianci, M.
Deposited on : 2022-06-01
Resolution : 1.63 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

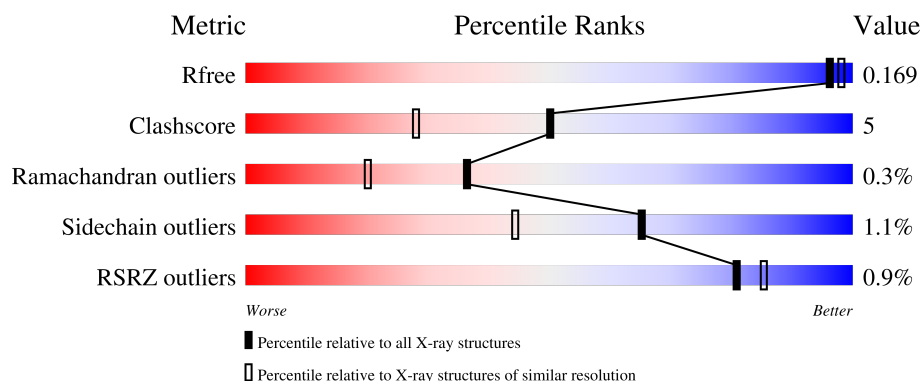
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

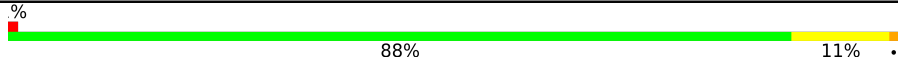
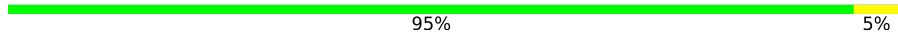
The reported resolution of this entry is 1.63 Å.

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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	AAA	100	
2	BBB	122	
3	CCC	570	

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	EDO	CCC	614	-	-	X	-
5	SO4	AAA	308	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7210 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 Urease subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	100	Total	C	N	O	S	0	8	0
			842	528	144	162	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	20	ALA	LEU	variant	UNP P41022
AAA	22	LYS	ARG	variant	UNP P41022

- Molecule 2 is a protein called Urease subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	122	Total	C	N	O	S	0	4	0
			983	607	177	198	1			

- Molecule 3 is a protein called Urease subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	570	Total	C	N	O	S	0	30	0
			4535	2849	779	878	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	35	TYR	-	insertion	UNP P41020
CCC	?	-	VAL	deletion	UNP P41020

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



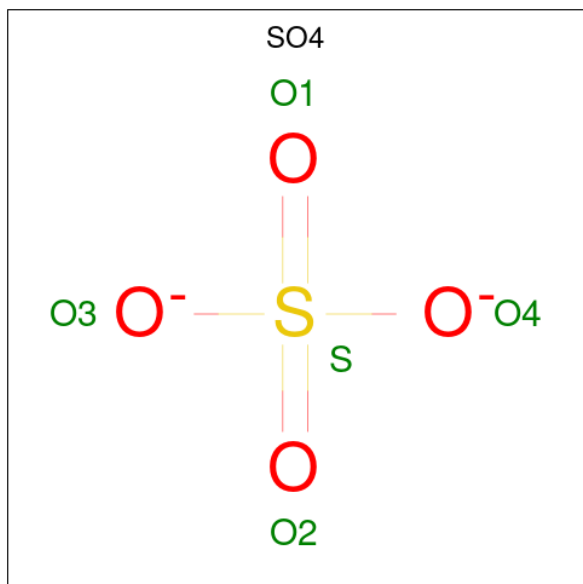
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		

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

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



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

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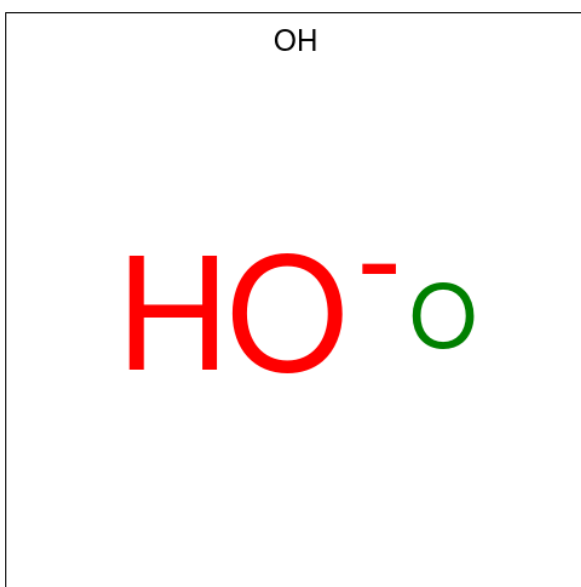
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1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

- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

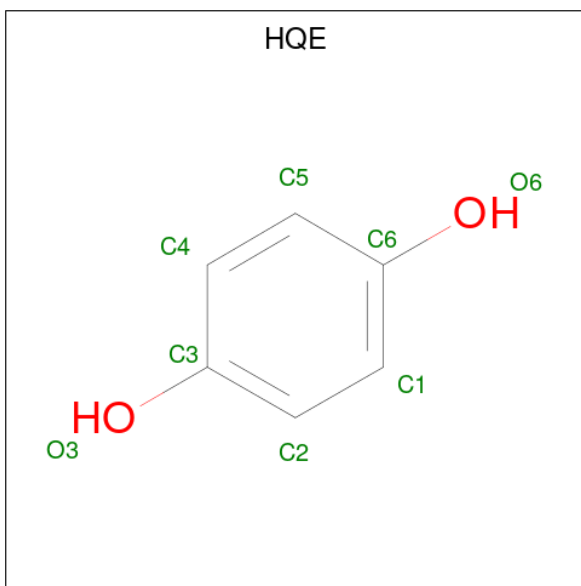
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	CCC	2	Total	Ni	0	0
			2	2		

- Molecule 7 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	CCC	1	Total	O		0	0
			1	1			

- Molecule 8 is benzene-1,4-diol (CCD ID: HQE) (formula: C₆H₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	CCC	1	Total	C	O	0	0
			8	6	2		
8	CCC	1	Total	C	O	0	0
			8	6	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	88	Total 88	O 88	0	0
9	BBB	123	Total 123	O 123	0	0
9	CCC	455	Total 455	O 455	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

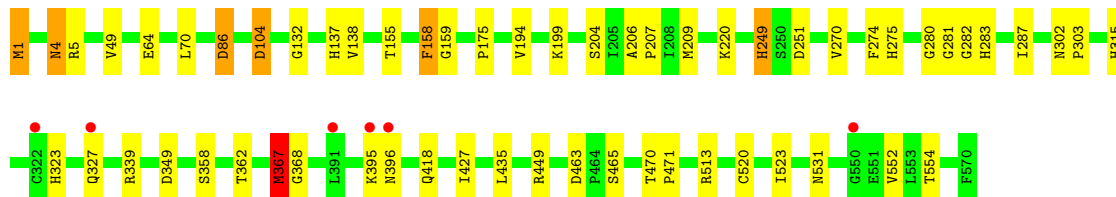
- Molecule 1: Urease subunit gamma



- Molecule 2: Urease subunit beta



- Molecule 3: Urease subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.67Å 131.67Å 189.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	114.29 – 1.63 114.03 – 1.63	Depositor EDS
% Data completeness (in resolution range)	99.9 (114.29-1.63) 99.9 (114.03-1.63)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.128 , 0.158 0.143 , 0.169	Depositor DCC
R_{free} test set	5968 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7210	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: KCX, NI, CXM, EDO, HQE, SO4, OH

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	AAA	1.02	1/849 (0.1%)	1.09	0/1141
2	BBB	1.01	0/998	1.10	0/1342
3	CCC	1.06	2/4630 (0.0%)	1.16	8/6269 (0.1%)
All	All	1.05	3/6477 (0.0%)	1.14	8/8752 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	315	HIS	CE1-NE2	6.31	1.38	1.32
1	AAA	43	ILE	C-O	5.04	1.29	1.24
3	CCC	204	SER	C-O	5.03	1.30	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	520	CYS	CB-CA-C	-12.25	88.34	109.65
3	CCC	104	ASP	CA-CB-CG	8.27	120.87	112.60
3	CCC	251	ASP	CA-CB-CG	7.53	120.13	112.60
3	CCC	194	VAL	CA-C-N	6.56	126.11	121.65
3	CCC	194	VAL	C-N-CA	6.56	126.11	121.65
3	CCC	349	ASP	CA-CB-CG	5.88	118.48	112.60
3	CCC	463	ASP	CA-CB-CG	5.67	118.27	112.60
3	CCC	86	ASP	CA-CB-CG	5.09	117.69	112.60

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	AAA	842	0	852	12	0
2	BBB	983	0	964	6	0
3	CCC	4535	0	4522	53	0
4	AAA	20	0	30	4	1
4	CCC	60	0	90	8	1
5	AAA	15	0	0	2	0
5	BBB	30	0	0	0	0
5	CCC	40	0	0	0	0
6	CCC	2	0	0	0	0
7	CCC	1	0	0	0	0
8	CCC	16	0	10	1	0
9	AAA	88	0	0	1	0
9	BBB	123	0	0	1	0
9	CCC	455	0	0	17	0
All	All	7210	0	6468	69	2

