



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 05:55 PM EDT

PDB ID : 6VK8
Title : Crystal Structure of Methylosinus trichosporium OB3b Soluble Methane Monooxygenase Hydroxylase and Regulatory Component Complex with small organic carboxylate at active center
Authors : Jones, J.C.; Banerjee, R.; Shi, K.; Aihara, H.; Lipscomb, J.D.
Deposited on : 2020-01-18
Resolution : 2.03 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:

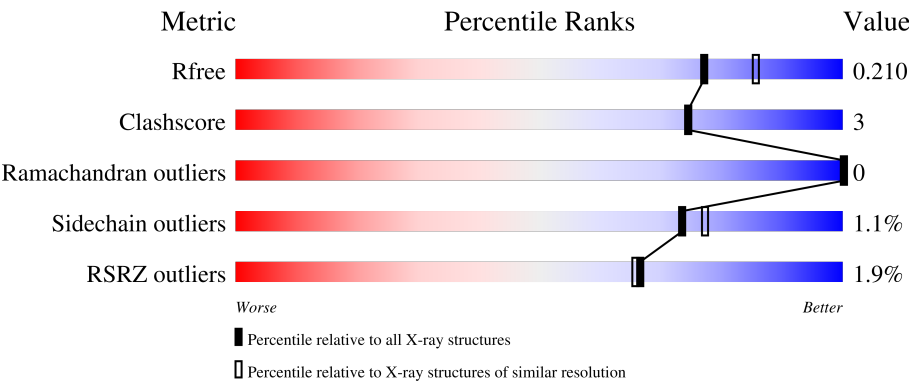
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.03 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	526	<div><div>2%</div><div>86%</div><div>11%</div><div>.</div></div>
1	E	526	<div><div>2%</div><div>87%</div><div>10%</div><div>.</div></div>
2	B	395	<div><div>%</div><div>95%</div><div>.</div><div>..</div></div>
2	F	395	<div><div></div><div>92%</div><div>7%</div><div>.</div></div>
3	C	169	<div><div>2%</div><div>93%</div><div>7%</div><div>.</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	169	<div><div></div><div>2%</div><div>95%</div><div></div></div>
4	D	138	<div><div></div><div>4%</div><div>91%</div><div></div></div>
4	H	138	<div><div></div><div>4%</div><div>94%</div><div>5%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21000 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 Methane monooxygenase component A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			4175	2676	723	764	12			
1	E	515	Total	C	N	O	S	0	1	0
			4183	2682	724	765	12			

- Molecule 2 is a protein called Methane monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	392	Total	C	N	O	S	0	0	0
			3185	2033	556	591	5			
2	F	392	Total	C	N	O	S	0	1	0
			3193	2037	558	593	5			

- Molecule 3 is a protein called Methane monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	168	Total	C	N	O	S	0	0	0
			1362	874	234	253	1			
3	G	168	Total	C	N	O	S	0	0	0
			1362	874	234	253	1			

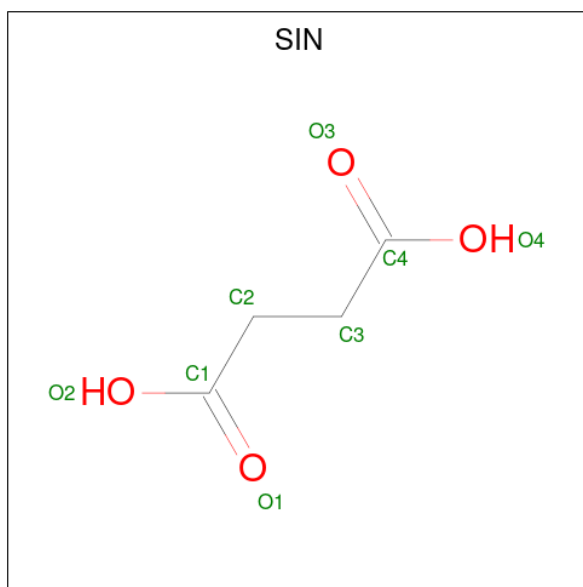
- Molecule 4 is a protein called Methane monooxygenase regulatory protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	132	Total	C	N	O	S	0	0	0
			1002	639	162	198	3			
4	H	137	Total	C	N	O	S	0	0	0
			1038	662	167	206	3			

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

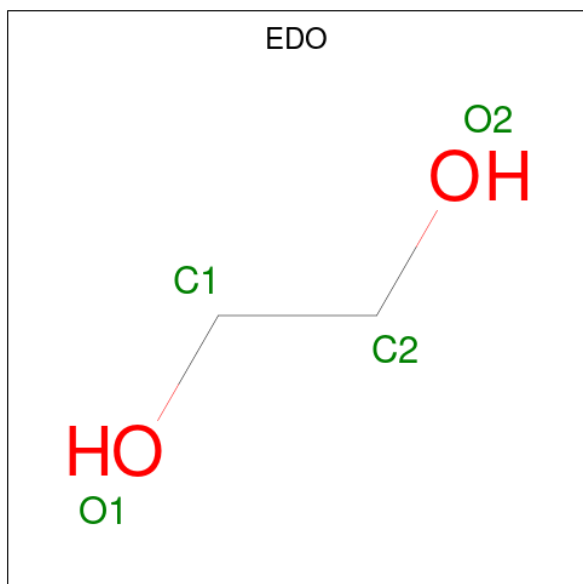
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Fe	0	0
			2	2		
5	E	2	Total	Fe	0	0
			2	2		

- Molecule 6 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



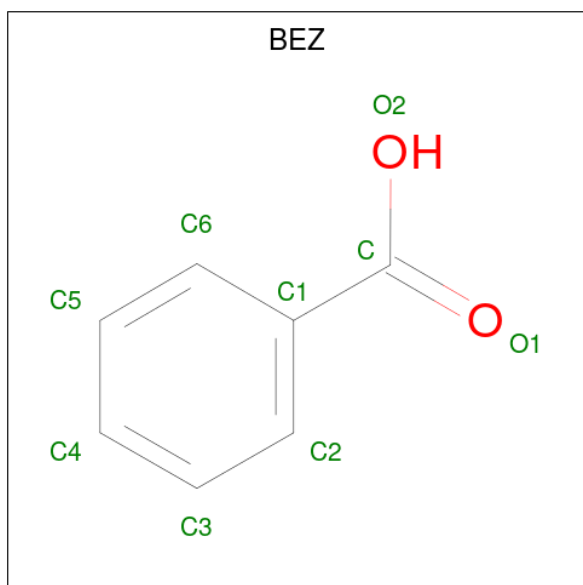
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 8 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			9	7	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	291	Total	O	0	0
			291	291		
9	B	255	Total	O	0	1
			256	256		
9	C	104	Total	O	0	0
			104	104		
9	D	42	Total	O	0	0
			42	42		
9	E	282	Total	O	0	0
			282	282		
9	F	244	Total	O	0	0
			244	244		

Continued on next page...

