wwPDB X-ray Structure Validation Summary Report (i)

Sep 9, 2026 – 03:43 pm BST

PDB ID	:	9I0F / pdb_00009i0f
Title	:	Revisited AvNifEN crystal structure
Authors	:	Paya Tormo, L.; Nguyen, T.Q.; Fyfe, C.; Basbous, H.; Dobrzynska, K.; Echavarri-Erasun, C.; Martin, L.; Caserta, G.; Legrand, P.; Thorn, A.; Amara, P.; Schoehn, G.; Cherrier, M.V.; Rubio, L.M.; Nicolet, Y.
Deposited on	:	2025-01-15
Resolution	:	2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

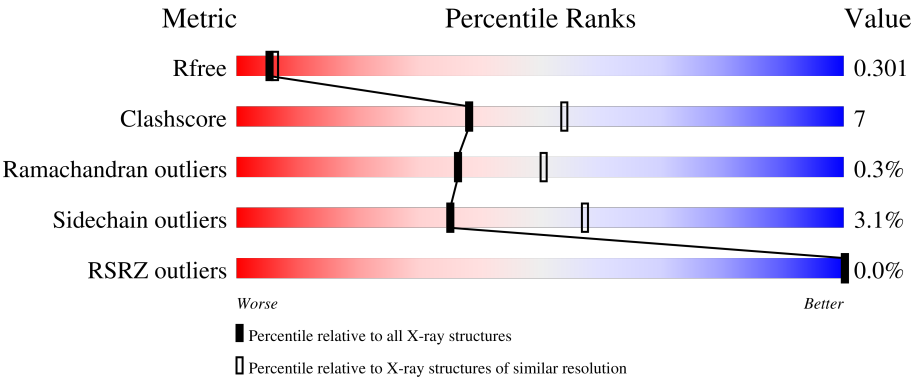
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	483	79% 16%
1	C	483	82% 14%
1	E	483	82% 14%
1	G	483	84% 11%

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Mol	Chain	Length	Quality of chain
2	B	458	81% 16%
2	D	458	83% 15%
2	F	458	81% 16%
2	H	458	82% 16%

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	S5Q	A	502	-	-	X	-
4	S5Q	C	502	-	-	X	-
4	S5Q	E	502	-	-	X	-
4	S5Q	G	502	-	-	X	-
5	PEG	A	503	-	-	X	-
5	PEG	B	503	-	-	X	-
5	PEG	D	507	-	-	X	-
5	PEG	G	506	-	-	X	-
5	PEG	H	504	-	-	X	-
6	EDO	B	505	-	-	X	-
6	EDO	B	513	-	-	X	-
6	EDO	G	503	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 29802 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 Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3591	2257	640	671	23			
1	C	465	Total	C	N	O	S	0	0	0
			3591	2257	640	671	23			
1	E	465	Total	C	N	O	S	0	0	0
			3591	2257	640	671	23			
1	G	465	Total	C	N	O	S	0	0	0
			3591	2257	640	671	23			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP C1DH03
A	-6	HIS	-	expression tag	UNP C1DH03
A	-5	HIS	-	expression tag	UNP C1DH03
A	-4	HIS	-	expression tag	UNP C1DH03
A	-3	HIS	-	expression tag	UNP C1DH03
A	-2	HIS	-	expression tag	UNP C1DH03
A	-1	HIS	-	expression tag	UNP C1DH03
A	0	HIS	-	expression tag	UNP C1DH03
C	-7	MET	-	initiating methionine	UNP C1DH03
C	-6	HIS	-	expression tag	UNP C1DH03
C	-5	HIS	-	expression tag	UNP C1DH03
C	-4	HIS	-	expression tag	UNP C1DH03
C	-3	HIS	-	expression tag	UNP C1DH03
C	-2	HIS	-	expression tag	UNP C1DH03
C	-1	HIS	-	expression tag	UNP C1DH03
C	0	HIS	-	expression tag	UNP C1DH03
E	-7	MET	-	initiating methionine	UNP C1DH03
E	-6	HIS	-	expression tag	UNP C1DH03
E	-5	HIS	-	expression tag	UNP C1DH03
E	-4	HIS	-	expression tag	UNP C1DH03

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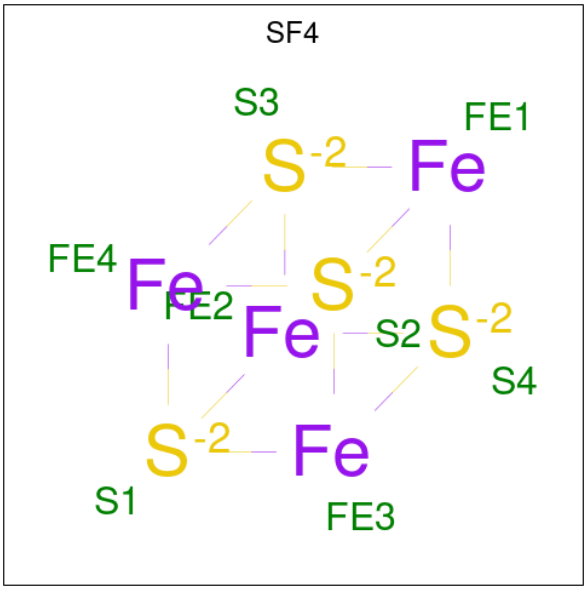
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	HIS	-	expression tag	UNP C1DH03
E	-2	HIS	-	expression tag	UNP C1DH03
E	-1	HIS	-	expression tag	UNP C1DH03
E	0	HIS	-	expression tag	UNP C1DH03
G	-7	MET	-	initiating methionine	UNP C1DH03
G	-6	HIS	-	expression tag	UNP C1DH03
G	-5	HIS	-	expression tag	UNP C1DH03
G	-4	HIS	-	expression tag	UNP C1DH03
G	-3	HIS	-	expression tag	UNP C1DH03
G	-2	HIS	-	expression tag	UNP C1DH03
G	-1	HIS	-	expression tag	UNP C1DH03
G	0	HIS	-	expression tag	UNP C1DH03

- Molecule 2 is a protein called Nitrogenase iron-molybdenum cofactor biosynthesis protein NifN.

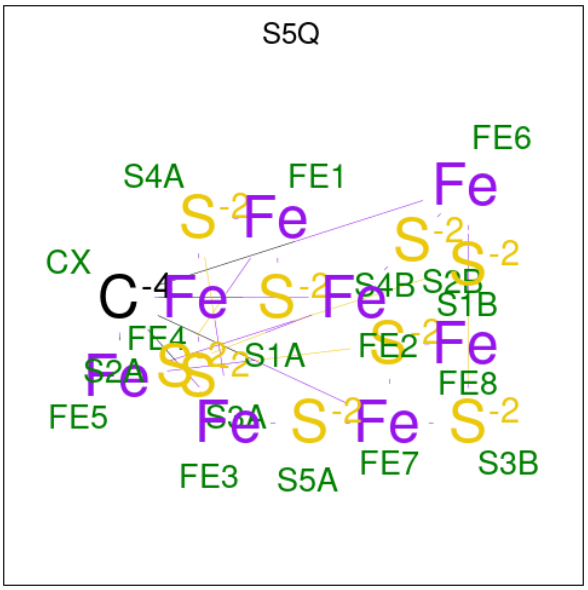
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	450	Total	C	N	O	S	0	0	0
			3386	2129	603	639	15			
2	D	450	Total	C	N	O	S	0	0	0
			3386	2129	603	639	15			
2	F	451	Total	C	N	O	S	0	0	0
			3394	2134	604	640	16			
2	H	450	Total	C	N	O	S	0	0	0
			3386	2129	603	639	15			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



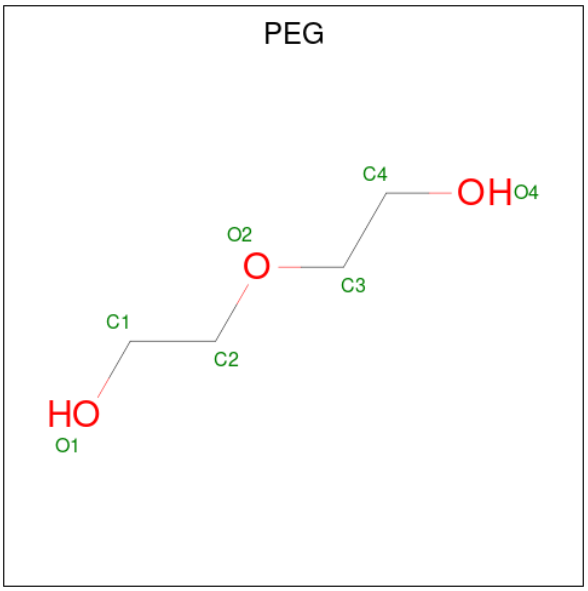
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	E	1	Total Fe S 8 4 4	0	0
3	G	1	Total Fe S 8 4 4	0	0

- Molecule 4 is FeFe cofactor (CCD ID: S5Q) (formula: CFe_8S_9) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Fe S 18 1 8 9	0	0
4	C	1	Total C Fe S 18 1 8 9	0	0
4	E	1	Total C Fe S 18 1 8 9	0	0
4	G	1	Total C Fe S 18 1 8 9	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

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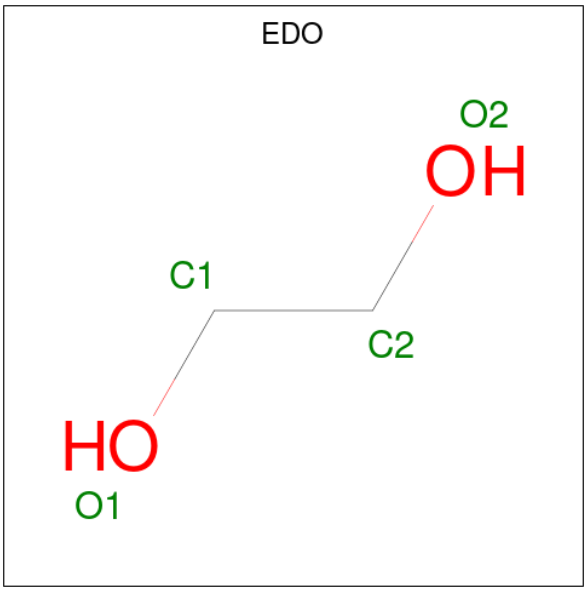
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0
5	G	1	Total C O 7 4 3	0	0
5	G	1	Total C O 7 4 3	0	0
5	H	1	Total C O 7 4 3	0	0
5	H	1	Total C O 7 4 3	0	0
5	H	1	Total C O 7 4 3	0	0
5	H	1	Total C O 7 4 3	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		

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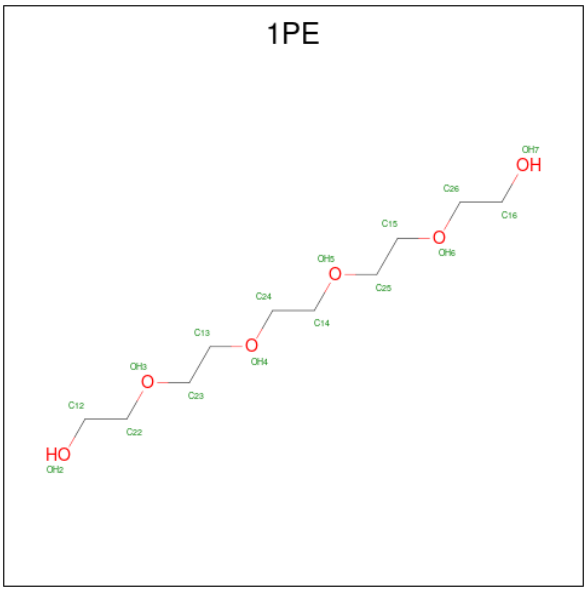
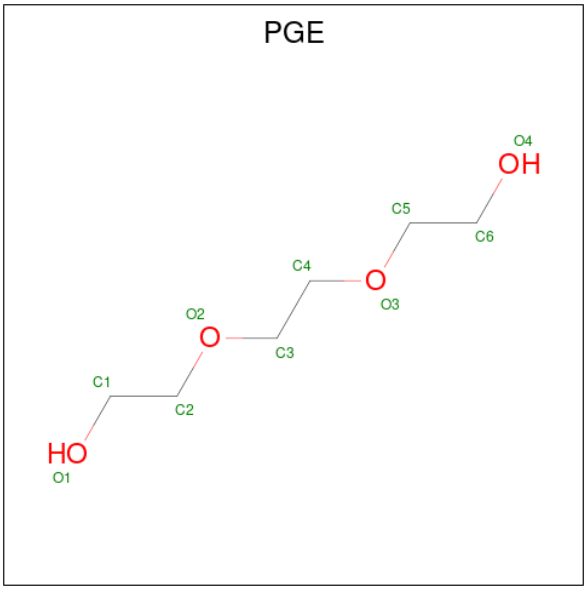
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 16 10 6	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

