Full wwPDB X-ray Structure Validation Report (i)

Jul 26, 2022 – 04:18 pm BST

PDB ID	:	7PTJ
Title	:	C54S mutant of choline-sulfatase from E. meliloti CECT4857 bound to HEPES
Authors	:	Gavira, J.A.; Martinez-Rodriguez, S.
Deposited on	:	2021-09-27
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

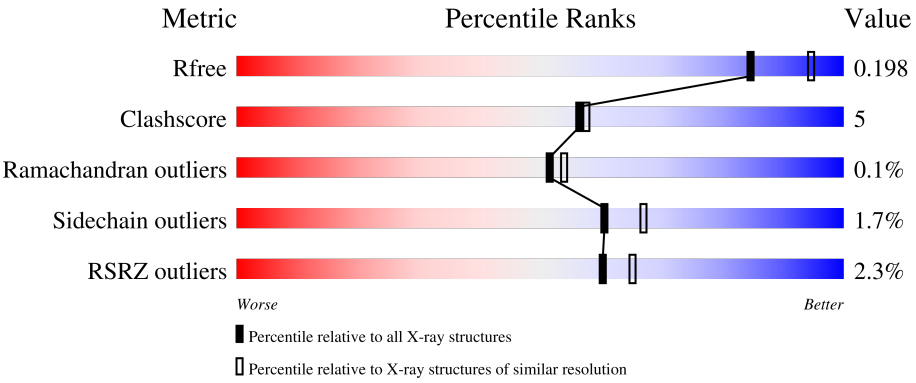
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	520	88% 11%
1	B	520	88% 10%
1	C	520	4% 87% 11%
1	D	520	3% 88% 9%

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	GOL	C	611	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18837 atoms, of which 48 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 Choline sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	9	0
			4189	2646	729	793	21			
1	B	512	Total	C	N	O	S	0	12	0
			4199	2655	735	788	21			
1	C	511	Total	C	N	O	S	0	14	0
			4206	2657	733	794	22			
1	D	509	Total	C	N	O	S	0	4	0
			4122	2603	719	779	21			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	SER	CYS	engineered mutation	UNP A0A410NSD4
A	513	GLY	-	expression tag	UNP A0A410NSD4
A	514	SER	-	expression tag	UNP A0A410NSD4
A	515	HIS	-	expression tag	UNP A0A410NSD4
A	516	HIS	-	expression tag	UNP A0A410NSD4
A	517	HIS	-	expression tag	UNP A0A410NSD4
A	518	HIS	-	expression tag	UNP A0A410NSD4
A	519	HIS	-	expression tag	UNP A0A410NSD4
A	520	HIS	-	expression tag	UNP A0A410NSD4
B	54	SER	CYS	engineered mutation	UNP A0A410NSD4
B	513	GLY	-	expression tag	UNP A0A410NSD4
B	514	SER	-	expression tag	UNP A0A410NSD4
B	515	HIS	-	expression tag	UNP A0A410NSD4
B	516	HIS	-	expression tag	UNP A0A410NSD4
B	517	HIS	-	expression tag	UNP A0A410NSD4
B	518	HIS	-	expression tag	UNP A0A410NSD4
B	519	HIS	-	expression tag	UNP A0A410NSD4
B	520	HIS	-	expression tag	UNP A0A410NSD4
C	54	SER	CYS	engineered mutation	UNP A0A410NSD4
C	513	GLY	-	expression tag	UNP A0A410NSD4
C	514	SER	-	expression tag	UNP A0A410NSD4

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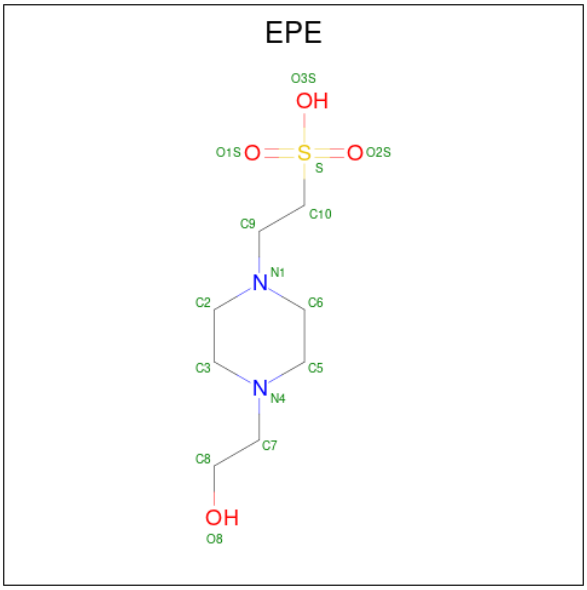
Chain	Residue	Modelled	Actual	Comment	Reference
C	515	HIS	-	expression tag	UNP A0A410NSD4
C	516	HIS	-	expression tag	UNP A0A410NSD4
C	517	HIS	-	expression tag	UNP A0A410NSD4
C	518	HIS	-	expression tag	UNP A0A410NSD4
C	519	HIS	-	expression tag	UNP A0A410NSD4
C	520	HIS	-	expression tag	UNP A0A410NSD4
D	54	SER	CYS	engineered mutation	UNP A0A410NSD4
D	513	GLY	-	expression tag	UNP A0A410NSD4
D	514	SER	-	expression tag	UNP A0A410NSD4
D	515	HIS	-	expression tag	UNP A0A410NSD4
D	516	HIS	-	expression tag	UNP A0A410NSD4
D	517	HIS	-	expression tag	UNP A0A410NSD4
D	518	HIS	-	expression tag	UNP A0A410NSD4
D	519	HIS	-	expression tag	UNP A0A410NSD4
D	520	HIS	-	expression tag	UNP A0A410NSD4

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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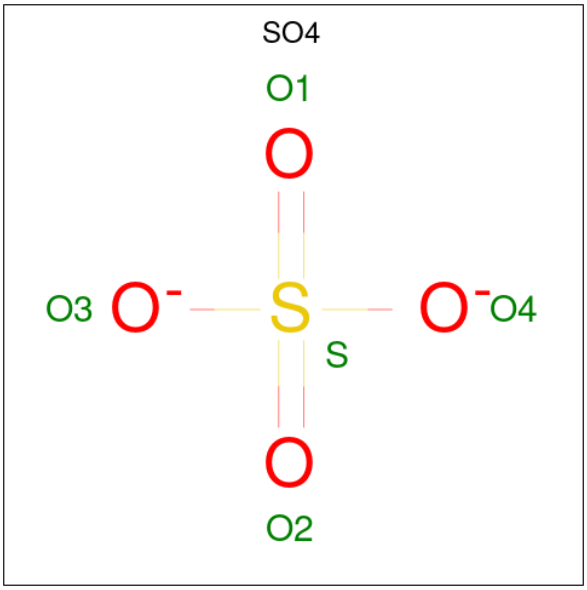
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O S 15 8 2 4 1	0	0
2	D	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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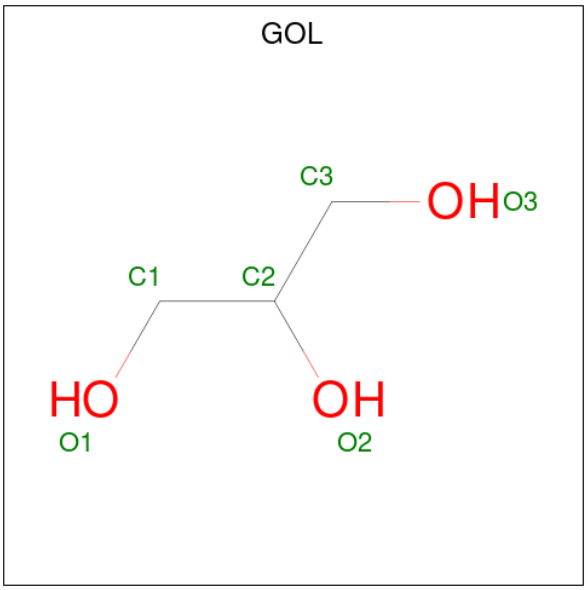
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C H O 14 3 8 3	0	0
4	B	1	Total C H O 14 3 8 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C H O 14 3 8 3	0	0
4	C	1	Total C H O 14 3 8 3	0	0
4	C	1	Total C H O 14 3 8 3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	488	Total O 488 488	0	0
6	B	484	Total O 484 484	0	0
6	C	497	Total O 497 497	0	0

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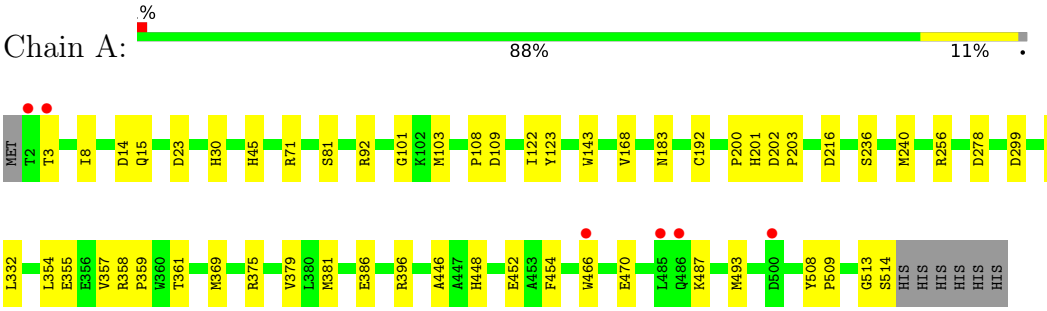
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	358	Total 358	O 358	0	0

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.