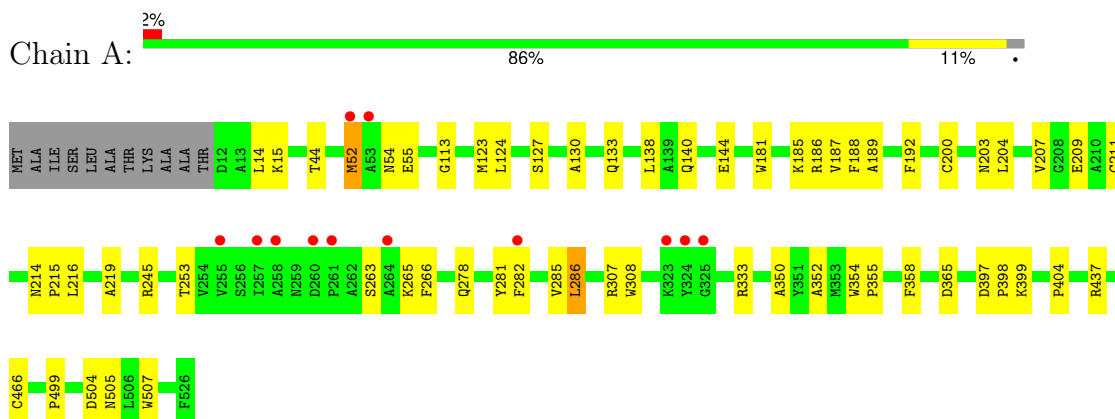
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	110	Total 110	O 110	0	0
9	H	54	Total 54	O 54	0	0

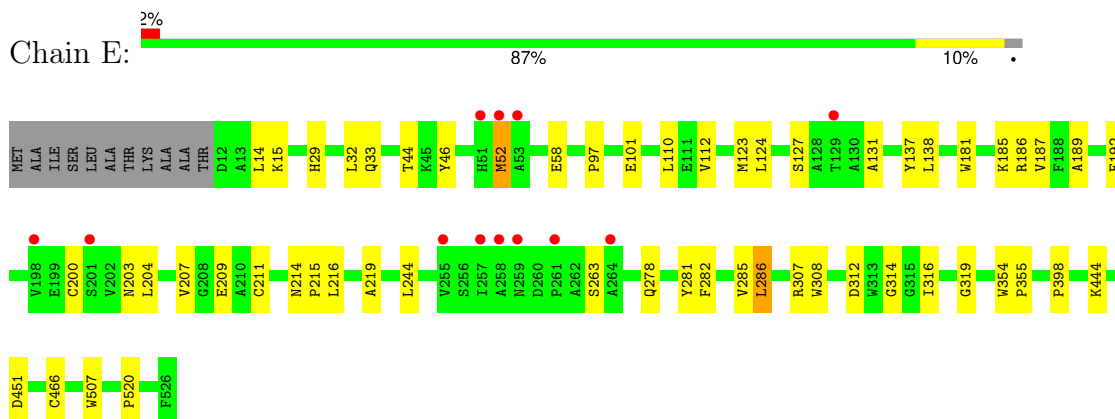
3 Residue-property plots [i](#)

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.

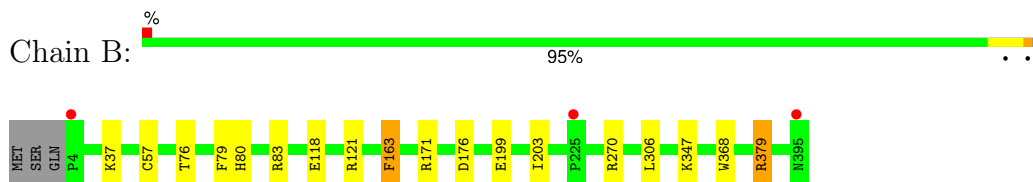
- Molecule 1: Methane monooxygenase component A alpha chain



- Molecule 1: Methane monooxygenase component A alpha chain

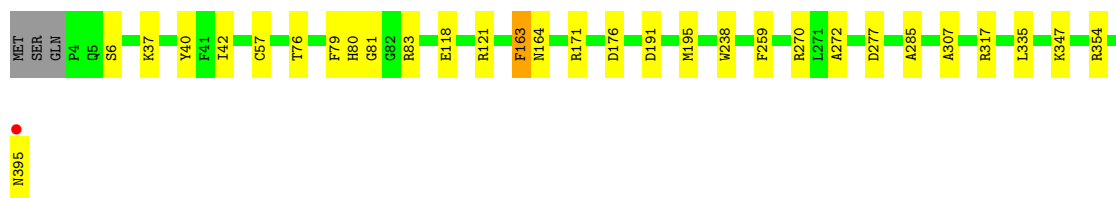


- Molecule 2: Methane monooxygenase

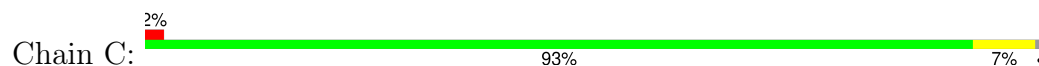


- Molecule 2: Methane monooxygenase





- Molecule 3: Methane monooxygenase



- Molecule 3: Methane monooxygenase



- Molecule 4: Methane monooxygenase regulatory protein B



- Molecule 4: Methane monooxygenase regulatory protein B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.87Å 105.35Å 297.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.99 – 2.03 85.99 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.8 (85.99-2.03) 97.9 (85.99-2.03)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.167 , 0.207 0.172 , 0.210	Depositor DCC
R_{free} test set	10354 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21000	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, FE, BEZ, SIN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/4305	0.55	0/5850
1	E	0.41	0/4313	0.56	0/5861
2	B	0.40	0/3278	0.52	0/4457
2	F	0.40	0/3286	0.53	0/4468
3	C	0.36	0/1388	0.51	0/1877
3	G	0.36	0/1388	0.53	0/1877
4	D	0.37	0/1018	0.53	0/1376
4	H	0.38	0/1054	0.53	0/1426
All	All	0.40	0/20030	0.54	0/27192

There are no bond length outliers.