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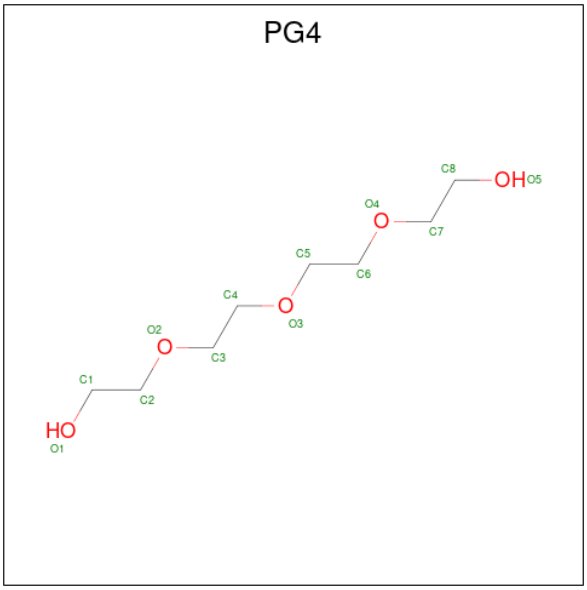
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C O 10 6 4	0	0
8	F	1	Total C O 10 6 4	0	0
8	F	1	Total C O 10 6 4	0	0
8	F	1	Total C O 10 6 4	0	0
8	G	1	Total C O 10 6 4	0	0
8	H	1	Total C O 10 6 4	0	0
8	H	1	Total C O 10 6 4	0	0

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	0	0
9	D	1	Total Mg 1 1	0	0
9	F	2	Total Mg 2 2	0	0

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 11 is water.

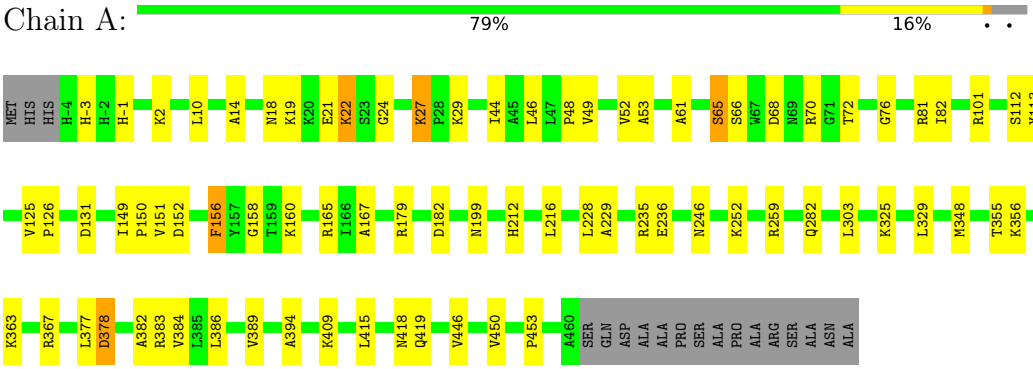
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	146	Total O 146 146	0	0
11	B	169	Total O 169 169	0	0
11	C	114	Total O 114 114	0	0
11	D	141	Total O 141 141	0	0
11	E	112	Total O 112 112	0	0
11	F	113	Total O 113 113	0	0
11	G	90	Total O 90 90	0	0
11	H	90	Total O 90 90	0	0

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.

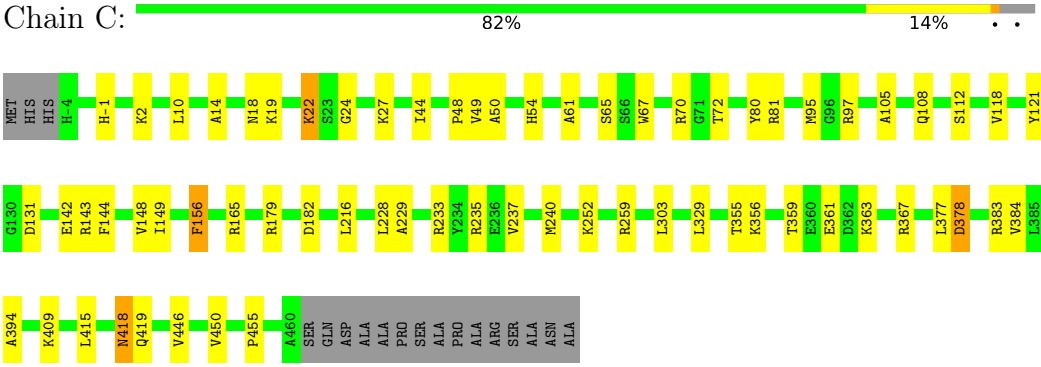
• Molecule 1: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE

Chain A:



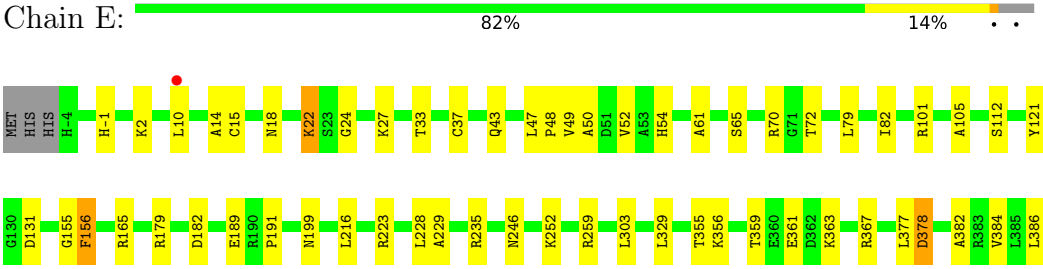
• Molecule 1: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE

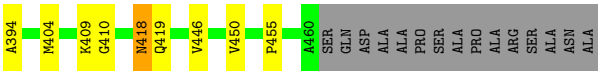
Chain C:



• Molecule 1: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE

Chain E:





• Molecule 1: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE

Chain G:

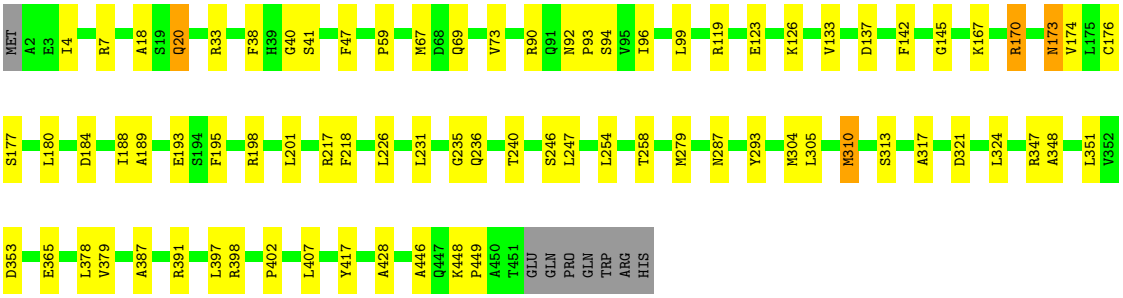




• Molecule 2: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifN

Chain B:

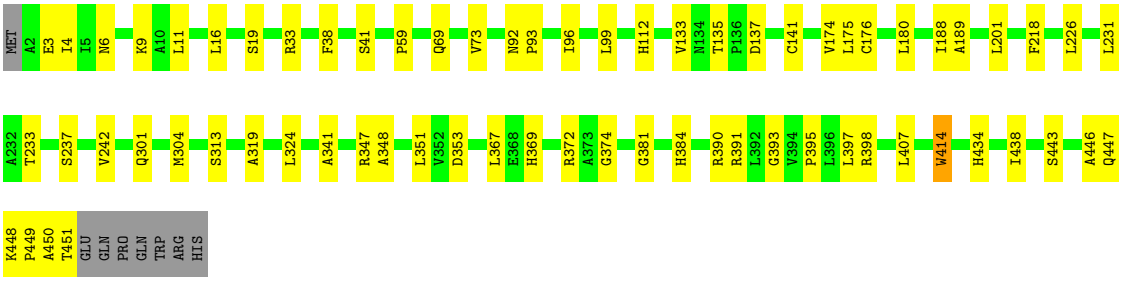




• Molecule 2: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifN

Chain D:

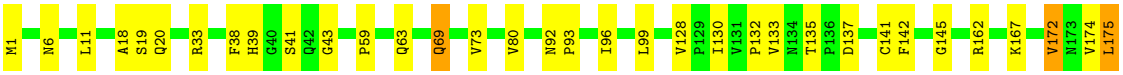


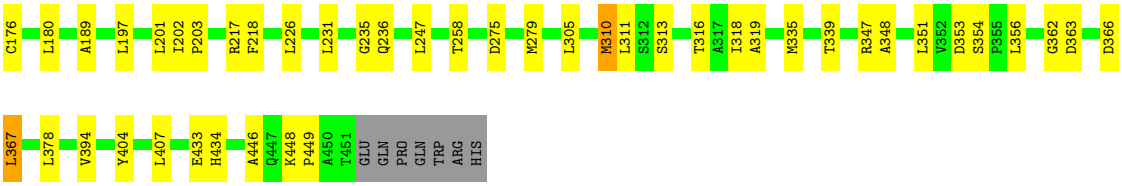


• Molecule 2: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifN

Chain F:



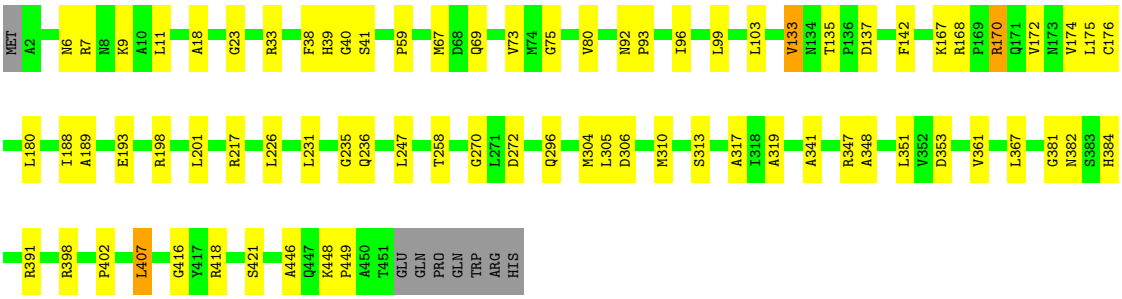




• Molecule 2: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifN

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	146.07Å 95.22Å 149.98Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	39.83 – 2.40 39.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.2 (39.83-2.40) 87.2 (39.83-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.4 (10-JUL-2024)	Depositor
R, R_{free}	0.249 , 0.304 0.245 , 0.301	Depositor DCC
R_{free} test set	13821 reflections (8.61%)	wwPDB-VP
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.075 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	29802	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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: PG4, S5Q, PEG, EDO, PGE, 1PE, MG, SF4

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	0.71	0/3665	1.03	3/4968 (0.1%)
1	C	0.64	0/3665	1.03	5/4968 (0.1%)
1	E	0.65	0/3665	1.02	5/4968 (0.1%)
1	G	0.62	0/3665	1.00	5/4968 (0.1%)
2	B	0.72	0/3451	1.08	2/4693 (0.0%)
2	D	0.74	0/3451	1.11	10/4693 (0.2%)
2	F	0.71	1/3459 (0.0%)	1.08	7/4703 (0.1%)
2	H	0.70	0/3451	1.06	2/4693 (0.0%)
All	All	0.69	1/28472 (0.0%)	1.05	39/38654 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	394	VAL	CA-C	6.74	1.58	1.52

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	49	VAL	CA-C-N	9.03	132.75	120.38
1	C	49	VAL	C-N-CA	9.03	132.75	120.38
2	F	362	GLY	N-CA-C	8.05	123.58	111.42
1	A	49	VAL	CA-C-N	7.30	131.78	120.82
1	A	49	VAL	C-N-CA	7.30	131.78	120.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3591	0	3571	61	0
1	C	3591	0	3571	50	0
1	E	3591	0	3571	46	0
1	G	3591	0	3571	54	0
2	B	3386	0	3379	72	0
2	D	3386	0	3379	56	0
2	F	3394	0	3391	46	0
2	H	3386	0	3379	67	0
3	A	8	0	0	1	0
3	C	8	0	0	1	0
3	E	8	0	0	1	0
3	G	8	0	0	0	0
4	A	18	0	0	5	0
4	C	18	0	0	5	0
4	E	18	0	0	5	0
4	G	18	0	0	5	0
5	A	42	0	60	6	0
5	B	42	0	60	7	0
5	C	7	0	10	0	0
5	D	49	0	70	12	0
5	F	7	0	10	0	0
5	G	14	0	20	6	0
5	H	28	0	40	7	0
6	A	100	0	150	10	0
6	B	84	0	126	22	0
6	C	28	0	42	5	0
6	D	72	0	108	13	0
6	E	36	0	54	3	0
6	F	72	0	108	1	0
6	G	48	0	72	6	0
6	H	32	0	48	5	0
7	A	16	0	22	5	0
8	A	20	0	28	3	0
8	C	10	0	14	0	0
8	E	10	0	14	0	0
8	F	30	0	42	1	0
8	G	10	0	14	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	20	0	28	6	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
9	F	2	0	0	0	0
10	B	13	0	18	0	0
10	F	13	0	18	0	0
11	A	146	0	0	2	0
11	B	169	0	0	1	0
11	C	114	0	0	2	0
11	D	141	0	0	1	0
11	E	112	0	0	1	0
11	F	113	0	0	1	0
11	G	90	0	0	1	0
11	H	90	0	0	1	0
All	All	29802	0	28988	397	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 7.