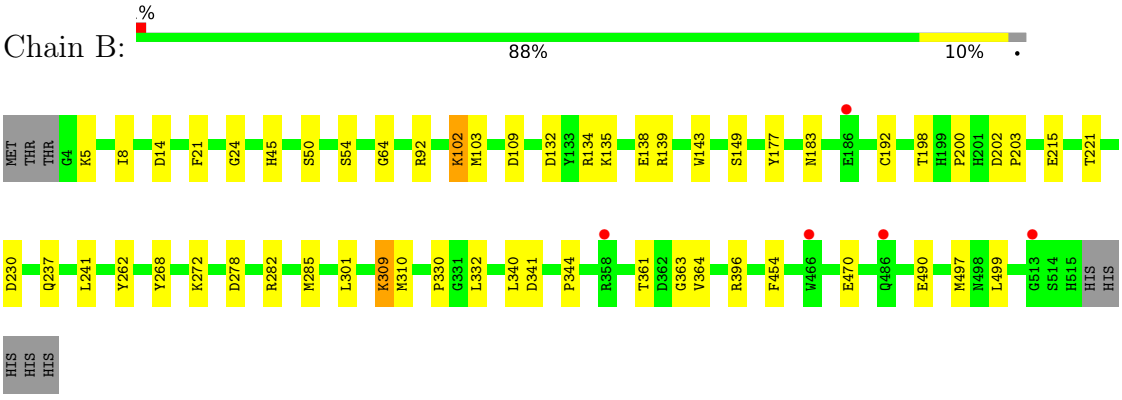
• Molecule 1: Choline sulfatase

Chain A:



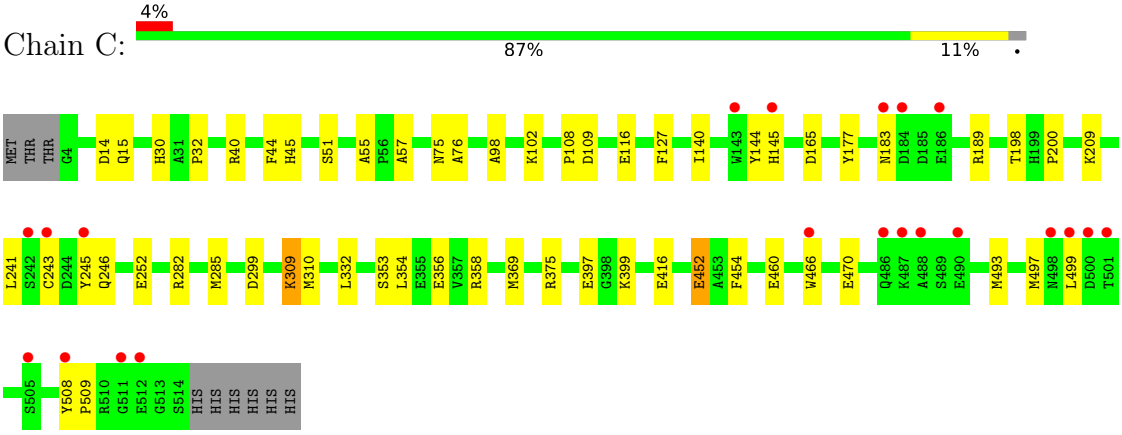
• Molecule 1: Choline sulfatase

Chain B:



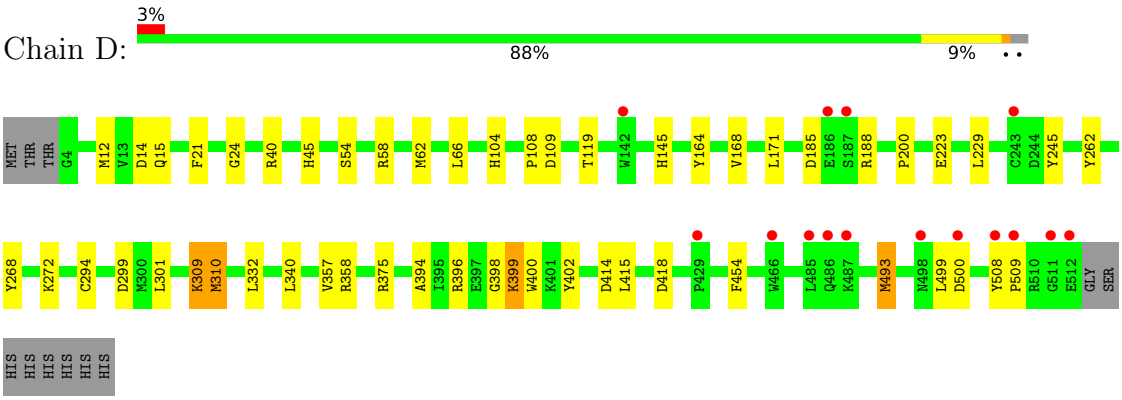
• Molecule 1: Choline sulfatase

Chain C:



• Molecule 1: Choline sulfatase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.52Å 207.01Å 116.83Å 90.00° 110.29° 90.00°	Depositor
Resolution (Å)	75.25 – 2.10 109.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.9 (75.25-2.10) 94.9 (109.58-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19-4092, REFMAC 5	Depositor
R, R_{free}	0.162 , 0.200 0.161 , 0.198	Depositor DCC
R_{free} test set	7964 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18837	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, EPE, SO4, GOL

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	0.41	0/4320	0.63	0/5879
1	B	0.43	2/4335 (0.0%)	0.63	2/5896 (0.0%)
1	C	0.43	0/4342	0.63	0/5906
1	D	0.37	0/4242	0.59	0/5774
All	All	0.41	2/17239 (0.0%)	0.62	2/23455 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102[A]	LYS	C-O	6.36	1.35	1.23
1	B	102[B]	LYS	C-O	6.36	1.35	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	102[A]	LYS	CA-C-O	5.02	130.64	120.10
1	B	102[B]	LYS	CA-C-O	5.02	130.64	120.10

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	4189	0	4001	36	0
1	B	4199	0	4039	46	0
1	C	4206	0	4034	54	0
1	D	4122	0	3936	33	0
2	A	30	0	35	2	0
2	B	15	0	17	4	0
2	C	15	0	17	0	0
2	D	15	0	17	0	0
3	A	20	0	0	1	0
3	B	10	0	0	0	0
3	C	25	0	0	1	0
3	D	10	0	0	0	0
4	A	18	8	24	4	0
4	B	42	16	56	1	0
4	C	42	24	56	6	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	488	0	0	7	0
6	B	484	0	0	7	0
6	C	497	0	0	12	0
6	D	358	0	0	5	1
All	All	18789	48	16232	165	1

