



Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2026 – 09:53 am 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

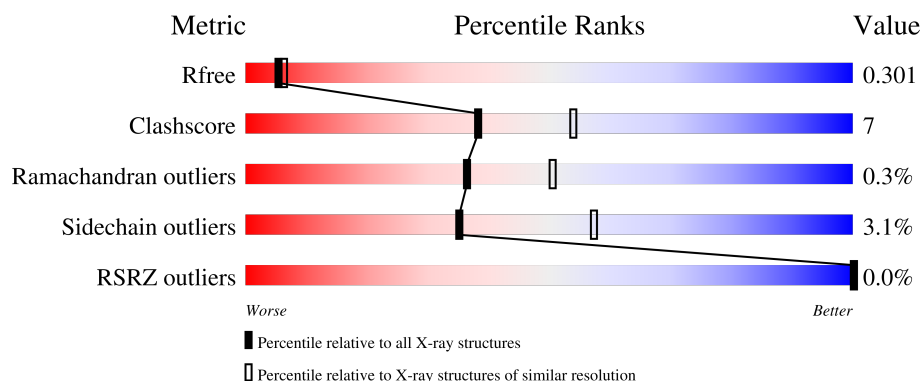
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




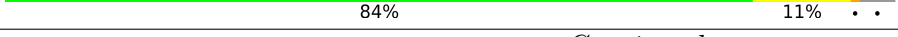
The reported resolution of this entry is 2.40 Å.

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	483	
1	C	483	
1	E	483	
1	G	483	

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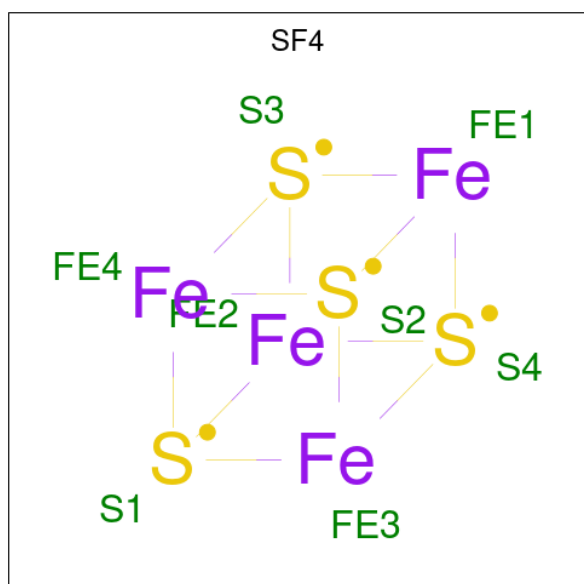
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	HIS	-	expression tag	UNP C1DH03
E	-2	HIS	-	expression tag	UNP C1DH03
E	-1	HIS	-	expression tag	UNP C1DH03
E	0	HIS	-	expression tag	UNP C1DH03
G	-7	MET	-	initiating methionine	UNP C1DH03
G	-6	HIS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

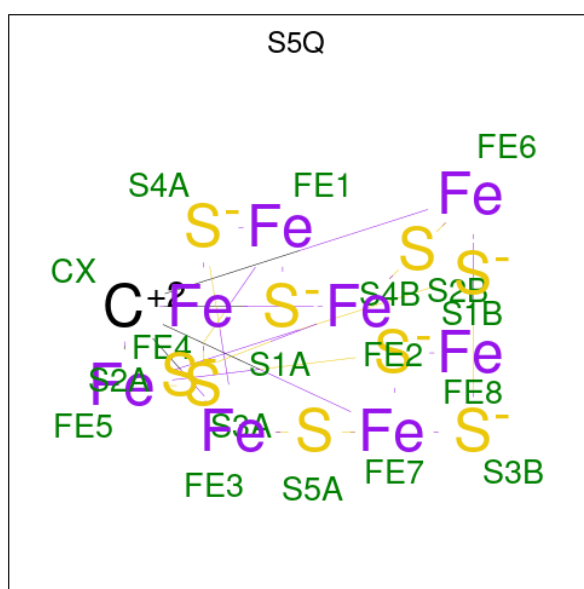
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	450	Total	C	N	O	S	0	0	0
			3386	2129	603	639	15			
2	D	450	Total	C	N	O	S	0	0	0
			3386	2129	603	639	15			
2	F	451	Total	C	N	O	S	0	0	0
			3394	2134	604	640	16			
2	H	450	Total	C	N	O	S	0	0	0
			3386	2129	603	639	15			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- 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	0	0
			18	1	8	9		
4	C	1	Total	C	Fe	S	0	0
			18	1	8	9		
4	E	1	Total	C	Fe	S	0	0
			18	1	8	9		
4	G	1	Total	C	Fe	S	0	0
			18	1	8	9		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $\text{C}_4\text{H}_{10}\text{O}_3$).



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	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: C₂H₆O₂).



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		

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

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

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

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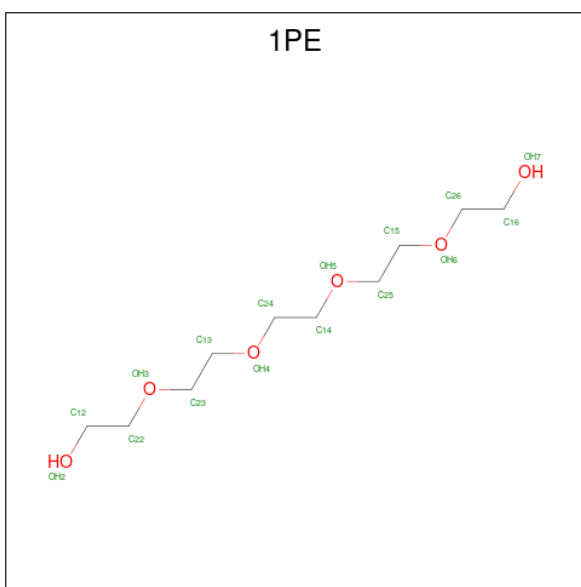
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0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

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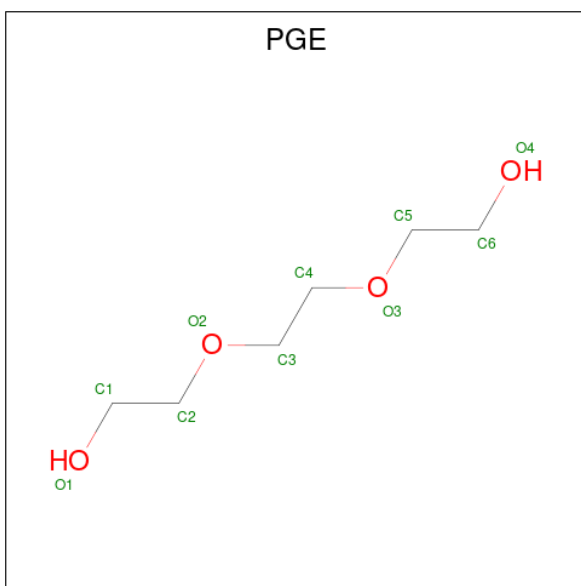
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0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

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



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

- 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	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		
8	C	1	Total	C	O	0	0
			10	6	4		

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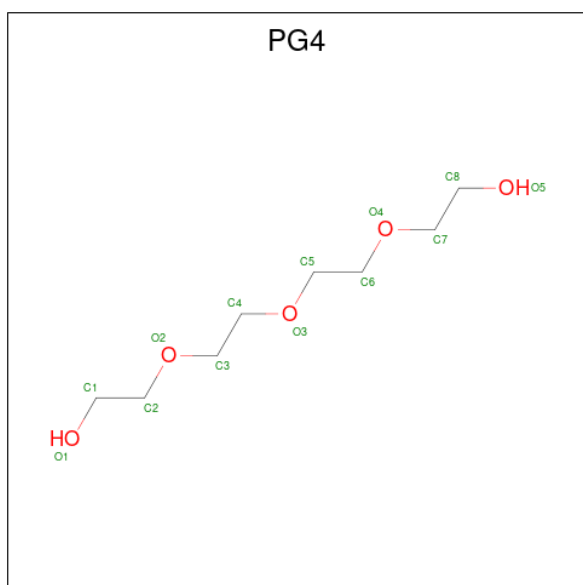
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			10	6	4		
8	F	1	Total	C	O	0	0
			10	6	4		
8	F	1	Total	C	O	0	0
			10	6	4		
8	F	1	Total	C	O	0	0
			10	6	4		
8	G	1	Total	C	O	0	0
			10	6	4		
8	H	1	Total	C	O	0	0
			10	6	4		
8	H	1	Total	C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

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

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

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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

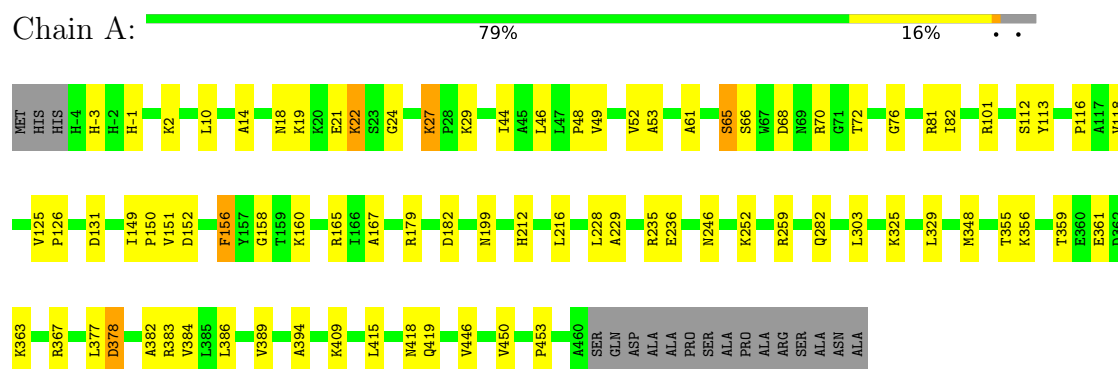
- Molecule 11 is water.

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

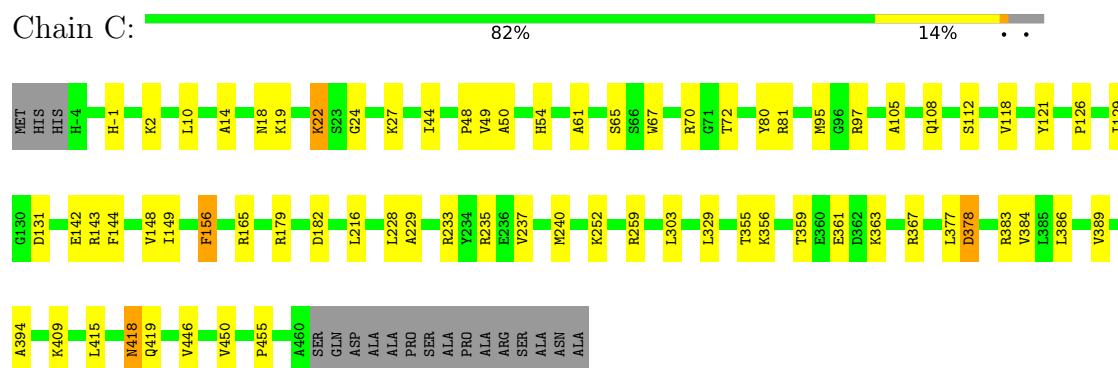
3 Residue-property plots

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

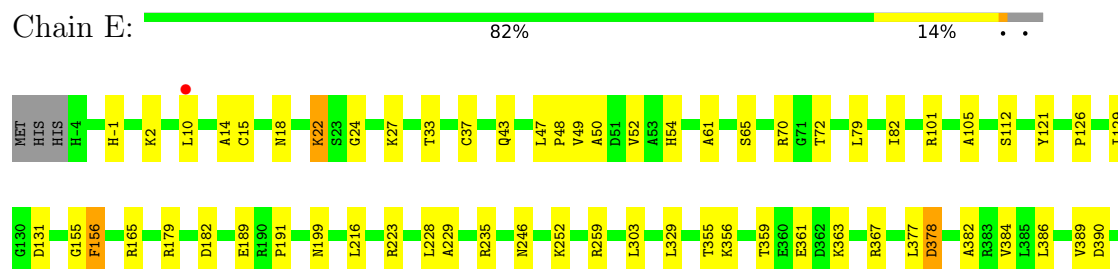
- Molecule 1: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE

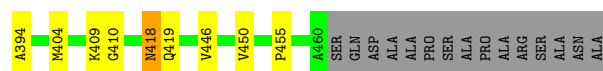


- Molecule 1: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE



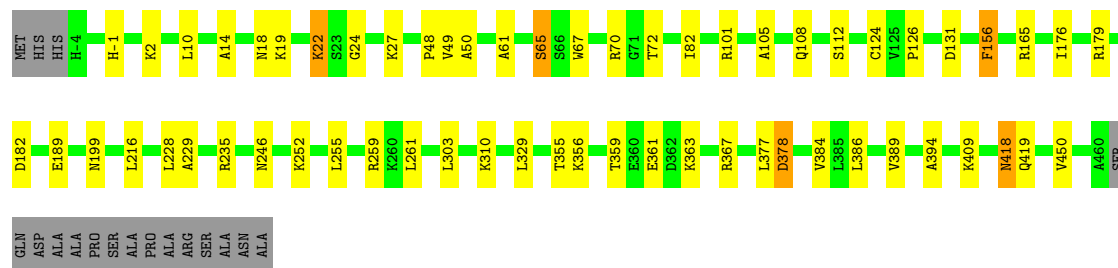
- Molecule 1: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE





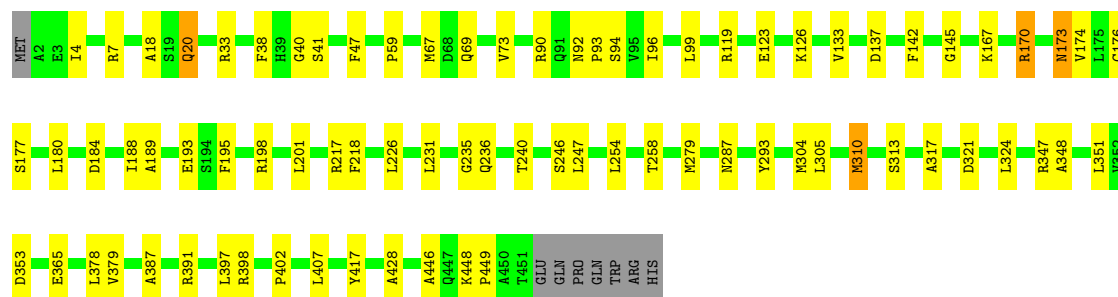
- Molecule 1: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE

Chain G: 84% 11% ..



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

Chain B: 81% 16% ..



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

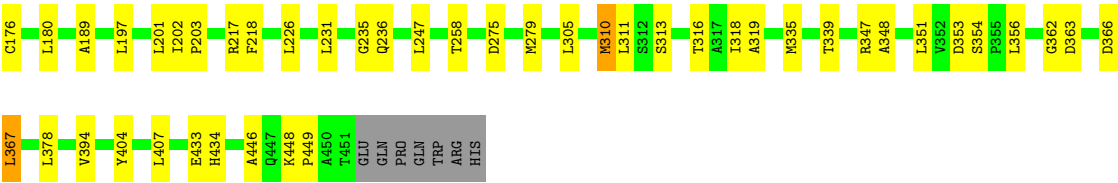
Chain D: 83% 15% .