The worst 5 of 397 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)
2:D:384:HIS:HA	6:D:520:EDO:H21	1.22	1.11
1:C:97:ARG:HA	6:C:506:EDO:H21	1.12	1.07
2:H:198:ARG:HA	8:H:514:PGE:H2	1.42	1.02
2:B:195:PHE:HA	5:B:503:PEG:H11	1.41	1.00
2:H:167:LYS:HB3	2:H:236:GLN:HB3	1.43	1.00

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	463/483 (96%)	439 (95%)	20 (4%)	4 (1%)	14	22
1	C	463/483 (96%)	440 (95%)	21 (4%)	2 (0%)	30	43
1	E	463/483 (96%)	441 (95%)	20 (4%)	2 (0%)	30	43
1	G	463/483 (96%)	440 (95%)	21 (4%)	2 (0%)	30	43
2	B	448/458 (98%)	436 (97%)	12 (3%)	0	100	100
2	D	448/458 (98%)	434 (97%)	13 (3%)	1 (0%)	43	58
2	F	449/458 (98%)	434 (97%)	15 (3%)	0	100	100
2	H	448/458 (98%)	432 (96%)	16 (4%)	0	100	100
All	All	3645/3764 (97%)	3496 (96%)	138 (4%)	11 (0%)	36	50

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	131	ASP
1	C	22	LYS
2	D	450	ALA
1	G	22	LYS

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	376/388 (97%)	362 (96%)	14 (4%)	30	51
1	C	376/388 (97%)	364 (97%)	12 (3%)	34	56
1	E	376/388 (97%)	365 (97%)	11 (3%)	37	60
1	G	376/388 (97%)	367 (98%)	9 (2%)	43	65
2	B	355/363 (98%)	341 (96%)	14 (4%)	28	48
2	D	355/363 (98%)	347 (98%)	8 (2%)	44	66
2	F	356/363 (98%)	345 (97%)	11 (3%)	35	57
2	H	355/363 (98%)	343 (97%)	12 (3%)	32	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2925/3004 (97%)	2834 (97%)	91 (3%)	35 57