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 (69) 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)
3:CCC:303[B]:PRO:HG2	9:CCC:1043:HOH:O	1.70	0.91
1:AAA:96[B]:HIS:NE2	5:AAA:308:SO4:O2	2.06	0.87
3:CCC:4[B]:ASN:ND2	9:CCC:702:HOH:O	2.07	0.86
3:CCC:64[B]:GLU:HG2	4:CCC:614:EDO:C2	2.11	0.80
3:CCC:64[B]:GLU:HG2	4:CCC:614:EDO:H22	1.64	0.80
1:AAA:66[B]:ARG:NH1	1:AAA:100:SER:OXT	2.14	0.80
3:CCC:287[B]:ILE:O	3:CCC:287[B]:ILE:HD13	1.86	0.75
3:CCC:270[B]:VAL:HG11	3:CCC:523:ILE:O	1.90	0.71
3:CCC:4[B]:ASN:CG	9:CCC:707:HOH:O	2.32	0.70
3:CCC:64[B]:GLU:CG	4:CCC:614:EDO:H22	2.26	0.66
1:AAA:79[B]:ASP:OD1	1:AAA:96[B]:HIS:ND1	2.30	0.64
3:CCC:270[B]:VAL:HG12	9:CCC:903:HOH:O	1.97	0.62
1:AAA:1:CXM:ON1	4:AAA:304:EDO:H12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:111[A]:GLU:CD	2:BBB:111[A]:GLU:H	2.07	0.60
1:AAA:32:TYR:OH	4:AAA:305:EDO:H22	2.06	0.56
3:CCC:303[B]:PRO:HG3	3:CCC:367[B]:MET:O	2.06	0.56
3:CCC:552:VAL:HG12	3:CCC:554[B]:THR:HG23	1.88	0.56
3:CCC:64[B]:GLU:HG2	4:CCC:614:EDO:H21	1.85	0.56
2:BBB:17:GLY:O	3:CCC:5[A]:ARG:HG2	2.05	0.56
2:BBB:71:SER:OG	3:CCC:49[A]:VAL:HG21	2.06	0.55
3:CCC:427[B]:ILE:CD1	3:CCC:435:LEU:CD2	2.86	0.54
8:CCC:619:HQE:H4	9:CCC:977:HOH:O	2.09	0.52
3:CCC:4[B]:ASN:ND2	9:CCC:707:HOH:O	2.41	0.52
2:BBB:95:GLU:O	3:CCC:104:ASP:HB3	2.10	0.51
3:CCC:4[B]:ASN:ND2	9:CCC:714:HOH:O	2.43	0.51
2:BBB:111[A]:GLU:OE1	9:BBB:301:HOH:O	2.19	0.50
3:CCC:64[B]:GLU:CG	4:CCC:614:EDO:C2	2.85	0.49
1:AAA:81[B]:GLN:HG2	1:AAA:94:THR:OG1	2.12	0.49
3:CCC:1[B]:MET:N	9:CCC:719:HOH:O	2.47	0.48
3:CCC:362:THR:O	3:CCC:368:GLY:HA3	2.13	0.48
3:CCC:132:GLY:HA3	3:CCC:155:THR:OG1	2.13	0.48
3:CCC:327:GLN:HG2	9:CCC:988:HOH:O	2.11	0.48
3:CCC:339:ARG:NH2	3:CCC:367[B]:MET:HE1	2.29	0.47
3:CCC:249:HIS:CE1	3:CCC:281:GLY:HA3	2.49	0.47
3:CCC:367[B]:MET:HE2	9:CCC:1063:HOH:O	2.14	0.47
3:CCC:302:ASN:N	3:CCC:303[B]:PRO:CD	2.78	0.47
4:CCC:615:EDO:H11	9:CCC:911:HOH:O	2.13	0.47
3:CCC:137:HIS:CE1	3:CCC:274:PHE:CD2	3.03	0.46
3:CCC:158:PHE:CE2	3:CCC:418[A]:GLN:CG	2.99	0.46
3:CCC:287[B]:ILE:HD13	3:CCC:287[B]:ILE:C	2.39	0.46
3:CCC:367[B]:MET:O	3:CCC:367[B]:MET:HG2	2.16	0.45
3:CCC:70:LEU:HD11	3:CCC:86:ASP:HB3	1.99	0.45
3:CCC:358:SER:HA	3:CCC:531:ASN:HB3	1.99	0.44
3:CCC:175:PRO:HB3	3:CCC:199:LYS:HE3	2.00	0.44
1:AAA:1:CXM:ON1	4:AAA:304:EDO:C1	2.64	0.44
1:AAA:66[B]:ARG:NH1	1:AAA:100:SER:C	2.76	0.44
1:AAA:77:ILE:HA	4:AAA:305:EDO:H21	2.01	0.43
3:CCC:449:ARG:NH2	9:CCC:721:HOH:O	2.48	0.43
1:AAA:62:HIS:HD2	9:AAA:478:HOH:O	2.01	0.43
3:CCC:206:ALA:N	3:CCC:207[B]:PRO:HD2	2.34	0.43
2:BBB:19:ILE:HG12	3:CCC:5[A]:ARG:HD2	2.00	0.42
3:CCC:64[B]:GLU:CD	9:CCC:712:HOH:O	2.61	0.42
3:CCC:274:PHE:O	3:CCC:275:HIS:C	2.62	0.42
4:CCC:615:EDO:H21	9:CCC:911:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CCC:138:VAL:O	3:CCC:159:GLY:HA3	2.20	0.42
3:CCC:470:THR:N	3:CCC:471:PRO:CD	2.83	0.42
3:CCC:4[B]:ASN:CG	9:CCC:714:HOH:O	2.62	0.41
3:CCC:280:GLY:HA2	3:CCC:367[B]:MET:SD	2.60	0.41
3:CCC:1[B]:MET:HB2	3:CCC:1[B]:MET:HE3	1.47	0.41
3:CCC:367[B]:MET:CE	9:CCC:1063:HOH:O	2.69	0.41
3:CCC:270[B]:VAL:CG1	3:CCC:523:ILE:O	2.64	0.41
3:CCC:513[B]:ARG:NH2	9:CCC:732:HOH:O	2.53	0.41
1:AAA:96[B]:HIS:NE2	5:AAA:308:SO4:S	2.89	0.41
3:CCC:209[B]:MET:HE3	3:CCC:209[B]:MET:HB2	1.82	0.41
3:CCC:282:GLY:O	3:CCC:283:HIS:C	2.64	0.40
3:CCC:513[B]:ARG:HH11	3:CCC:513[B]:ARG:HD3	1.75	0.40
3:CCC:323:HIS:CE1	4:CCC:610:EDO:H11	2.55	0.40
1:AAA:6:ALA:HB2	3:CCC:465[B]:SER:OG	2.22	0.40
3:CCC:339:ARG:HH21	3:CCC:367[B]:MET:HE1	1.86	0.40