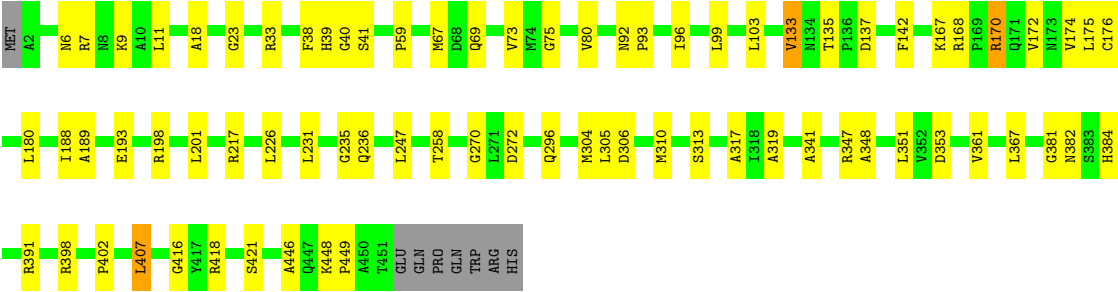
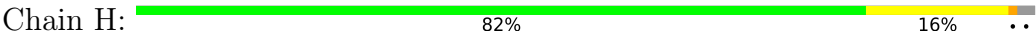
- Molecule 2: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifN

Chain F: 81% 16% ..





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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, 1PE, SF4, PG4, MG, EDO, PGE, S5Q