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	386	LEU
1	G	27	LYS
2	F	69	GLN
2	F	313	SER
1	G	189	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	164	ASN
2	H	92	ASN
2	H	403	GLN
2	D	121	GLN
2	D	112	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 170 ligands modelled in this entry, 4 are monoatomic - leaving 166 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	$\#\|Z\| > 2$
6	EDO	F	514	-	3,3,3	0.41	0	2,2,2	0.03	0
6	EDO	E	509	-	3,3,3	0.31	0	2,2,2	0.29	0
6	EDO	B	509	-	3,3,3	0.21	0	2,2,2	0.32	0
6	EDO	B	525	-	3,3,3	0.40	0	2,2,2	0.05	0
6	EDO	C	507	-	3,3,3	0.36	0	2,2,2	0.24	0
6	EDO	D	516	-	3,3,3	0.30	0	2,2,2	0.20	0
6	EDO	A	524	-	3,3,3	0.32	0	2,2,2	0.19	0
5	PEG	C	505	-	6,6,6	0.13	0	5,5,5	0.12	0
6	EDO	B	516	-	3,3,3	0.26	0	2,2,2	0.32	0
3	SF4	E	501	1,2	0,12,12	-	-	-		
6	EDO	A	515	-	3,3,3	0.34	0	2,2,2	0.04	0
6	EDO	E	508	-	3,3,3	0.35	0	2,2,2	0.27	0
6	EDO	G	507	-	3,3,3	0.27	0	2,2,2	0.32	0
6	EDO	E	503	-	3,3,3	0.31	0	2,2,2	0.33	0
6	EDO	D	523	-	3,3,3	0.25	0	2,2,2	0.28	0
6	EDO	B	507	-	3,3,3	0.28	0	2,2,2	0.29	0
6	EDO	H	505	-	3,3,3	0.54	0	2,2,2	0.34	0
6	EDO	H	506	-	3,3,3	0.31	0	2,2,2	0.38	0
7	1PE	A	532	-	15,15,15	0.23	0	14,14,14	0.29	0
6	EDO	B	524	-	3,3,3	0.50	0	2,2,2	0.25	0
8	PGE	C	503	-	9,9,9	0.23	0	8,8,8	0.08	0
5	PEG	B	503	-	6,6,6	0.21	0	5,5,5	0.15	0
5	PEG	D	506	-	6,6,6	0.23	0	5,5,5	0.07	0
6	EDO	A	530	-	3,3,3	0.28	0	2,2,2	0.23	0
6	EDO	G	514	-	3,3,3	0.30	0	2,2,2	0.19	0
6	EDO	A	512	-	3,3,3	0.36	0	2,2,2	0.15	0
5	PEG	G	508	-	6,6,6	0.21	0	5,5,5	0.13	0
6	EDO	H	509	-	3,3,3	0.55	0	2,2,2	0.11	0
5	PEG	A	531	-	6,6,6	0.13	0	5,5,5	0.10	0
8	PGE	H	514	-	9,9,9	0.18	0	8,8,8	0.14	0
6	EDO	B	514	-	3,3,3	0.56	0	2,2,2	0.07	0
6	EDO	A	518	-	3,3,3	0.42	0	2,2,2	0.05	0
6	EDO	C	508	-	3,3,3	0.25	0	2,2,2	0.42	0
6	EDO	F	504	-	3,3,3	0.31	0	2,2,2	0.26	0
6	EDO	D	521	-	3,3,3	0.31	0	2,2,2	0.20	0
6	EDO	G	505	-	3,3,3	0.25	0	2,2,2	0.23	0
5	PEG	F	507	-	6,6,6	0.23	0	5,5,5	0.14	0
6	EDO	F	510	-	3,3,3	0.46	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PEG	H	503	-	6,6,6	0.16	0	5,5,5	0.08	0
6	EDO	F	505	-	3,3,3	0.35	0	2,2,2	0.14	0
8	PGE	F	520	-	9,9,9	0.21	0	8,8,8	0.12	0
6	EDO	E	505	-	3,3,3	0.34	0	2,2,2	0.13	0
6	EDO	E	506	-	3,3,3	0.45	0	2,2,2	0.32	0
6	EDO	G	513	-	3,3,3	0.27	0	2,2,2	0.31	0
8	PGE	A	536	-	9,9,9	0.17	0	8,8,8	0.12	0
6	EDO	G	504	-	3,3,3	0.33	0	2,2,2	0.25	0
8	PGE	E	507	-	9,9,9	0.16	0	8,8,8	0.12	0
6	EDO	F	509	-	3,3,3	0.38	0	2,2,2	0.26	0
5	PEG	D	504	-	6,6,6	0.14	0	5,5,5	0.23	0
6	EDO	H	510	-	3,3,3	0.49	0	2,2,2	0.09	0
6	EDO	A	521	-	3,3,3	0.35	0	2,2,2	0.07	0
6	EDO	D	509	-	3,3,3	0.28	0	2,2,2	0.30	0
3	SF4	G	501	1,2	0,12,12	-	-	-		
6	EDO	D	520	-	3,3,3	0.30	0	2,2,2	0.13	0
6	EDO	D	503	-	3,3,3	0.21	0	2,2,2	0.31	0
6	EDO	B	526	-	3,3,3	0.20	0	2,2,2	0.28	0
6	EDO	B	508	-	3,3,3	0.26	0	2,2,2	0.18	0
8	PGE	A	535	-	9,9,9	0.17	0	8,8,8	0.09	0
6	EDO	A	507	-	3,3,3	0.34	0	2,2,2	0.11	0
6	EDO	A	527	-	3,3,3	0.32	0	2,2,2	0.23	0
6	EDO	F	508	-	3,3,3	0.25	0	2,2,2	0.33	0
6	EDO	B	519	-	3,3,3	0.42	0	2,2,2	0.13	0
6	EDO	E	504	-	3,3,3	0.39	0	2,2,2	0.21	0
5	PEG	B	502	-	6,6,6	0.13	0	5,5,5	0.11	0
6	EDO	D	525	-	3,3,3	0.47	0	2,2,2	0.15	0
6	EDO	C	504	-	3,3,3	0.55	0	2,2,2	0.27	0
6	EDO	A	513	-	3,3,3	0.36	0	2,2,2	0.13	0
6	EDO	B	517	-	3,3,3	0.29	0	2,2,2	0.26	0
6	EDO	D	514	-	3,3,3	0.40	0	2,2,2	0.27	0
6	EDO	G	515	-	3,3,3	0.41	0	2,2,2	0.21	0
6	EDO	F	506	-	3,3,3	0.23	0	2,2,2	0.31	0
6	EDO	A	523	-	3,3,3	0.36	0	2,2,2	0.17	0
6	EDO	D	518	-	3,3,3	0.32	0	2,2,2	0.19	0
6	EDO	F	515	-	3,3,3	0.33	0	2,2,2	0.17	0
6	EDO	G	510	-	3,3,3	0.39	0	2,2,2	0.14	0
6	EDO	F	516	-	3,3,3	0.26	0	2,2,2	0.36	0
6	EDO	G	509	-	3,3,3	0.26	0	2,2,2	0.18	0
5	PEG	G	506	-	6,6,6	0.11	0	5,5,5	0.12	0
10	PG4	B	520	-	12,12,12	0.21	0	11,11,11	0.35	0
6	EDO	E	511	-	3,3,3	0.41	0	2,2,2	0.26	0
6	EDO	A	509	-	3,3,3	0.23	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PEG	B	529	-	6,6,6	0.14	0	5,5,5	0.11	0
6	EDO	F	513	-	3,3,3	0.35	0	2,2,2	0.18	0
6	EDO	A	529	-	3,3,3	0.29	0	2,2,2	0.29	0
6	EDO	A	514	-	3,3,3	0.45	0	2,2,2	0.09	0
3	SF4	C	501	1,2	0,12,12	-	-	-		
6	EDO	A	516	-	3,3,3	0.37	0	2,2,2	0.25	0
6	EDO	B	528	-	3,3,3	0.45	0	2,2,2	0.19	0
6	EDO	D	510	-	3,3,3	0.38	0	2,2,2	0.11	0
6	EDO	F	511	-	3,3,3	0.36	0	2,2,2	0.27	0
6	EDO	H	507	-	3,3,3	0.21	0	2,2,2	0.33	0
3	SF4	A	501	1,2	0,12,12	-	-	-		
6	EDO	A	508	-	3,3,3	0.33	0	2,2,2	0.23	0
6	EDO	B	515	-	3,3,3	0.42	0	2,2,2	0.07	0
6	EDO	D	508	-	3,3,3	0.26	0	2,2,2	0.39	0
4	S5Q	C	502	1	18,30,30	2.33	11 (61%)	-		
6	EDO	A	528	-	3,3,3	0.30	0	2,2,2	0.14	0
6	EDO	A	519	-	3,3,3	0.33	0	2,2,2	0.20	0
5	PEG	A	503	-	6,6,6	0.18	0	5,5,5	0.12	0
6	EDO	G	512	-	3,3,3	0.39	0	2,2,2	0.04	0
5	PEG	B	521	-	6,6,6	0.24	0	5,5,5	0.11	0
6	EDO	A	525	-	3,3,3	0.30	0	2,2,2	0.25	0
6	EDO	F	518	-	3,3,3	0.23	0	2,2,2	0.35	0
6	EDO	D	522	-	3,3,3	0.36	0	2,2,2	0.30	0
4	S5Q	G	502	1	18,30,30	2.38	11 (61%)	-		
6	EDO	B	512	-	3,3,3	0.31	0	2,2,2	0.18	0
8	PGE	G	517	-	9,9,9	0.18	0	8,8,8	0.12	0
6	EDO	G	503	-	3,3,3	0.36	0	2,2,2	0.19	0
6	EDO	F	512	-	3,3,3	0.42	0	2,2,2	0.26	0
6	EDO	H	511	-	3,3,3	0.32	0	2,2,2	0.27	0
5	PEG	A	533	-	6,6,6	0.15	0	5,5,5	0.13	0
5	PEG	B	522	-	6,6,6	0.25	0	5,5,5	0.15	0
6	EDO	B	510	-	3,3,3	0.27	0	2,2,2	0.19	0
6	EDO	D	519	-	3,3,3	0.34	0	2,2,2	0.14	0
5	PEG	D	526	-	6,6,6	0.14	0	5,5,5	0.08	0
4	S5Q	A	502	1	18,30,30	2.35	11 (61%)	-		
6	EDO	F	503	-	3,3,3	0.45	0	2,2,2	0.16	0
6	EDO	B	505	-	3,3,3	0.46	0	2,2,2	0.35	0
6	EDO	B	506	-	3,3,3	0.31	0	2,2,2	0.19	0
6	EDO	A	520	-	3,3,3	0.40	0	2,2,2	0.28	0
5	PEG	D	511	-	6,6,6	0.14	0	5,5,5	0.10	0
6	EDO	H	512	-	3,3,3	0.29	0	2,2,2	0.31	0
6	EDO	E	510	-	3,3,3	0.23	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	A	517	-	3,3,3	0.31	0	2,2,2	0.47	0
6	EDO	A	506	-	3,3,3	0.41	0	2,2,2	0.11	0
6	EDO	B	527	-	3,3,3	0.33	0	2,2,2	0.15	0
6	EDO	C	510	-	3,3,3	0.22	0	2,2,2	0.41	0
10	PG4	F	517	-	12,12,12	0.14	0	11,11,11	0.08	0
5	PEG	B	504	-	6,6,6	0.21	0	5,5,5	0.11	0
6	EDO	A	522	-	3,3,3	0.37	0	2,2,2	0.22	0
6	EDO	E	512	-	3,3,3	0.30	0	2,2,2	0.33	0
6	EDO	G	516	-	3,3,3	0.28	0	2,2,2	0.26	0
5	PEG	H	502	-	6,6,6	0.19	0	5,5,5	0.14	0
5	PEG	D	505	-	6,6,6	0.16	0	5,5,5	0.06	0
5	PEG	A	504	-	6,6,6	0.16	0	5,5,5	0.09	0
5	PEG	A	505	-	6,6,6	0.19	0	5,5,5	0.06	0
6	EDO	G	511	-	3,3,3	0.25	0	2,2,2	0.29	0
8	PGE	F	525	-	9,9,9	0.20	0	8,8,8	0.10	0
6	EDO	A	534	-	3,3,3	0.33	0	2,2,2	0.37	0
6	EDO	F	521	-	3,3,3	0.22	0	2,2,2	0.38	0
6	EDO	A	526	-	3,3,3	0.43	0	2,2,2	0.15	0
6	EDO	B	511	-	3,3,3	0.50	0	2,2,2	0.11	0
6	EDO	F	519	-	3,3,3	0.33	0	2,2,2	0.10	0
6	EDO	D	515	-	3,3,3	0.26	0	2,2,2	0.20	0
6	EDO	C	511	-	3,3,3	0.47	0	2,2,2	0.17	0
6	EDO	B	523	-	3,3,3	0.25	0	2,2,2	0.31	0
5	PEG	D	517	-	6,6,6	0.17	0	5,5,5	0.22	0
6	EDO	A	511	-	3,3,3	0.23	0	2,2,2	0.06	0
6	EDO	F	522	-	3,3,3	0.38	0	2,2,2	0.09	0
6	EDO	F	523	-	3,3,3	0.28	0	2,2,2	0.25	0
8	PGE	F	524	-	9,9,9	0.19	0	8,8,8	0.06	0
6	EDO	C	509	-	3,3,3	0.34	0	2,2,2	0.06	0
6	EDO	D	512	-	3,3,3	0.27	0	2,2,2	0.28	0
6	EDO	D	513	-	3,3,3	0.32	0	2,2,2	0.19	0
4	S5Q	E	502	1	18,30,30	2.37	10 (55%)	-		
6	EDO	D	502	-	3,3,3	0.35	0	2,2,2	0.16	0
6	EDO	B	513	-	3,3,3	0.70	0	2,2,2	0.54	0
6	EDO	D	524	-	3,3,3	0.35	0	2,2,2	0.19	0
8	PGE	H	513	-	9,9,9	0.18	0	8,8,8	0.10	0
5	PEG	D	507	-	6,6,6	0.20	0	5,5,5	0.20	0
6	EDO	B	518	-	3,3,3	0.26	0	2,2,2	0.41	0
5	PEG	H	504	-	6,6,6	0.17	0	5,5,5	0.23	0
5	PEG	H	501	-	6,6,6	0.17	0	5,5,5	0.03	0
6	EDO	C	506	-	3,3,3	0.52	0	2,2,2	0.34	0
5	PEG	A	510	-	6,6,6	0.24	0	5,5,5	0.07	0
6	EDO	H	508	-	3,3,3	0.41	0	2,2,2	0.11	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	EDO	F	514	-	-	0/1/1/1	-
6	EDO	E	509	-	-	1/1/1/1	-
6	EDO	B	509	-	-	1/1/1/1	-
6	EDO	B	525	-	-	1/1/1/1	-
6	EDO	C	507	-	-	1/1/1/1	-
6	EDO	D	516	-	-	1/1/1/1	-
6	EDO	A	524	-	-	1/1/1/1	-
5	PEG	C	505	-	-	3/4/4/4	-
6	EDO	B	516	-	-	0/1/1/1	-
6	EDO	A	515	-	-	1/1/1/1	-
6	EDO	E	508	-	-	1/1/1/1	-
3	SF4	E	501	1,2	-	-	0/6/5/5
6	EDO	G	507	-	-	0/1/1/1	-
6	EDO	E	503	-	-	1/1/1/1	-
6	EDO	D	523	-	-	1/1/1/1	-
6	EDO	B	507	-	-	1/1/1/1	-
6	EDO	H	505	-	-	0/1/1/1	-
6	EDO	H	506	-	-	1/1/1/1	-
7	1PE	A	532	-	-	8/13/13/13	-
6	EDO	B	524	-	-	1/1/1/1	-
8	PGE	C	503	-	-	6/7/7/7	-
5	PEG	B	503	-	-	2/4/4/4	-
5	PEG	D	506	-	-	3/4/4/4	-
6	EDO	A	530	-	-	1/1/1/1	-
6	EDO	G	514	-	-	1/1/1/1	-
6	EDO	A	512	-	-	0/1/1/1	-
5	PEG	G	508	-	-	2/4/4/4	-
6	EDO	H	509	-	-	1/1/1/1	-
5	PEG	A	531	-	-	4/4/4/4	-
8	PGE	H	514	-	-	3/7/7/7	-
6	EDO	B	514	-	-	1/1/1/1	-
6	EDO	A	518	-	-	0/1/1/1	-
6	EDO	C	508	-	-	1/1/1/1	-
6	EDO	F	504	-	-	1/1/1/1	-
6	EDO	D	521	-	-	1/1/1/1	-
6	EDO	G	505	-	-	1/1/1/1	-
5	PEG	F	507	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	F	510	-	-	1/1/1/1	-
5	PEG	H	503	-	-	2/4/4/4	-
6	EDO	F	505	-	-	1/1/1/1	-
8	PGE	F	520	-	-	4/7/7/7	-
6	EDO	E	505	-	-	0/1/1/1	-
6	EDO	E	506	-	-	1/1/1/1	-
6	EDO	G	513	-	-	1/1/1/1	-
8	PGE	A	536	-	-	3/7/7/7	-
6	EDO	G	504	-	-	1/1/1/1	-
8	PGE	E	507	-	-	3/7/7/7	-
6	EDO	F	509	-	-	1/1/1/1	-
5	PEG	D	504	-	-	1/4/4/4	-
6	EDO	H	510	-	-	1/1/1/1	-
6	EDO	A	521	-	-	1/1/1/1	-
6	EDO	D	509	-	-	1/1/1/1	-
3	SF4	G	501	1,2	-	-	0/6/5/5
6	EDO	D	520	-	-	0/1/1/1	-
6	EDO	D	503	-	-	1/1/1/1	-
6	EDO	B	526	-	-	1/1/1/1	-
6	EDO	B	508	-	-	1/1/1/1	-
8	PGE	A	535	-	-	3/7/7/7	-
6	EDO	A	507	-	-	0/1/1/1	-
6	EDO	A	527	-	-	1/1/1/1	-
6	EDO	F	508	-	-	1/1/1/1	-
6	EDO	B	519	-	-	1/1/1/1	-
6	EDO	E	504	-	-	0/1/1/1	-
5	PEG	B	502	-	-	1/4/4/4	-
6	EDO	D	525	-	-	0/1/1/1	-
6	EDO	C	504	-	-	1/1/1/1	-
6	EDO	A	513	-	-	1/1/1/1	-
6	EDO	B	517	-	-	0/1/1/1	-
6	EDO	D	514	-	-	1/1/1/1	-
6	EDO	G	515	-	-	1/1/1/1	-
6	EDO	F	506	-	-	1/1/1/1	-
6	EDO	A	523	-	-	1/1/1/1	-
6	EDO	D	518	-	-	0/1/1/1	-
6	EDO	F	515	-	-	1/1/1/1	-
6	EDO	G	510	-	-	1/1/1/1	-
6	EDO	F	516	-	-	0/1/1/1	-
6	EDO	G	509	-	-	0/1/1/1	-
5	PEG	G	506	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PG4	B	520	-	-	7/10/10/10	-
6	EDO	E	511	-	-	1/1/1/1	-
6	EDO	A	509	-	-	1/1/1/1	-
5	PEG	B	529	-	-	3/4/4/4	-
6	EDO	F	513	-	-	1/1/1/1	-
6	EDO	A	529	-	-	1/1/1/1	-
6	EDO	A	514	-	-	0/1/1/1	-
6	EDO	A	516	-	-	1/1/1/1	-
3	SF4	C	501	1,2	-	-	0/6/5/5
6	EDO	B	528	-	-	1/1/1/1	-
6	EDO	D	510	-	-	1/1/1/1	-
6	EDO	F	511	-	-	1/1/1/1	-
6	EDO	H	507	-	-	1/1/1/1	-
6	EDO	D	508	-	-	1/1/1/1	-
6	EDO	A	508	-	-	1/1/1/1	-
6	EDO	B	515	-	-	1/1/1/1	-
3	SF4	A	501	1,2	-	-	0/6/5/5
6	EDO	A	528	-	-	1/1/1/1	-
6	EDO	A	519	-	-	0/1/1/1	-
5	PEG	A	503	-	-	3/4/4/4	-
6	EDO	G	512	-	-	1/1/1/1	-
5	PEG	B	521	-	-	2/4/4/4	-
6	EDO	A	525	-	-	1/1/1/1	-
6	EDO	F	518	-	-	1/1/1/1	-
6	EDO	D	522	-	-	1/1/1/1	-
6	EDO	B	512	-	-	1/1/1/1	-
8	PGE	G	517	-	-	3/7/7/7	-
6	EDO	G	503	-	-	1/1/1/1	-
6	EDO	F	512	-	-	1/1/1/1	-
6	EDO	H	511	-	-	1/1/1/1	-
5	PEG	A	533	-	-	1/4/4/4	-
5	PEG	B	522	-	-	2/4/4/4	-
6	EDO	B	510	-	-	1/1/1/1	-
6	EDO	D	519	-	-	1/1/1/1	-
5	PEG	D	526	-	-	4/4/4/4	-
6	EDO	F	503	-	-	0/1/1/1	-
6	EDO	B	505	-	-	1/1/1/1	-
6	EDO	B	506	-	-	1/1/1/1	-
6	EDO	A	520	-	-	0/1/1/1	-
5	PEG	D	511	-	-	1/4/4/4	-
6	EDO	H	512	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	E	510	-	-	1/1/1/1	-
6	EDO	A	517	-	-	0/1/1/1	-
6	EDO	A	506	-	-	1/1/1/1	-
6	EDO	B	527	-	-	1/1/1/1	-
6	EDO	C	510	-	-	0/1/1/1	-
10	PG4	F	517	-	-	8/10/10/10	-
5	PEG	B	504	-	-	2/4/4/4	-
6	EDO	A	522	-	-	1/1/1/1	-
6	EDO	E	512	-	-	1/1/1/1	-
6	EDO	G	516	-	-	0/1/1/1	-
5	PEG	H	502	-	-	3/4/4/4	-
5	PEG	D	505	-	-	1/4/4/4	-
5	PEG	A	505	-	-	3/4/4/4	-
5	PEG	A	504	-	-	3/4/4/4	-
6	EDO	G	511	-	-	1/1/1/1	-
8	PGE	F	525	-	-	3/7/7/7	-
6	EDO	A	534	-	-	1/1/1/1	-
6	EDO	F	521	-	-	0/1/1/1	-
6	EDO	A	526	-	-	1/1/1/1	-
6	EDO	B	511	-	-	1/1/1/1	-
6	EDO	F	519	-	-	0/1/1/1	-
6	EDO	D	515	-	-	0/1/1/1	-
6	EDO	C	511	-	-	1/1/1/1	-
6	EDO	B	523	-	-	0/1/1/1	-
5	PEG	D	517	-	-	2/4/4/4	-
6	EDO	A	511	-	-	1/1/1/1	-
6	EDO	F	522	-	-	1/1/1/1	-
6	EDO	F	523	-	-	1/1/1/1	-
8	PGE	F	524	-	-	2/7/7/7	-
6	EDO	C	509	-	-	1/1/1/1	-
6	EDO	D	512	-	-	0/1/1/1	-
6	EDO	D	513	-	-	0/1/1/1	-
6	EDO	D	502	-	-	1/1/1/1	-
6	EDO	B	513	-	-	1/1/1/1	-
6	EDO	D	524	-	-	1/1/1/1	-
8	PGE	H	513	-	-	2/7/7/7	-
5	PEG	D	507	-	-	1/4/4/4	-
6	EDO	B	518	-	-	1/1/1/1	-
5	PEG	H	504	-	-	2/4/4/4	-
5	PEG	H	501	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	C	506	-	-	0/1/1/1	-
5	PEG	A	510	-	-	1/4/4/4	-
6	EDO	H	508	-	-	1/1/1/1	-