All (2) 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)
4:AAA:304:EDO:O2	4:AAA:305:EDO:O2[2_665]	1.82	0.38
4:CCC:618:EDO:O1	4:CCC:618:EDO:O1[11_555]	2.02	0.18

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	AAA	106/100 (106%)	106 (100%)	0	0	100	100
2	BBB	124/122 (102%)	120 (97%)	3 (2%)	1 (1%)	16	3
3	CCC	596/570 (105%)	571 (96%)	23 (4%)	2 (0%)	36	20
All	All	826/792 (104%)	797 (96%)	26 (3%)	3 (0%)	36	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	CCC	367[A]	MET
3	CCC	367[B]	MET
2	BBB	99	ILE

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	AAA	91/83 (110%)	91 (100%)	0	100	100
2	BBB	105/101 (104%)	105 (100%)	0	100	100
3	CCC	487/458 (106%)	477 (98%)	10 (2%)	47	19
All	All	683/642 (106%)	673 (98%)	10 (2%)	65	32

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CCC	1[A]	MET
3	CCC	1[B]	MET
3	CCC	4[A]	ASN
3	CCC	4[B]	ASN
3	CCC	158	PHE
3	CCC	249	HIS
3	CCC	367[A]	MET
3	CCC	367[B]	MET
3	CCC	395	LYS
3	CCC	396	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CXM	AAA	1	1	9,10,11	1.87	1 (11%)	9,11,13	1.47	1 (11%)
3	KCX	CCC	220	6,3	10,11,12	0.61	0	6,12,14	1.33	1 (16%)

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
1	CXM	AAA	1	1	-	5/9/10/12	-
3	KCX	CCC	220	6,3	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	1	CXM	ON1-CN	4.78	1.30	1.21

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	1	CXM	ON1-CN-N	-3.67	118.84	124.86
3	CCC	220	KCX	OQ1-CX-NZ	-2.50	121.12	124.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	1	CXM	O-C-CA-CB
1	AAA	1	CXM	CB-CA-N-CN