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

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	G	49	VAL	CA-C-N	6.58	129.40	120.38
1	G	49	VAL	C-N-CA	6.58	129.40	120.38
2	D	414	TRP	CA-C-N	6.54	131.20	120.94
2	D	414	TRP	C-N-CA	6.54	131.20	120.94
1	E	49	VAL	CA-C-N	6.46	129.24	120.38
1	E	49	VAL	C-N-CA	6.46	129.24	120.38
1	E	156	PHE	CA-CB-CG	6.42	120.22	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	50	ALA	N-CA-C	6.29	118.94	111.33
1	E	50	ALA	N-CA-C	6.28	118.93	111.33
1	C	156	PHE	CA-CB-CG	6.26	120.06	113.80
2	H	38	PHE	CA-CB-CG	6.17	119.97	113.80
2	F	38	PHE	CA-CB-CG	6.08	119.88	113.80
2	F	394	VAL	N-CA-C	5.95	114.45	107.84
1	G	50	ALA	N-CA-C	5.95	118.53	111.33
2	D	38	PHE	CA-CB-CG	5.94	119.74	113.80
2	B	38	PHE	CA-CB-CG	5.87	119.67	113.80
1	G	156	PHE	CA-CB-CG	5.78	119.58	113.80
2	H	306	ASP	CA-CB-CG	5.75	118.35	112.60
2	F	19	SER	CA-C-N	5.70	128.48	120.28
2	F	19	SER	C-N-CA	5.70	128.48	120.28
1	A	156	PHE	CA-CB-CG	5.53	119.33	113.80
2	D	16	LEU	CA-C-N	5.46	128.46	120.71
2	D	16	LEU	C-N-CA	5.46	128.46	120.71
2	D	19	SER	CA-C-N	5.43	127.55	120.28
2	D	19	SER	C-N-CA	5.43	127.55	120.28
2	D	4	ILE	N-CA-C	5.39	116.04	109.30
2	F	141	CYS	CA-C-N	5.38	127.48	120.28
2	F	141	CYS	C-N-CA	5.38	127.48	120.28
2	D	141	CYS	CA-C-N	5.25	127.31	120.28
2	D	141	CYS	C-N-CA	5.25	127.31	120.28
1	E	418	ASN	CA-CB-CG	5.21	117.81	112.60
1	G	418	ASN	CA-CB-CG	5.17	117.77	112.60
1	C	418	ASN	CA-CB-CG	5.07	117.67	112.60
2	B	184	ASP	CA-CB-CG	5.03	117.62	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3591	0	3571	61	0
1	C	3591	0	3571	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
2:D:369:HIS:HA	5:D:507:PEG:H11	1.47	0.96
2:D:369:HIS:HA	5:D:507:PEG:C1	1.97	0.95
1:G:310:LYS:NZ	6:G:503:EDO:H21	1.81	0.94
7:A:532:1PE:H131	2:B:391:ARG:HD3	1.50	0.94
2:B:119:ARG:HD2	6:B:505:EDO:H21	1.50	0.92
2:H:319:ALA:HB2	2:H:367:LEU:HD22	1.52	0.92
1:C:97:ARG:HA	6:C:506:EDO:C2	1.99	0.90
1:A:68:ASP:HA	5:A:503:PEG:H32	1.55	0.88
1:A:325:LYS:HB2	1:A:348:MET:HE3	1.56	0.88
2:D:319:ALA:HB2	2:D:367:LEU:HD22	1.57	0.87
7:A:532:1PE:H242	2:B:391:ARG:HH21	1.40	0.87
2:B:293:TYR:HD1	6:B:509:EDO:H22	1.40	0.86
1:A:101:ARG:NH2	2:B:7:ARG:NH1	2.25	0.83
1:A:22:LYS:HB3	4:A:502:S5Q:S4A	2.19	0.83
1:A:453:PRO:HA	6:A:522:EDO:H21	1.59	0.82
2:B:195:PHE:HA	5:B:503:PEG:C1	2.09	0.82
1:G:22:LYS:HB3	4:G:502:S5Q:S4A	2.19	0.82
1:C:22:LYS:HB3	4:C:502:S5Q:S4A	2.20	0.82
1:E:22:LYS:HB3	4:E:502:S5Q:S4A	2.20	0.81
1:G:310:LYS:HZ2	6:G:503:EDO:H21	1.44	0.79
3:C:501:SF4:S3	2:D:41:SER:HB3	2.23	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:TYR:CD1	6:B:509:EDO:H22	2.19	0.77
2:D:384:HIS:CA	6:D:520:EDO:H21	2.10	0.77
2:F:1:MET:HB2	2:F:354:SER:O	1.84	0.76
2:F:319:ALA:HB2	2:F:367:LEU:HD13	1.69	0.74
2:D:414:TRP:NE1	5:D:504:PEG:H21	2.02	0.74
2:H:272:ASP:HB2	6:H:507:EDO:H22	1.68	0.74
2:H:168:ARG:HH22	2:H:198:ARG:NH2	1.87	0.73
2:D:384:HIS:HA	6:D:520:EDO:C2	2.12	0.73
2:F:128:VAL:HG12	11:F:602:HOH:O	1.87	0.72
1:A:101:ARG:HH22	2:B:7:ARG:NH1	1.84	0.72
5:G:506:PEG:H32	2:H:391:ARG:HH12	1.55	0.72
7:A:532:1PE:H242	2:B:391:ARG:NH2	2.05	0.71
1:E:47:LEU:HD21	6:E:508:EDO:H21	1.71	0.71
1:A:101:ARG:NH2	2:B:7:ARG:HH12	1.87	0.70
1:E:-1:HIS:ND1	2:F:73:VAL:HG21	2.06	0.70
1:E:48:PRO:HB3	1:E:72:THR:HG21	1.75	0.69
1:A:48:PRO:HB3	1:A:72:THR:HG21	1.74	0.69
2:B:123:GLU:HA	6:B:505:EDO:H11	1.75	0.69
2:D:372:ARG:NH2	5:D:507:PEG:O1	2.25	0.69
1:G:-1:HIS:ND1	2:H:73:VAL:HG21	2.09	0.68
1:A:235:ARG:NH1	6:A:516:EDO:O2	2.27	0.68
2:H:296:GLN:OE1	5:H:504:PEG:C1	2.42	0.68
1:G:48:PRO:HB3	1:G:72:THR:HG21	1.76	0.68
1:G:310:LYS:HZ3	6:G:503:EDO:H21	1.57	0.68
1:C:48:PRO:HB3	1:C:72:THR:HG21	1.75	0.67
1:C:97:ARG:CA	6:C:506:EDO:H21	2.07	0.67
5:G:506:PEG:H32	2:H:391:ARG:NH1	2.10	0.67
2:B:398:ARG:NH1	6:B:513:EDO:H11	2.08	0.67
1:E:15:CYS:SG	1:E:252:LYS:NZ	2.67	0.67
1:C:95:MET:SD	1:C:97:ARG:NH1	2.69	0.66
1:G:101:ARG:HH22	2:H:7:ARG:NH1	1.93	0.65
1:C:126:PRO:HA	1:C:129:ILE:HG12	1.78	0.65
2:D:369:HIS:HA	5:D:507:PEG:H12	1.76	0.65
2:H:296:GLN:OE1	5:H:504:PEG:H11	1.97	0.64
1:C:252:LYS:NZ	1:C:361:GLU:CD	2.56	0.64
2:H:198:ARG:CA	8:H:514:PGE:H2	2.22	0.64
1:A:101:ARG:HH21	2:B:7:ARG:HH12	1.46	0.64
2:D:390:ARG:HE	6:D:513:EDO:C2	2.10	0.64
1:E:-1:HIS:ND1	2:F:73:VAL:CG2	2.62	0.63
1:A:252:LYS:HD2	1:A:361:GLU:HG3	1.81	0.63
2:H:226:LEU:HD21	2:H:231:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:ARG:NH1	4:G:502:S5Q:S1B	2.72	0.63
1:C:216:LEU:HD22	1:C:303:LEU:HD21	1.81	0.62
1:A:48:PRO:HB2	1:A:229:ALA:O	1.99	0.62
1:A:282:GLN:HG2	6:A:521:EDO:H22	1.82	0.62
1:E:165:ARG:NH1	4:E:502:S5Q:S1B	2.73	0.62
1:C:165:ARG:NH1	4:C:502:S5Q:S1B	2.73	0.62
2:B:226:LEU:HD21	2:B:231:LEU:HD13	1.81	0.62
8:G:517:PGE:H52	2:H:402:PRO:HD3	1.83	0.61
1:C:252:LYS:HZ1	1:C:361:GLU:CD	2.08	0.61
2:D:226:LEU:HD21	2:D:231:LEU:HD13	1.83	0.61
1:E:216:LEU:HD22	1:E:303:LEU:HD21	1.83	0.61
3:A:501:SF4:S3	2:B:41:SER:HB3	2.41	0.61
1:G:101:ARG:NH2	2:H:7:ARG:NH1	2.48	0.61
1:A:325:LYS:HB2	1:A:348:MET:CE	2.28	0.60
1:C:252:LYS:HZ3	1:C:361:GLU:HG3	1.66	0.60
1:G:216:LEU:HD22	1:G:303:LEU:HD21	1.83	0.60
1:A:68:ASP:HA	5:A:503:PEG:C3	2.30	0.60
2:B:193:GLU:HG2	6:B:511:EDO:H21	1.83	0.60
1:G:101:ARG:NH2	2:H:7:ARG:HH12	1.98	0.60
1:C:48:PRO:HB2	1:C:229:ALA:O	2.02	0.60
1:A:359:THR:HG22	4:A:502:S5Q:S2A	2.41	0.60
2:B:195:PHE:CA	5:B:503:PEG:H11	2.26	0.60
1:C:356:LYS:H	1:C:378:ASP:HA	1.67	0.60
1:E:48:PRO:HB2	1:E:229:ALA:O	2.01	0.60
1:G:48:PRO:HB2	1:G:229:ALA:O	2.02	0.60
2:B:126:LYS:HA	6:B:505:EDO:H22	1.84	0.60
1:A:165:ARG:NH1	4:A:502:S5Q:S1B	2.74	0.59
1:C:359:THR:HG22	4:C:502:S5Q:S2A	2.42	0.59
1:E:356:LYS:H	1:E:378:ASP:HA	1.67	0.59
1:A:356:LYS:H	1:A:378:ASP:HA	1.66	0.59
2:D:372:ARG:HD2	5:D:507:PEG:H22	1.84	0.59
1:E:359:THR:HG22	4:E:502:S5Q:S2A	2.43	0.59
1:G:105:ALA:HB1	2:H:11:LEU:HD13	1.84	0.59
2:B:310:MET:HG3	2:B:428:ALA:HB1	1.85	0.59
2:F:434:HIS:HE1	8:F:525:PGE:O3	1.86	0.59
1:G:252:LYS:NZ	1:G:361:GLU:HG3	2.18	0.59
1:G:409:LYS:HZ3	2:H:59:PRO:HD3	1.68	0.59
1:A:216:LEU:HD22	1:A:303:LEU:HD21	1.85	0.58
1:G:24:GLY:HA3	4:G:502:S5Q:S2A	2.44	0.58
1:G:356:LYS:H	1:G:378:ASP:HA	1.67	0.58
1:G:359:THR:HG22	4:G:502:S5Q:S2A	2.42	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLY:HA3	4:A:502:S5Q:S2A	2.44	0.58
2:B:123:GLU:HA	6:B:505:EDO:C1	2.34	0.58
1:G:310:LYS:NZ	6:G:503:EDO:C2	2.64	0.57
1:G:-1:HIS:ND1	2:H:73:VAL:CG2	2.67	0.57
2:D:112:HIS:HD2	11:D:719:HOH:O	1.88	0.57
1:E:24:GLY:HA3	4:E:502:S5Q:S2A	2.45	0.57
1:G:108:GLN:HE22	2:H:9:LYS:HD2	1.69	0.57
1:C:24:GLY:HA3	4:C:502:S5Q:S2A	2.44	0.57
1:A:76:GLY:HA2	5:A:533:PEG:H42	1.85	0.57
1:C:70:ARG:HH22	1:C:419:GLN:HB2	1.70	0.57
1:C:54:HIS:ND1	1:C:121:TYR:OH	2.30	0.56
1:A:-1:HIS:ND1	2:B:73:VAL:HG21	2.20	0.56
1:A:70:ARG:HH22	1:A:419:GLN:HB2	1.70	0.56
1:A:116:PRO:HD3	8:A:535:PGE:H5	1.85	0.56
2:F:226:LEU:HD21	2:F:231:LEU:HD13	1.88	0.56
1:G:70:ARG:HH22	1:G:419:GLN:HB2	1.71	0.56
2:B:4:ILE:HD11	2:B:351:LEU:HB3	1.87	0.55
2:B:417:TYR:HB2	6:B:509:EDO:H21	1.87	0.55
1:E:70:ARG:HH22	1:E:419:GLN:HB2	1.71	0.55
1:G:82:ILE:HD13	5:G:506:PEG:H21	1.87	0.55
2:B:398:ARG:HH21	5:B:504:PEG:H22	1.72	0.55
1:A:389:VAL:HG13	1:A:394:ALA:HB3	1.89	0.55
1:E:37:CYS:SG	2:F:43:GLY:HA3	2.47	0.54
1:C:126:PRO:O	1:C:131:ASP:HB2	2.07	0.54
1:C:144:PHE:HB2	11:C:650:HOH:O	2.07	0.54
1:G:409:LYS:HZ1	2:H:59:PRO:HD2	1.73	0.54
1:A:150:PRO:HG3	6:A:520:EDO:H22	1.90	0.54
2:D:319:ALA:CB	2:D:367:LEU:HD22	2.35	0.54
1:E:355:THR:HG22	1:E:377:LEU:HB2	1.90	0.54
1:C:355:THR:HG22	1:C:377:LEU:HB2	1.90	0.54
1:C:389:VAL:HG13	1:C:394:ALA:HB3	1.90	0.53
1:G:65:SER:HA	8:G:517:PGE:H42	1.89	0.53
1:A:355:THR:HG22	1:A:377:LEU:HB2	1.91	0.53
1:E:33:THR:H	2:F:63:GLN:HE22	1.56	0.53
2:D:390:ARG:HD3	6:D:521:EDO:H12	1.90	0.53
1:G:355:THR:HG22	1:G:377:LEU:HB2	1.90	0.53
1:G:389:VAL:HG13	1:G:394:ALA:HB3	1.91	0.53
2:B:94:SER:HA	6:B:506:EDO:H21	1.90	0.53
1:A:149:ILE:HD11	11:A:611:HOH:O	2.08	0.53
1:A:158:GLY:HA3	11:A:647:HOH:O	2.08	0.53
1:E:54:HIS:HB3	1:E:121:TYR:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:HIS:NE2	2:D:438:ILE:HD13	2.25	0.52
2:F:316:THR:HG22	2:F:378:LEU:HB3	1.92	0.52
2:B:4:ILE:HG21	2:B:347:ARG:HG2	1.90	0.52
2:H:235:GLY:HA2	2:H:258:THR:HB	1.90	0.52
1:E:382:ALA:HB3	2:F:218:PHE:CE1	2.46	0.51
2:H:361:VAL:HG11	6:H:509:EDO:H11	1.92	0.51
1:C:-1:HIS:ND1	2:D:73:VAL:HG21	2.25	0.51
2:D:133:VAL:HG22	2:D:135:THR:HG23	1.93	0.51
1:E:191:PRO:HA	6:E:504:EDO:H22	1.91	0.51
2:B:20:GLN:HG2	2:B:145:GLY:CA	2.41	0.51
1:A:446:VAL:HG23	2:D:304:MET:HE2	1.93	0.51
2:F:133:VAL:HG22	2:F:135:THR:HG23	1.93	0.51
1:G:310:LYS:HZ3	6:G:503:EDO:C2	2.21	0.51
2:B:324:LEU:HD12	6:B:518:EDO:H12	1.93	0.51
1:E:389:VAL:HG13	1:E:394:ALA:HB3	1.92	0.50
2:H:193:GLU:HG2	8:H:514:PGE:H22	1.91	0.50
1:C:142:GLU:HG3	11:C:677:HOH:O	2.11	0.50
1:C:233:ARG:HH11	6:C:507:EDO:HO1	1.56	0.50
1:E:446:VAL:HG23	2:H:304:MET:HE2	1.93	0.50
2:H:381:GLY:O	2:H:398:ARG:HA	2.12	0.50
1:A:-1:HIS:ND1	2:B:73:VAL:CG2	2.75	0.50
1:A:44:ILE:HD12	1:A:160:LYS:HE3	1.93	0.50
2:D:397:LEU:HD12	6:D:522:EDO:H21	1.94	0.50
1:C:67:TRP:CH2	6:D:503:EDO:H21	2.47	0.49
2:H:341:ALA:HA	5:H:503:PEG:H12	1.95	0.49
1:A:235:ARG:HD3	2:D:449:PRO:HD3	1.94	0.49
2:B:173:ASN:ND2	2:B:240:THR:OG1	2.46	0.49
2:F:363:ASP:OD1	2:F:366:ASP:OD1	2.30	0.49
1:E:252:LYS:HG3	1:E:361:GLU:HG3	1.94	0.49
2:F:93:PRO:HG2	2:F:96:ILE:HD11	1.95	0.49
2:H:40:GLY:HA2	2:H:67:MET:SD	2.52	0.49
1:A:53:ALA:HB3	1:A:118:VAL:HG22	1.94	0.49
2:D:451:THR:HB	5:D:526:PEG:C4	2.42	0.49
2:D:175:LEU:HD12	2:D:242:VAL:HG22	1.94	0.49
2:B:167:LYS:HB3	2:B:236:GLN:HG2	1.95	0.49
2:H:168:ARG:NH2	2:H:198:ARG:NH2	2.57	0.49
1:E:182:ASP:O	1:E:223:ARG:NH1	2.46	0.49
2:F:189:ALA:HB2	2:F:201:LEU:HD11	1.93	0.49
2:F:448:LYS:HB3	6:G:505:EDO:H12	1.94	0.49
2:H:175:LEU:HB3	2:H:247:LEU:HD13	1.95	0.48
2:B:446:ALA:HB1	2:B:448:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:93:PRO:HG2	2:H:96:ILE:HD11	1.96	0.48
2:B:348:ALA:HB1	6:B:528:EDO:H12	1.96	0.48
2:F:446:ALA:HB1	2:F:448:LYS:HG3	1.94	0.48
2:H:449:PRO:HD2	8:H:513:PGE:H6	1.96	0.48
1:C:-1:HIS:ND1	2:D:73:VAL:CG2	2.77	0.48
1:C:80:TYR:OH	1:C:81:ARG:NH2	2.46	0.48
1:C:377:LEU:HD22	1:C:384:VAL:HG12	1.96	0.48
2:D:393:GLY:HA2	6:D:521:EDO:H22	1.96	0.48
1:C:228:LEU:HA	1:C:229:ALA:HA	1.70	0.48
1:E:105:ALA:HB1	2:F:11:LEU:HD13	1.96	0.48
1:A:46:LEU:HD21	1:A:167:ALA:HB1	1.96	0.48
2:D:384:HIS:O	6:D:503:EDO:O1	2.27	0.48
8:G:517:PGE:H32	2:H:384:HIS:NE2	2.29	0.48
2:B:176:CYS:HB3	2:B:180:LEU:HD12	1.96	0.48
1:A:377:LEU:HD22	1:A:384:VAL:HG12	1.96	0.47
2:H:133:VAL:HG22	2:H:135:THR:HG23	1.96	0.47
2:D:451:THR:HB	5:D:526:PEG:H41	1.95	0.47
1:E:377:LEU:HD22	1:E:384:VAL:HG12	1.96	0.47
2:F:172:VAL:HG21	2:F:197:LEU:HD13	1.95	0.47
1:G:377:LEU:HD22	1:G:384:VAL:HG12	1.96	0.47
2:H:449:PRO:O	8:H:513:PGE:O3	2.32	0.47
2:D:390:ARG:HE	6:D:513:EDO:H21	1.77	0.47
1:G:14:ALA:HB2	1:G:259:ARG:HD3	1.96	0.47
1:G:67:TRP:HH2	5:G:506:PEG:H41	1.79	0.47
2:D:93:PRO:HG2	2:D:96:ILE:HD11	1.95	0.47
2:B:18:ALA:HB3	2:B:142:PHE:HB2	1.96	0.47
2:B:33:ARG:NH1	2:B:92:ASN:O	2.48	0.47
1:G:61:ALA:HB2	2:H:137:ASP:CG	2.39	0.47
1:A:27:LYS:NZ	8:A:536:PGE:O2	2.34	0.47
2:D:446:ALA:HB1	2:D:448:LYS:HG3	1.95	0.47
2:B:397:LEU:HD12	5:B:504:PEG:H11	1.96	0.47
1:C:61:ALA:HB2	2:D:137:ASP:CG	2.40	0.47
2:D:33:ARG:NH1	2:D:92:ASN:O	2.48	0.47
2:D:176:CYS:HB3	2:D:180:LEU:HD12	1.97	0.47
1:E:-1:HIS:HA	1:E:2:LYS:HD3	1.96	0.47
1:A:66:SER:O	6:A:511:EDO:O2	2.25	0.47
1:A:14:ALA:HB2	1:A:259:ARG:HD3	1.97	0.47
1:A:453:PRO:HA	6:A:522:EDO:C2	2.39	0.47
2:B:33:ARG:HH22	6:B:512:EDO:HO1	1.62	0.47
1:C:14:ALA:HB2	1:C:259:ARG:HD3	1.97	0.47
1:G:409:LYS:NZ	2:H:59:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:PRO:HG2	2:B:96:ILE:HD11	1.96	0.46
2:B:321:ASP:H	6:B:518:EDO:H11	1.80	0.46
1:C:105:ALA:HB1	2:D:11:LEU:HD13	1.96	0.46
2:H:33:ARG:NH1	2:H:92:ASN:O	2.48	0.46
6:A:511:EDO:H12	6:A:512:EDO:H21	1.97	0.46
1:G:252:LYS:NZ	1:G:361:GLU:CG	2.78	0.46
2:D:324:LEU:HD21	5:D:504:PEG:H11	1.98	0.46
2:H:317:ALA:HB1	2:H:367:LEU:HD11	1.98	0.46
2:B:235:GLY:HA2	2:B:258:THR:HB	1.97	0.46
1:C:149:ILE:HD12	1:C:149:ILE:N	2.31	0.46
2:D:189:ALA:HB2	2:D:201:LEU:HD11	1.97	0.46
1:E:390:ASP:OD2	2:F:217:ARG:NH2	2.47	0.46
2:F:167:LYS:HB3	2:F:236:GLN:HB3	1.96	0.46
1:G:179:ARG:NH1	1:G:182:ASP:OD1	2.49	0.46
1:A:82:ILE:HD13	6:A:517:EDO:H12	1.98	0.46
1:E:14:ALA:HB2	1:E:259:ARG:HD3	1.97	0.46
1:G:124:CYS:HB3	2:H:103:LEU:HD13	1.98	0.46
1:E:410:GLY:HA2	2:F:217:ARG:HB3	1.98	0.46
1:E:228:LEU:HA	1:E:229:ALA:HA	1.71	0.46
1:A:68:ASP:OD1	5:A:503:PEG:H32	2.16	0.45
2:D:414:TRP:HE1	5:D:504:PEG:H21	1.77	0.45
2:F:305:LEU:HD21	1:G:450:VAL:HG21	1.98	0.45
2:F:348:ALA:HB3	2:F:351:LEU:HG	1.98	0.45
1:G:199:ASN:HB2	1:G:246:ASN:OD1	2.16	0.45
1:A:10:LEU:O	4:A:502:S5Q:S3A	2.74	0.45
2:B:348:ALA:HB3	2:B:351:LEU:HG	1.97	0.45
2:F:33:ARG:NH1	2:F:92:ASN:O	2.50	0.45
2:F:175:LEU:HB3	2:F:247:LEU:HD13	1.98	0.45
2:B:398:ARG:NH1	6:B:513:EDO:C1	2.79	0.45
1:G:252:LYS:HZ3	1:G:361:GLU:CG	2.30	0.45
6:A:517:EDO:H11	2:B:387:ALA:CB	2.47	0.45
1:A:179:ARG:NH1	1:A:182:ASP:OD1	2.50	0.45
7:A:532:1PE:H252	11:B:717:HOH:O	2.17	0.45
2:F:6:ASN:HD21	2:F:347:ARG:HH21	1.65	0.45
2:H:189:ALA:HB2	2:H:201:LEU:HD11	1.99	0.45
1:E:61:ALA:HB2	2:F:137:ASP:CG	2.41	0.45
1:G:252:LYS:HZ2	1:G:361:GLU:HG3	1.78	0.45
1:G:252:LYS:O	1:G:255:LEU:HB2	2.16	0.45
6:A:512:EDO:H22	6:A:513:EDO:H12	1.97	0.45
2:B:304:MET:HB3	1:C:446:VAL:HG23	1.99	0.45
1:C:179:ARG:NH1	1:C:182:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ALA:HB3	2:B:218:PHE:CE1	2.51	0.45
2:B:398:ARG:HH12	6:B:513:EDO:H11	1.82	0.45
1:E:-1:HIS:HB3	2:F:69:GLN:HE22	1.80	0.45
1:E:126:PRO:HA	1:E:129:ILE:HG12	1.98	0.45
2:F:404:TYR:HE1	6:F:513:EDO:H22	1.81	0.45
2:H:75:GLY:HA3	5:H:502:PEG:O2	2.16	0.45
2:H:382:ASN:OD1	2:H:384:HIS:HB2	2.16	0.45
2:B:170:ARG:HH22	6:B:511:EDO:H12	1.81	0.45
1:C:118:VAL:HB	1:C:148:VAL:HG13	1.99	0.45
1:A:383:ARG:HB3	2:B:218:PHE:CD2	2.52	0.44
2:H:446:ALA:HB1	2:H:448:LYS:HG3	1.99	0.44
2:B:174:VAL:HB	2:B:201:LEU:HD23	1.99	0.44
2:F:20:GLN:HG3	2:F:145:GLY:CA	2.47	0.44
2:H:416:GLY:HA3	5:H:504:PEG:H22	1.99	0.44
1:A:65:SER:HB2	2:B:47:PHE:HB3	1.99	0.44
1:C:10:LEU:O	4:C:502:S5Q:S3A	2.75	0.44
2:H:319:ALA:CB	2:H:367:LEU:HD22	2.36	0.44
1:C:252:LYS:HZ3	1:C:361:GLU:CG	2.28	0.44
1:G:126:PRO:O	1:G:131:ASP:HB2	2.17	0.44
2:H:270:GLY:HA3	6:H:507:EDO:H11	1.99	0.44
2:H:348:ALA:HB3	2:H:351:LEU:HG	2.00	0.44
2:B:246:SER:HA	6:B:528:EDO:H11	1.99	0.44
2:B:317:ALA:HB3	2:B:379:VAL:HG22	1.99	0.44
1:E:37:CYS:HB2	1:E:155:GLY:HA2	2.00	0.44
1:E:199:ASN:HB2	1:E:246:ASN:OD1	2.18	0.44
1:A:409:LYS:HZ3	2:B:59:PRO:HD3	1.81	0.43
2:B:189:ALA:HB2	2:B:201:LEU:HD11	1.99	0.43
1:C:108:GLN:HE22	2:D:9:LYS:HD2	1.82	0.43
6:C:504:EDO:HO2	2:D:391:ARG:HH22	1.65	0.43
2:D:348:ALA:HB3	2:D:351:LEU:HG	1.99	0.43
1:E:126:PRO:O	1:E:131:ASP:HB2	2.18	0.43
2:F:176:CYS:HB3	2:F:180:LEU:HD12	2.00	0.43
1:C:67:TRP:HH2	6:D:503:EDO:H21	1.80	0.43
1:E:179:ARG:NH1	1:E:182:ASP:OD1	2.51	0.43
1:E:235:ARG:HD3	2:H:449:PRO:HD3	2.01	0.43
1:A:18:ASN:HA	1:A:22:LYS:NZ	2.33	0.43
1:A:125:VAL:HB	1:A:126:PRO:HD3	2.00	0.43
1:C:409:LYS:HZ1	2:D:59:PRO:HD2	1.82	0.43
1:E:10:LEU:O	4:E:502:S5Q:S3A	2.76	0.43
7:A:532:1PE:H142	2:B:391:ARG:HG3	2.00	0.43
1:C:363:LYS:O	1:C:367:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:443:SER:HB3	2:D:446:ALA:HB2	1.99	0.43
1:G:10:LEU:O	4:G:502:S5Q:S3A	2.76	0.43
1:G:176:ILE:HG21	1:G:261:LEU:HD21	2.00	0.43
1:C:252:LYS:HZ3	1:C:361:GLU:CD	2.27	0.43
2:D:174:VAL:HB	2:D:201:LEU:HD23	2.00	0.43
1:G:363:LYS:O	1:G:367:ARG:HG2	2.19	0.43
1:G:409:LYS:NZ	2:H:59:PRO:HD3	2.32	0.43
2:B:398:ARG:HH12	6:B:513:EDO:C1	2.31	0.43
1:E:450:VAL:HG21	2:H:305:LEU:HD21	2.01	0.43
1:G:18:ASN:HA	1:G:22:LYS:NZ	2.34	0.43
1:G:252:LYS:NZ	1:G:361:GLU:CD	2.77	0.43
1:A:450:VAL:HG12	2:D:301:GLN:HB3	2.00	0.43
2:D:374:GLY:HA2	6:D:508:EDO:O1	2.19	0.43
1:A:61:ALA:HB2	2:B:137:ASP:CG	2.44	0.42
1:A:228:LEU:HA	1:A:229:ALA:HA	1.72	0.42
2:B:305:LEU:HD21	1:C:450:VAL:HG21	2.00	0.42
1:E:363:LYS:O	1:E:367:ARG:HG2	2.19	0.42
2:H:296:GLN:OE1	5:H:504:PEG:H12	2.18	0.42
1:A:212:HIS:NE2	2:D:438:ILE:CD1	2.83	0.42
2:F:39:HIS:CE1	2:F:80:VAL:HG23	2.54	0.42
2:F:339:THR:HB	2:F:356:LEU:HD21	2.01	0.42
2:H:176:CYS:HB3	2:H:180:LEU:HD12	2.01	0.42
5:A:510:PEG:H42	6:B:510:EDO:H21	2.01	0.42
1:C:237:VAL:O	1:C:240:MET:HG3	2.19	0.42
1:E:404:MET:HE2	11:E:602:HOH:O	2.18	0.42
1:G:-1:HIS:HA	1:G:2:LYS:HD3	2.00	0.42
2:H:18:ALA:HB3	2:H:142:PHE:HB2	2.02	0.42
1:C:18:ASN:HA	1:C:22:LYS:NZ	2.34	0.42
2:D:174:VAL:HG11	2:D:188:ILE:HG21	2.00	0.42
1:E:18:ASN:HA	1:E:22:LYS:NZ	2.35	0.42
2:D:381:GLY:O	2:D:398:ARG:HA	2.20	0.42
2:B:4:ILE:HD11	2:B:351:LEU:CB	2.49	0.42
2:B:119:ARG:CD	6:B:505:EDO:H21	2.36	0.42
2:F:310:MET:HE2	2:H:407:LEU:HD11	2.01	0.42
2:H:418:ARG:H	5:H:504:PEG:H12	1.84	0.42
1:A:199:ASN:HB2	1:A:246:ASN:OD1	2.19	0.42
2:B:449:PRO:HD3	1:C:235:ARG:HD3	2.00	0.42
2:H:193:GLU:HB3	11:H:666:HOH:O	2.20	0.42
1:A:236:GLU:HG2	2:D:447:GLN:HB2	2.02	0.42
2:B:177:SER:HB3	2:B:247:LEU:HD11	2.02	0.42
2:F:235:GLY:HA2	2:F:258:THR:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:341:ALA:HA	5:D:511:PEG:H41	2.01	0.41
1:E:79:LEU:HD12	1:E:82:ILE:HD12	2.02	0.41
2:F:174:VAL:HB	2:F:201:LEU:HD23	2.01	0.41
2:D:6:ASN:HD21	2:D:347:ARG:HH21	1.68	0.41
1:G:252:LYS:HD3	1:G:255:LEU:HD22	2.02	0.41
2:H:174:VAL:HG11	2:H:188:ILE:HG21	2.02	0.41
1:A:29:LYS:NZ	2:B:90:ARG:NH1	2.68	0.41
5:G:506:PEG:O4	2:H:384:HIS:O	2.35	0.41
2:B:174:VAL:HG11	2:B:188:ILE:HG21	2.01	0.41
1:E:455:PRO:HG3	6:E:509:EDO:H12	2.01	0.41
5:G:506:PEG:C3	2:H:391:ARG:NH1	2.83	0.41
2:B:279:MET:SD	1:C:455:PRO:HB2	2.60	0.41
2:D:397:LEU:HA	6:D:522:EDO:H21	2.02	0.41
1:G:67:TRP:O	8:G:517:PGE:O1	2.36	0.41
2:H:39:HIS:CE1	2:H:80:VAL:HG23	2.55	0.41
2:H:198:ARG:HA	8:H:514:PGE:C2	2.32	0.41
1:A:363:LYS:O	1:A:367:ARG:HG2	2.20	0.41
2:B:198:ARG:HG3	6:B:511:EDO:H22	2.02	0.41
2:F:449:PRO:HD3	1:G:235:ARG:HD3	2.02	0.41
1:A:113:TYR:O	8:A:535:PGE:O2	2.39	0.41
2:F:202:ILE:HA	2:F:203:PRO:HA	1.94	0.41
2:H:6:ASN:HD21	2:H:347:ARG:HH21	1.69	0.41
2:B:287:ASN:CB	5:B:503:PEG:H12	2.51	0.41
1:A:81:ARG:HG2	5:A:503:PEG:H31	2.02	0.41
2:B:40:GLY:HA2	2:B:67:MET:SD	2.61	0.41
2:H:23:GLY:HA3	2:H:142:PHE:O	2.21	0.41
2:H:170:ARG:CZ	2:H:198:ARG:HD2	2.50	0.41
2:H:174:VAL:HB	2:H:201:LEU:HD23	2.02	0.41
2:B:195:PHE:HA	5:B:503:PEG:O1	2.20	0.41
2:F:130:ILE:O	2:F:132:PRO:HD3	2.21	0.40
2:F:311:LEU:HD12	2:F:335:MET:HE2	2.03	0.40
2:B:240:THR:HG21	2:B:254:LEU:HD23	2.03	0.40
1:C:383:ARG:HB3	2:D:218:PHE:CD2	2.56	0.40
2:F:18:ALA:HB3	2:F:142:PHE:HB2	2.02	0.40
2:F:275:ASP:O	2:F:279:MET:HG2	2.22	0.40
2:D:395:PRO:HB3	2:D:434:HIS:CE1	2.56	0.40
1:E:409:LYS:HZ1	2:F:59:PRO:HD2	1.87	0.40
1:G:419:GLN:HB3	11:G:643:HOH:O	2.22	0.40
2:D:451:THR:HB	5:D:526:PEG:O4	2.21	0.40
3:E:501:SF4:S3	2:F:41:SER:HB3	2.61	0.40
2:F:433:GLU:HG3	6:H:510:EDO:H21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:LEU:HA	1:G:229:ALA:HA	1.71	0.40
2:H:391:ARG:HG2	6:H:511:EDO:H11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