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	S5Q	S2A-FE2	-4.27	2.21	2.32
4	E	502	S5Q	S2A-FE2	-4.13	2.22	2.32
4	G	502	S5Q	S2A-FE2	-4.01	2.22	2.32
4	C	502	S5Q	S2A-FE2	-4.00	2.22	2.32
4	G	502	S5Q	S1A-FE4	-3.89	2.22	2.32

There are no bond angle outliers.

There are no chirality outliers.

5 of 204 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	504	PEG	O1-C1-C2-O2
10	B	520	PG4	O3-C5-C6-O4
8	A	535	PGE	O2-C3-C4-O3
5	H	503	PEG	O1-C1-C2-O2
8	E	507	PGE	O2-C3-C4-O3

There are no ring outliers.

63 monomers are involved in 144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	509	EDO	1	0
6	B	509	EDO	3	0
6	C	507	EDO	1	0
3	E	501	SF4	1	0
6	E	508	EDO	1	0
7	A	532	1PE	5	0
5	B	503	PEG	5	0
6	A	512	EDO	2	0
6	H	509	EDO	1	0
8	H	514	PGE	4	0
6	D	521	EDO	2	0
6	G	505	EDO	1	0
5	H	503	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	536	PGE	1	0
5	D	504	PEG	3	0
6	H	510	EDO	1	0
6	A	521	EDO	1	0
6	D	520	EDO	3	0
6	D	503	EDO	3	0
8	A	535	PGE	2	0
6	E	504	EDO	1	0
6	C	504	EDO	1	0
6	A	513	EDO	1	0
5	G	506	PEG	6	0
6	F	513	EDO	1	0
3	C	501	SF4	1	0
6	A	516	EDO	1	0
6	B	528	EDO	2	0
6	H	507	EDO	2	0
3	A	501	SF4	1	0
6	D	508	EDO	1	0
4	C	502	S5Q	5	0
5	A	503	PEG	4	0
6	D	522	EDO	2	0
4	G	502	S5Q	5	0
6	B	512	EDO	1	0
8	G	517	PGE	4	0
6	G	503	EDO	5	0
6	H	511	EDO	1	0
5	A	533	PEG	1	0
6	B	510	EDO	1	0
5	D	526	PEG	3	0
4	A	502	S5Q	5	0
6	B	505	EDO	5	0
6	B	506	EDO	1	0
6	A	520	EDO	1	0
5	D	511	PEG	1	0
6	A	517	EDO	2	0
5	B	504	PEG	2	0
6	A	522	EDO	2	0
5	H	502	PEG	1	0
8	F	525	PGE	1	0
6	B	511	EDO	3	0
6	A	511	EDO	2	0
6	D	513	EDO	2	0

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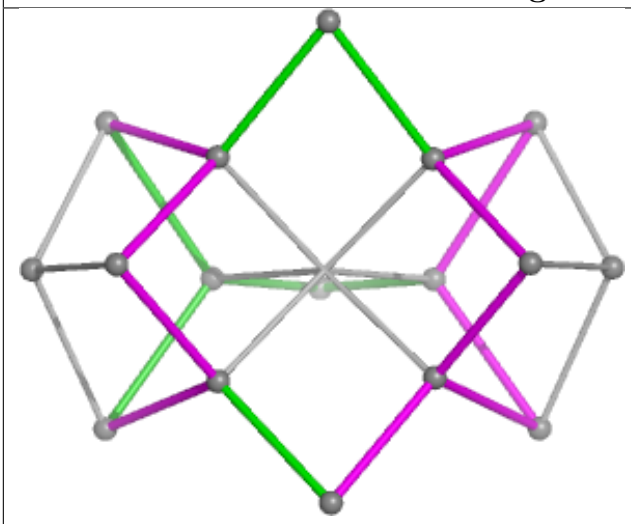
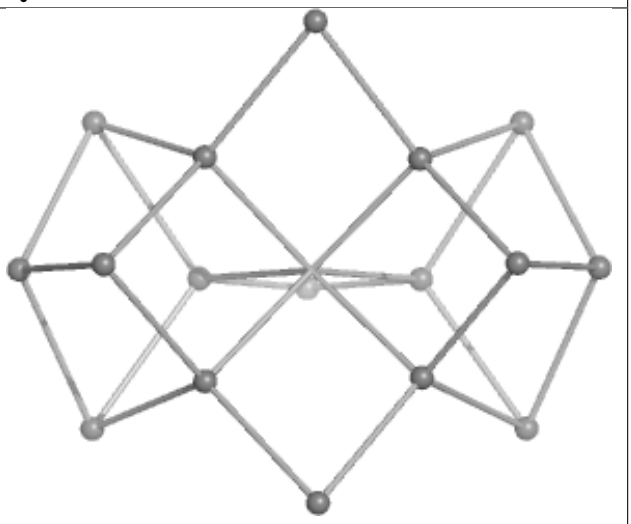
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	502	S5Q	5	0
6	B	513	EDO	4	0
8	H	513	PGE	2	0
5	D	507	PEG	5	0
6	B	518	EDO	2	0
5	H	504	PEG	5	0
6	C	506	EDO	3	0
5	A	510	PEG	1	0

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.