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

All (165) 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:C:243[A]:CYS:HB2	1:C:245[A]:TYR:CE1	2.05	0.91
1:A:143:TRP:O	2:A:1101:EPE:H52	1.82	0.79
1:A:278[A]:ASP:OD1	6:A:1201:HOH:O	2.03	0.76
1:B:361[B]:THR:HG22	1:B:363:GLY:H	1.50	0.76
1:B:344:PRO:HD3	1:B:361[B]:THR:HG21	1.68	0.74
1:C:397[A]:GLU:OE2	6:C:701:HOH:O	2.05	0.73
1:C:354:LEU:HD23	6:C:1075:HOH:O	1.88	0.73
1:C:32:PRO:HB3	4:C:609:GOL:H12	1.73	0.70
1:C:243[A]:CYS:SG	1:C:245[A]:TYR:HE1	2.15	0.70
1:D:493:MET:HG3	1:D:499:LEU:HD22	1.73	0.70
1:C:243[A]:CYS:HB2	1:C:245[A]:TYR:CD1	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243[A]:CYS:HB2	1:C:245[A]:TYR:HE1	1.55	0.69
1:C:30:HIS:CD2	4:C:609:GOL:H32	2.28	0.68
1:A:466[A]:TRP:HA	1:A:466[A]:TRP:CE3	2.27	0.68
1:B:135[B]:LYS:HB3	1:B:138[B]:GLU:OE1	1.93	0.68
1:A:103:MET:HG3	1:A:103:MET:O	1.94	0.68
1:A:446:ALA:O	6:A:1202:HOH:O	2.12	0.68
1:B:183:ASN:HD21	1:B:285:MET:HG2	1.63	0.63
1:A:513:GLY:O	1:A:514:SER:HB2	1.99	0.63
1:B:143:TRP:O	2:B:602:EPE:H61	1.99	0.62
1:D:229:LEU:HD22	1:D:245:TYR:OH	1.99	0.62
1:C:243[A]:CYS:CB	1:C:245[A]:TYR:HE1	2.13	0.61
1:D:14:ASP:O	1:D:200:PRO:HD2	1.99	0.61
1:B:143:TRP:HA	2:B:602:EPE:H72	1.83	0.61
1:C:245[B]:TYR:CE1	1:C:246[B]:GLN:HG3	2.36	0.60
1:A:452:GLU:HG2	3:A:1103:SO4:O2	2.02	0.60
1:B:497:MET:O	1:B:499:LEU:HD13	2.03	0.59
1:B:50[A]:SER:OG	1:B:340:LEU:HG	2.04	0.58
2:A:1101:EPE:H51	2:A:1101:EPE:O8	2.02	0.58
1:C:183:ASN:HD21	1:C:285:MET:HG2	1.67	0.58
1:B:138[B]:GLU:HG2	1:B:139:ARG:N	2.18	0.57
1:C:353:SER:HB2	4:C:611:GOL:H32	1.86	0.57
1:C:358:ARG:HG2	1:C:358:ARG:HH11	1.69	0.57
1:C:108:PRO:HG2	1:D:108:PRO:HG2	1.86	0.57
1:B:341:ASP:HB3	1:B:364:VAL:O	2.06	0.56
1:A:312:PHE:CD1	1:A:381:MET:HE3	2.41	0.56
1:B:268:TYR:CZ	1:B:272:LYS:HE2	2.40	0.56
1:C:44:PHE:HE1	1:C:369:MET:HE2	1.71	0.55
1:D:54[B]:SER:HB2	1:D:104:HIS:HD1	1.71	0.55
1:D:357:VAL:HG11	6:D:919:HOH:O	2.07	0.55
1:D:399:LYS:HE3	1:D:400:TRP:CZ2	2.42	0.55
1:C:353:SER:HA	4:C:611:GOL:H11	1.88	0.55
1:B:344:PRO:CD	1:B:361[B]:THR:HG21	2.37	0.54
1:A:256[B]:ARG:HH21	4:A:1108:GOL:C1	2.21	0.54
1:B:45:HIS:HB2	1:B:332:LEU:HD11	1.90	0.54
1:D:262:TYR:CE1	1:D:301:LEU:HD11	2.44	0.53
1:A:466[A]:TRP:HA	1:A:466[A]:TRP:HE3	1.71	0.53
1:A:216:ASP:OD1	1:A:216:ASP:N	2.38	0.53
1:A:386:GLU:HG3	6:A:1463:HOH:O	2.08	0.52
1:A:81:SER:HB2	1:A:109:ASP:OD2	2.08	0.52
1:A:101:GLY:HA2	1:A:168:VAL:HG22	1.92	0.52
1:A:369:MET:HG3	6:A:1394:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:TRP:O	2:B:602:EPE:H72	2.10	0.52
1:D:396:ARG:CZ	1:D:415:LEU:HD12	2.40	0.52
1:A:92:ARG:NH1	1:B:470:GLU:OE1	2.42	0.52
1:D:268:TYR:CZ	1:D:272:LYS:HE2	2.45	0.52
1:C:282:ARG:HD3	6:C:1135:HOH:O	2.10	0.51
1:C:252:GLU:OE1	6:C:702:HOH:O	2.19	0.51
1:A:236:SER:O	1:A:240:MET:HG3	2.11	0.51
1:B:132:ASP:OD1	1:B:134:ARG:HB2	2.11	0.51
1:B:183:ASN:HD21	1:B:285:MET:CG	2.23	0.50
1:C:358:ARG:HG2	1:C:358:ARG:NH1	2.25	0.50
1:C:241[B]:LEU:HD23	1:C:245[B]:TYR:CE1	2.47	0.50
1:D:12:MET:HG2	6:D:731:HOH:O	2.11	0.50
1:C:108:PRO:HG3	1:D:109:ASP:HB2	1.93	0.50
1:D:66:LEU:HD21	1:D:340:LEU:HD11	1.93	0.50
1:B:102[B]:LYS:HG2	1:B:103:MET:N	2.27	0.50
1:C:177:TYR:OH	1:C:282:ARG:NH2	2.39	0.50
1:C:493:MET:HG3	1:C:499:LEU:HD22	1.94	0.50
1:C:109:ASP:HB2	1:D:108:PRO:HG3	1.93	0.49
1:C:140:ILE:HD12	1:C:144:TYR:CE1	2.47	0.49
1:C:15:GLN:HG2	1:C:299:ASP:HB2	1.94	0.49
1:D:185:ASP:O	1:D:188:ARG:HG2	2.12	0.49
1:B:8:ILE:O	1:B:192:CYS:HA	2.11	0.49
1:B:14:ASP:O	1:B:200:PRO:HD2	2.12	0.49
1:B:278:ASP:OD1	1:B:282[B]:ARG:HD2	2.12	0.49
1:C:508:TYR:HA	1:C:509:PRO:C	2.33	0.49
1:C:466:TRP:O	1:C:470:GLU:HG3	2.12	0.49
1:C:399:LYS:HB2	1:C:416:GLU:HG3	1.95	0.48
1:D:310:MET:HE3	6:D:1006:HOH:O	2.13	0.48
1:B:221:THR:HB	6:B:954:HOH:O	2.13	0.48
1:C:140:ILE:HD12	1:C:144:TYR:HE1	1.76	0.48
1:A:513:GLY:O	1:A:514:SER:CB	2.61	0.48
1:A:354:LEU:HD12	6:A:1291:HOH:O	2.13	0.48
1:B:490:GLU:OE2	6:B:701:HOH:O	2.20	0.48
1:C:102[A]:LYS:HD3	1:C:198:THR:HA	1.96	0.47
1:A:379:VAL:HB	1:A:396:ARG:HB3	1.97	0.47
1:A:15:GLN:HG2	1:A:299:ASP:HB2	1.96	0.47
1:B:361[A]:THR:HG23	6:B:836:HOH:O	2.14	0.47
1:D:58:ARG:O	1:D:62[A]:MET:HG3	2.14	0.47
1:A:14:ASP:O	1:A:200:PRO:HD2	2.15	0.47
1:D:396:ARG:NH1	1:D:398:GLY:O	2.46	0.47
1:B:268:TYR:OH	1:B:272:LYS:HE2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:LEU:CD2	1:D:340:LEU:HD11	2.44	0.47
1:C:55:ALA:HB3	1:C:75:ASN:HA	1.97	0.47
1:C:40[B]:ARG:NH1	6:C:723:HOH:O	2.47	0.47
1:C:356:GLU:OE1	6:C:703:HOH:O	2.21	0.47
1:D:164:TYR:O	1:D:168:VAL:HG23	2.15	0.46
1:C:252:GLU:HG2	6:C:782:HOH:O	2.13	0.46
1:C:44:PHE:CE1	1:C:369:MET:HE2	2.51	0.46
1:D:394:ALA:HA	1:D:402:TYR:O	2.16	0.46
1:B:282[B]:ARG:NH1	6:B:725:HOH:O	2.48	0.46
1:C:14:ASP:O	1:C:200:PRO:HD2	2.15	0.46
1:C:140:ILE:HD12	6:C:945:HOH:O	2.16	0.46
1:C:243[A]:CYS:HG	1:C:245[A]:TYR:HE1	1.63	0.46
1:B:344:PRO:HG3	1:B:361[B]:THR:HG21	1.98	0.45
1:A:448:HIS:HB3	6:A:1393:HOH:O	2.16	0.45
1:D:358:ARG:HH11	1:D:358:ARG:HG2	1.82	0.45
1:D:21:PHE:HA	1:D:24:GLY:O	2.15	0.45
1:A:256[B]:ARG:HH21	4:A:1108:GOL:H11	1.81	0.45
1:B:64:GLY:O	1:B:361[B]:THR:HG23	2.16	0.45
1:B:177:TYR:OH	1:B:282[A]:ARG:NH2	2.43	0.45
1:A:30:HIS:HE1	6:A:1589:HOH:O	1.99	0.45
1:B:135[B]:LYS:CB	1:B:138[B]:GLU:OE1	2.62	0.44
1:B:237:GLN:O	1:B:241:LEU:HG	2.17	0.44
1:C:45:HIS:HB2	1:C:332:LEU:HD11	1.98	0.44
1:B:330:PRO:HD2	6:B:989:HOH:O	2.17	0.44
1:C:243[A]:CYS:CB	1:C:245[A]:TYR:CE1	2.85	0.44
1:B:309:LYS:O	1:B:310:MET:HB2	2.18	0.44
1:A:357:VAL:O	1:A:361:THR:HG22	2.18	0.44
1:B:21:PHE:HA	1:B:24:GLY:O	2.17	0.43
1:A:470:GLU:HG2	1:B:92:ARG:HG3	2.00	0.43
1:C:452[A]:GLU:OE1	3:C:604:SO4:O3	2.36	0.43
1:A:202:ASP:HA	1:A:203:PRO:C	2.39	0.43
1:B:262:TYR:CE1	1:B:301:LEU:HD11	2.54	0.42
1:D:294:CYS:HB2	6:D:813:HOH:O	2.19	0.42
1:A:8:ILE:O	1:A:192:CYS:HA	2.19	0.42
1:B:202:ASP:HA	1:B:203:PRO:C	2.40	0.42
1:D:414:ASP:O	1:D:418:ASP:HB3	2.18	0.42
1:C:98:ALA:HA	1:C:116:GLU:O	2.19	0.42
1:B:396:ARG:HH22	4:B:608:GOL:C3	2.32	0.42
1:A:108:PRO:HG3	1:B:109:ASP:HB2	2.01	0.42
1:B:202:ASP:HB2	1:B:203:PRO:HA	2.01	0.42
1:D:493:MET:HG3	1:D:499:LEU:CD2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:608:GOL:H11	6:C:724:HOH:O	2.20	0.42
1:D:223:GLU:HG3	6:D:899:HOH:O	2.20	0.42
1:A:71:ARG:HH22	4:A:1109:GOL:H11	1.85	0.42
1:B:14:ASP:HB3	1:B:198:THR:O	2.20	0.42
1:A:358:ARG:HB3	1:A:359:PRO:HD3	2.01	0.42
1:C:309:LYS:O	1:C:310:MET:HB2	2.20	0.41
1:C:493:MET:HE2	1:C:493:MET:HB2	1.93	0.41
1:A:45:HIS:HB2	1:A:332:LEU:HD11	2.02	0.41
1:C:189:ARG:HB2	4:C:613:GOL:H32	2.01	0.41
1:C:369:MET:HG3	6:C:1025:HOH:O	2.18	0.41
1:D:119:THR:HG22	1:D:171:LEU:HD12	2.03	0.41
1:C:140:ILE:CD1	6:C:945:HOH:O	2.69	0.41
1:D:309:LYS:O	1:D:310:MET:HB2	2.20	0.41
1:D:396:ARG:HD2	1:D:400:TRP:O	2.20	0.41
1:B:361[A]:THR:CG2	6:B:836:HOH:O	2.69	0.41
1:C:76:ALA:HB1	1:C:127:PHE:HA	2.03	0.41
1:A:508:TYR:CD1	1:A:509:PRO:HA	2.55	0.41
1:C:165:ASP:OD1	1:C:198:THR:HG22	2.21	0.41
1:C:241[B]:LEU:HD23	1:C:245[B]:TYR:CD1	2.55	0.41
1:B:5:LYS:NZ	6:B:708:HOH:O	2.34	0.41
1:C:102[B]:LYS:HB2	1:C:102[B]:LYS:HE2	1.71	0.41
1:A:122:ILE:HG23	1:A:123:TYR:CD1	2.55	0.41
1:C:209:LYS:NZ	6:C:736:HOH:O	2.52	0.41
1:D:508:TYR:HA	1:D:509:PRO:C	2.41	0.40
1:B:344:PRO:CG	1:B:361[B]:THR:HG21	2.51	0.40
1:D:45:HIS:HB2	1:D:332:LEU:HD11	2.03	0.40
1:A:256[B]:ARG:HE	4:A:1108:GOL:C1	2.35	0.40
1:B:143:TRP:CA	2:B:602:EPE:H72	2.51	0.40
1:D:15:GLN:HG2	1:D:299:ASP:HB2	2.03	0.40
1:C:51:SER:O	1:C:57:ALA:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:896:HOH:O	6:D:999:HOH:O[2_657]	2.17	0.03