There are no bond angle outliers.

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	4175	0	3972	42	0
1	E	4183	0	3982	38	0
2	B	3185	0	3025	14	0
2	F	3193	0	3030	23	0
3	C	1362	0	1400	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1362	0	1400	5	0
4	D	1002	0	995	6	0
4	H	1038	0	1033	6	0
5	A	2	0	0	0	0
5	E	2	0	0	0	0
6	A	8	0	4	0	0
7	A	24	0	36	4	0
7	B	12	0	18	1	0
7	C	4	0	6	0	0
7	D	12	0	18	1	0
7	E	24	0	36	2	0
7	F	12	0	18	2	0
7	G	8	0	12	0	0
8	E	9	0	5	1	0
9	A	291	0	0	3	0
9	B	256	0	0	2	0
9	C	104	0	0	0	0
9	D	42	0	0	0	0
9	E	282	0	0	5	0
9	F	244	0	0	3	0
9	G	110	0	0	1	0
9	H	54	0	0	2	0
All	All	21000	0	18990	125	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 3.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:GLU:OE1	9:E:901:HOH:O	2.02	0.77
1:A:54:ASN:HD21	1:A:253:THR:HG22	1.51	0.74
2:F:354:ARG:HH21	2:F:395:ASN:HD21	1.38	0.72
1:E:192:PHE:O	9:E:902:HOH:O	2.11	0.68
4:H:7:ALA:O	9:H:201:HOH:O	2.11	0.68
1:A:187:VAL:HG23	1:A:278:GLN:HA	1.79	0.64
4:H:79:LYS:NZ	9:H:202:HOH:O	2.28	0.62
1:A:354:TRP:HA	7:A:808:EDO:H21	1.81	0.62
3:G:71:GLU:OE1	9:G:301:HOH:O	2.16	0.60
2:F:354:ARG:NH2	2:F:395:ASN:HD21	1.98	0.60
1:A:358:PHE:CE1	7:A:807:EDO:H22	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ASP:OD2	1:A:505:ASN:ND2	2.34	0.60
1:A:181:TRP:CE2	1:A:185:LYS:HD2	2.36	0.59
1:A:466:CYS:HB2	2:B:76:THR:HA	1.84	0.59
1:E:187:VAL:HG23	1:E:278:GLN:HA	1.83	0.59
1:A:350:ALA:HA	7:A:808:EDO:H11	1.86	0.57
1:A:14:LEU:HB2	1:A:15:LYS:HD2	1.88	0.56
1:E:138:LEU:HD22	2:F:163:PHE:CE1	2.41	0.56
1:E:282:PHE:CE2	1:E:286:LEU:HD22	2.41	0.56
1:E:316[A]:ILE:HD12	4:H:37:ALA:O	2.06	0.56
1:A:245:ARG:NH2	9:A:901:HOH:O	2.02	0.55
1:E:123:MET:HG3	2:F:171:ARG:HD3	1.88	0.55
1:E:451:ASP:HB3	7:E:809:EDO:H22	1.88	0.55
1:A:333:ARG:NH2	4:D:27:GLU:OE2	2.39	0.55
1:A:207:VAL:O	1:A:211:CYS:HB3	2.05	0.55
1:A:181:TRP:NE1	1:A:185:LYS:HD2	2.20	0.55
1:E:14:LEU:HB2	1:E:15:LYS:HD2	1.89	0.55
1:A:282:PHE:CE2	1:A:286:LEU:HD22	2.44	0.53
1:E:52:MET:HB3	1:E:263:SER:OG	2.10	0.52
1:E:207:VAL:O	1:E:211:CYS:HB3	2.09	0.52
1:A:138:LEU:HD22	2:B:163:PHE:CE1	2.45	0.52
1:A:185:LYS:O	1:A:189:ALA:HB3	2.09	0.52
2:F:285:ALA:HB2	7:F:401:EDO:H12	1.93	0.51
1:E:181:TRP:CE2	1:E:185:LYS:HD2	2.45	0.51
1:E:185:LYS:O	1:E:189:ALA:HB3	2.10	0.51
1:E:200:CYS:HA	1:E:203:ASN:OD1	2.11	0.51
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.46	0.50
2:F:42:ILE:HD13	2:F:57:CYS:HB2	1.93	0.50
1:A:123:MET:HG3	2:B:171:ARG:HD3	1.94	0.50
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.46	0.50
2:F:80:HIS:CD2	3:G:141:MET:HG2	2.47	0.49
1:E:520:PRO:HB3	7:E:806:EDO:H12	1.94	0.49
1:E:181:TRP:NE1	1:E:185:LYS:HD2	2.27	0.49
1:E:44:THR:HB	1:E:127:SER:HA	1.93	0.49
1:E:33:GLN:HA	1:E:131:ALA:HB3	1.95	0.49
2:F:191:ASP:O	2:F:195:MET:HG2	2.13	0.48
1:A:44:THR:HB	1:A:127:SER:HA	1.95	0.48
2:B:121:ARG:HD3	2:F:118:GLU:OE2	2.14	0.48
1:A:124:LEU:HD21	1:A:200:CYS:HB2	1.96	0.48
2:B:347:LYS:HD3	2:B:347:LYS:HA	1.70	0.47
2:F:317:ARG:NH2	9:F:506:HOH:O	2.46	0.47
1:E:354:TRP:CG	1:E:355:PRO:HD3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:116:ARG:O	3:G:120:LYS:HB2	2.14	0.47
4:D:2:SER:N	4:D:5:HIS:HE2	2.12	0.47
1:E:203:ASN:OD1	1:E:204:LEU:N	2.47	0.47
1:E:316[A]:ILE:HD13	4:H:35:SER:HB3	1.96	0.47
3:C:163:LYS:HD2	3:C:165:LEU:HD21	1.96	0.47
1:E:138:LEU:HD22	2:F:163:PHE:HE1	1.79	0.47
1:E:137:TYR:OH	9:E:903:HOH:O	2.20	0.47
2:F:307:ALA:O	2:F:317:ARG:HD2	2.14	0.47
1:A:215:PRO:HG2	1:A:282:PHE:CZ	2.50	0.47
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.97	0.47
2:F:57:CYS:HB3	9:F:731:HOH:O	2.14	0.47