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Mol	Chain	Res	Type	Atoms
1	AAA	1	CXM	C-CA-N-CN
1	AAA	1	CXM	ON1-CN-N-CA
1	AAA	1	CXM	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AAA	1	CXM	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 39 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	EDO	CCC	618	-	3,3,3	0.95	0	2,2,2	0.69	0
4	EDO	AAA	303	-	3,3,3	0.54	0	2,2,2	0.55	0
4	EDO	AAA	305	-	3,3,3	0.45	0	2,2,2	1.00	0
5	SO4	BBB	206	-	4,4,4	0.38	0	6,6,6	0.09	0
5	SO4	CCC	628	-	4,4,4	0.38	0	6,6,6	0.38	0
4	EDO	CCC	617	-	3,3,3	0.59	0	2,2,2	0.45	0
5	SO4	CCC	627	-	4,4,4	0.32	0	6,6,6	0.12	0
5	SO4	CCC	626	-	4,4,4	0.32	0	6,6,6	0.09	0
4	EDO	CCC	604	-	3,3,3	0.39	0	2,2,2	0.43	0
4	EDO	CCC	614	-	3,3,3	0.30	0	2,2,2	0.72	0
8	HQE	CCC	620	3	8,8,8	0.63	0	10,10,10	0.41	0
5	SO4	BBB	203	-	4,4,4	0.27	0	6,6,6	0.08	0
5	SO4	AAA	307	-	4,4,4	0.39	0	6,6,6	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	CCC	612	-	3,3,3	1.03	0	2,2,2	0.29	0
5	SO4	BBB	202	-	4,4,4	0.54	0	6,6,6	0.18	0
5	SO4	BBB	205	-	4,4,4	0.30	0	6,6,6	0.09	0
4	EDO	CCC	606	-	3,3,3	0.77	0	2,2,2	0.47	0
4	EDO	CCC	615	-	3,3,3	0.98	0	2,2,2	1.07	0
5	SO4	CCC	624	-	4,4,4	0.67	0	6,6,6	0.26	0
5	SO4	AAA	308	-	4,4,4	0.30	0	6,6,6	0.16	0
4	EDO	CCC	616	-	3,3,3	0.58	0	2,2,2	0.47	0
5	SO4	CCC	621	-	4,4,4	0.29	0	6,6,6	0.12	0
4	EDO	CCC	611	-	3,3,3	0.58	0	2,2,2	0.24	0
4	EDO	CCC	605	-	3,3,3	0.24	0	2,2,2	0.74	0
4	EDO	AAA	302	-	3,3,3	0.89	0	2,2,2	0.53	0
4	EDO	CCC	610	-	3,3,3	0.51	0	2,2,2	0.34	0
4	EDO	CCC	609	-	3,3,3	0.50	0	2,2,2	0.78	0
4	EDO	AAA	301	-	3,3,3	1.19	0	2,2,2	0.50	0
5	SO4	BBB	201	-	4,4,4	0.40	0	6,6,6	0.14	0
5	SO4	CCC	625	-	4,4,4	0.31	0	6,6,6	0.46	0
5	SO4	AAA	306	-	4,4,4	0.62	0	6,6,6	0.35	0
4	EDO	AAA	304	-	3,3,3	1.10	0	2,2,2	1.00	0
5	SO4	CCC	622	-	4,4,4	0.31	0	6,6,6	0.16	0
5	SO4	BBB	204	-	4,4,4	0.33	0	6,6,6	0.10	0
4	EDO	CCC	613	-	3,3,3	0.58	0	2,2,2	0.37	0
4	EDO	CCC	607	-	3,3,3	0.47	0	2,2,2	1.10	0
8	HQE	CCC	619	3	8,8,8	0.46	0	10,10,10	0.45	0
5	SO4	CCC	623	-	4,4,4	0.28	0	6,6,6	0.05	0
4	EDO	CCC	608	-	3,3,3	0.26	0	2,2,2	1.36	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	EDO	CCC	618	-	-	0/1/1/1	-
4	EDO	AAA	303	-	-	0/1/1/1	-
4	EDO	AAA	305	-	-	1/1/1/1	-
4	EDO	CCC	617	-	-	1/1/1/1	-
4	EDO	CCC	604	-	-	0/1/1/1	-
4	EDO	CCC	614	-	-	0/1/1/1	-
8	HQE	CCC	620	3	-	-	0/1/1/1
4	EDO	CCC	612	-	-	0/1/1/1	-
4	EDO	CCC	606	-	-	0/1/1/1	-
4	EDO	CCC	615	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	CCC	616	-	-	0/1/1/1	-
4	EDO	CCC	611	-	-	0/1/1/1	-
4	EDO	CCC	605	-	-	0/1/1/1	-
4	EDO	AAA	302	-	-	0/1/1/1	-
4	EDO	CCC	610	-	-	0/1/1/1	-
4	EDO	CCC	609	-	-	0/1/1/1	-
4	EDO	AAA	301	-	-	0/1/1/1	-
4	EDO	AAA	304	-	-	1/1/1/1	-
4	EDO	CCC	613	-	-	0/1/1/1	-
4	EDO	CCC	607	-	-	1/1/1/1	-
8	HQE	CCC	619	3	-	-	0/1/1/1
4	EDO	CCC	608	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	CCC	607	EDO	O1-C1-C2-O2
4	AAA	304	EDO	O1-C1-C2-O2
4	CCC	615	EDO	O1-C1-C2-O2
4	AAA	305	EDO	O1-C1-C2-O2
4	CCC	617	EDO	O1-C1-C2-O2