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	520/520 (100%)	504 (97%)	14 (3%)	2 (0%)	34	32
1	B	522/520 (100%)	506 (97%)	15 (3%)	1 (0%)	47	49
1	C	523/520 (101%)	504 (96%)	19 (4%)	0	100	100
1	D	511/520 (98%)	496 (97%)	15 (3%)	0	100	100
All	All	2076/2080 (100%)	2010 (97%)	63 (3%)	3 (0%)	51	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	B	54	SER
1	A	201	HIS

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	445/443 (100%)	437 (98%)	8 (2%)	59	65
1	B	447/443 (101%)	442 (99%)	5 (1%)	73	79
1	C	448/443 (101%)	440 (98%)	8 (2%)	59	65
1	D	437/443 (99%)	427 (98%)	10 (2%)	50	55
All	All	1777/1772 (100%)	1746 (98%)	31 (2%)	60	67

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	183	ASN
1	A	309	LYS
1	A	355	GLU
1	A	375	ARG
1	A	454	PHE
1	A	487	LYS
1	A	493	MET
1	B	149	SER
1	B	215	GLU
1	B	230	ASP
1	B	309	LYS
1	B	454	PHE
1	C	145	HIS
1	C	309	LYS
1	C	375	ARG
1	C	452[A]	GLU
1	C	452[B]	GLU
1	C	454	PHE
1	C	460	GLU
1	C	497	MET
1	D	40	ARG
1	D	145	HIS
1	D	309	LYS
1	D	310	MET
1	D	375	ARG
1	D	399	LYS
1	D	454	PHE
1	D	493	MET
1	D	500[A]	ASP
1	D	500[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	B	183	ASN
1	C	30	HIS
1	C	183	ASN
1	D	428	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
4	GOL	B	605	-	5,5,5	0.75	0	5,5,5	1.18	0
4	GOL	B	606	-	5,5,5	1.07	0	5,5,5	0.87	0
3	SO4	A	1104	-	4,4,4	0.13	0	6,6,6	0.18	0
2	EPE	A	1101	-	15,15,15	0.93	1 (6%)	18,20,20	2.04	5 (27%)
4	GOL	B	610	-	5,5,5	0.95	0	5,5,5	1.01	0
4	GOL	A	1109	-	5,5,5	0.76	0	5,5,5	1.07	0
3	SO4	C	602	-	4,4,4	0.19	0	6,6,6	0.25	0
2	EPE	D	601	-	15,15,15	0.93	1 (6%)	18,20,20	2.16	5 (27%)
3	SO4	A	1106	-	4,4,4	0.20	0	6,6,6	0.17	0
4	GOL	B	608	-	5,5,5	1.04	0	5,5,5	0.92	0
4	GOL	C	609	-	5,5,5	1.30	0	5,5,5	0.95	0
4	GOL	C	612	-	5,5,5	0.92	0	5,5,5	1.34	1 (20%)
3	SO4	C	603	-	4,4,4	0.14	0	6,6,6	0.30	0
4	GOL	C	613	-	5,5,5	0.76	0	5,5,5	1.05	0
3	SO4	C	604	-	4,4,4	0.18	0	6,6,6	0.16	0
3	SO4	C	606	-	4,4,4	0.19	0	6,6,6	0.15	0
2	EPE	C	601	-	15,15,15	0.99	1 (6%)	18,20,20	2.08	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	C	607	-	5,5,5	0.80	0	5,5,5	1.23	0
3	SO4	B	601	-	4,4,4	0.13	0	6,6,6	0.14	0
3	SO4	B	603	-	4,4,4	0.19	0	6,6,6	0.09	0
2	EPE	A	1102	-	15,15,15	0.91	1 (6%)	18,20,20	2.05	6 (33%)
4	GOL	C	610	-	5,5,5	1.01	0	5,5,5	0.75	0
3	SO4	A	1105	-	4,4,4	0.15	0	6,6,6	0.11	0
4	GOL	A	1107	-	5,5,5	0.78	0	5,5,5	1.04	0
3	SO4	A	1103	-	4,4,4	0.17	0	6,6,6	0.14	0
4	GOL	B	604	-	5,5,5	1.00	0	5,5,5	1.00	0
2	EPE	B	602	5	15,15,15	0.93	1 (6%)	18,20,20	2.10	5 (27%)
4	GOL	B	607	-	5,5,5	0.94	0	5,5,5	1.07	0
3	SO4	D	602	-	4,4,4	0.17	0	6,6,6	0.12	0
3	SO4	D	603	-	4,4,4	0.12	0	6,6,6	0.18	0
3	SO4	C	605	-	4,4,4	0.13	0	6,6,6	0.20	0
4	GOL	A	1108	-	5,5,5	0.99	0	5,5,5	0.97	0
4	GOL	C	611	-	5,5,5	0.83	0	5,5,5	1.20	1 (20%)
4	GOL	C	608	-	5,5,5	0.85	0	5,5,5	1.13	0
4	GOL	B	609	-	5,5,5	0.70	0	5,5,5	0.91	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	GOL	B	605	-	-	3/4/4/4	-
4	GOL	B	606	-	-	2/4/4/4	-
2	EPE	A	1101	-	-	4/9/19/19	0/1/1/1
4	GOL	B	610	-	-	3/4/4/4	-
4	GOL	A	1109	-	-	1/4/4/4	-
2	EPE	D	601	-	-	7/9/19/19	0/1/1/1
4	GOL	B	608	-	-	2/4/4/4	-
4	GOL	C	609	-	-	0/4/4/4	-
4	GOL	C	612	-	-	0/4/4/4	-
4	GOL	C	613	-	-	0/4/4/4	-
2	EPE	C	601	-	-	2/9/19/19	0/1/1/1
4	GOL	C	607	-	-	0/4/4/4	-
2	EPE	A	1102	-	-	2/9/19/19	0/1/1/1
4	GOL	C	610	-	-	0/4/4/4	-
4	GOL	A	1107	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	604	-	-	0/4/4/4	-
2	EPE	B	602	5	-	3/9/19/19	0/1/1/1
4	GOL	B	607	-	-	2/4/4/4	-
4	GOL	A	1108	-	-	0/4/4/4	-
4	GOL	C	611	-	-	2/4/4/4	-
4	GOL	C	608	-	-	0/4/4/4	-
4	GOL	B	609	-	-	4/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	EPE	C10-S	3.28	1.82	1.77
2	A	1102	EPE	C10-S	3.20	1.82	1.77
2	A	1101	EPE	C10-S	3.15	1.82	1.77
2	D	601	EPE	C10-S	3.07	1.81	1.77
2	B	602	EPE	C10-S	2.95	1.81	1.77

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	602	EPE	O2S-S-C10	5.60	113.66	106.92
2	C	601	EPE	O1S-S-C10	5.00	112.94	106.92
2	A	1101	EPE	O3S-S-C10	4.48	113.01	105.77
2	D	601	EPE	O3S-S-C10	4.37	112.83	105.77
2	D	601	EPE	C7-N4-C5	4.16	121.88	111.23
2	A	1102	EPE	C5-N4-C3	4.16	118.18	108.83
2	B	602	EPE	C7-N4-C3	4.08	121.67	111.23
2	A	1101	EPE	C5-N4-C3	4.07	118.00	108.83
2	A	1101	EPE	C7-N4-C3	4.06	121.62	111.23
2	D	601	EPE	C7-N4-C3	3.93	121.27	111.23
2	A	1102	EPE	C7-N4-C5	3.88	121.17	111.23
2	C	601	EPE	C5-N4-C3	3.55	116.82	108.83
2	D	601	EPE	C5-N4-C3	3.53	116.78	108.83
2	C	601	EPE	C7-N4-C3	3.39	119.91	111.23
2	D	601	EPE	O1S-S-C10	3.35	110.94	106.92
2	A	1102	EPE	C7-N4-C3	3.24	119.52	111.23
2	B	602	EPE	C7-N4-C5	3.08	119.12	111.23
2	A	1101	EPE	C7-N4-C5	3.04	119.02	111.23
2	A	1102	EPE	C6-N1-C2	2.84	115.22	108.83
2	C	601	EPE	C7-N4-C5	2.79	118.37	111.23
2	B	602	EPE	C5-N4-C3	2.60	114.69	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	612	GOL	C3-C2-C1	-2.39	102.42	111.70
4	C	611	GOL	C3-C2-C1	-2.36	102.54	111.70
2	A	1102	EPE	O2S-S-C10	2.25	109.62	106.92
2	C	601	EPE	O2S-S-C10	2.23	109.60	106.92
2	B	602	EPE	O3S-S-C10	2.22	109.36	105.77
2	C	601	EPE	C2-C3-N4	2.17	115.09	110.64
2	A	1102	EPE	O1S-S-C10	2.10	109.44	106.92
2	A	1101	EPE	O2S-S-C10	2.06	109.39	106.92