2:B:57:CYS:HB3	9:B:736:HOH:O	2.14	0.47
2:B:79:PHE:HB2	2:B:83:ARG:HB3	1.96	0.46
2:F:347:LYS:HD3	2:F:347:LYS:HA	1.68	0.46
1:E:124:LEU:HD21	1:E:200:CYS:HB2	1.97	0.46
1:E:215:PRO:HA	1:E:219:ALA:HB3	1.98	0.45
2:B:118:GLU:OE2	2:F:121:ARG:HD3	2.16	0.45
4:D:2:SER:HA	4:D:3:SER:HA	1.78	0.45
2:B:37:LYS:NZ	9:B:509:HOH:O	2.48	0.45
2:F:259:PHE:HA	2:F:335:LEU:HD21	1.99	0.45
1:A:398:PRO:HA	1:A:507:TRP:CE2	2.51	0.44
2:F:164:ASN:HB3	2:F:238:TRP:CE2	2.53	0.44
3:C:116:ARG:O	3:C:120:LYS:HB2	2.17	0.44
1:E:466:CYS:HB2	2:F:76:THR:HA	1.99	0.44
1:A:215:PRO:HG2	1:A:282:PHE:HZ	1.82	0.44
1:A:192:PHE:CE1	1:A:204:LEU:HA	2.53	0.44
1:A:203:ASN:OD1	1:A:204:LEU:N	2.51	0.44
1:A:215:PRO:HA	1:A:219:ALA:HB3	2.00	0.44
1:E:281:TYR:CZ	1:E:285:VAL:HG21	2.53	0.44
1:E:192:PHE:CE1	1:E:204:LEU:HA	2.53	0.43
1:A:399:LYS:HA	1:A:399:LYS:HD3	1.84	0.43
1:A:365:ASP:HB2	9:A:1146:HOH:O	2.18	0.43
2:B:80:HIS:CD2	3:C:141:MET:HG2	2.53	0.43
2:F:6:SER:HB3	4:H:7:ALA:HB1	2.00	0.43
1:E:312:ASP:O	1:E:316[A]:ILE:HG12	2.18	0.43
2:F:79:PHE:HB2	2:F:83:ARG:HB3	2.00	0.43
1:A:52:MET:HB3	1:A:263:SER:OG	2.19	0.43
1:A:265:LYS:HE2	1:A:266:PHE:CZ	2.53	0.42
1:A:214:ASN:HB3	1:A:308:TRP:CE3	2.54	0.42
1:E:444:LYS:NZ	9:E:916:HOH:O	2.47	0.42
1:A:140:GLN:O	1:A:144:GLU:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:PRO:HD3	3:C:129:PHE:CG	2.54	0.42
1:A:55:GLU:HA	1:A:130:ALA:HB2	2.01	0.42
1:E:314:GLY:O	1:E:319:GLY:N	2.50	0.42
1:A:200:CYS:HA	1:A:203:ASN:OD1	2.20	0.42
4:D:129:MET:HE3	4:D:129:MET:HB2	1.86	0.42
1:E:29:HIS:CD2	1:E:32:LEU:HD12	2.55	0.42
2:B:306:LEU:HD23	2:B:306:LEU:HA	1.92	0.41
2:B:379:ARG:HA	2:B:379:ARG:HD3	1.79	0.41
2:B:368:TRP:HA	7:B:403:EDO:H21	2.01	0.41
4:D:5:HIS:H	4:D:5:HIS:CD2	2.38	0.41
1:A:216:LEU:HD13	1:A:286:LEU:HD11	2.02	0.41
3:C:57:ILE:O	3:C:61:ILE:HG13	2.20	0.41
2:F:81:GLY:HA3	3:G:112:HIS:CE1	2.55	0.41
1:A:397:ASP:OD1	9:A:902:HOH:O	2.21	0.41
3:G:119:TYR:HB3	3:G:124:LEU:HD22	2.02	0.41
4:H:3:SER:HB3	4:H:66:SER:HA	2.02	0.41
3:C:58:GLU:O	3:C:62:GLU:HG3	2.21	0.41
4:D:99:PHE:HE1	7:D:202:EDO:H11	1.84	0.41
1:A:113:GLY:HA2	1:A:188:PHE:O	2.21	0.41
1:E:110:LEU:HD13	1:E:216:LEU:HD21	2.02	0.41
1:E:214:ASN:HB3	1:E:308:TRP:CE3	2.56	0.41
2:F:37:LYS:HB3	2:F:40:TYR:HB3	2.03	0.41
1:E:46:TYR:HB3	9:E:1018:HOH:O	2.19	0.41
1:E:209:GLU:HG2	8:E:803:BEZ:O1	2.21	0.41
1:A:204:LEU:O	1:A:209:GLU:HG3	2.21	0.40
2:B:199:GLU:O	2:B:203:ILE:HG13	2.21	0.40
2:F:272:ALA:HB1	2:F:277:ASP:HB3	2.03	0.40
1:E:398:PRO:HA	1:E:507:TRP:CE2	2.56	0.40
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.56	0.40
1:A:358:PHE:CD1	7:A:807:EDO:H22	2.56	0.40
7:F:402:EDO:H11	9:F:538:HOH:O	2.20	0.40
1:E:97:PRO:O	1:E:101:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	513/526 (98%)	495 (96%)	18 (4%)	0	100	100
1	E	514/526 (98%)	500 (97%)	14 (3%)	0	100	100
2	B	390/395 (99%)	379 (97%)	11 (3%)	0	100	100
2	F	391/395 (99%)	379 (97%)	12 (3%)	0	100	100
3	C	166/169 (98%)	164 (99%)	2 (1%)	0	100	100
3	G	166/169 (98%)	164 (99%)	2 (1%)	0	100	100
4	D	130/138 (94%)	126 (97%)	4 (3%)	0	100	100
4	H	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
All	All	2405/2456 (98%)	2337 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	426/433 (98%)	420 (99%)	6 (1%)	67	70
1	E	427/433 (99%)	421 (99%)	6 (1%)	67	70
2	B	324/327 (99%)	320 (99%)	4 (1%)	71	75
2	F	325/327 (99%)	322 (99%)	3 (1%)	78	82
3	C	145/146 (99%)	145 (100%)	0	100	100
3	G	145/146 (99%)	145 (100%)	0	100	100
4	D	105/110 (96%)	103 (98%)	2 (2%)	57	59
4	H	109/110 (99%)	108 (99%)	1 (1%)	78	82
All	All	2006/2032 (99%)	1984 (99%)	22 (1%)	73	77