All (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
1	E	22	LYS
1	A	152	ASP
1	A	378	ASP

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Mol	Chain	Res	Type
1	C	378	ASP
1	E	378	ASP
1	G	378	ASP

5.3.2 Protein sidechains ⓘ

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

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

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

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	HIS
1	A	2	LYS
1	A	19	LYS
1	A	21	GLU
1	A	27	LYS
1	A	52	VAL
1	A	65	SER
1	A	112	SER
1	A	151	VAL
1	A	156	PHE
1	A	329	LEU
1	A	386	LEU

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Mol	Chain	Res	Type
1	A	415	LEU
1	A	418	ASN
2	B	20	GLN
2	B	69	GLN
2	B	99	LEU
2	B	133	VAL
2	B	170	ARG
2	B	173	ASN
2	B	217	ARG
2	B	310	MET
2	B	313	SER
2	B	353	ASP
2	B	365	GLU
2	B	378	LEU
2	B	402	PRO
2	B	407	LEU
1	C	2	LYS
1	C	19	LYS
1	C	27	LYS
1	C	44	ILE
1	C	65	SER
1	C	112	SER
1	C	143	ARG
1	C	156	PHE
1	C	329	LEU
1	C	386	LEU
1	C	415	LEU
1	C	418	ASN
2	D	3	GLU
2	D	69	GLN
2	D	99	LEU
2	D	233	THR
2	D	237	SER
2	D	313	SER
2	D	353	ASP
2	D	407	LEU
1	E	27	LYS
1	E	43	GLN
1	E	52	VAL
1	E	65	SER
1	E	101	ARG
1	E	112	SER

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Mol	Chain	Res	Type
1	E	156	PHE
1	E	189	GLU
1	E	329	LEU
1	E	386	LEU
1	E	418	ASN
2	F	69	GLN
2	F	99	LEU
2	F	162	ARG
2	F	172	VAL
2	F	175	LEU
2	F	310	MET
2	F	313	SER
2	F	318	ILE
2	F	353	ASP
2	F	367	LEU
2	F	407	LEU
1	G	19	LYS
1	G	27	LYS
1	G	65	SER
1	G	112	SER
1	G	156	PHE
1	G	189	GLU
1	G	329	LEU
1	G	386	LEU
1	G	418	ASN
2	H	41	SER
2	H	69	GLN
2	H	99	LEU
2	H	133	VAL
2	H	170	ARG
2	H	172	VAL
2	H	217	ARG
2	H	310	MET
2	H	313	SER
2	H	353	ASP
2	H	407	LEU
2	H	421	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS