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	EPE	C8-C7-N4-C5
2	A	1101	EPE	S-C10-C9-N1
2	A	1102	EPE	C10-C9-N1-C2
2	A	1102	EPE	C10-C9-N1-C6
2	B	602	EPE	C10-C9-N1-C2
2	B	602	EPE	C10-C9-N1-C6
2	B	602	EPE	S-C10-C9-N1
2	C	601	EPE	S-C10-C9-N1
2	D	601	EPE	S-C10-C9-N1
2	D	601	EPE	C9-C10-S-O1S
4	A	1107	GOL	O1-C1-C2-C3
4	B	605	GOL	C1-C2-C3-O3
4	B	607	GOL	C1-C2-C3-O3
4	B	607	GOL	O2-C2-C3-O3
2	D	601	EPE	C9-C10-S-O3S
2	C	601	EPE	C8-C7-N4-C3
4	A	1107	GOL	C1-C2-C3-O3
4	B	606	GOL	O1-C1-C2-C3
4	B	608	GOL	O1-C1-C2-C3
4	B	609	GOL	C1-C2-C3-O3
4	B	610	GOL	O1-C1-C2-C3
4	C	611	GOL	O1-C1-C2-C3
4	A	1107	GOL	O1-C1-C2-O2
4	B	606	GOL	O1-C1-C2-O2
4	B	609	GOL	O2-C2-C3-O3
4	A	1107	GOL	O2-C2-C3-O3
4	B	605	GOL	O2-C2-C3-O3
2	A	1101	EPE	C10-C9-N1-C2
2	A	1101	EPE	C10-C9-N1-C6

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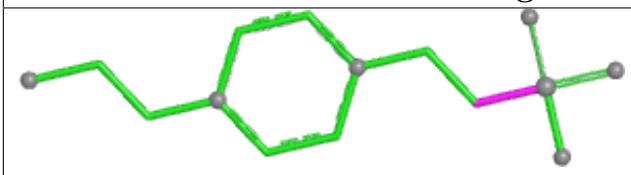
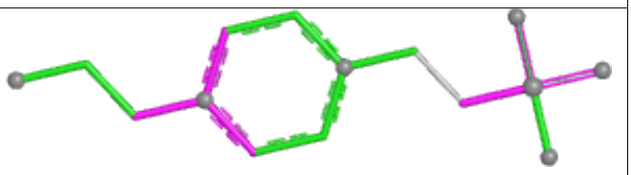
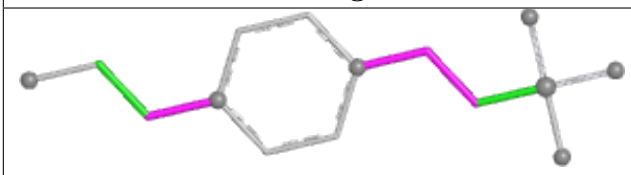
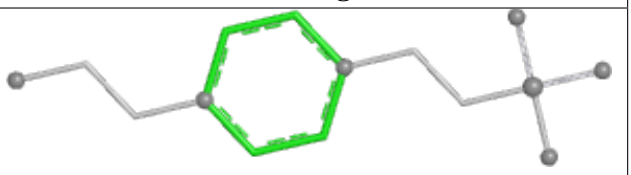
Mol	Chain	Res	Type	Atoms
2	D	601	EPE	C10-C9-N1-C2
2	D	601	EPE	C10-C9-N1-C6
2	D	601	EPE	C8-C7-N4-C3
4	B	609	GOL	O1-C1-C2-O2
4	B	605	GOL	O1-C1-C2-C3
4	B	610	GOL	C1-C2-C3-O3
2	D	601	EPE	C9-C10-S-O2S
4	B	610	GOL	O2-C2-C3-O3
4	C	611	GOL	O1-C1-C2-O2
4	B	609	GOL	O1-C1-C2-C3
4	A	1109	GOL	O2-C2-C3-O3
4	B	608	GOL	O1-C1-C2-O2

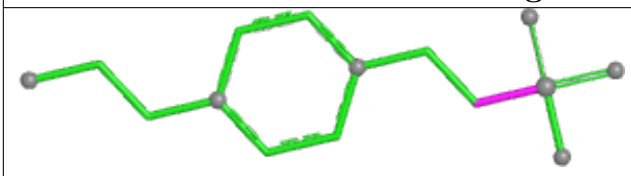
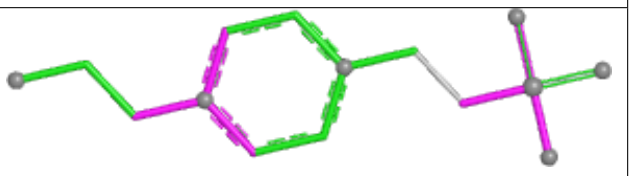
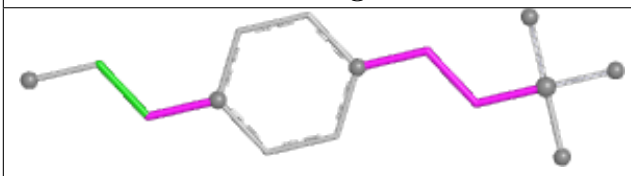
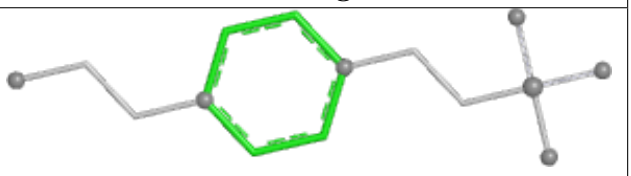
There are no ring outliers.

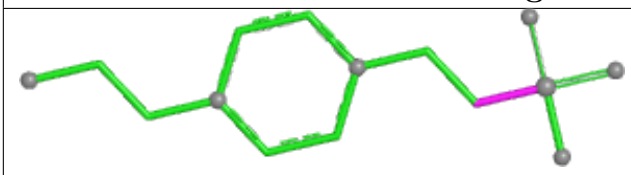
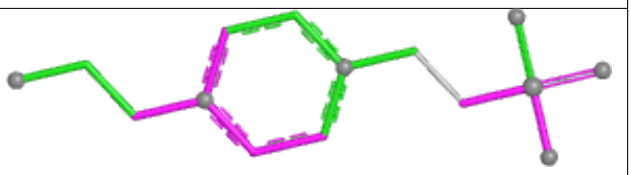
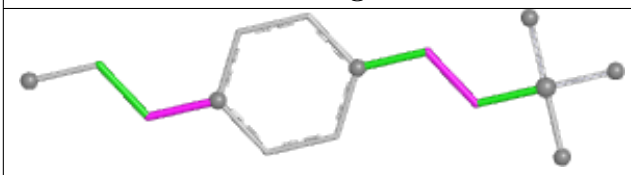
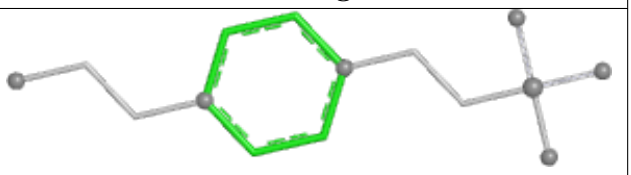
11 monomers are involved in 19 short contacts:

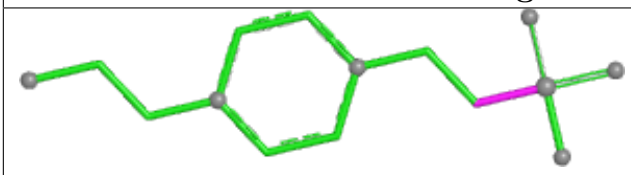
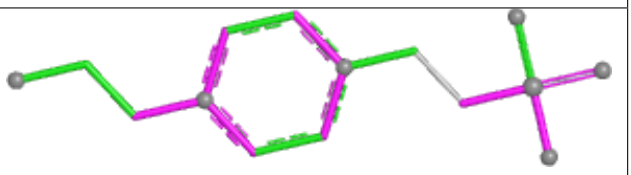
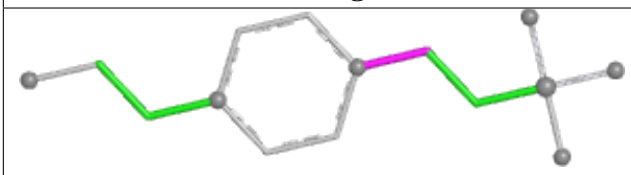
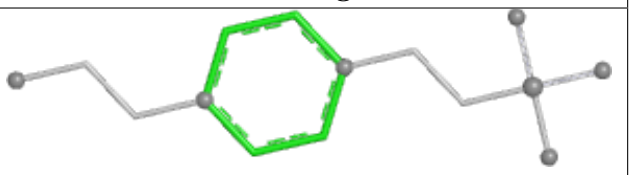
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	EPE	2	0
4	A	1109	GOL	1	0
4	B	608	GOL	1	0
4	C	609	GOL	2	0
4	C	613	GOL	1	0
3	C	604	SO4	1	0
3	A	1103	SO4	1	0
2	B	602	EPE	4	0
4	A	1108	GOL	3	0
4	C	611	GOL	2	0
4	C	608	GOL	1	0