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	MET
1	A	133	GLN
1	A	186	ARG
1	A	286	LEU
1	A	307	ARG
1	A	437	ARG
2	B	163	PHE
2	B	176	ASP
2	B	270	ARG
2	B	379	ARG
4	D	114	ARG
4	D	129	MET
1	E	52	MET
1	E	112	VAL
1	E	186	ARG
1	E	244	LEU
1	E	286	LEU
1	E	307	ARG
2	F	163	PHE
2	F	176	ASP
2	F	270	ARG
4	H	129	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	395	ASN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 4 are monoatomic - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	EDO	B	401	-	3,3,3	0.51	0	2,2,2	0.31	0
7	EDO	A	807	-	3,3,3	0.37	0	2,2,2	0.39	0
6	SIN	A	803	5	7,7,7	1.17	0	8,8,8	1.62	1 (12%)
7	EDO	G	201	-	3,3,3	0.50	0	2,2,2	0.40	0
7	EDO	A	808	-	3,3,3	0.47	0	2,2,2	0.20	0
7	EDO	F	402	-	3,3,3	0.44	0	2,2,2	0.42	0
7	EDO	A	806	-	3,3,3	0.47	0	2,2,2	0.22	0
7	EDO	D	201	-	3,3,3	0.39	0	2,2,2	0.35	0
7	EDO	D	202	-	3,3,3	0.54	0	2,2,2	0.27	0
7	EDO	D	203	-	3,3,3	0.49	0	2,2,2	0.20	0
7	EDO	A	809	-	3,3,3	0.48	0	2,2,2	0.33	0
7	EDO	B	402	-	3,3,3	0.44	0	2,2,2	0.49	0
8	BEZ	E	803	5	9,9,9	0.89	0	11,11,11	0.94	0
7	EDO	C	201	-	3,3,3	0.41	0	2,2,2	0.31	0
7	EDO	E	807	-	3,3,3	0.44	0	2,2,2	0.34	0
7	EDO	F	403	-	3,3,3	0.42	0	2,2,2	0.44	0
7	EDO	B	403	-	3,3,3	0.54	0	2,2,2	0.23	0
7	EDO	E	808	-	3,3,3	0.40	0	2,2,2	0.50	0
7	EDO	E	805	-	3,3,3	0.54	0	2,2,2	0.22	0
7	EDO	F	401	-	3,3,3	0.50	0	2,2,2	0.39	0
7	EDO	E	806	-	3,3,3	0.51	0	2,2,2	0.26	0
7	EDO	A	804	-	3,3,3	0.43	0	2,2,2	0.39	0
7	EDO	G	202	-	3,3,3	0.44	0	2,2,2	0.27	0
7	EDO	E	809	-	3,3,3	0.53	0	2,2,2	0.28	0
7	EDO	E	804	-	3,3,3	0.45	0	2,2,2	0.35	0
7	EDO	A	805	-	3,3,3	0.39	0	2,2,2	0.54	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
7	EDO	B	401	-	-	1/1/1/1	-
7	EDO	A	807	-	-	0/1/1/1	-
6	SIN	A	803	5	-	0/5/5/5	-
7	EDO	G	201	-	-	0/1/1/1	-
7	EDO	A	808	-	-	1/1/1/1	-
7	EDO	F	402	-	-	1/1/1/1	-
7	EDO	A	806	-	-	0/1/1/1	-
7	EDO	D	201	-	-	0/1/1/1	-
7	EDO	D	202	-	-	1/1/1/1	-
7	EDO	D	203	-	-	1/1/1/1	-
7	EDO	A	809	-	-	0/1/1/1	-
7	EDO	B	402	-	-	0/1/1/1	-
8	BEZ	E	803	5	-	0/4/4/4	0/1/1/1
7	EDO	C	201	-	-	0/1/1/1	-
7	EDO	E	807	-	-	0/1/1/1	-
7	EDO	F	403	-	-	0/1/1/1	-
7	EDO	B	403	-	-	0/1/1/1	-
7	EDO	E	808	-	-	0/1/1/1	-
7	EDO	E	805	-	-	1/1/1/1	-
7	EDO	F	401	-	-	1/1/1/1	-
7	EDO	E	806	-	-	1/1/1/1	-
7	EDO	A	804	-	-	0/1/1/1	-
7	EDO	G	202	-	-	0/1/1/1	-
7	EDO	E	809	-	-	0/1/1/1	-
7	EDO	E	804	-	-	0/1/1/1	-
7	EDO	A	805	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	803	SIN	O1-C1-C2	-2.31	115.76	123.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	808	EDO	O1-C1-C2-O2
7	B	401	EDO	O1-C1-C2-O2
7	F	401	EDO	O1-C1-C2-O2
7	E	806	EDO	O1-C1-C2-O2
7	D	202	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	D	203	EDO	O1-C1-C2-O2
7	E	805	EDO	O1-C1-C2-O2
7	F	402	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	807	EDO	2	0
7	A	808	EDO	2	0
7	F	402	EDO	1	0
7	D	202	EDO	1	0
8	E	803	BEZ	1	0
7	B	403	EDO	1	0
7	F	401	EDO	1	0
7	E	806	EDO	1	0
7	E	809	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	515/526 (97%)	0.10	12 (2%) 60 59	23, 32, 54, 82	0
1	E	515/526 (97%)	0.05	12 (2%) 60 59	23, 33, 55, 87	0
2	B	392/395 (99%)	0.00	3 (0%) 86 85	24, 31, 47, 82	0
2	F	392/395 (99%)	-0.03	1 (0%) 94 93	25, 32, 45, 88	0
3	C	168/169 (99%)	0.08	3 (1%) 68 67	27, 37, 51, 74	0
3	G	168/169 (99%)	0.07	3 (1%) 68 67	28, 36, 51, 61	0
4	D	132/138 (95%)	0.22	5 (3%) 40 40	30, 41, 62, 102	0
4	H	137/138 (99%)	0.39	6 (4%) 34 33	31, 43, 69, 101	0
All	All	2419/2456 (98%)	0.07	45 (1%) 66 66	23, 34, 55, 102	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	133	ARG	6.2
4	H	135	LEU	6.0
4	D	133	ARG	5.9
4	H	134	ALA	5.3
4	H	2	SER	4.5
4	H	138	ILE	4.5
1	E	53	ALA	4.4
1	A	255	VAL	4.3
1	A	261	PRO	4.1
1	A	260	ASP	3.9
1	E	52	MET	3.9
1	E	259	ASN	3.9
4	H	136	THR	3.8
1	A	52	MET	3.8
4	D	36	ASN	3.7
1	E	255	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	257	ILE	3.5
3	G	79	ILE	3.5
4	D	2	SER	3.4
1	A	53	ALA	3.3
1	E	261	PRO	3.2
1	A	258	ALA	3.0
3	C	169	ALA	2.9
1	A	282	PHE	2.8
4	D	3	SER	2.7
1	E	51	HIS	2.7
2	B	395	ASN	2.7
1	A	264	ALA	2.4
3	G	158	LYS	2.4
3	C	2	ALA	2.4
2	B	4	PRO	2.4
2	F	395	ASN	2.4
1	A	257	ILE	2.3
1	A	325	GLY	2.2
1	A	324	TYR	2.2
1	E	258	ALA	2.2
4	D	56	VAL	2.2
1	A	323	LYS	2.2
1	E	198	VAL	2.2
1	E	201	SER	2.2
1	E	264	ALA	2.1
3	G	93	ALA	2.1
3	C	91	VAL	2.0
2	B	225	PRO	2.0
1	E	129	THR	2.0