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Mol	Chain	Res	Type
1	A	164	ASN
2	B	8	ASN
2	B	42	GLN
2	B	92	ASN
2	B	121	GLN
2	B	173	ASN
2	B	179	ASN
2	B	236	GLN
2	B	411	GLN
2	D	8	ASN
2	D	112	HIS
2	D	121	GLN
2	D	236	GLN
2	D	369	HIS
2	D	375	GLN
2	D	436	GLN
1	E	69	ASN
1	E	164	ASN
2	F	63	GLN
2	F	69	GLN
2	F	92	ASN
2	F	121	GLN
2	F	171	GLN
2	F	179	ASN
2	F	236	GLN
2	F	403	GLN
2	F	434	HIS
1	G	164	ASN
2	H	92	ASN
2	H	121	GLN
2	H	236	GLN
2	H	403	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	A	527	-	3,3,3	0.32	0	2,2,2	0.23	0
5	PEG	H	503	-	6,6,6	0.16	0	5,5,5	0.08	0
6	EDO	G	510	-	3,3,3	0.39	0	2,2,2	0.14	0
5	PEG	D	506	-	6,6,6	0.23	0	5,5,5	0.07	0
6	EDO	B	525	-	3,3,3	0.40	0	2,2,2	0.05	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	A	528	-	3,3,3	0.30	0	2,2,2	0.14	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
6	EDO	E	504	-	3,3,3	0.39	0	2,2,2	0.21	0
5	PEG	A	531	-	6,6,6	0.13	0	5,5,5	0.10	0
3	SF4	G	501	1,2	0,12,12	-	-	-	-	-
6	EDO	A	520	-	3,3,3	0.40	0	2,2,2	0.28	0
6	EDO	G	504	-	3,3,3	0.33	0	2,2,2	0.25	0
6	EDO	D	525	-	3,3,3	0.47	0	2,2,2	0.15	0
6	EDO	G	513	-	3,3,3	0.27	0	2,2,2	0.31	0
6	EDO	F	513	-	3,3,3	0.35	0	2,2,2	0.18	0
6	EDO	B	510	-	3,3,3	0.27	0	2,2,2	0.19	0
5	PEG	B	502	-	6,6,6	0.13	0	5,5,5	0.11	0
4	S5Q	C	502	1	18,30,30	2.33	11 (61%)	-	-	-
6	EDO	C	509	-	3,3,3	0.34	0	2,2,2	0.06	0
6	EDO	F	518	-	3,3,3	0.23	0	2,2,2	0.35	0
6	EDO	F	510	-	3,3,3	0.46	0	2,2,2	0.14	0
10	PG4	F	517	-	12,12,12	0.14	0	11,11,11	0.08	0
6	EDO	A	523	-	3,3,3	0.36	0	2,2,2	0.17	0
5	PEG	B	521	-	6,6,6	0.24	0	5,5,5	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	B	526	-	3,3,3	0.20	0	2,2,2	0.28	0
6	EDO	A	509	-	3,3,3	0.23	0	2,2,2	0.36	0
6	EDO	D	508	-	3,3,3	0.26	0	2,2,2	0.39	0
6	EDO	B	518	-	3,3,3	0.26	0	2,2,2	0.41	0
6	EDO	H	512	-	3,3,3	0.29	0	2,2,2	0.31	0
5	PEG	D	507	-	6,6,6	0.20	0	5,5,5	0.20	0
6	EDO	B	523	-	3,3,3	0.25	0	2,2,2	0.31	0
6	EDO	E	512	-	3,3,3	0.30	0	2,2,2	0.33	0
6	EDO	A	515	-	3,3,3	0.34	0	2,2,2	0.04	0
6	EDO	F	523	-	3,3,3	0.28	0	2,2,2	0.25	0
6	EDO	F	521	-	3,3,3	0.22	0	2,2,2	0.38	0
8	PGE	F	524	-	9,9,9	0.19	0	8,8,8	0.06	0
5	PEG	B	504	-	6,6,6	0.21	0	5,5,5	0.11	0
6	EDO	F	506	-	3,3,3	0.23	0	2,2,2	0.31	0
5	PEG	D	526	-	6,6,6	0.14	0	5,5,5	0.08	0
6	EDO	D	513	-	3,3,3	0.32	0	2,2,2	0.19	0
6	EDO	C	508	-	3,3,3	0.25	0	2,2,2	0.42	0
5	PEG	A	503	-	6,6,6	0.18	0	5,5,5	0.12	0
6	EDO	D	512	-	3,3,3	0.27	0	2,2,2	0.28	0
6	EDO	D	518	-	3,3,3	0.32	0	2,2,2	0.19	0
6	EDO	G	509	-	3,3,3	0.26	0	2,2,2	0.18	0
6	EDO	B	515	-	3,3,3	0.42	0	2,2,2	0.07	0
6	EDO	C	511	-	3,3,3	0.47	0	2,2,2	0.17	0
6	EDO	D	502	-	3,3,3	0.35	0	2,2,2	0.16	0
3	SF4	A	501	1,2	0,12,12	-	-	-	-	-
6	EDO	B	527	-	3,3,3	0.33	0	2,2,2	0.15	0
5	PEG	A	504	-	6,6,6	0.16	0	5,5,5	0.09	0
6	EDO	H	510	-	3,3,3	0.49	0	2,2,2	0.09	0
6	EDO	E	510	-	3,3,3	0.23	0	2,2,2	0.28	0
6	EDO	B	517	-	3,3,3	0.29	0	2,2,2	0.26	0
6	EDO	A	512	-	3,3,3	0.36	0	2,2,2	0.15	0
6	EDO	B	514	-	3,3,3	0.56	0	2,2,2	0.07	0
6	EDO	A	508	-	3,3,3	0.33	0	2,2,2	0.23	0
6	EDO	G	515	-	3,3,3	0.41	0	2,2,2	0.21	0
6	EDO	F	522	-	3,3,3	0.38	0	2,2,2	0.09	0
6	EDO	A	522	-	3,3,3	0.37	0	2,2,2	0.22	0
6	EDO	B	516	-	3,3,3	0.26	0	2,2,2	0.32	0
6	EDO	D	523	-	3,3,3	0.25	0	2,2,2	0.28	0
6	EDO	F	516	-	3,3,3	0.26	0	2,2,2	0.36	0
6	EDO	B	508	-	3,3,3	0.26	0	2,2,2	0.18	0
6	EDO	H	508	-	3,3,3	0.41	0	2,2,2	0.11	0
10	PG4	B	520	-	12,12,12	0.21	0	11,11,11	0.35	0
4	S5Q	E	502	1	18,30,30	2.37	10 (55%)	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	B	522	-	6,6,6	0.25	0	5,5,5	0.15	0
6	EDO	B	512	-	3,3,3	0.31	0	2,2,2	0.18	0
6	EDO	D	516	-	3,3,3	0.30	0	2,2,2	0.20	0
6	EDO	F	508	-	3,3,3	0.25	0	2,2,2	0.33	0
6	EDO	H	505	-	3,3,3	0.54	0	2,2,2	0.34	0
6	EDO	F	505	-	3,3,3	0.35	0	2,2,2	0.14	0
6	EDO	H	507	-	3,3,3	0.21	0	2,2,2	0.33	0
6	EDO	D	524	-	3,3,3	0.35	0	2,2,2	0.19	0
6	EDO	A	524	-	3,3,3	0.32	0	2,2,2	0.19	0
6	EDO	D	509	-	3,3,3	0.28	0	2,2,2	0.30	0
8	PGE	A	536	-	9,9,9	0.17	0	8,8,8	0.12	0
6	EDO	A	506	-	3,3,3	0.41	0	2,2,2	0.11	0
5	PEG	H	504	-	6,6,6	0.17	0	5,5,5	0.23	0
8	PGE	E	507	-	9,9,9	0.16	0	8,8,8	0.12	0
6	EDO	D	510	-	3,3,3	0.38	0	2,2,2	0.11	0
6	EDO	G	503	-	3,3,3	0.36	0	2,2,2	0.19	0
6	EDO	G	514	-	3,3,3	0.30	0	2,2,2	0.19	0
6	EDO	B	528	-	3,3,3	0.45	0	2,2,2	0.19	0
6	EDO	G	512	-	3,3,3	0.39	0	2,2,2	0.04	0
6	EDO	B	519	-	3,3,3	0.42	0	2,2,2	0.13	0
5	PEG	D	517	-	6,6,6	0.17	0	5,5,5	0.22	0
6	EDO	C	506	-	3,3,3	0.52	0	2,2,2	0.34	0
5	PEG	D	504	-	6,6,6	0.14	0	5,5,5	0.23	0
8	PGE	C	503	-	9,9,9	0.23	0	8,8,8	0.08	0
6	EDO	E	511	-	3,3,3	0.41	0	2,2,2	0.26	0
6	EDO	A	534	-	3,3,3	0.33	0	2,2,2	0.37	0
5	PEG	B	529	-	6,6,6	0.14	0	5,5,5	0.11	0
6	EDO	C	510	-	3,3,3	0.22	0	2,2,2	0.41	0
5	PEG	D	511	-	6,6,6	0.14	0	5,5,5	0.10	0
6	EDO	A	513	-	3,3,3	0.36	0	2,2,2	0.13	0
6	EDO	D	515	-	3,3,3	0.26	0	2,2,2	0.20	0
5	PEG	F	507	-	6,6,6	0.23	0	5,5,5	0.14	0
5	PEG	G	506	-	6,6,6	0.11	0	5,5,5	0.12	0
6	EDO	A	518	-	3,3,3	0.42	0	2,2,2	0.05	0
5	PEG	C	505	-	6,6,6	0.13	0	5,5,5	0.12	0
4	S5Q	G	502	1	18,30,30	2.38	11 (61%)	-		
6	EDO	F	512	-	3,3,3	0.42	0	2,2,2	0.26	0
6	EDO	H	506	-	3,3,3	0.31	0	2,2,2	0.38	0
6	EDO	B	511	-	3,3,3	0.50	0	2,2,2	0.11	0
6	EDO	D	503	-	3,3,3	0.21	0	2,2,2	0.31	0
5	PEG	H	501	-	6,6,6	0.17	0	5,5,5	0.03	0
6	EDO	D	514	-	3,3,3	0.40	0	2,2,2	0.27	0
6	EDO	G	516	-	3,3,3	0.28	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	514	-	3,3,3	0.45	0	2,2,2	0.09	0
6	EDO	D	521	-	3,3,3	0.31	0	2,2,2	0.20	0
6	EDO	E	509	-	3,3,3	0.31	0	2,2,2	0.29	0
6	EDO	B	505	-	3,3,3	0.46	0	2,2,2	0.35	0
6	EDO	B	507	-	3,3,3	0.28	0	2,2,2	0.29	0
6	EDO	F	504	-	3,3,3	0.31	0	2,2,2	0.26	0
6	EDO	A	529	-	3,3,3	0.29	0	2,2,2	0.29	0
6	EDO	F	514	-	3,3,3	0.41	0	2,2,2	0.03	0
8	PGE	H	514	-	9,9,9	0.18	0	8,8,8	0.14	0
6	EDO	C	504	-	3,3,3	0.55	0	2,2,2	0.27	0
5	PEG	H	502	-	6,6,6	0.19	0	5,5,5	0.14	0
6	EDO	H	511	-	3,3,3	0.32	0	2,2,2	0.27	0
6	EDO	A	530	-	3,3,3	0.28	0	2,2,2	0.23	0
6	EDO	A	526	-	3,3,3	0.43	0	2,2,2	0.15	0
6	EDO	G	511	-	3,3,3	0.25	0	2,2,2	0.29	0
5	PEG	A	533	-	6,6,6	0.15	0	5,5,5	0.13	0
6	EDO	E	506	-	3,3,3	0.45	0	2,2,2	0.32	0
6	EDO	F	519	-	3,3,3	0.33	0	2,2,2	0.10	0
3	SF4	C	501	1,2	0,12,12	-	-	-	-	-
6	EDO	E	508	-	3,3,3	0.35	0	2,2,2	0.27	0
6	EDO	B	506	-	3,3,3	0.31	0	2,2,2	0.19	0
6	EDO	A	516	-	3,3,3	0.37	0	2,2,2	0.25	0
6	EDO	E	503	-	3,3,3	0.31	0	2,2,2	0.33	0
5	PEG	A	510	-	6,6,6	0.24	0	5,5,5	0.07	0
8	PGE	H	513	-	9,9,9	0.18	0	8,8,8	0.10	0
4	S5Q	A	502	1	18,30,30	2.35	11 (61%)	-	-	-
6	EDO	G	507	-	3,3,3	0.27	0	2,2,2	0.32	0
6	EDO	D	520	-	3,3,3	0.30	0	2,2,2	0.13	0
6	EDO	D	519	-	3,3,3	0.34	0	2,2,2	0.14	0
8	PGE	A	535	-	9,9,9	0.17	0	8,8,8	0.09	0
6	EDO	C	507	-	3,3,3	0.36	0	2,2,2	0.24	0
6	EDO	B	509	-	3,3,3	0.21	0	2,2,2	0.32	0
5	PEG	D	505	-	6,6,6	0.16	0	5,5,5	0.06	0
5	PEG	A	505	-	6,6,6	0.19	0	5,5,5	0.06	0
6	EDO	F	509	-	3,3,3	0.38	0	2,2,2	0.26	0
3	SF4	E	501	1,2	0,12,12	-	-	-	-	-
6	EDO	A	517	-	3,3,3	0.31	0	2,2,2	0.47	0
6	EDO	F	515	-	3,3,3	0.33	0	2,2,2	0.17	0
8	PGE	G	517	-	9,9,9	0.18	0	8,8,8	0.12	0
6	EDO	A	507	-	3,3,3	0.34	0	2,2,2	0.11	0
6	EDO	A	521	-	3,3,3	0.35	0	2,2,2	0.07	0
6	EDO	G	505	-	3,3,3	0.25	0	2,2,2	0.23	0
5	PEG	G	508	-	6,6,6	0.21	0	5,5,5	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	B	503	-	6,6,6	0.21	0	5,5,5	0.15	0
6	EDO	A	511	-	3,3,3	0.23	0	2,2,2	0.06	0
6	EDO	A	525	-	3,3,3	0.30	0	2,2,2	0.25	0
6	EDO	F	503	-	3,3,3	0.45	0	2,2,2	0.16	0
8	PGE	F	525	-	9,9,9	0.20	0	8,8,8	0.10	0
6	EDO	A	519	-	3,3,3	0.33	0	2,2,2	0.20	0
6	EDO	H	509	-	3,3,3	0.55	0	2,2,2	0.11	0
6	EDO	B	513	-	3,3,3	0.70	0	2,2,2	0.54	0
6	EDO	D	522	-	3,3,3	0.36	0	2,2,2	0.30	0
6	EDO	F	511	-	3,3,3	0.36	0	2,2,2	0.27	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	A	527	-	-	1/1/1/1	-
5	PEG	H	503	-	-	2/4/4/4	-
6	EDO	G	510	-	-	1/1/1/1	-
5	PEG	D	506	-	-	3/4/4/4	-
6	EDO	B	525	-	-	1/1/1/1	-
8	PGE	F	520	-	-	4/7/7/7	-
6	EDO	E	505	-	-	0/1/1/1	-
6	EDO	A	528	-	-	1/1/1/1	-
7	1PE	A	532	-	-	8/13/13/13	-
6	EDO	B	524	-	-	1/1/1/1	-
6	EDO	E	504	-	-	0/1/1/1	-
5	PEG	A	531	-	-	4/4/4/4	-
3	SF4	G	501	1,2	-	-	0/6/5/5
6	EDO	A	520	-	-	0/1/1/1	-
6	EDO	G	504	-	-	1/1/1/1	-
6	EDO	D	525	-	-	0/1/1/1	-
6	EDO	G	513	-	-	1/1/1/1	-
6	EDO	F	513	-	-	1/1/1/1	-
6	EDO	B	510	-	-	1/1/1/1	-
5	PEG	B	502	-	-	1/4/4/4	-
6	EDO	C	509	-	-	1/1/1/1	-
6	EDO	F	518	-	-	1/1/1/1	-
6	EDO	F	510	-	-	1/1/1/1	-
10	PG4	F	517	-	-	8/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	523	-	-	1/1/1/1	-
5	PEG	B	521	-	-	2/4/4/4	-
6	EDO	B	526	-	-	1/1/1/1	-
6	EDO	A	509	-	-	1/1/1/1	-
6	EDO	D	508	-	-	1/1/1/1	-
6	EDO	B	518	-	-	1/1/1/1	-
6	EDO	H	512	-	-	1/1/1/1	-
5	PEG	D	507	-	-	1/4/4/4	-
6	EDO	B	523	-	-	0/1/1/1	-
6	EDO	E	512	-	-	1/1/1/1	-
6	EDO	A	515	-	-	1/1/1/1	-
6	EDO	F	523	-	-	1/1/1/1	-
6	EDO	F	521	-	-	0/1/1/1	-
8	PGE	F	524	-	-	2/7/7/7	-
5	PEG	B	504	-	-	2/4/4/4	-
6	EDO	F	506	-	-	1/1/1/1	-
5	PEG	D	526	-	-	4/4/4/4	-
6	EDO	D	513	-	-	0/1/1/1	-
6	EDO	C	508	-	-	1/1/1/1	-
5	PEG	A	503	-	-	3/4/4/4	-
6	EDO	D	512	-	-	0/1/1/1	-
6	EDO	D	518	-	-	0/1/1/1	-
6	EDO	G	509	-	-	0/1/1/1	-
6	EDO	B	515	-	-	1/1/1/1	-
6	EDO	C	511	-	-	1/1/1/1	-
6	EDO	D	502	-	-	1/1/1/1	-
6	EDO	H	510	-	-	1/1/1/1	-
6	EDO	B	527	-	-	1/1/1/1	-
5	PEG	A	504	-	-	3/4/4/4	-
3	SF4	A	501	1,2	-	-	0/6/5/5
6	EDO	E	510	-	-	1/1/1/1	-
6	EDO	B	517	-	-	0/1/1/1	-
6	EDO	A	512	-	-	0/1/1/1	-
6	EDO	B	514	-	-	1/1/1/1	-
6	EDO	A	508	-	-	1/1/1/1	-
6	EDO	G	515	-	-	1/1/1/1	-
6	EDO	F	522	-	-	1/1/1/1	-
6	EDO	A	522	-	-	1/1/1/1	-
6	EDO	B	516	-	-	0/1/1/1	-
6	EDO	D	523	-	-	1/1/1/1	-
6	EDO	F	516	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	508	-	-	1/1/1/1	-
6	EDO	H	508	-	-	1/1/1/1	-
10	PG4	B	520	-	-	7/10/10/10	-
5	PEG	B	522	-	-	2/4/4/4	-
6	EDO	B	512	-	-	1/1/1/1	-
6	EDO	D	516	-	-	1/1/1/1	-
6	EDO	F	508	-	-	1/1/1/1	-
6	EDO	H	505	-	-	0/1/1/1	-
6	EDO	F	505	-	-	1/1/1/1	-
6	EDO	H	507	-	-	1/1/1/1	-
6	EDO	D	524	-	-	1/1/1/1	-
6	EDO	A	524	-	-	1/1/1/1	-
6	EDO	D	509	-	-	1/1/1/1	-
8	PGE	A	536	-	-	3/7/7/7	-
6	EDO	A	506	-	-	1/1/1/1	-
5	PEG	H	504	-	-	2/4/4/4	-
8	PGE	E	507	-	-	3/7/7/7	-
6	EDO	D	510	-	-	1/1/1/1	-
6	EDO	G	503	-	-	1/1/1/1	-
6	EDO	G	514	-	-	1/1/1/1	-
6	EDO	B	528	-	-	1/1/1/1	-
6	EDO	G	512	-	-	1/1/1/1	-
6	EDO	B	519	-	-	1/1/1/1	-
5	PEG	D	517	-	-	2/4/4/4	-
6	EDO	C	506	-	-	0/1/1/1	-
5	PEG	D	504	-	-	1/4/4/4	-
8	PGE	C	503	-	-	6/7/7/7	-
6	EDO	E	511	-	-	1/1/1/1	-
6	EDO	A	534	-	-	1/1/1/1	-
5	PEG	B	529	-	-	3/4/4/4	-
6	EDO	C	510	-	-	0/1/1/1	-
5	PEG	D	511	-	-	1/4/4/4	-
6	EDO	A	513	-	-	1/1/1/1	-
6	EDO	D	515	-	-	0/1/1/1	-
5	PEG	F	507	-	-	2/4/4/4	-
5	PEG	G	506	-	-	4/4/4/4	-
6	EDO	A	518	-	-	0/1/1/1	-
5	PEG	C	505	-	-	3/4/4/4	-
6	EDO	F	512	-	-	1/1/1/1	-
6	EDO	H	506	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	511	-	-	1/1/1/1	-
6	EDO	D	503	-	-	1/1/1/1	-
5	PEG	H	501	-	-	2/4/4/4	-
6	EDO	D	514	-	-	1/1/1/1	-
6	EDO	G	516	-	-	0/1/1/1	-
6	EDO	A	514	-	-	0/1/1/1	-
6	EDO	D	521	-	-	1/1/1/1	-
6	EDO	E	509	-	-	1/1/1/1	-
6	EDO	B	505	-	-	1/1/1/1	-
6	EDO	B	507	-	-	1/1/1/1	-
6	EDO	F	504	-	-	1/1/1/1	-
6	EDO	A	529	-	-	1/1/1/1	-
6	EDO	F	514	-	-	0/1/1/1	-
8	PGE	H	514	-	-	3/7/7/7	-
6	EDO	C	504	-	-	1/1/1/1	-
5	PEG	H	502	-	-	3/4/4/4	-
6	EDO	H	511	-	-	1/1/1/1	-
6	EDO	A	530	-	-	1/1/1/1	-
6	EDO	A	526	-	-	1/1/1/1	-
6	EDO	G	511	-	-	1/1/1/1	-
5	PEG	A	533	-	-	1/4/4/4	-
6	EDO	E	506	-	-	1/1/1/1	-
6	EDO	F	519	-	-	0/1/1/1	-
3	SF4	C	501	1,2	-	-	0/6/5/5
6	EDO	E	508	-	-	1/1/1/1	-
6	EDO	B	506	-	-	1/1/1/1	-
6	EDO	A	516	-	-	1/1/1/1	-
6	EDO	E	503	-	-	1/1/1/1	-
5	PEG	A	510	-	-	1/4/4/4	-
8	PGE	H	513	-	-	2/7/7/7	-
6	EDO	G	507	-	-	0/1/1/1	-
6	EDO	D	520	-	-	0/1/1/1	-
6	EDO	D	519	-	-	1/1/1/1	-
8	PGE	A	535	-	-	3/7/7/7	-
6	EDO	C	507	-	-	1/1/1/1	-
6	EDO	B	509	-	-	1/1/1/1	-
5	PEG	D	505	-	-	1/4/4/4	-
5	PEG	A	505	-	-	3/4/4/4	-
6	EDO	F	509	-	-	1/1/1/1	-
6	EDO	A	517	-	-	0/1/1/1	-
3	SF4	E	501	1,2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	F	515	-	-	1/1/1/1	-
8	PGE	G	517	-	-	3/7/7/7	-
6	EDO	A	507	-	-	0/1/1/1	-
6	EDO	A	521	-	-	1/1/1/1	-
6	EDO	G	505	-	-	1/1/1/1	-
5	PEG	G	508	-	-	2/4/4/4	-
5	PEG	B	503	-	-	2/4/4/4	-
6	EDO	A	511	-	-	1/1/1/1	-
6	EDO	A	525	-	-	1/1/1/1	-
6	EDO	F	503	-	-	0/1/1/1	-
8	PGE	F	525	-	-	3/7/7/7	-
6	EDO	A	519	-	-	0/1/1/1	-
6	EDO	H	509	-	-	1/1/1/1	-
6	EDO	B	513	-	-	1/1/1/1	-
6	EDO	D	522	-	-	1/1/1/1	-
6	EDO	F	511	-	-	1/1/1/1	-