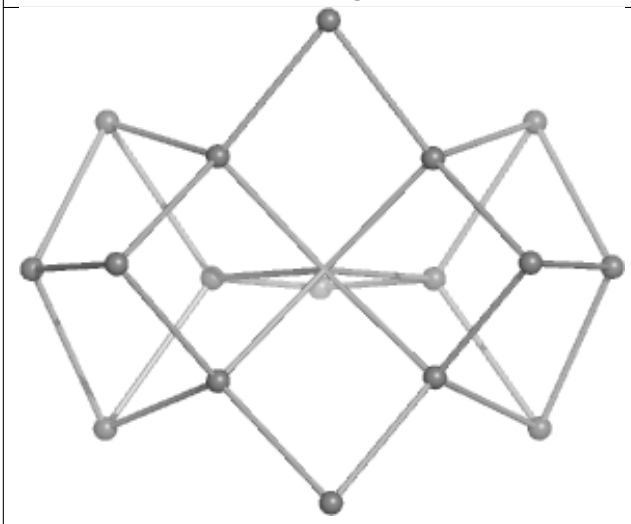
Ligand S5Q C 502



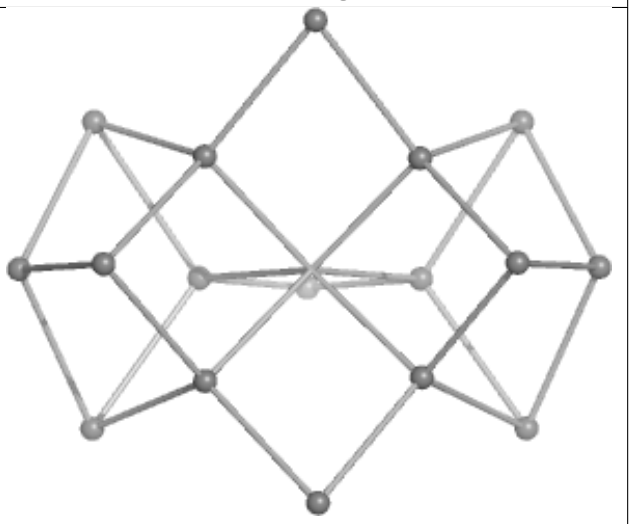
Bond lengths



Bond angles

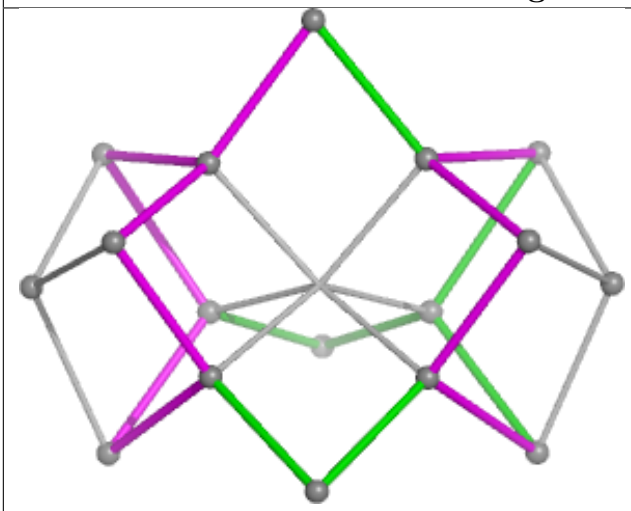


Torsions

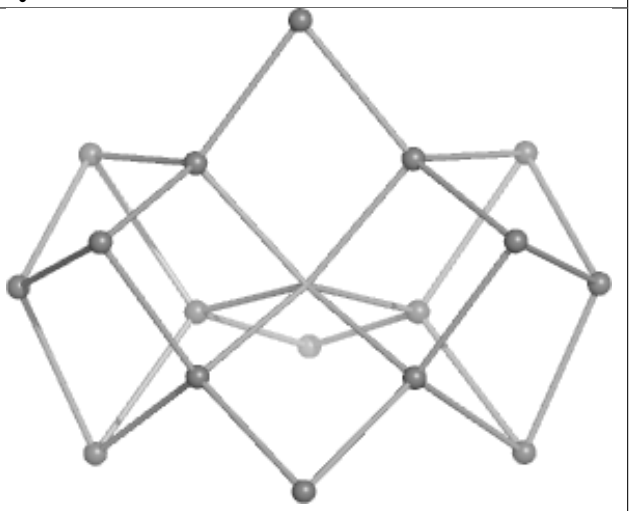


Rings

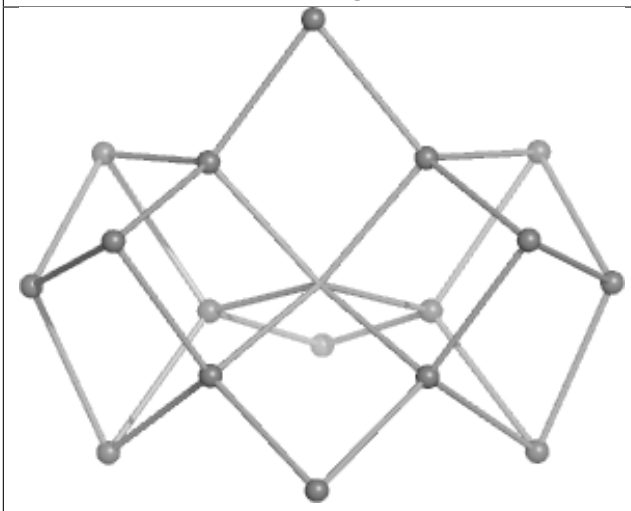
Ligand S5Q G 502



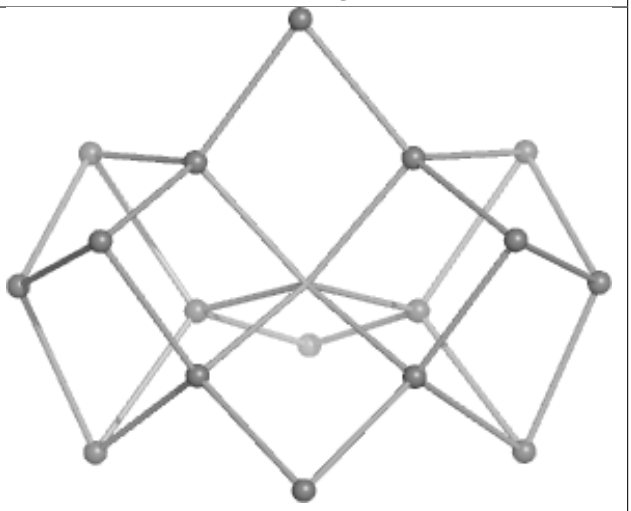
Bond lengths



Bond angles

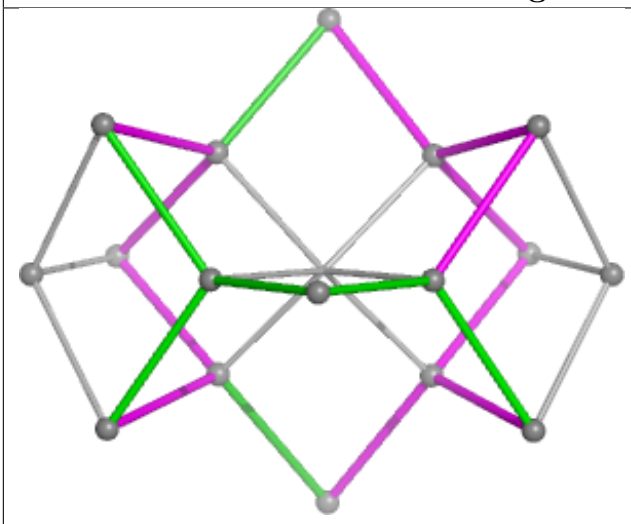


Torsions

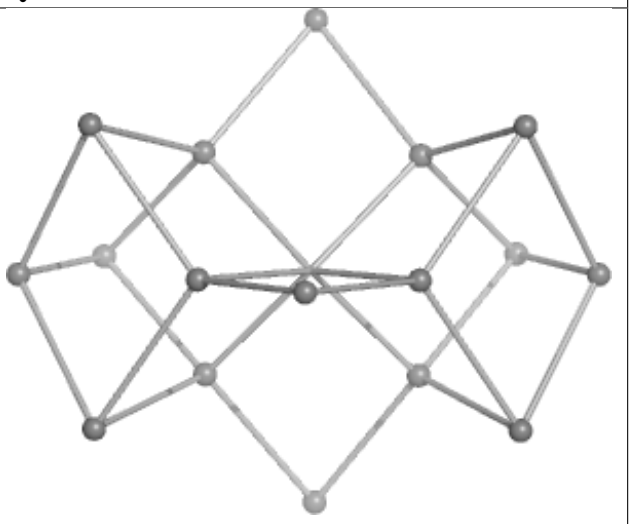


Rings

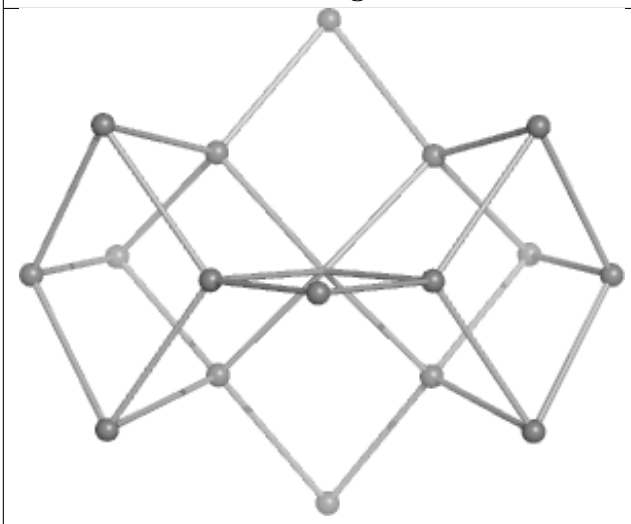
Ligand S5Q A 502



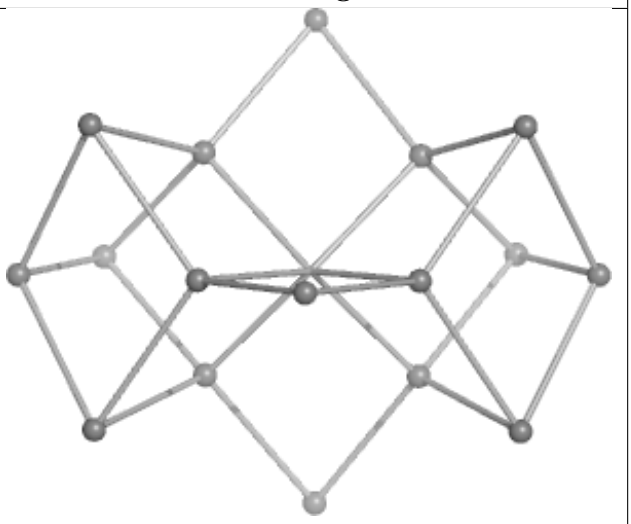
Bond lengths



Bond angles

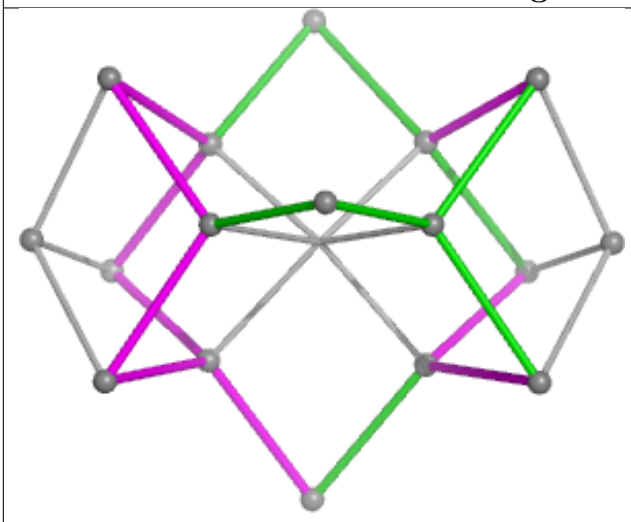


Torsions

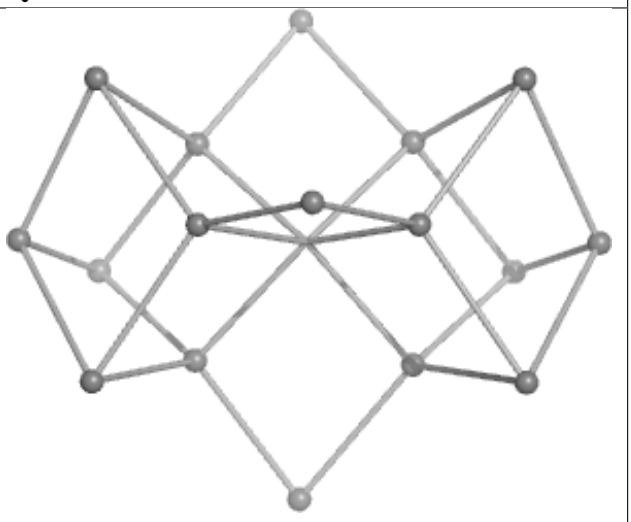


Rings

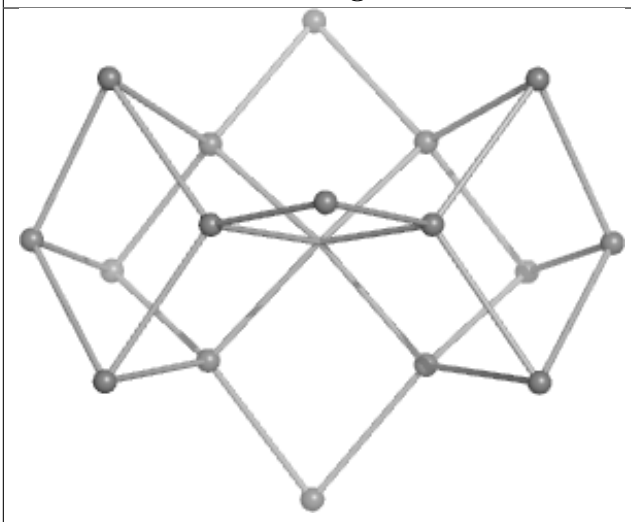
Ligand S5Q E 502



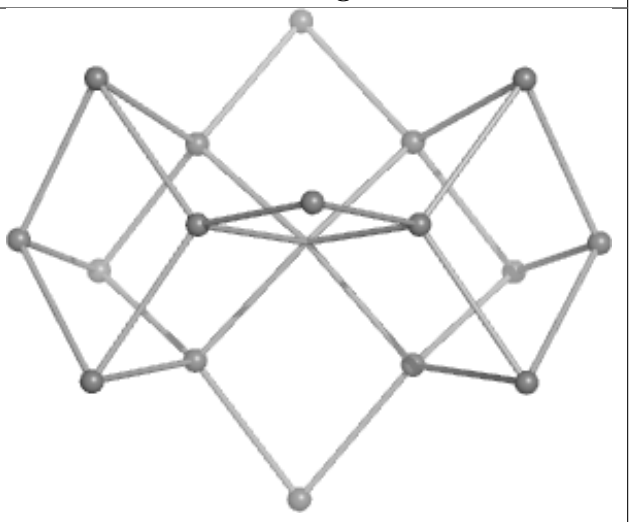
Bond lengths



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, 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	465/483 (96%)	-1.10	0 100 100	17, 42, 85, 104	0
1	C	465/483 (96%)	-0.89	0 100 100	28, 60, 120, 137	0
1	E	465/483 (96%)	-0.78	1 (0%) 91 89	32, 63, 142, 187	0
1	G	465/483 (96%)	-0.73	0 100 100	32, 72, 229, 250	0
2	B	450/458 (98%)	-1.11	0 100 100	10, 46, 72, 89	0
2	D	450/458 (98%)	-1.11	0 100 100	18, 49, 84, 91	0
2	F	451/458 (98%)	-0.88	0 100 100	28, 59, 95, 104	0
2	H	450/458 (98%)	-0.96	0 100 100	28, 58, 87, 99	0
All	All	3661/3764 (97%)	-0.94	1 (0%) 100 100	10, 56, 117, 250	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	10	LEU	2.1