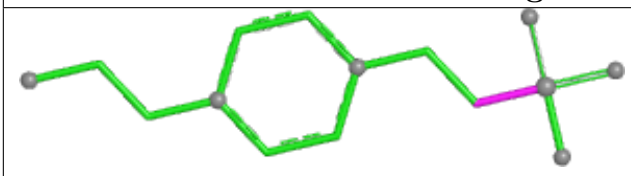
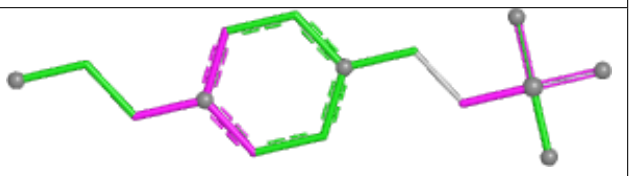
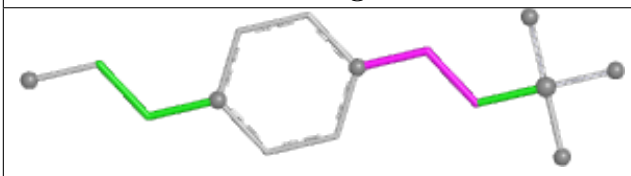
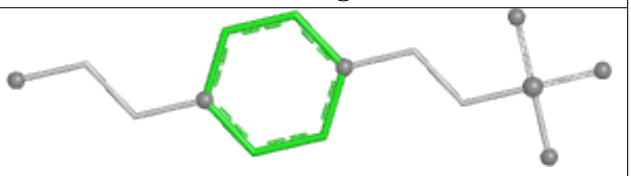
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand EPE A 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EPE D 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EPE C 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EPE A 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EPE B 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	513/520 (98%)	0.05	6 (1%)	79	82	19, 27, 48, 104	0
1	B	512/520 (98%)	0.07	5 (0%)	82	85	20, 29, 49, 100	0
1	C	511/520 (98%)	0.22	21 (4%)	37	43	17, 26, 56, 128	0
1	D	509/520 (97%)	0.19	15 (2%)	51	57	25, 37, 61, 126	0
All	All	2045/2080 (98%)	0.13	47 (2%)	60	65	17, 30, 54, 128	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	486	GLN	6.3
1	D	500[A]	ASP	6.2
1	C	500	ASP	6.0
1	C	501	THR	5.1
1	D	186	GLU	5.0
1	A	486	GLN	4.2
1	A	3	THR	4.2
1	B	466	TRP	4.1
1	A	2	THR	3.9
1	D	486	GLN	3.9
1	D	485	LEU	3.8
1	C	498	ASN	3.8
1	A	500	ASP	3.5
1	C	488	ALA	3.3
1	D	509	PRO	3.3
1	C	487	LYS	3.2
1	B	513	GLY	3.2
1	C	183	ASN	3.1
1	C	508	TYR	3.0
1	B	186	GLU	3.0
1	A	485	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	243[A]	CYS	2.9
1	C	511	GLY	2.9
1	C	184	ASP	2.9
1	C	499	LEU	2.9
1	C	245[A]	TYR	2.9
1	D	508	TYR	2.8
1	C	505	SER	2.8
1	D	243	CYS	2.8
1	D	512	GLU	2.7
1	C	512	GLU	2.6
1	A	466[A]	TRP	2.6
1	C	143	TRP	2.6
1	D	466	TRP	2.6
1	C	186	GLU	2.5
1	D	511	GLY	2.5
1	D	498[A]	ASN	2.4
1	D	142	TRP	2.4
1	B	486	GLN	2.4
1	B	358	ARG	2.3
1	C	145	HIS	2.3
1	D	487	LYS	2.3
1	C	242[A]	SER	2.2
1	D	429	PRO	2.1
1	C	466	TRP	2.1
1	D	187	SER	2.1
1	C	490	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

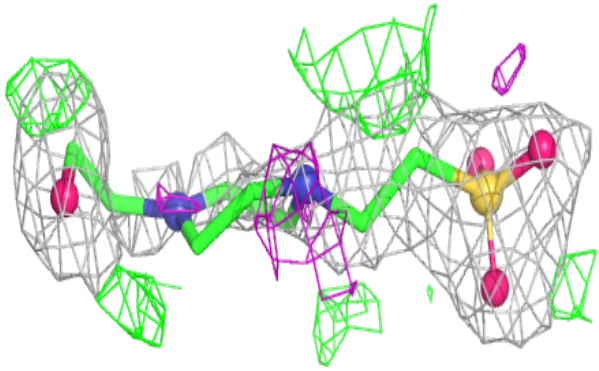
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

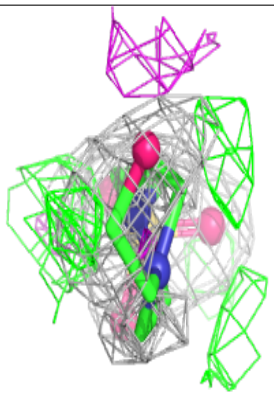
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	C	611	6/6	0.71	0.48	53,66,79,87	0
4	GOL	B	609	6/6	0.76	0.13	52,63,80,81	0
4	GOL	A	1109	6/6	0.79	0.31	64,77,89,94	0
4	GOL	C	610	6/6	0.82	0.25	39,44,49,67	0
4	GOL	B	608	6/6	0.82	0.18	40,42,48,49	0
4	GOL	C	612	6/6	0.82	0.28	42,55,71,71	0
3	SO4	A	1106	5/5	0.83	0.25	66,69,77,93	0
4	GOL	C	613	6/6	0.84	0.29	51,61,71,82	0
2	EPE	D	601	15/15	0.85	0.25	30,49,62,63	15
4	GOL	B	604	6/6	0.85	0.16	37,44,48,51	0
3	SO4	B	603	5/5	0.88	0.29	63,80,94,104	0
4	GOL	B	610	6/6	0.88	0.20	33,53,64,65	0
2	EPE	B	602	15/15	0.90	0.24	26,41,49,53	15
3	SO4	D	603	5/5	0.91	0.32	50,66,74,75	0
3	SO4	A	1105	5/5	0.91	0.18	59,64,87,90	0
3	SO4	C	603	5/5	0.91	0.14	57,58,61,72	0
4	GOL	C	607	6/6	0.91	0.15	26,29,39,42	0
2	EPE	A	1102	15/15	0.92	0.29	26,44,56,57	15
4	GOL	B	605	6/6	0.92	0.16	39,42,48,54	0
3	SO4	C	605	5/5	0.92	0.25	52,53,75,78	5
4	GOL	C	609	6/6	0.92	0.16	28,41,44,44	0
5	CA	B	611	1/1	0.92	0.11	46,46,46,46	1
2	EPE	A	1101	15/15	0.93	0.15	27,38,46,48	15
4	GOL	C	608	6/6	0.93	0.14	41,52,57,57	0
3	SO4	D	602	5/5	0.93	0.21	76,81,97,104	0
4	GOL	B	606	6/6	0.93	0.17	32,36,38,42	0
5	CA	D	604	1/1	0.93	0.16	48,48,48,48	1
3	SO4	C	606	5/5	0.94	0.18	38,59,76,76	0
4	GOL	A	1108	6/6	0.94	0.14	34,40,44,44	0
2	EPE	C	601	15/15	0.94	0.20	28,47,55,57	15
4	GOL	A	1107	6/6	0.95	0.12	32,35,39,46	0
5	CA	A	1110	1/1	0.95	0.08	46,46,46,46	1
3	SO4	A	1104	5/5	0.95	0.12	56,57,63,75	0
5	CA	C	614	1/1	0.95	0.24	56,56,56,56	1
3	SO4	C	604	5/5	0.95	0.21	46,51,61,70	0
3	SO4	A	1103	5/5	0.96	0.13	41,52,58,63	0
4	GOL	B	607	6/6	0.96	0.10	45,48,49,50	0
3	SO4	C	602	5/5	0.99	0.17	27,27,28,30	5
3	SO4	B	601	5/5	0.99	0.13	49,51,53,54	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 EPE D 601:

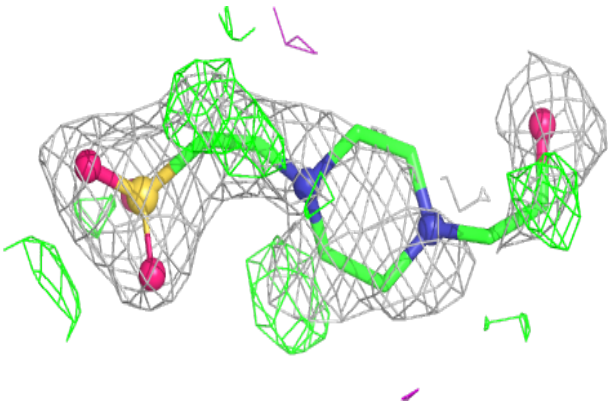
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

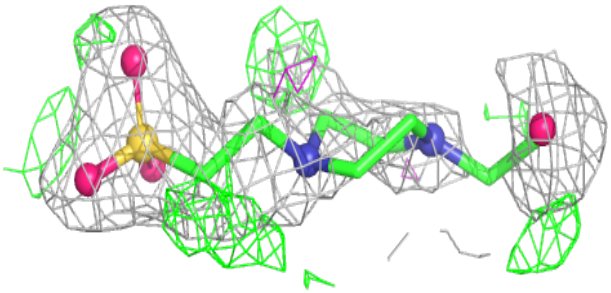


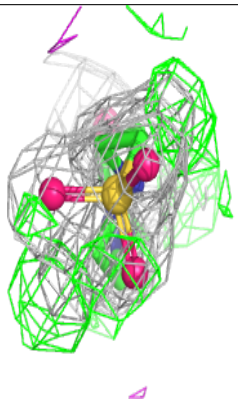


Electron density around EPE B 602:

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

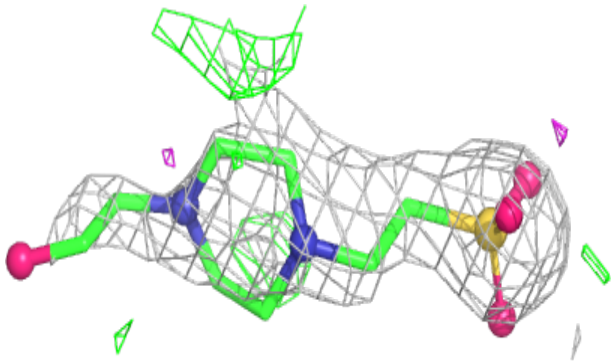


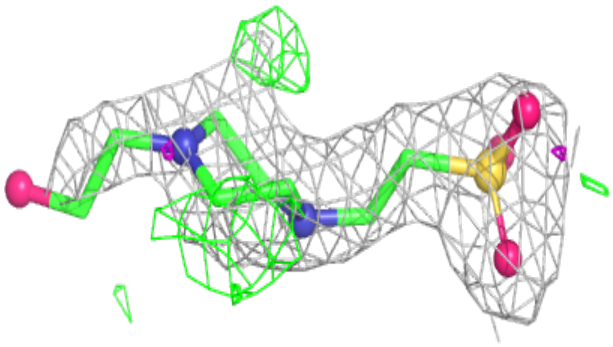


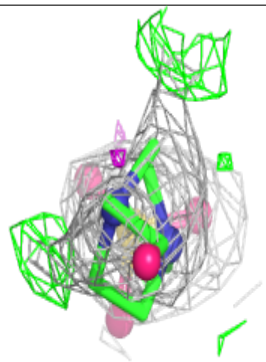


Electron density around EPE A 1102:

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

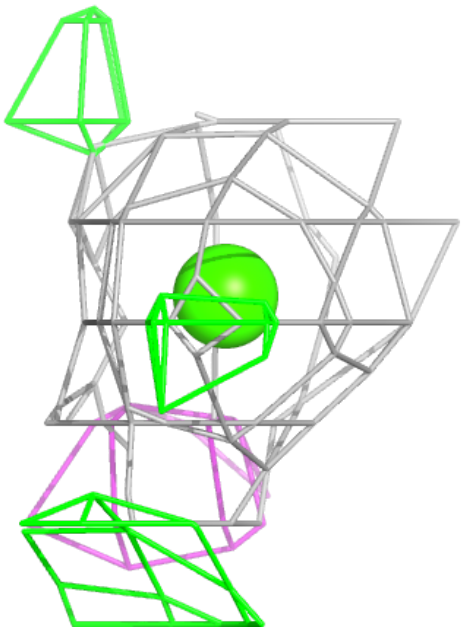


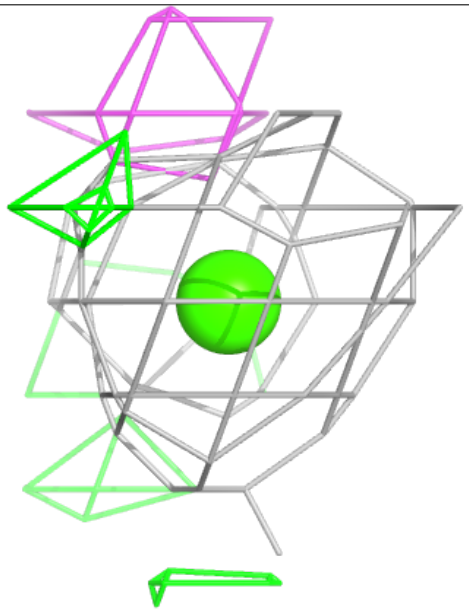


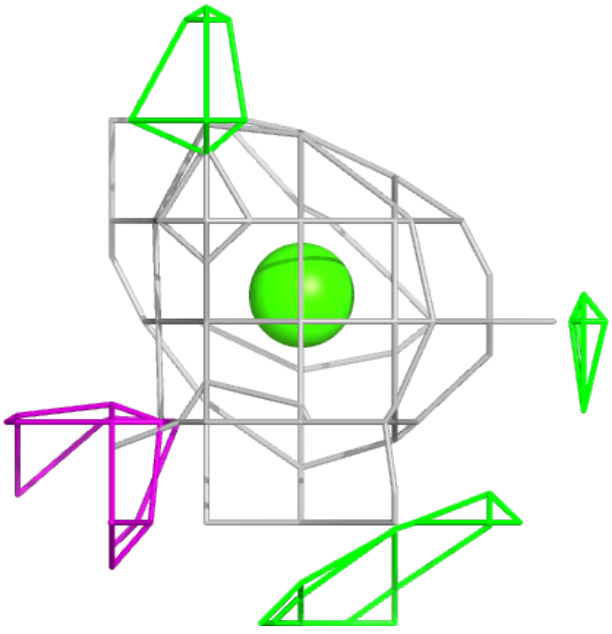


Electron density around CA B 611:

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

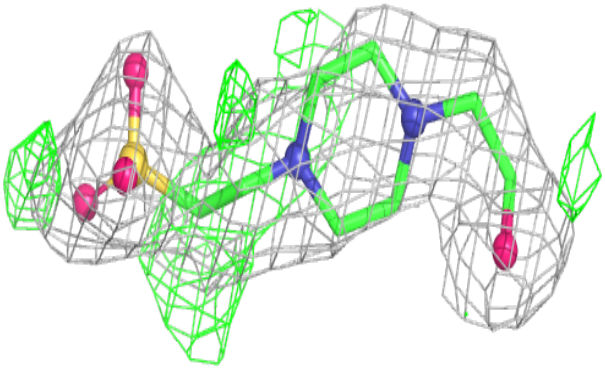


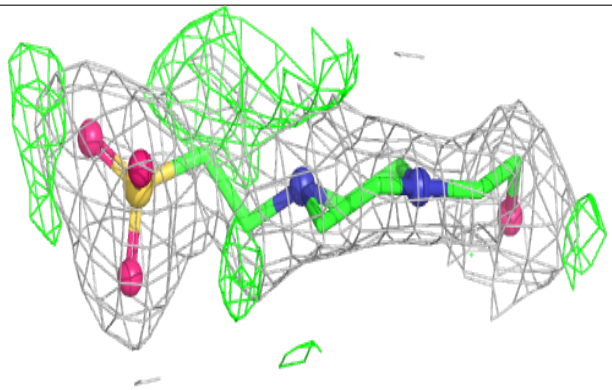


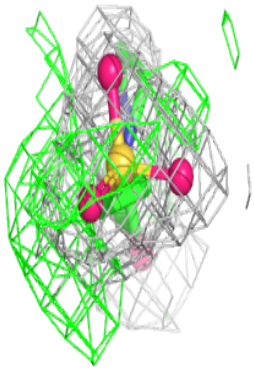


Electron density around EPE A 1101:

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

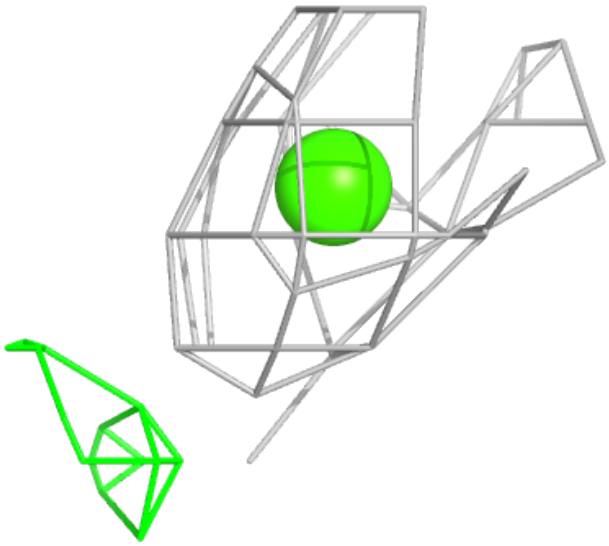


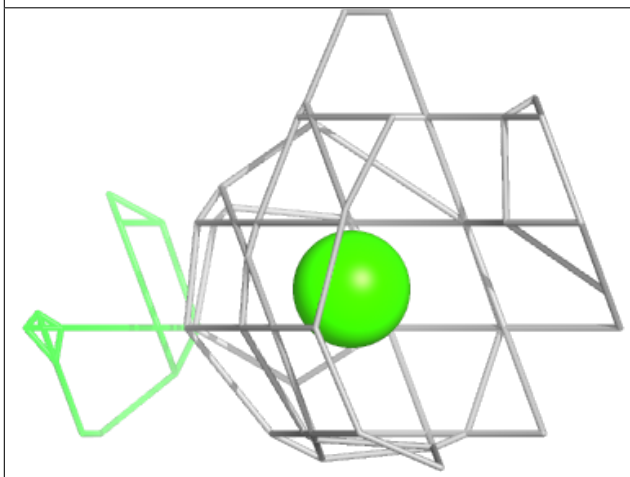


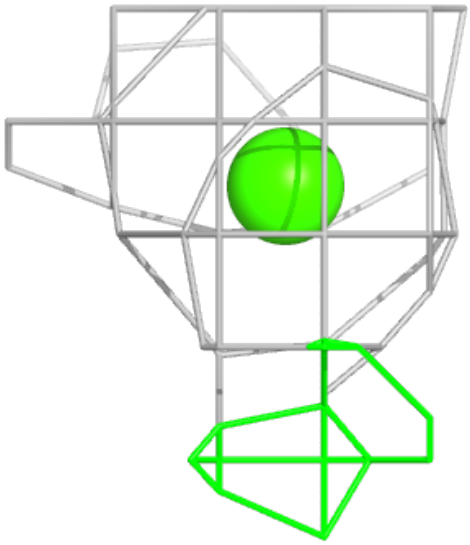


Electron density around CA D 604:

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

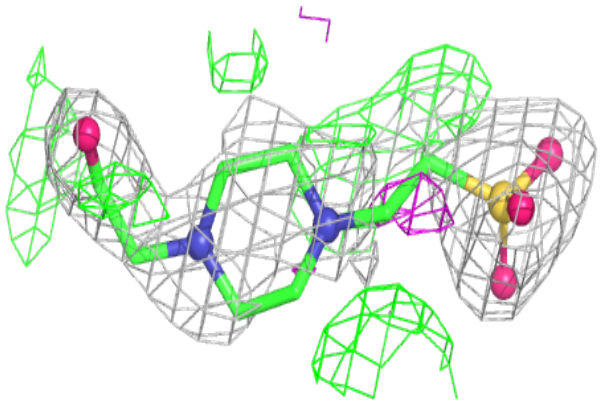


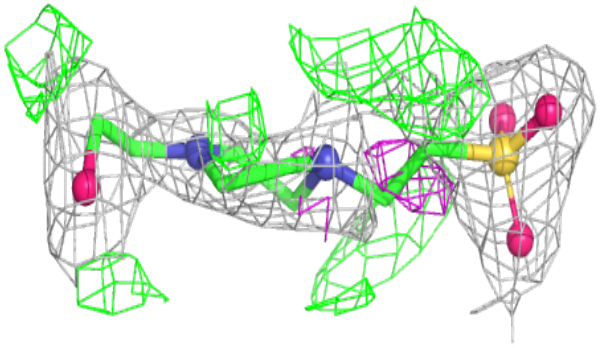


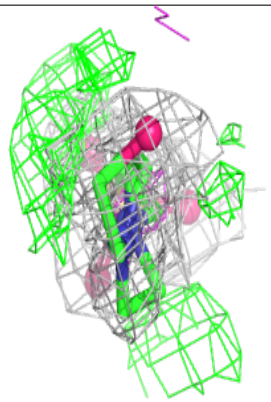


Electron density around EPE C 601:

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

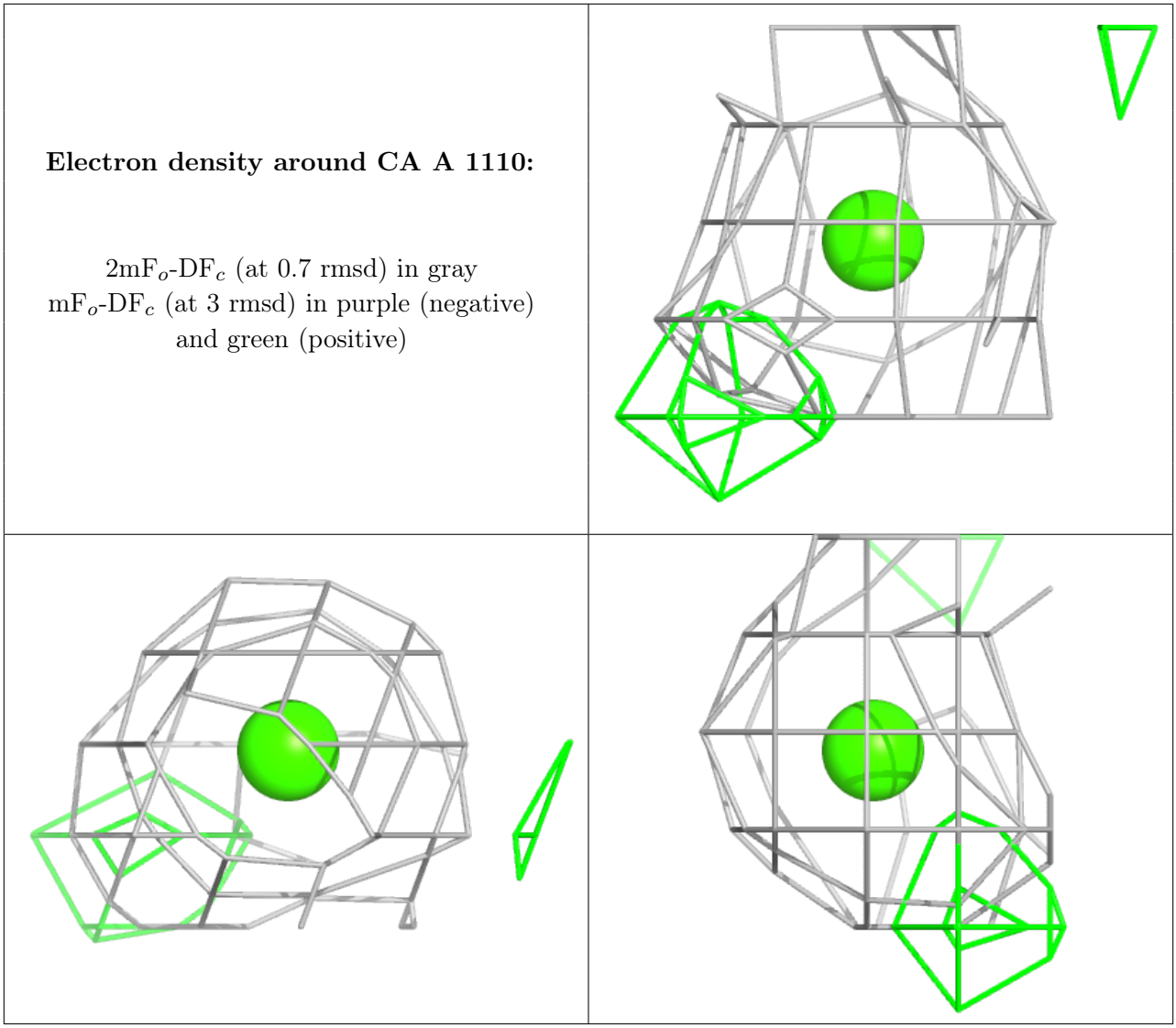






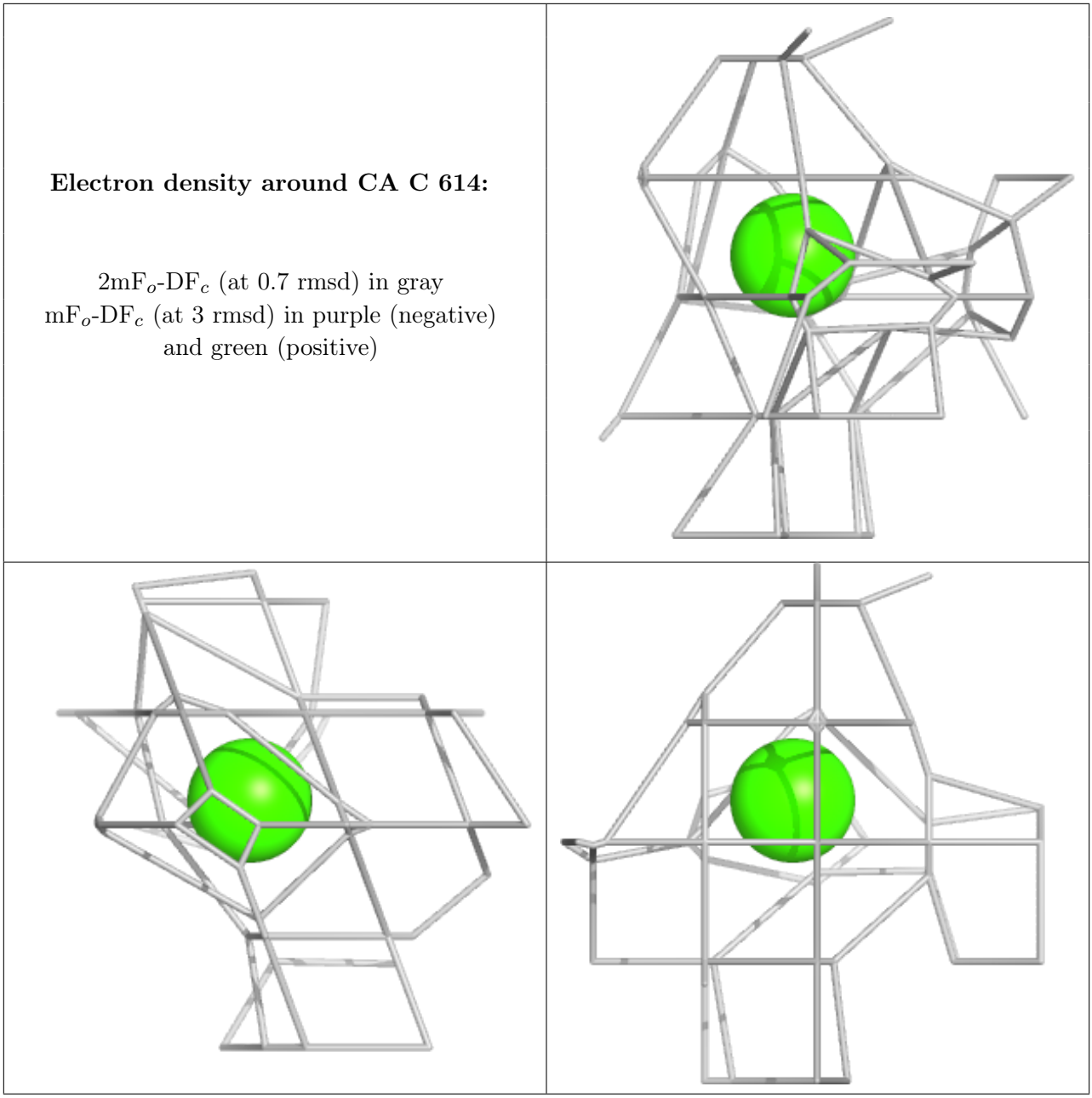
Electron density around CA A 1110:

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



Electron density around CA C 614:

$2mF_o$-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.