All (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
4	E	502	S5Q	S1A-FE4	-3.78	2.23	2.32
4	C	502	S5Q	S1A-FE4	-3.77	2.23	2.32
4	A	502	S5Q	S1A-FE4	-3.59	2.23	2.32
4	E	502	S5Q	S4A-FE4	-3.39	2.24	2.32
4	C	502	S5Q	S4A-FE4	-3.32	2.24	2.32
4	A	502	S5Q	S4A-FE4	-3.14	2.24	2.32
4	G	502	S5Q	S4A-FE4	-3.12	2.24	2.32
4	A	502	S5Q	S1B-FE6	-3.06	2.24	2.32
4	E	502	S5Q	S3A-FE4	-2.83	2.18	2.24
4	G	502	S5Q	S1B-FE5	-2.76	2.25	2.32
4	G	502	S5Q	S3B-FE6	-2.76	2.25	2.32
4	G	502	S5Q	S3A-FE4	-2.75	2.18	2.24
4	G	502	S5Q	S1A-FE2	-2.74	2.25	2.32
4	C	502	S5Q	S3A-FE4	-2.73	2.18	2.24
4	E	502	S5Q	S1B-FE5	-2.67	2.25	2.32
4	C	502	S5Q	S3B-FE6	-2.63	2.25	2.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	502	S5Q	S1A-FE2	-2.63	2.25	2.32
4	C	502	S5Q	S1B-FE5	-2.62	2.25	2.32
4	E	502	S5Q	S3B-FE6	-2.61	2.25	2.32
4	A	502	S5Q	S1B-FE5	-2.60	2.25	2.32
4	C	502	S5Q	S1A-FE2	-2.59	2.26	2.32
4	E	502	S5Q	S2A-FE3	-2.42	2.26	2.32
4	G	502	S5Q	S2A-FE3	-2.38	2.26	2.32
4	G	502	S5Q	S4A-FE3	-2.35	2.26	2.32
4	C	502	S5Q	S2A-FE3	-2.35	2.26	2.32
4	G	502	S5Q	S4B-FE5	-2.34	2.26	2.32
4	A	502	S5Q	S4A-FE3	-2.31	2.26	2.32
4	C	502	S5Q	S4A-FE3	-2.29	2.26	2.32
4	A	502	S5Q	S4B-FE5	-2.29	2.26	2.32
4	A	502	S5Q	S3A-FE4	-2.28	2.19	2.24
4	G	502	S5Q	S1B-FE6	-2.26	2.26	2.32
4	A	502	S5Q	S1A-FE2	-2.21	2.26	2.32
4	E	502	S5Q	S4B-FE5	-2.20	2.26	2.32
4	E	502	S5Q	S4A-FE3	-2.18	2.27	2.32
4	A	502	S5Q	S3B-FE6	-2.12	2.27	2.32
4	C	502	S5Q	S1B-FE6	-2.10	2.27	2.32
4	A	502	S5Q	S2B-FE2	-2.04	2.20	2.24
4	C	502	S5Q	S4B-FE5	-2.04	2.27	2.32

There are no bond angle outliers.

There are no chirality outliers.

All (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
8	A	536	PGE	O2-C3-C4-O3
5	A	505	PEG	O1-C1-C2-O2
5	B	503	PEG	O1-C1-C2-O2
5	B	521	PEG	O2-C3-C4-O4
5	D	517	PEG	O1-C1-C2-O2
5	G	506	PEG	O1-C1-C2-O2
5	G	506	PEG	O2-C3-C4-O4
5	H	501	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
5	H	502	PEG	O2-C3-C4-O4
5	H	504	PEG	O2-C3-C4-O4
8	A	535	PGE	O1-C1-C2-O2
8	A	535	PGE	O3-C5-C6-O4
8	A	536	PGE	O1-C1-C2-O2
8	G	517	PGE	O3-C5-C6-O4
10	B	520	PG4	O1-C1-C2-O2
6	B	526	EDO	O1-C1-C2-O2
6	G	511	EDO	O1-C1-C2-O2
10	F	517	PG4	O3-C5-C6-O4
5	B	522	PEG	O1-C1-C2-O2
5	B	529	PEG	O1-C1-C2-O2
5	D	504	PEG	O2-C3-C4-O4
5	D	517	PEG	O2-C3-C4-O4
5	H	502	PEG	O1-C1-C2-O2
8	E	507	PGE	O1-C1-C2-O2
8	G	517	PGE	O1-C1-C2-O2
8	F	524	PGE	O2-C3-C4-O3
5	A	503	PEG	O1-C1-C2-O2
5	A	504	PEG	O2-C3-C4-O4
5	B	503	PEG	O2-C3-C4-O4
5	B	504	PEG	O2-C3-C4-O4
5	G	508	PEG	O1-C1-C2-O2
8	C	503	PGE	O1-C1-C2-O2
10	B	520	PG4	O4-C7-C8-O5
8	G	517	PGE	O2-C3-C4-O3
10	B	520	PG4	O2-C3-C4-O3
5	A	531	PEG	O1-C1-C2-O2
6	A	509	EDO	O1-C1-C2-O2
6	A	511	EDO	O1-C1-C2-O2
6	A	513	EDO	O1-C1-C2-O2
6	A	515	EDO	O1-C1-C2-O2
6	A	516	EDO	O1-C1-C2-O2
6	A	521	EDO	O1-C1-C2-O2
6	A	522	EDO	O1-C1-C2-O2
6	A	527	EDO	O1-C1-C2-O2
6	A	528	EDO	O1-C1-C2-O2
6	A	529	EDO	O1-C1-C2-O2
6	A	530	EDO	O1-C1-C2-O2
6	B	507	EDO	O1-C1-C2-O2
6	B	509	EDO	O1-C1-C2-O2
6	B	513	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	B	514	EDO	O1-C1-C2-O2
6	B	518	EDO	O1-C1-C2-O2
6	B	519	EDO	O1-C1-C2-O2
6	B	527	EDO	O1-C1-C2-O2
6	B	528	EDO	O1-C1-C2-O2
6	C	511	EDO	O1-C1-C2-O2
6	D	502	EDO	O1-C1-C2-O2
6	D	503	EDO	O1-C1-C2-O2
6	D	519	EDO	O1-C1-C2-O2
6	D	521	EDO	O1-C1-C2-O2
6	D	522	EDO	O1-C1-C2-O2
6	E	503	EDO	O1-C1-C2-O2
6	E	510	EDO	O1-C1-C2-O2
6	E	511	EDO	O1-C1-C2-O2
6	F	505	EDO	O1-C1-C2-O2
6	F	506	EDO	O1-C1-C2-O2
6	F	508	EDO	O1-C1-C2-O2
6	F	509	EDO	O1-C1-C2-O2
6	F	512	EDO	O1-C1-C2-O2
6	F	515	EDO	O1-C1-C2-O2
6	F	522	EDO	O1-C1-C2-O2
6	G	505	EDO	O1-C1-C2-O2
6	G	512	EDO	O1-C1-C2-O2
6	G	513	EDO	O1-C1-C2-O2
6	G	515	EDO	O1-C1-C2-O2
6	H	506	EDO	O1-C1-C2-O2
6	H	507	EDO	O1-C1-C2-O2
6	H	508	EDO	O1-C1-C2-O2
6	H	510	EDO	O1-C1-C2-O2
6	H	512	EDO	O1-C1-C2-O2
5	A	503	PEG	O2-C3-C4-O4
5	A	504	PEG	O1-C1-C2-O2
5	A	531	PEG	O2-C3-C4-O4
5	C	505	PEG	O2-C3-C4-O4
5	D	505	PEG	O1-C1-C2-O2
5	H	504	PEG	O1-C1-C2-O2
5	D	511	PEG	O1-C1-C2-O2
5	F	507	PEG	O2-C3-C4-O4
5	H	503	PEG	O2-C3-C4-O4
8	F	524	PGE	O1-C1-C2-O2
10	F	517	PG4	O4-C7-C8-O5
8	H	514	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
6	A	523	EDO	O1-C1-C2-O2
6	A	534	EDO	O1-C1-C2-O2
6	B	506	EDO	O1-C1-C2-O2
6	D	509	EDO	O1-C1-C2-O2
6	D	523	EDO	O1-C1-C2-O2
6	E	509	EDO	O1-C1-C2-O2
5	F	507	PEG	O1-C1-C2-O2
8	F	525	PGE	O1-C1-C2-O2
6	A	506	EDO	O1-C1-C2-O2
6	A	524	EDO	O1-C1-C2-O2
6	A	526	EDO	O1-C1-C2-O2
6	B	510	EDO	O1-C1-C2-O2
6	B	525	EDO	O1-C1-C2-O2
6	C	508	EDO	O1-C1-C2-O2
6	D	508	EDO	O1-C1-C2-O2
6	F	511	EDO	O1-C1-C2-O2
6	F	513	EDO	O1-C1-C2-O2
6	F	518	EDO	O1-C1-C2-O2
6	F	523	EDO	O1-C1-C2-O2
6	H	509	EDO	O1-C1-C2-O2
7	A	532	1PE	OH6-C15-C25-OH5
8	H	514	PGE	C6-C5-O3-C4
5	A	533	PEG	C1-C2-O2-C3
5	B	522	PEG	C4-C3-O2-C2
5	A	531	PEG	C4-C3-O2-C2
8	F	520	PGE	C4-C3-O2-C2
5	D	526	PEG	C4-C3-O2-C2
5	D	507	PEG	C1-C2-O2-C3
5	G	508	PEG	C1-C2-O2-C3
5	H	501	PEG	C4-C3-O2-C2
7	A	532	1PE	C25-C15-OH6-C26
5	A	504	PEG	C1-C2-O2-C3
5	B	502	PEG	C4-C3-O2-C2
8	H	514	PGE	C1-C2-O2-C3
10	F	517	PG4	C1-C2-O2-C3
5	C	505	PEG	C1-C2-O2-C3
8	F	520	PGE	C6-C5-O3-C4
10	B	520	PG4	C8-C7-O4-C6
5	H	502	PEG	C1-C2-O2-C3
7	A	532	1PE	C14-C24-OH4-C13
8	C	503	PGE	C3-C4-O3-C5
8	F	525	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
10	F	517	PG4	C4-C3-O2-C2
5	A	503	PEG	C1-C2-O2-C3
5	D	506	PEG	O1-C1-C2-O2
8	F	525	PGE	O3-C5-C6-O4
8	E	507	PGE	C6-C5-O3-C4
5	G	506	PEG	C1-C2-O2-C3
6	B	505	EDO	O1-C1-C2-O2
6	B	511	EDO	O1-C1-C2-O2
6	C	507	EDO	O1-C1-C2-O2
6	D	514	EDO	O1-C1-C2-O2
6	E	512	EDO	O1-C1-C2-O2
6	F	504	EDO	O1-C1-C2-O2
10	F	517	PG4	C3-C4-O3-C5
10	F	517	PG4	C5-C6-O4-C7
5	D	526	PEG	O1-C1-C2-O2
7	A	532	1PE	OH2-C12-C22-OH3
5	D	506	PEG	C1-C2-O2-C3
5	A	505	PEG	C1-C2-O2-C3
8	C	503	PGE	C6-C5-O3-C4
5	B	529	PEG	C4-C3-O2-C2
5	A	510	PEG	C4-C3-O2-C2
5	B	529	PEG	O2-C3-C4-O4
5	A	505	PEG	C4-C3-O2-C2
6	B	508	EDO	O1-C1-C2-O2
6	B	515	EDO	O1-C1-C2-O2
6	B	524	EDO	O1-C1-C2-O2
6	G	504	EDO	O1-C1-C2-O2
5	C	505	PEG	C4-C3-O2-C2
5	D	526	PEG	O2-C3-C4-O4
7	A	532	1PE	C23-C13-OH4-C24
10	B	520	PG4	C3-C4-O3-C5
10	F	517	PG4	C6-C5-O3-C4
6	B	512	EDO	O1-C1-C2-O2
6	F	510	EDO	O1-C1-C2-O2
6	H	511	EDO	O1-C1-C2-O2
5	D	526	PEG	C1-C2-O2-C3
6	A	508	EDO	O1-C1-C2-O2
6	A	525	EDO	O1-C1-C2-O2
6	D	510	EDO	O1-C1-C2-O2
6	D	516	EDO	O1-C1-C2-O2
5	G	506	PEG	C4-C3-O2-C2
8	C	503	PGE	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
10	F	517	PG4	C8-C7-O4-C6
5	B	521	PEG	C1-C2-O2-C3
7	A	532	1PE	C15-C25-OH5-C14
7	A	532	1PE	OH4-C13-C23-OH3
8	C	503	PGE	C4-C3-O2-C2
10	B	520	PG4	C6-C5-O3-C4
6	C	504	EDO	O1-C1-C2-O2
6	E	508	EDO	O1-C1-C2-O2
6	G	503	EDO	O1-C1-C2-O2
6	G	510	EDO	O1-C1-C2-O2
6	G	514	EDO	O1-C1-C2-O2
5	A	531	PEG	C1-C2-O2-C3
5	D	506	PEG	O2-C3-C4-O4
8	F	520	PGE	C1-C2-O2-C3
8	A	536	PGE	C3-C4-O3-C5
6	C	509	EDO	O1-C1-C2-O2
6	D	524	EDO	O1-C1-C2-O2
6	E	506	EDO	O1-C1-C2-O2
8	F	520	PGE	O2-C3-C4-O3
8	H	513	PGE	C1-C2-O2-C3
8	C	503	PGE	O2-C3-C4-O3
7	A	532	1PE	C24-C14-OH5-C25
8	H	513	PGE	C3-C4-O3-C5

There are no ring outliers.