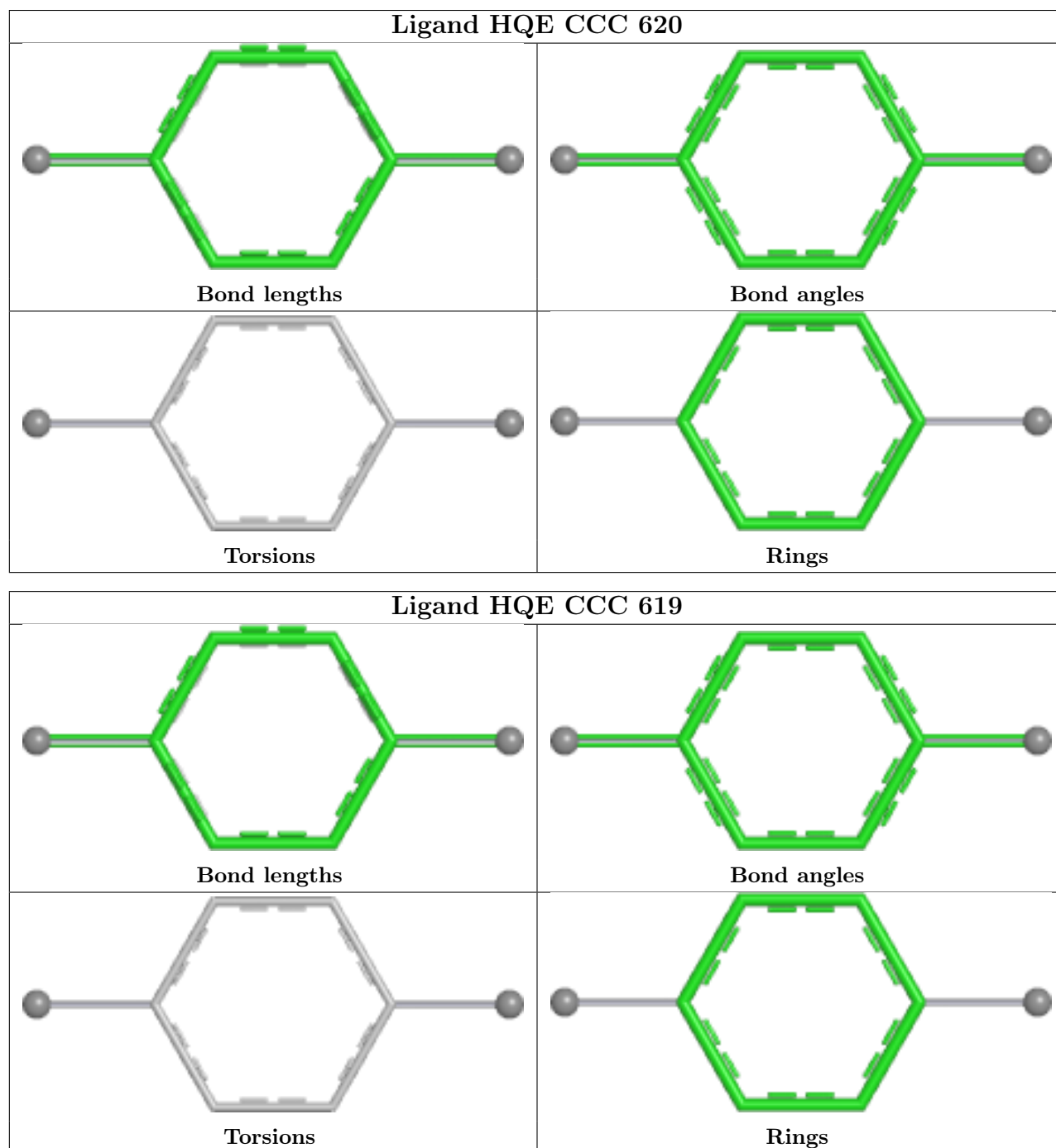
There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CCC	618	EDO	0	1
4	AAA	305	EDO	2	1
4	CCC	614	EDO	5	0
4	CCC	615	EDO	2	0
5	AAA	308	SO4	2	0
4	CCC	610	EDO	1	0
4	AAA	304	EDO	2	1
8	CCC	619	HQE	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	AAA	99/100 (99%)	-0.55	1 (1%) 79 84	10, 20, 28, 48	8 (8%)
2	BBB	122/122 (100%)	-0.33	0 100 100	11, 23, 39, 68	4 (3%)
3	CCC	569/570 (99%)	-0.47	6 (1%) 78 83	9, 20, 35, 82	30 (5%)
All	All	790/792 (99%)	-0.46	7 (0%) 81 85	9, 21, 35, 82	42 (5%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	100	SER	2.7
3	CCC	396	ASN	2.5
3	CCC	322	CYS	2.4
3	CCC	395	LYS	2.3
3	CCC	550	GLY	2.3
3	CCC	327	GLN	2.2
3	CCC	391	LEU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	CXM	AAA	1	11/12	0.97	0.07	21,23,29,29	0
3	KCX	CCC	220	12/13	0.98	0.05	16,17,19,20	0