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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	PEG	H	502	7/7	0.90	0.13	82,82,83,83	0
6	EDO	A	524	4/4	0.90	0.08	53,53,53,53	0
6	EDO	F	516	4/4	0.92	0.07	75,75,75,75	0
6	EDO	B	515	4/4	0.93	0.08	59,59,59,59	0
6	EDO	A	521	4/4	0.94	0.08	63,63,64,64	0
6	EDO	D	509	4/4	0.94	0.07	58,58,58,58	0
6	EDO	D	519	4/4	0.94	0.06	52,52,52,52	0
5	PEG	H	501	7/7	0.94	0.06	74,74,75,75	0
6	EDO	F	521	4/4	0.94	0.06	56,56,56,56	0
6	EDO	A	530	4/4	0.95	0.06	44,44,45,45	0
6	EDO	F	506	4/4	0.95	0.05	56,56,56,56	0
6	EDO	G	514	4/4	0.95	0.07	42,42,42,43	0
6	EDO	G	515	4/4	0.95	0.07	52,52,53,53	0
8	PGE	E	507	10/10	0.95	0.07	55,58,61,61	0
5	PEG	B	502	7/7	0.96	0.06	75,75,75,75	0
6	EDO	B	516	4/4	0.96	0.08	39,39,40,40	0
6	EDO	C	508	4/4	0.96	0.06	50,50,50,50	0
6	EDO	C	509	4/4	0.96	0.08	64,64,64,64	0
5	PEG	B	522	7/7	0.96	0.07	42,42,42,42	0
6	EDO	D	510	4/4	0.96	0.10	52,53,53,53	0
6	EDO	A	513	4/4	0.96	0.13	65,65,66,66	0
6	EDO	E	505	4/4	0.96	0.06	58,58,58,58	0
6	EDO	E	511	4/4	0.96	0.05	33,33,34,34	0
6	EDO	F	503	4/4	0.96	0.05	50,50,50,50	0
6	EDO	F	505	4/4	0.96	0.06	62,62,62,62	0
5	PEG	D	505	7/7	0.96	0.06	55,55,55,55	0
6	EDO	F	508	4/4	0.96	0.06	74,74,74,74	0
6	EDO	F	512	4/4	0.96	0.05	49,49,49,49	0
6	EDO	A	522	4/4	0.96	0.11	46,46,47,47	0
5	PEG	D	506	7/7	0.96	0.09	75,76,78,78	0
6	EDO	F	523	4/4	0.96	0.06	72,72,72,72	0
6	EDO	G	509	4/4	0.96	0.06	42,42,42,42	0
6	EDO	A	526	4/4	0.96	0.05	40,41,41,41	0
5	PEG	D	526	7/7	0.96	0.06	63,63,63,63	0
6	EDO	G	516	4/4	0.96	0.05	59,59,59,59	0
6	EDO	B	514	4/4	0.96	0.05	42,42,42,42	0
8	PGE	F	525	10/10	0.96	0.06	73,74,75,75	0
8	PGE	H	513	10/10	0.96	0.06	52,54,54,54	0
6	EDO	A	514	4/4	0.97	0.09	42,43,43,43	0
6	EDO	A	515	4/4	0.97	0.06	52,52,52,52	0
6	EDO	C	511	4/4	0.97	0.06	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	A	517	4/4	0.97	0.12	21,22,22,24	0
6	EDO	A	518	4/4	0.97	0.06	35,35,35,35	0
6	EDO	D	518	4/4	0.97	0.06	53,53,53,53	0
6	EDO	A	519	4/4	0.97	0.10	56,56,56,56	0
6	EDO	D	520	4/4	0.97	0.10	40,40,41,41	0
6	EDO	D	523	4/4	0.97	0.09	51,51,51,51	0
6	EDO	A	520	4/4	0.97	0.06	27,28,29,29	0
6	EDO	E	508	4/4	0.97	0.09	38,38,38,38	0
6	EDO	E	509	4/4	0.97	0.04	43,43,44,44	0
5	PEG	C	505	7/7	0.97	0.07	64,64,65,65	0
6	EDO	E	512	4/4	0.97	0.06	59,60,60,60	0
5	PEG	G	508	7/7	0.97	0.08	57,57,58,58	0
6	EDO	F	504	4/4	0.97	0.07	35,35,35,35	0
6	EDO	A	523	4/4	0.97	0.05	43,43,44,44	0
5	PEG	A	503	7/7	0.97	0.08	36,37,37,38	0
5	PEG	A	533	7/7	0.97	0.06	62,62,62,62	0
6	EDO	F	509	4/4	0.97	0.05	56,56,56,56	0
6	EDO	A	529	4/4	0.97	0.13	51,51,51,51	0
6	EDO	F	515	4/4	0.97	0.07	44,44,45,45	0
6	EDO	A	506	4/4	0.97	0.09	37,38,38,39	0
6	EDO	F	518	4/4	0.97	0.06	73,73,73,73	0
6	EDO	F	519	4/4	0.97	0.05	54,55,55,55	0
6	EDO	B	508	4/4	0.97	0.08	62,62,63,63	0
6	EDO	B	512	4/4	0.97	0.06	73,74,74,74	0
6	EDO	G	505	4/4	0.97	0.04	42,43,43,43	0
6	EDO	A	507	4/4	0.97	0.06	59,59,59,59	0
6	EDO	A	508	4/4	0.97	0.06	44,44,45,45	0
5	PEG	D	507	7/7	0.97	0.05	47,49,50,50	0
6	EDO	B	517	4/4	0.97	0.06	51,51,52,52	0
6	EDO	H	510	4/4	0.97	0.09	46,46,46,46	0
6	EDO	H	511	4/4	0.97	0.07	40,40,40,40	0
8	PGE	C	503	10/10	0.97	0.06	47,50,51,51	0
6	EDO	B	525	4/4	0.97	0.09	47,47,47,47	0
6	EDO	B	527	4/4	0.97	0.06	71,71,71,71	0
6	EDO	B	528	4/4	0.97	0.07	39,39,40,40	0
6	EDO	D	516	4/4	0.98	0.05	41,41,41,41	0
5	PEG	D	517	7/7	0.98	0.04	40,40,40,41	0
6	EDO	A	534	4/4	0.98	0.04	30,31,31,31	0
6	EDO	B	505	4/4	0.98	0.09	37,38,38,38	0
6	EDO	D	521	4/4	0.98	0.07	44,44,45,45	0
6	EDO	D	522	4/4	0.98	0.07	26,26,27,27	0
6	EDO	B	506	4/4	0.98	0.04	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	D	524	4/4	0.98	0.04	40,41,41,41	0
6	EDO	E	503	4/4	0.98	0.05	56,56,57,57	0
6	EDO	E	504	4/4	0.98	0.07	50,50,50,50	0
6	EDO	B	507	4/4	0.98	0.08	31,31,31,31	0
5	PEG	B	521	7/7	0.98	0.07	38,38,40,40	0
6	EDO	B	510	4/4	0.98	0.05	49,49,49,49	0
6	EDO	E	510	4/4	0.98	0.06	61,61,61,61	0
6	EDO	B	511	4/4	0.98	0.05	33,33,33,33	0
6	EDO	A	516	4/4	0.98	0.09	30,30,31,31	0
6	EDO	B	513	4/4	0.98	0.04	10,11,12,12	0
5	PEG	A	531	7/7	0.98	0.07	52,53,53,54	0
5	PEG	B	529	7/7	0.98	0.05	56,56,57,57	0
5	PEG	A	504	7/7	0.98	0.06	36,36,37,37	0
5	PEG	H	503	7/7	0.98	0.05	59,60,61,61	0
6	EDO	B	518	4/4	0.98	0.09	41,41,41,42	0
6	EDO	F	511	4/4	0.98	0.05	39,40,40,40	0
6	EDO	B	519	4/4	0.98	0.04	52,52,53,53	0
6	EDO	B	523	4/4	0.98	0.05	28,29,29,30	0
5	PEG	A	510	7/7	0.98	0.06	46,46,46,46	0
6	EDO	B	526	4/4	0.98	0.04	36,36,36,36	0
5	PEG	B	503	7/7	0.98	0.07	53,53,54,54	0
5	PEG	B	504	7/7	0.98	0.10	42,43,44,44	0
6	EDO	F	522	4/4	0.98	0.07	48,48,49,49	0
6	EDO	C	504	4/4	0.98	0.08	25,25,26,26	0
6	EDO	A	509	4/4	0.98	0.04	50,50,51,51	0
6	EDO	A	512	4/4	0.98	0.07	46,46,46,46	0
6	EDO	G	511	4/4	0.98	0.07	49,49,49,49	0
6	EDO	G	513	4/4	0.98	0.04	44,45,45,45	0
6	EDO	C	510	4/4	0.98	0.05	61,61,61,61	0
6	EDO	A	527	4/4	0.98	0.06	46,46,46,46	0
6	EDO	D	502	4/4	0.98	0.06	76,76,76,76	0
6	EDO	H	505	4/4	0.98	0.05	45,45,45,45	0
6	EDO	H	506	4/4	0.98	0.05	48,48,49,49	0
6	EDO	H	508	4/4	0.98	0.07	50,50,50,50	0
6	EDO	H	509	4/4	0.98	0.07	33,34,34,34	0
6	EDO	D	508	4/4	0.98	0.12	33,33,33,34	0
6	EDO	A	528	4/4	0.98	0.06	48,49,49,49	0
6	EDO	H	512	4/4	0.98	0.05	52,53,53,53	0
7	1PE	A	532	16/16	0.98	0.06	66,67,67,67	0
8	PGE	A	535	10/10	0.98	0.07	66,67,67,67	0
8	PGE	A	536	10/10	0.98	0.06	57,60,60,60	0
5	PEG	D	511	7/7	0.98	0.06	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	D	512	4/4	0.98	0.06	56,56,57,57	0
8	PGE	F	520	10/10	0.98	0.06	64,64,64,64	0
6	EDO	D	513	4/4	0.98	0.04	39,40,40,40	0
8	PGE	G	517	10/10	0.98	0.08	71,72,73,73	0
6	EDO	D	515	4/4	0.98	0.06	28,28,28,29	0
8	PGE	H	514	10/10	0.98	0.06	57,58,58,58	0
10	PG4	B	520	13/13	0.98	0.05	62,63,64,64	0
10	PG4	F	517	13/13	0.98	0.06	71,72,73,73	0
6	EDO	B	509	4/4	0.99	0.05	53,53,53,53	0
6	EDO	G	510	4/4	0.99	0.05	42,42,43,43	0
6	EDO	A	525	4/4	0.99	0.04	42,43,43,43	0
6	EDO	G	512	4/4	0.99	0.03	43,44,44,44	0
6	EDO	D	514	4/4	0.99	0.05	45,45,45,45	0
4	S5Q	C	502	18/18	0.99	0.03	128,128,128,128	0
5	PEG	H	504	7/7	0.99	0.05	44,44,45,45	0
5	PEG	A	505	7/7	0.99	0.06	57,58,59,59	0
6	EDO	C	506	4/4	0.99	0.03	30,31,32,32	0
6	EDO	C	507	4/4	0.99	0.03	27,28,28,28	0
6	EDO	H	507	4/4	0.99	0.05	41,42,42,42	0
5	PEG	D	504	7/7	0.99	0.06	57,59,59,59	0
6	EDO	F	510	4/4	0.99	0.05	48,49,49,49	0
5	PEG	F	507	7/7	0.99	0.04	50,50,50,50	0
5	PEG	G	506	7/7	0.99	0.07	32,33,34,34	0
6	EDO	F	513	4/4	0.99	0.06	63,63,63,63	0
6	EDO	F	514	4/4	0.99	0.04	44,44,45,45	0
6	EDO	A	511	4/4	0.99	0.09	75,75,76,76	0
6	EDO	D	525	4/4	0.99	0.04	38,38,39,39	0
4	S5Q	E	502	18/18	0.99	0.04	141,141,141,141	0
6	EDO	D	503	4/4	0.99	0.10	35,36,36,36	0
4	S5Q	G	502	18/18	0.99	0.03	153,153,153,153	0
8	PGE	F	524	10/10	0.99	0.06	64,65,65,65	0
6	EDO	E	506	4/4	0.99	0.05	36,36,37,37	0
3	SF4	E	501	8/8	0.99	0.03	57,58,58,59	0
6	EDO	G	503	4/4	0.99	0.06	61,61,61,61	0
6	EDO	G	504	4/4	0.99	0.03	51,51,51,51	0
6	EDO	B	524	4/4	0.99	0.03	25,26,26,27	0
6	EDO	G	507	4/4	0.99	0.05	43,43,44,44	0
3	SF4	A	501	8/8	1.00	0.02	29,29,30,31	0
3	SF4	G	501	8/8	1.00	0.02	49,49,50,50	0
9	MG	B	501	1/1	1.00	0.05	22,22,22,22	0
9	MG	D	501	1/1	1.00	0.01	32,32,32,32	0
9	MG	F	501	1/1	1.00	0.02	33,33,33,33	0