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 monosaccharides in this entry.

6.4 Ligands ⓘ

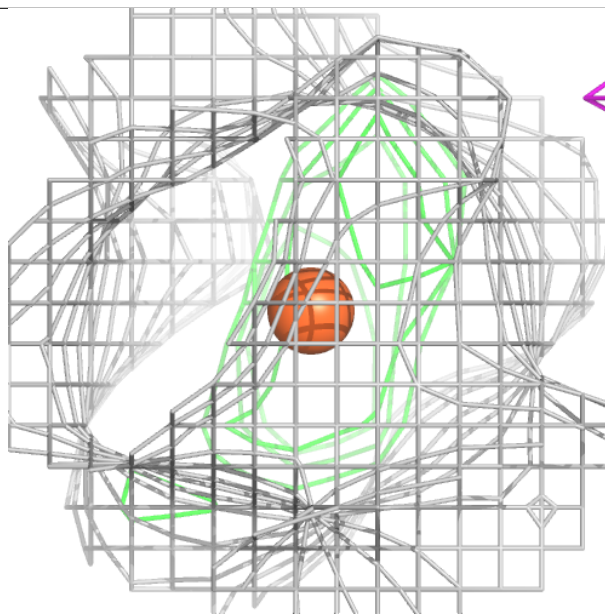
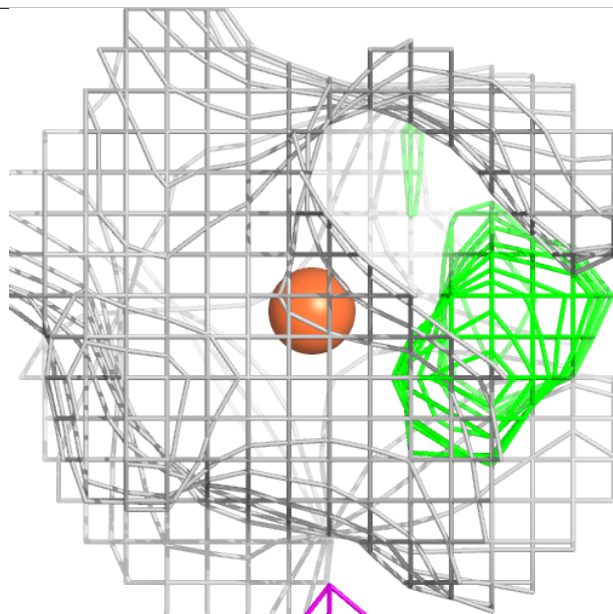
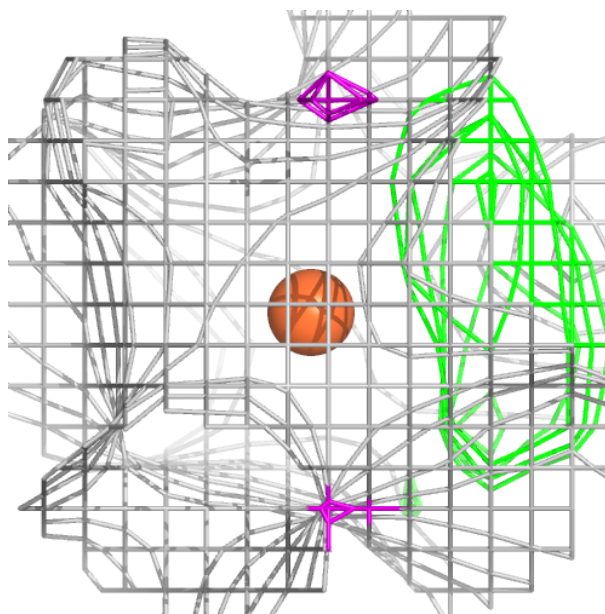
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	D	202	4/4	0.74	0.27	43,48,58,60	0
7	EDO	B	401	4/4	0.77	0.20	47,53,58,59	0
7	EDO	F	403	4/4	0.79	0.20	60,60,63,64	0
7	EDO	E	804	4/4	0.81	0.22	50,56,57,65	0
7	EDO	G	202	4/4	0.81	0.28	60,66,69,71	0
7	EDO	E	806	4/4	0.82	0.24	50,51,53,54	0
7	EDO	E	805	4/4	0.83	0.20	44,46,50,51	0
7	EDO	E	808	4/4	0.84	0.41	65,69,76,80	0
7	EDO	E	807	4/4	0.86	0.45	51,63,71,75	0
7	EDO	B	403	4/4	0.86	0.22	44,45,46,53	0
7	EDO	D	203	4/4	0.88	0.22	53,54,54,57	0
7	EDO	A	809	4/4	0.89	0.33	50,62,66,68	0
7	EDO	E	809	4/4	0.89	0.15	42,43,46,49	0
7	EDO	A	806	4/4	0.90	0.29	52,57,64,72	0
7	EDO	F	401	4/4	0.91	0.19	42,43,44,60	0
7	EDO	A	808	4/4	0.92	0.17	50,51,54,56	0
7	EDO	F	402	4/4	0.92	0.24	39,41,43,47	0
6	SIN	A	803	8/8	0.92	0.17	44,48,68,69	0
7	EDO	A	807	4/4	0.92	0.17	31,33,46,59	0
7	EDO	A	804	4/4	0.93	0.17	41,42,43,49	0
7	EDO	A	805	4/4	0.94	0.21	40,41,45,50	0
7	EDO	B	402	4/4	0.95	0.18	40,41,42,48	0
7	EDO	D	201	4/4	0.95	0.25	39,41,42,44	0
8	BEZ	E	803	9/9	0.95	0.14	37,47,56,56	0
7	EDO	C	201	4/4	0.96	0.18	34,39,41,42	0
7	EDO	G	201	4/4	0.97	0.15	34,36,38,42	0
5	FE	E	801	1/1	0.99	0.10	35,35,35,35	0
5	FE	E	802	1/1	1.00	0.07	39,39,39,39	0
5	FE	A	802	1/1	1.00	0.09	40,40,40,40	0
5	FE	A	801	1/1	1.00	0.09	34,34,34,34	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.