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	AAA	308	5/5	0.47	0.16	133,155,169,173	0
5	SO4	BBB	205	5/5	0.51	0.12	102,106,109,112	0
4	EDO	CCC	615	4/4	0.72	0.21	51,52,56,58	0
4	EDO	CCC	613	4/4	0.75	0.18	64,68,69,69	0
5	SO4	BBB	201	5/5	0.76	0.14	70,80,94,103	0
5	SO4	AAA	307	5/5	0.77	0.17	47,54,74,79	5
4	EDO	CCC	617	4/4	0.77	0.17	63,63,68,69	0
5	SO4	CCC	621	5/5	0.79	0.10	83,92,101,104	0
5	SO4	CCC	623	5/5	0.80	0.12	79,79,79,79	5
4	EDO	CCC	618	4/4	0.81	0.24	53,59,64,70	0
5	SO4	AAA	306	5/5	0.81	0.15	30,45,53,62	5
5	SO4	CCC	626	5/5	0.81	0.09	75,86,87,87	5
5	SO4	BBB	203	5/5	0.82	0.10	66,67,83,83	0
4	EDO	CCC	612	4/4	0.84	0.15	36,37,41,42	0
5	SO4	CCC	624	5/5	0.84	0.12	32,51,55,56	5
4	EDO	CCC	610	4/4	0.84	0.16	56,58,59,60	0
5	SO4	BBB	206	5/5	0.85	0.18	56,59,61,62	5
5	SO4	CCC	622	5/5	0.86	0.14	57,67,73,76	5
5	SO4	CCC	627	5/5	0.87	0.19	42,47,56,60	5
8	HQE	CCC	619	8/8	0.87	0.11	41,43,46,47	0
4	EDO	CCC	614	4/4	0.88	0.14	40,44,45,49	0
4	EDO	CCC	607	4/4	0.88	0.13	36,37,40,48	0
4	EDO	AAA	302	4/4	0.88	0.14	36,45,47,49	0
8	HQE	CCC	620	8/8	0.88	0.10	35,37,40,43	0
4	EDO	CCC	616	4/4	0.89	0.12	49,49,50,50	0
4	EDO	CCC	606	4/4	0.89	0.12	34,38,40,45	0
4	EDO	CCC	611	4/4	0.89	0.12	38,46,46,51	0
5	SO4	BBB	202	5/5	0.89	0.09	41,52,58,62	5
4	EDO	CCC	608	4/4	0.89	0.15	43,50,52,53	0
4	EDO	AAA	305	4/4	0.90	0.11	28,34,36,39	0
4	EDO	CCC	605	4/4	0.91	0.13	38,43,46,55	0
5	SO4	BBB	204	5/5	0.92	0.12	51,58,72,73	5