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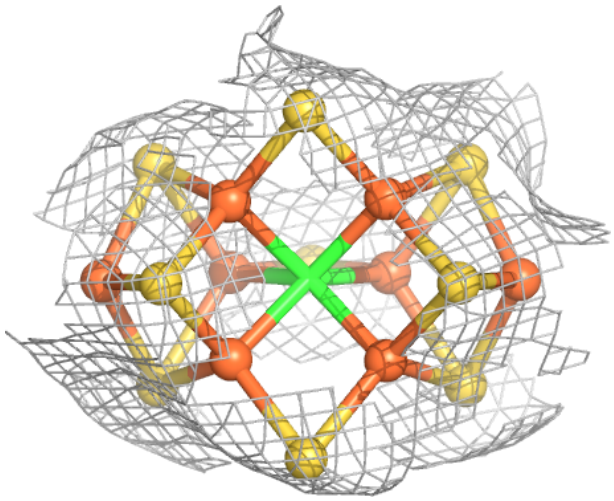
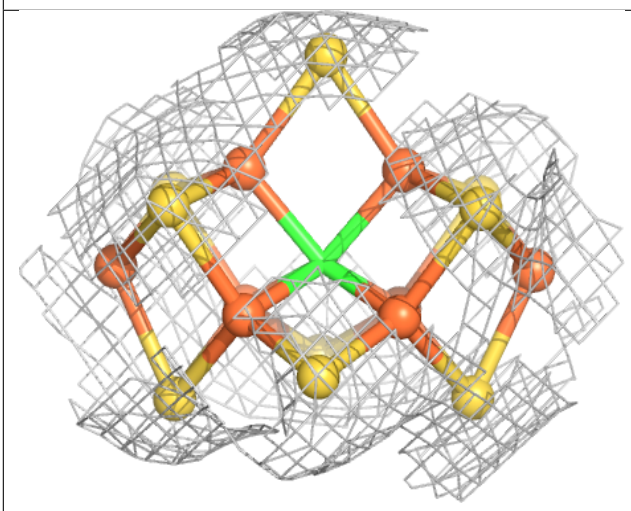
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MG	F	502	1/1	1.00	0.01	49,49,49,49	0
4	S5Q	A	502	18/18	1.00	0.02	52,53,53,53	0
3	SF4	C	501	8/8	1.00	0.02	36,36,37,37	0

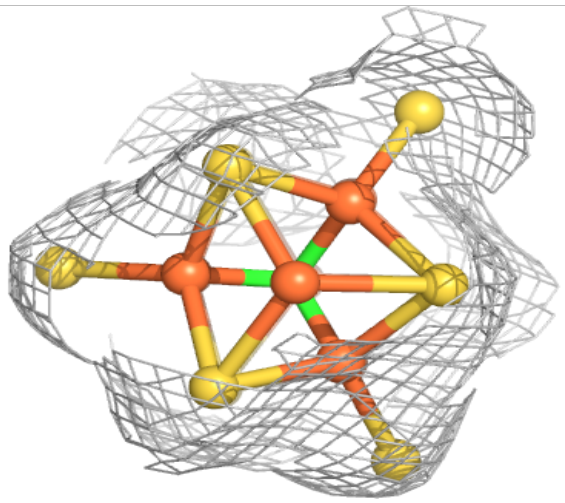
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around S5Q C 502:

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

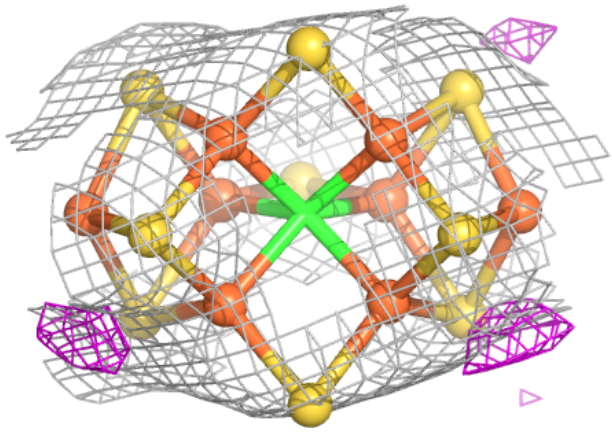


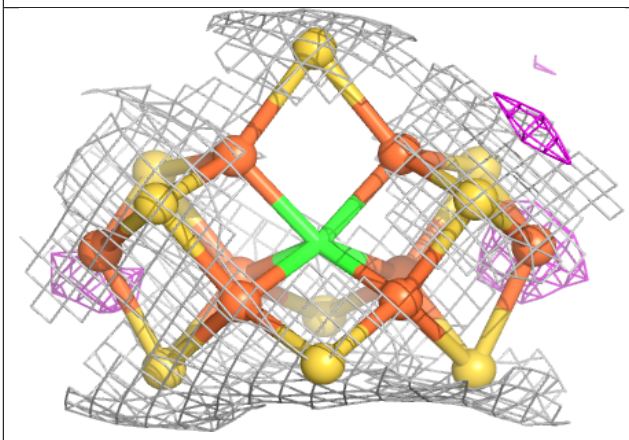


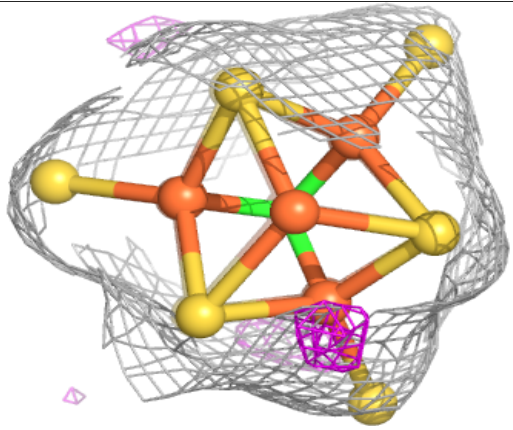


Electron density around S5Q E 502:

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

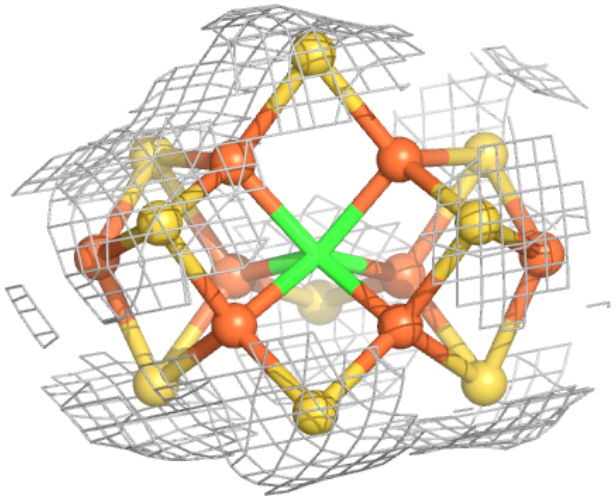


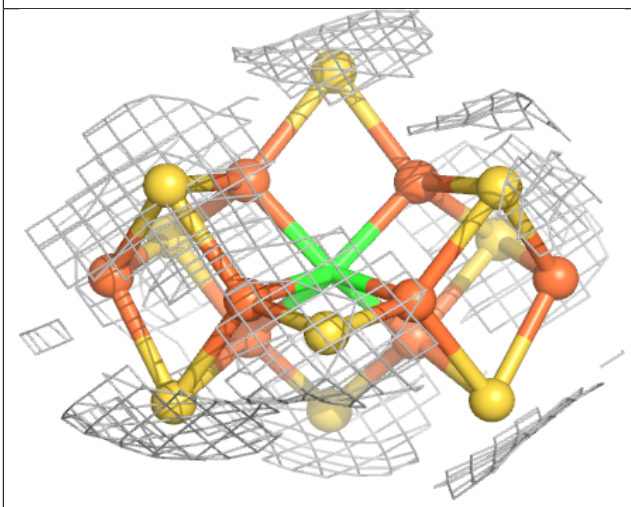


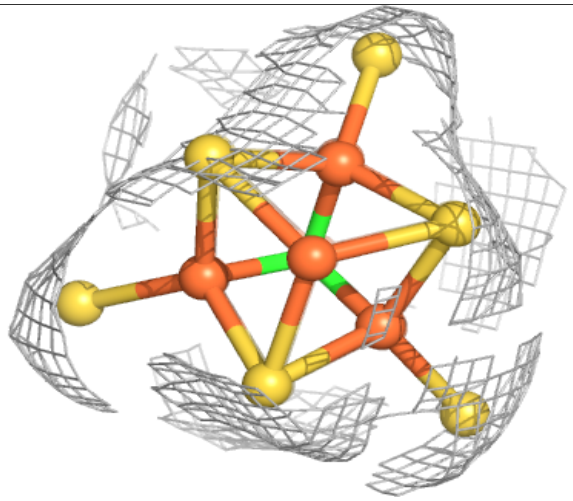


Electron density around S5Q G 502:

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

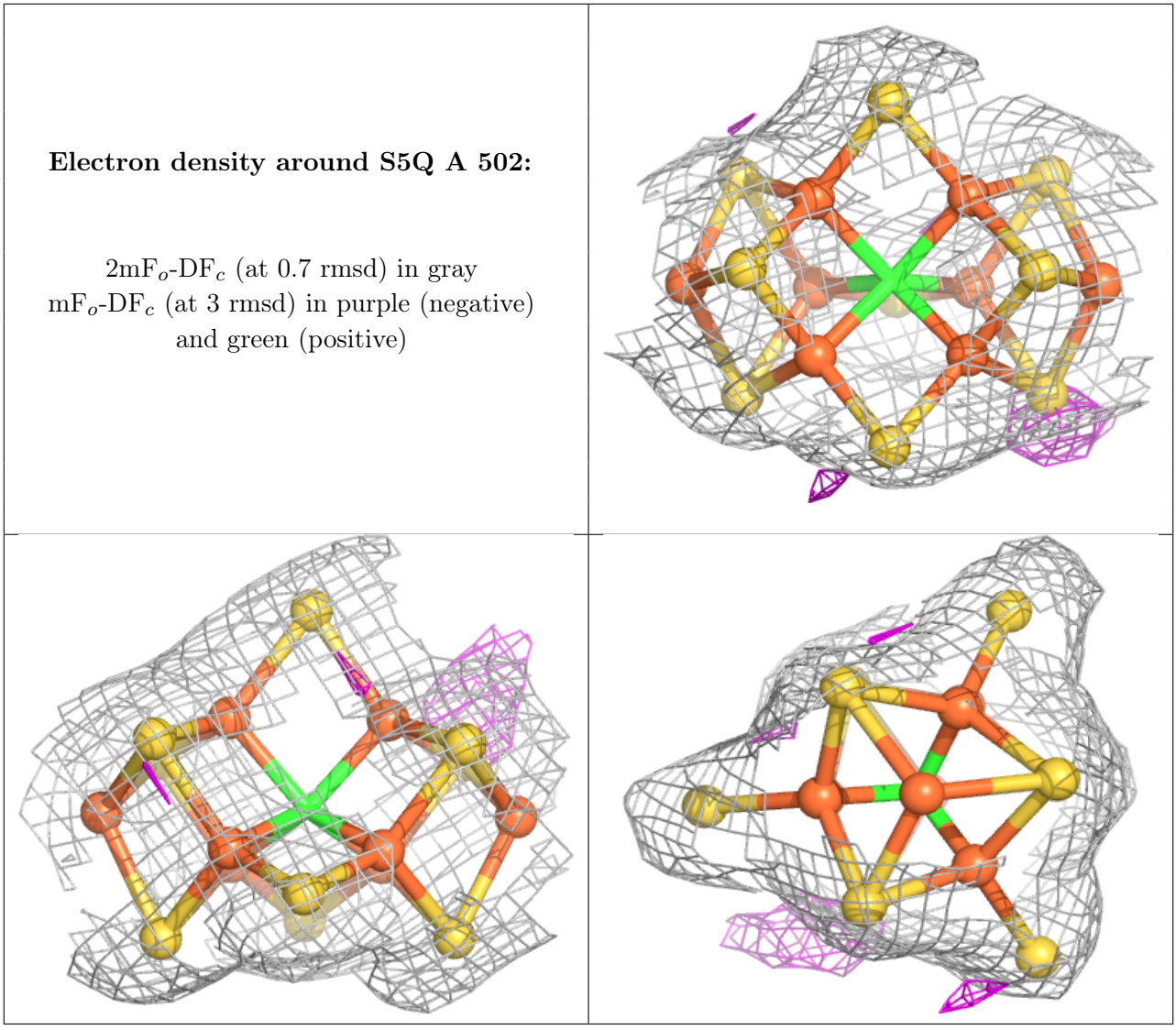






Electron density around S5Q A 502:

$2mF_o$-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.