63 monomers are involved in 144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	503	PEG	1	0
7	A	532	1PE	5	0
6	E	504	EDO	1	0
6	A	520	EDO	1	0
6	F	513	EDO	1	0
6	B	510	EDO	1	0
4	C	502	S5Q	5	0
6	D	508	EDO	1	0
6	B	518	EDO	2	0
5	D	507	PEG	5	0
5	B	504	PEG	2	0
5	D	526	PEG	3	0
6	D	513	EDO	2	0
5	A	503	PEG	4	0

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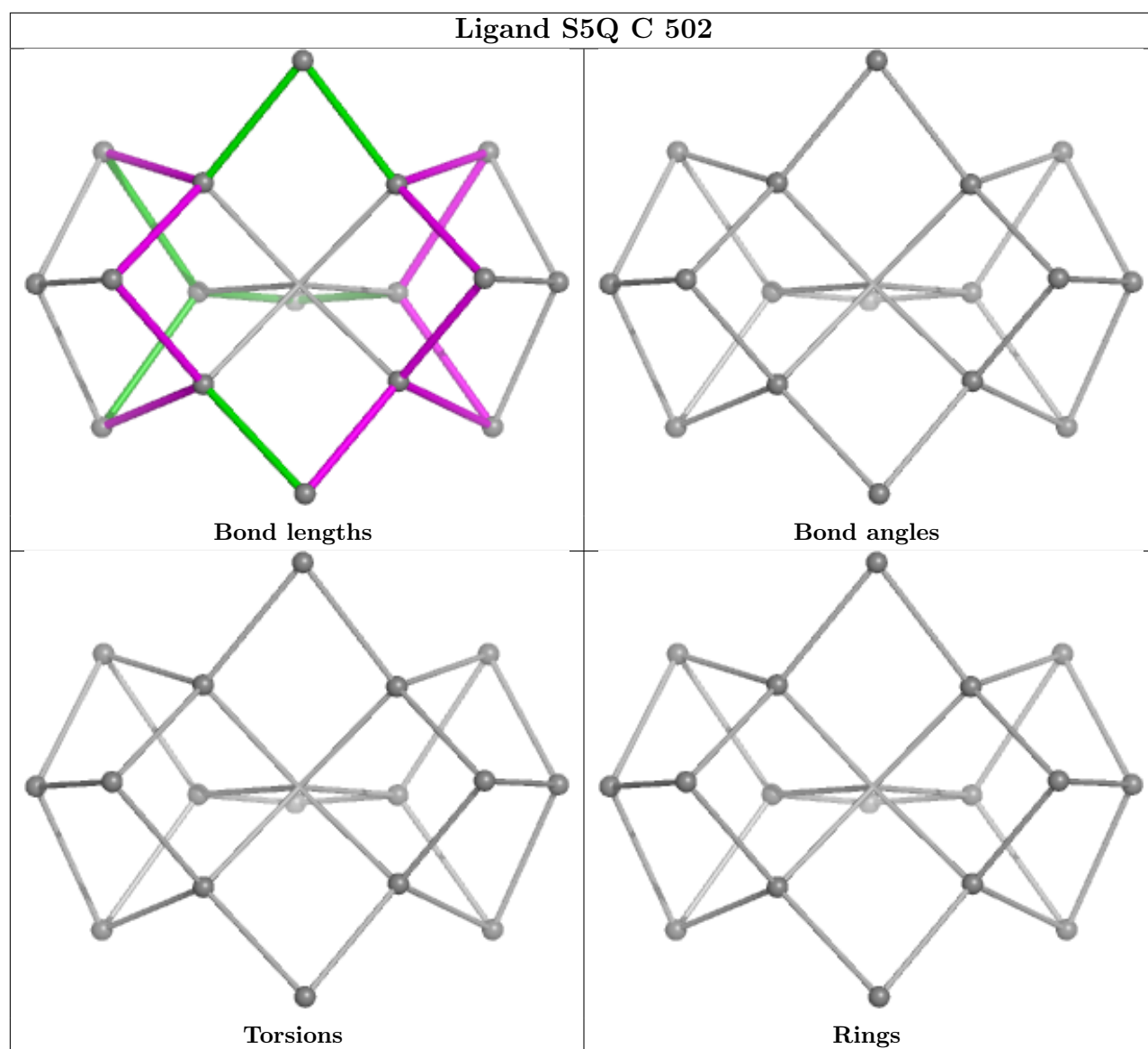
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	SF4	1	0
6	H	510	EDO	1	0
6	A	512	EDO	2	0
6	A	522	EDO	2	0
4	E	502	S5Q	5	0
6	B	512	EDO	1	0
6	H	507	EDO	2	0
8	A	536	PGE	1	0
5	H	504	PEG	5	0
6	G	503	EDO	5	0
6	B	528	EDO	2	0
6	C	506	EDO	3	0
5	D	504	PEG	3	0
5	D	511	PEG	1	0
6	A	513	EDO	1	0
5	G	506	PEG	6	0
4	G	502	S5Q	5	0
6	B	511	EDO	3	0
6	D	503	EDO	3	0
6	D	521	EDO	2	0
6	E	509	EDO	1	0
6	B	505	EDO	5	0
8	H	514	PGE	4	0
6	C	504	EDO	1	0
5	H	502	PEG	1	0
6	H	511	EDO	1	0
5	A	533	PEG	1	0
3	C	501	SF4	1	0
6	E	508	EDO	1	0
6	B	506	EDO	1	0
6	A	516	EDO	1	0
5	A	510	PEG	1	0
8	H	513	PGE	2	0
4	A	502	S5Q	5	0
6	D	520	EDO	3	0
8	A	535	PGE	2	0
6	C	507	EDO	1	0
6	B	509	EDO	3	0
3	E	501	SF4	1	0
6	A	517	EDO	2	0
8	G	517	PGE	4	0
6	A	521	EDO	1	0

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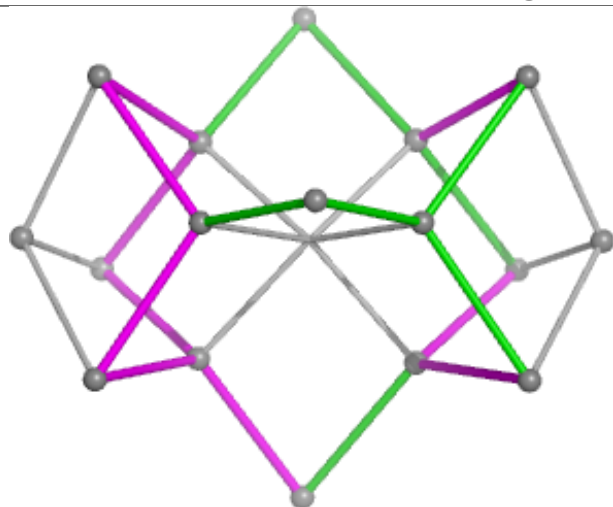
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	505	EDO	1	0
5	B	503	PEG	5	0
6	A	511	EDO	2	0
8	F	525	PGE	1	0
6	H	509	EDO	1	0
6	B	513	EDO	4	0
6	D	522	EDO	2	0

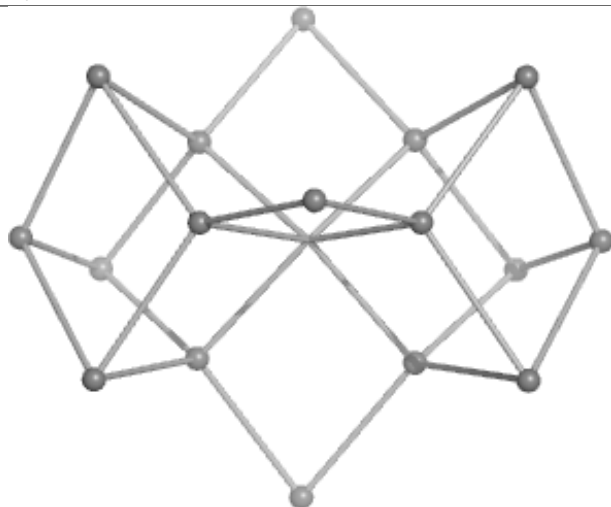
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