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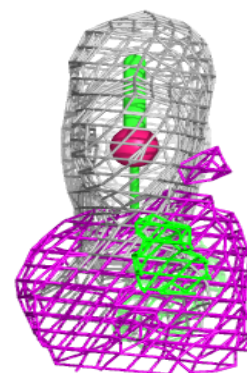
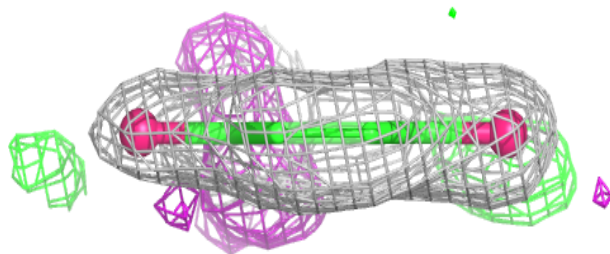
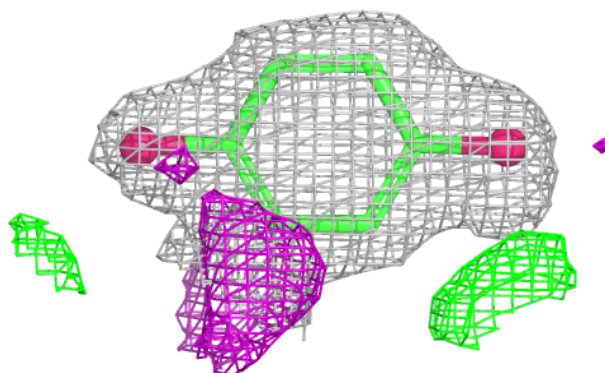
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	AAA	304	4/4	0.93	0.10	41,43,43,44	0
4	EDO	AAA	301	4/4	0.94	0.10	33,37,37,39	0
5	SO4	CCC	625	5/5	0.94	0.07	24,26,40,40	5
7	OH	CCC	603	1/1	0.96	0.07	20,20,20,20	0
4	EDO	CCC	609	4/4	0.96	0.08	28,32,35,37	0
5	SO4	CCC	628	5/5	0.96	0.08	36,36,40,51	0
4	EDO	AAA	303	4/4	0.97	0.07	24,28,29,30	0
4	EDO	CCC	604	4/4	0.97	0.06	33,34,35,35	0
6	NI	CCC	602	1/1	1.00	0.03	19,19,19,19	0
6	NI	CCC	601	1/1	1.00	0.02	20,20,20,20	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.

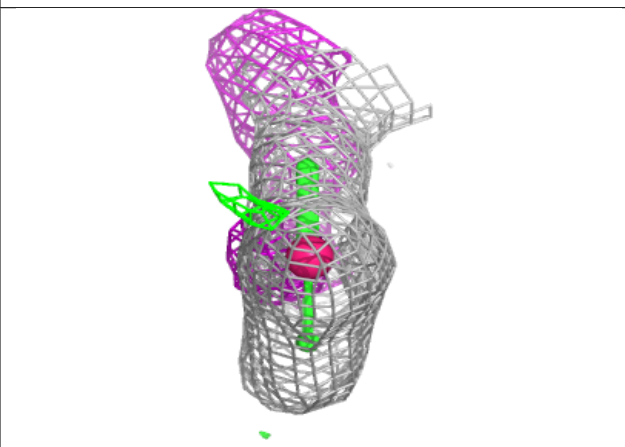
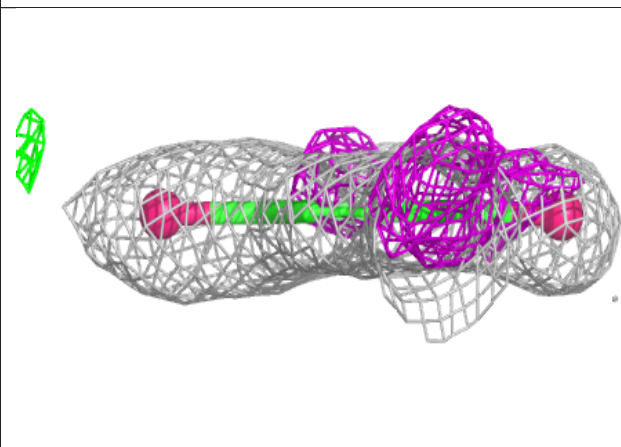
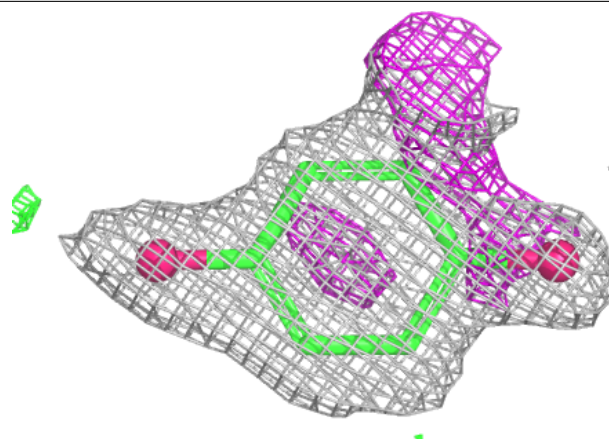
Electron density around HQE CCC 619:

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 HQE CCC 620:

$2mF_o - DF_c$ (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.