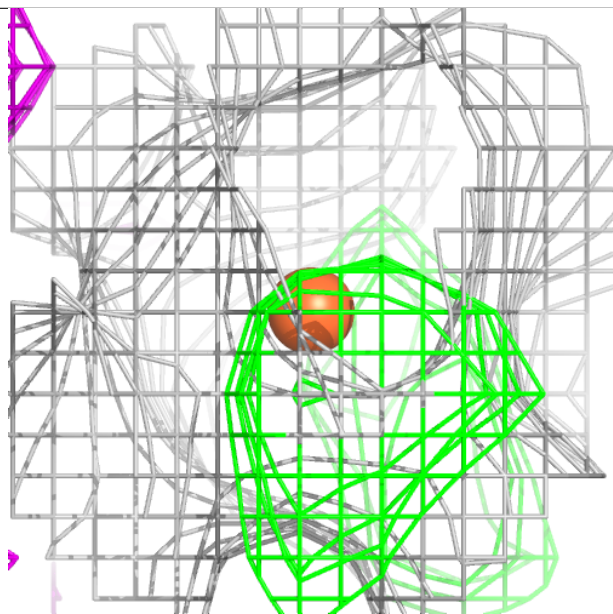
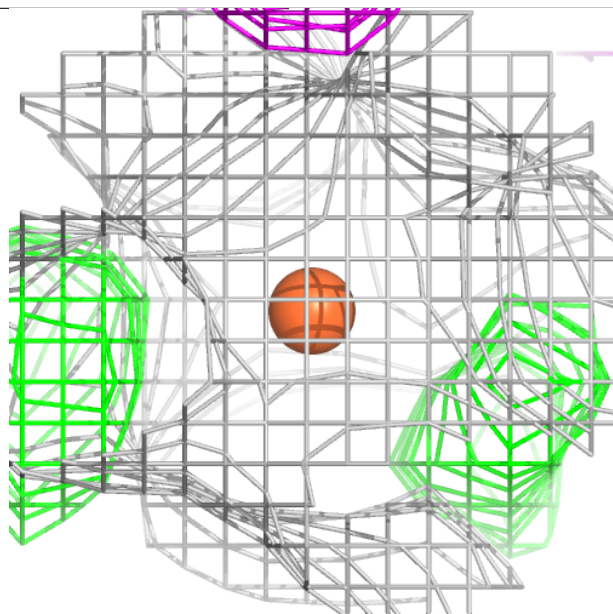
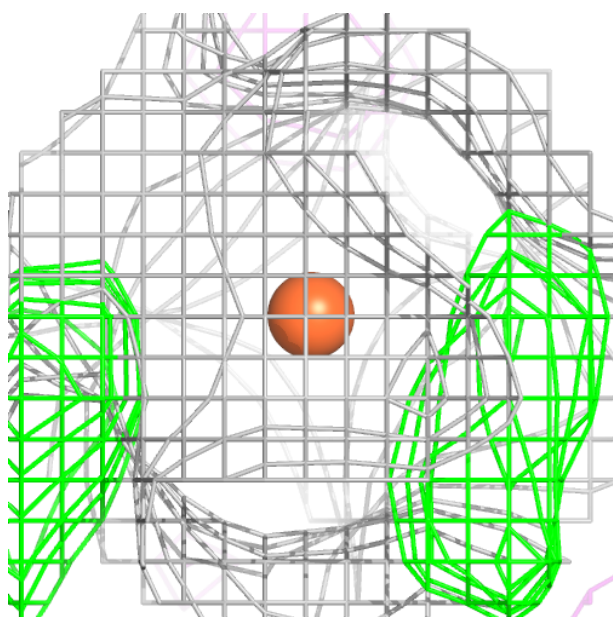
Electron density around FE E 801:

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



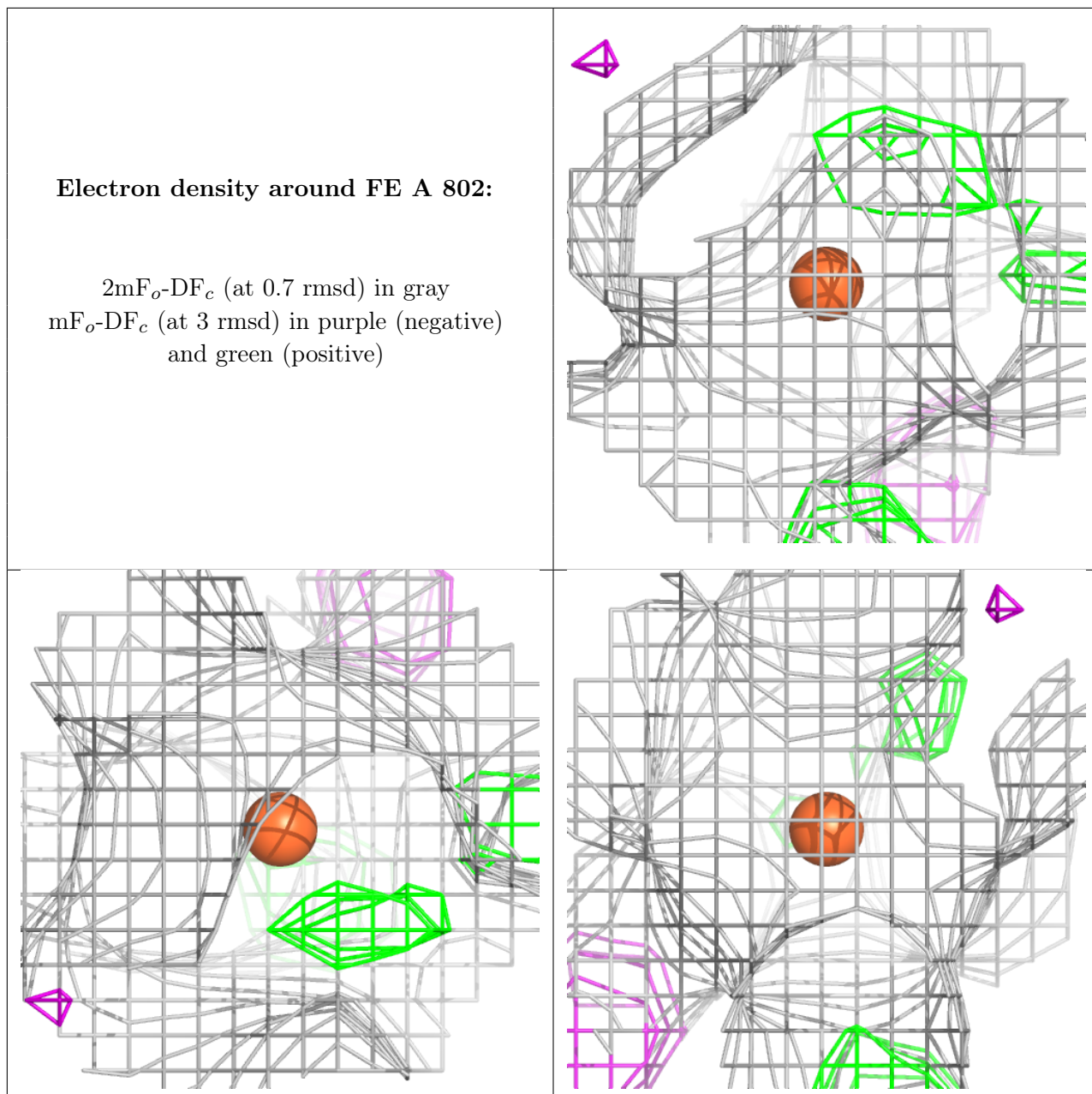
Electron density around FE E 802:

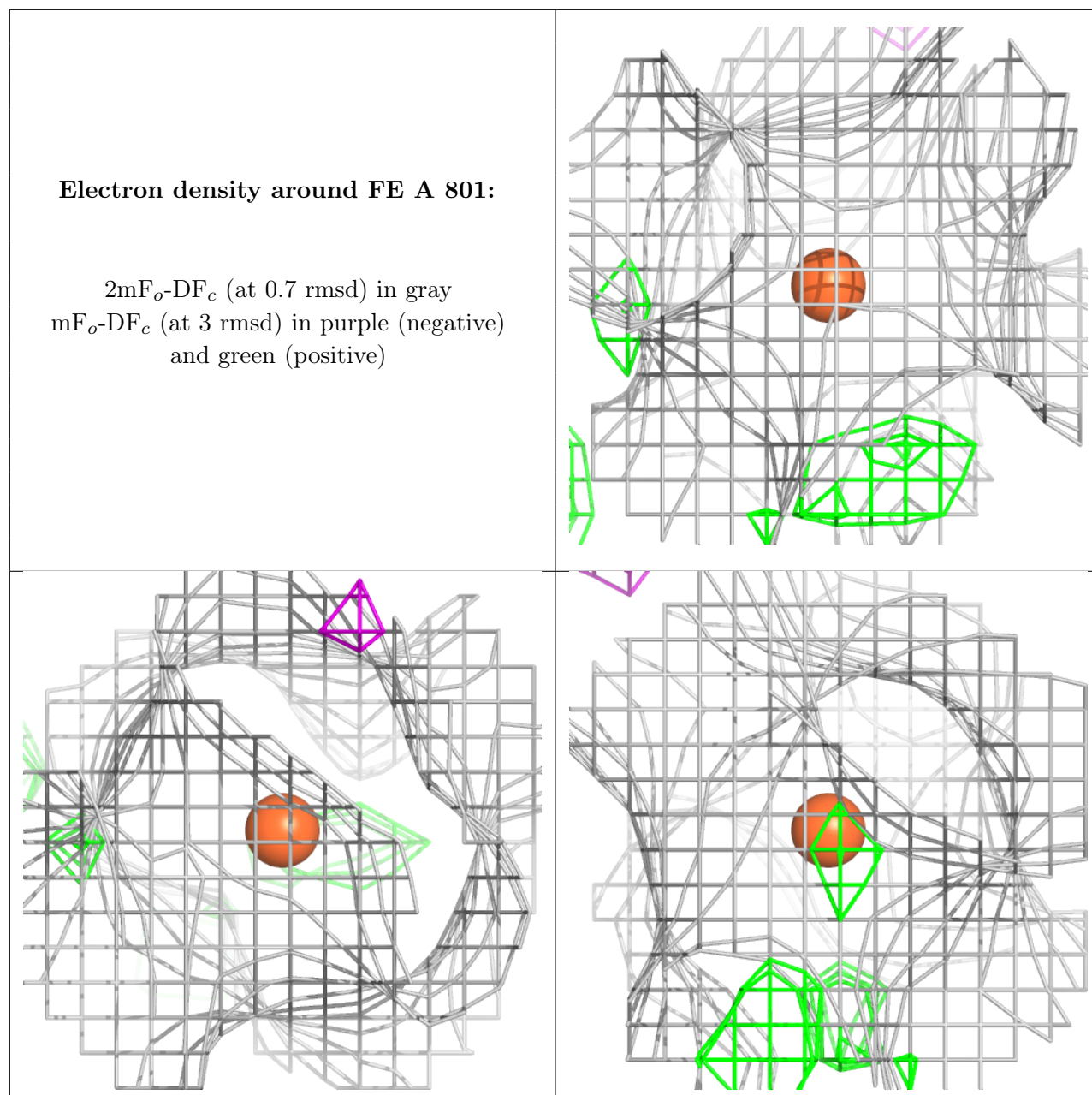
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE A 802:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.