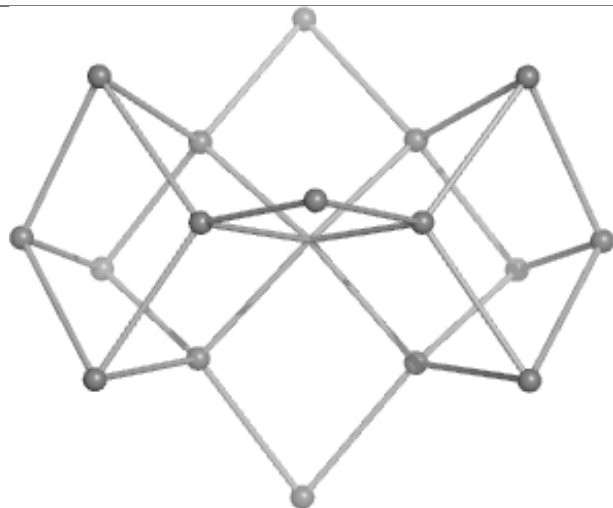
Ligand S5Q E 502



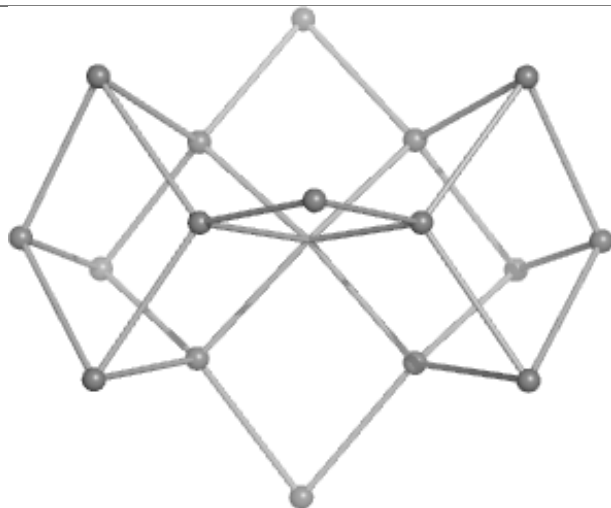
Bond lengths



Bond angles

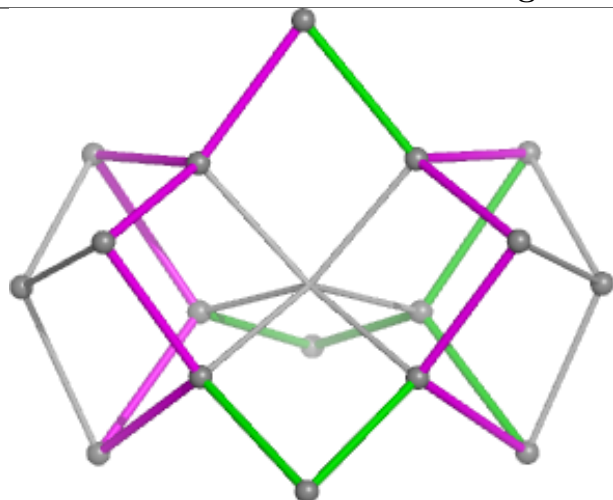


Torsions

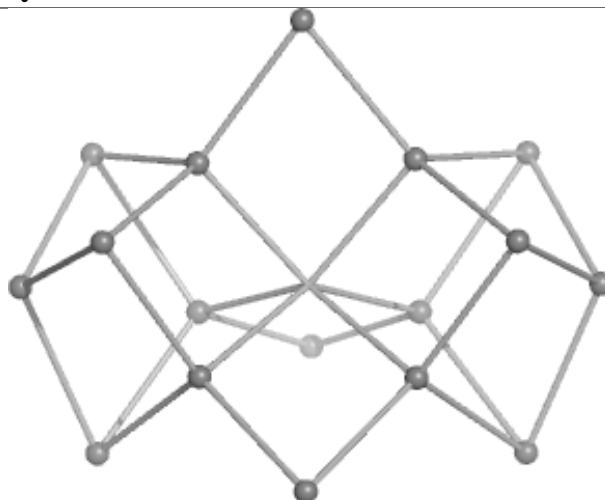


Rings

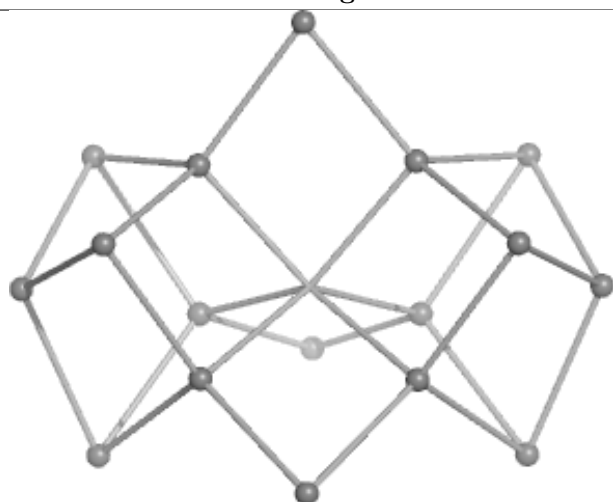
Ligand S5Q G 502



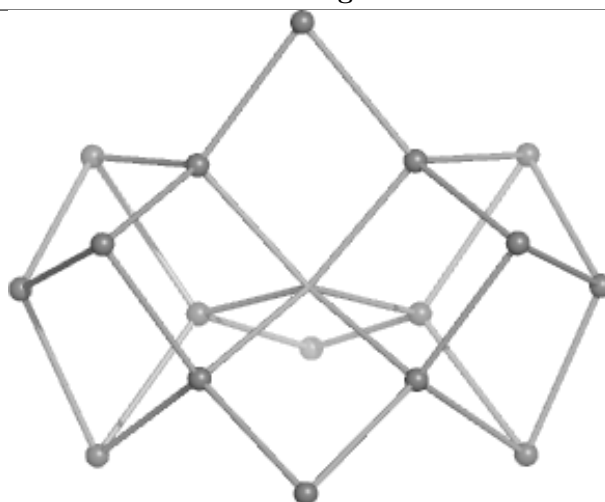
Bond lengths



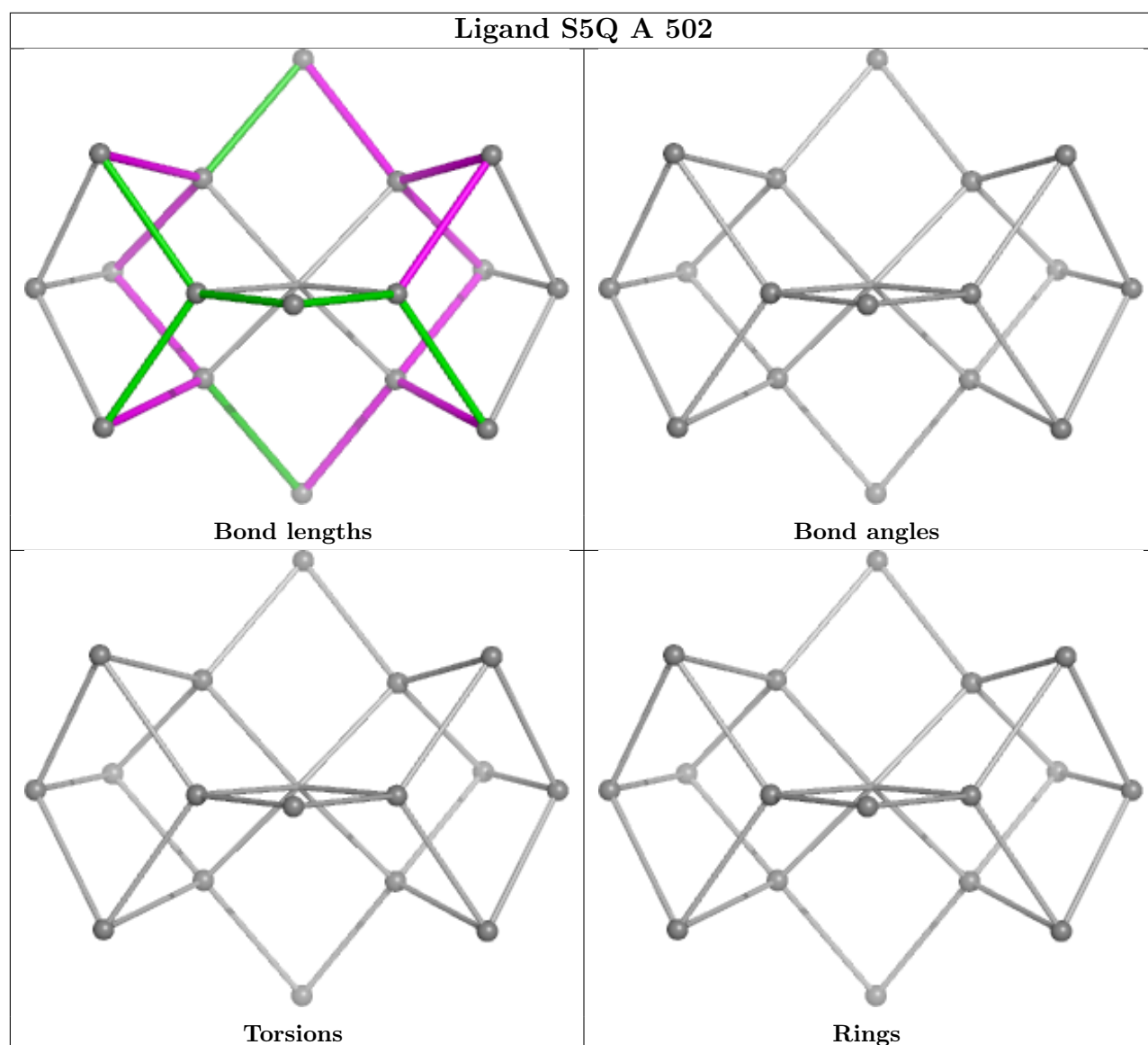
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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 [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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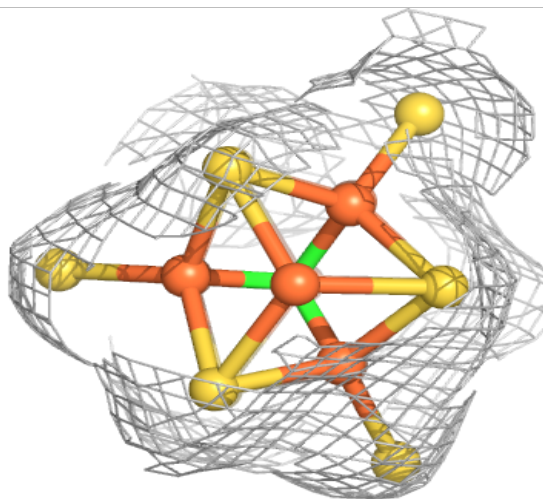
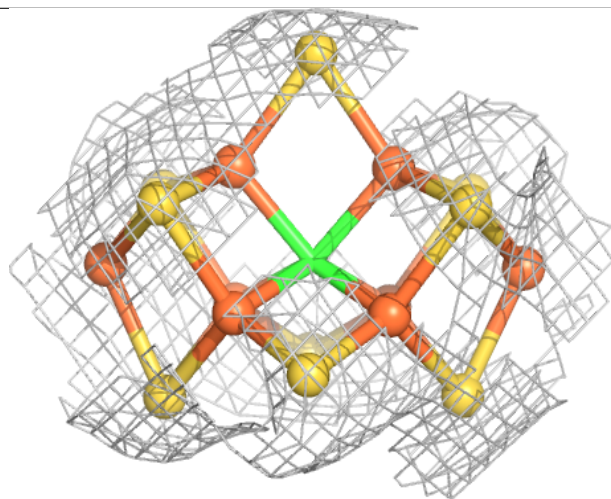
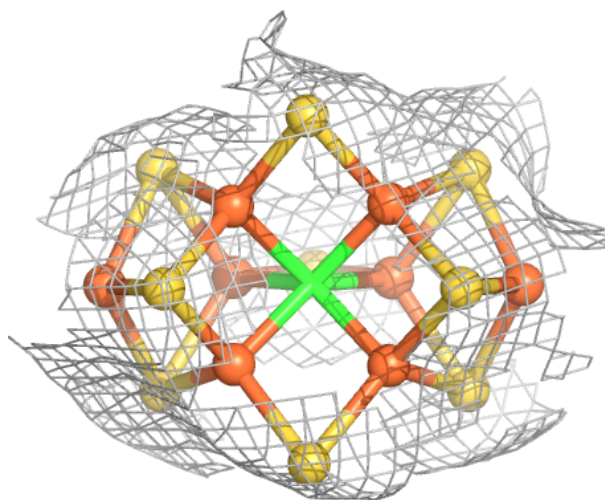
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	MG	F	502	1/1	1.00	0.01	49,49,49,49	0
4	S5Q	A	502	18/18	1.00	0.02	52,53,53,53	0
3	SF4	C	501	8/8	1.00	0.02	36,36,37,37	0

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.

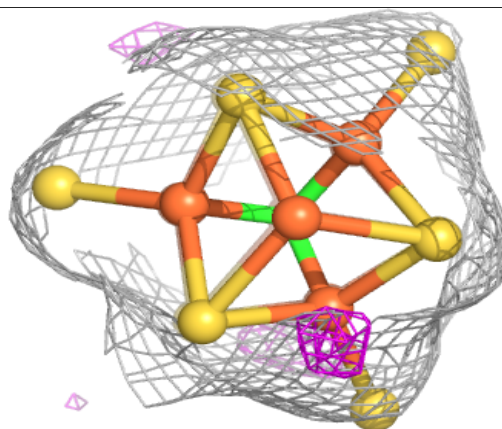
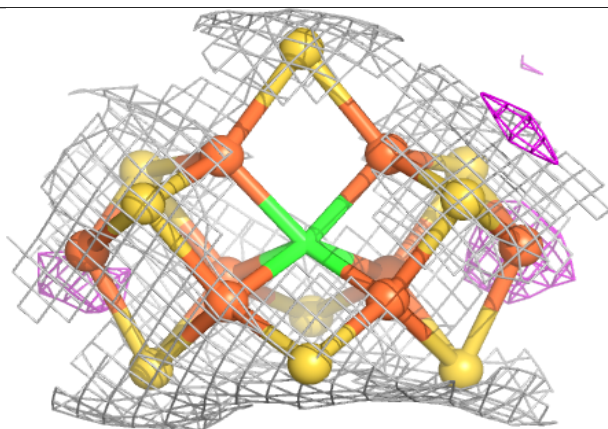
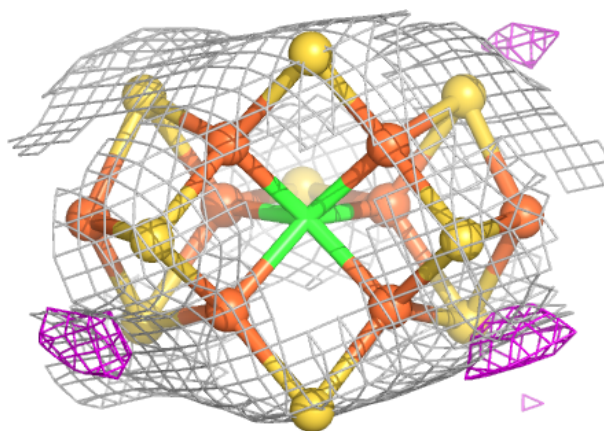
Electron density around S5Q C 502:

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



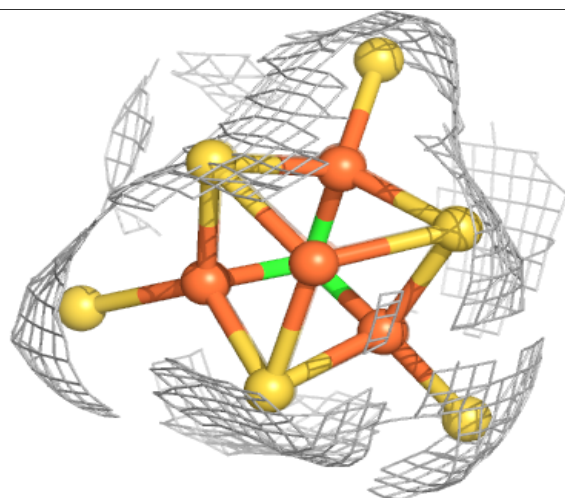
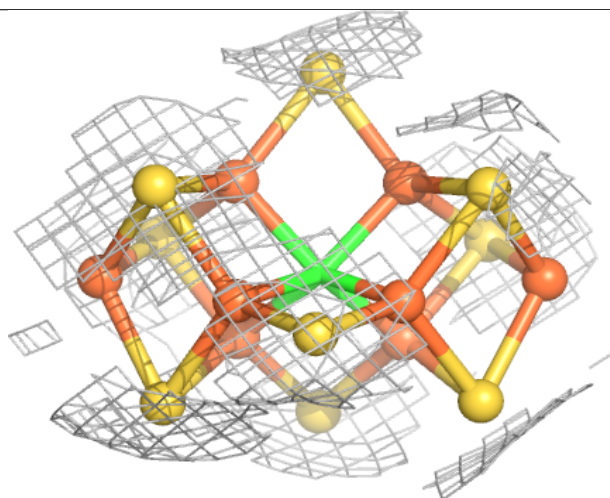
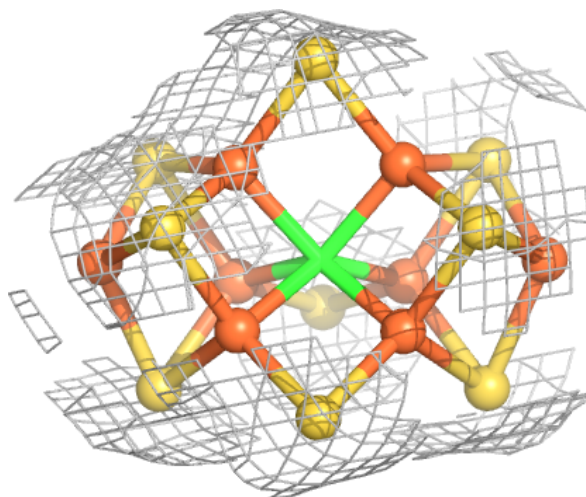
Electron density around S5Q E 502:

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



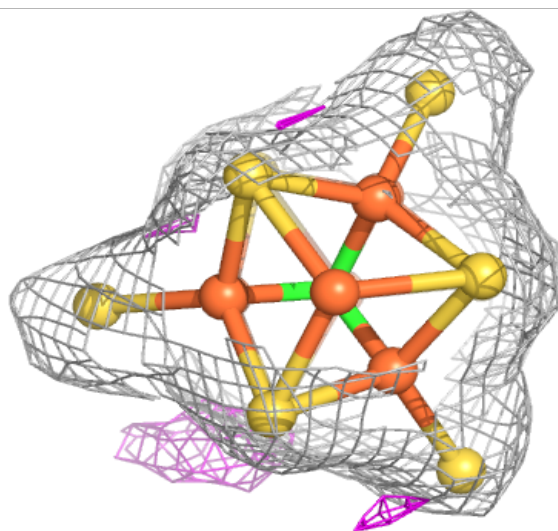
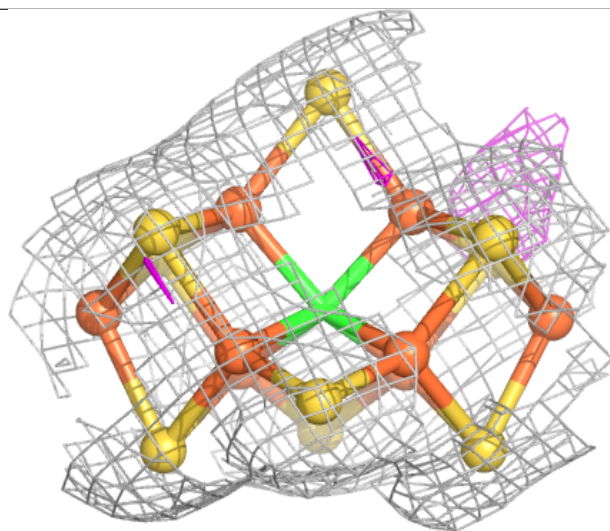
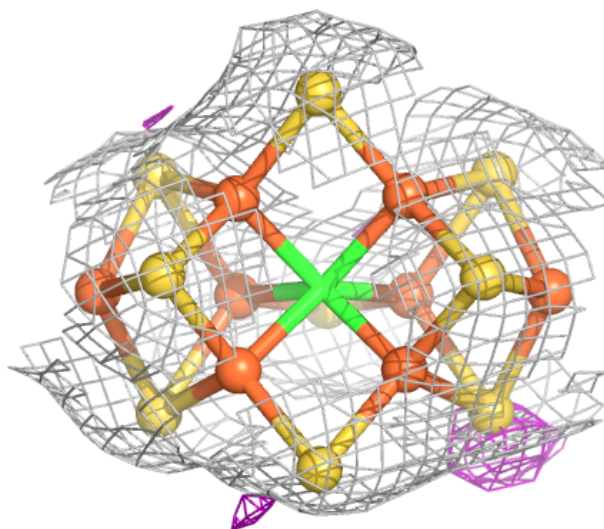
Electron density around S5Q G 502:

$2mF_o-DF_c$ (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.