Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 06:33 PM JST

PDB ID	:	7BUI / pdb_00007bui
Title	:	Complex of reduced oxygenase and oxidized ferredoxin in carbazole 1,9a- dioxygenase
Authors	:	Matsuzawa, J.; Wang, Y.X.; Suzuki-Minakuchi, C.; Nojiri, H.
Deposited on	:	2020-04-06
Resolution	:	2.15 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

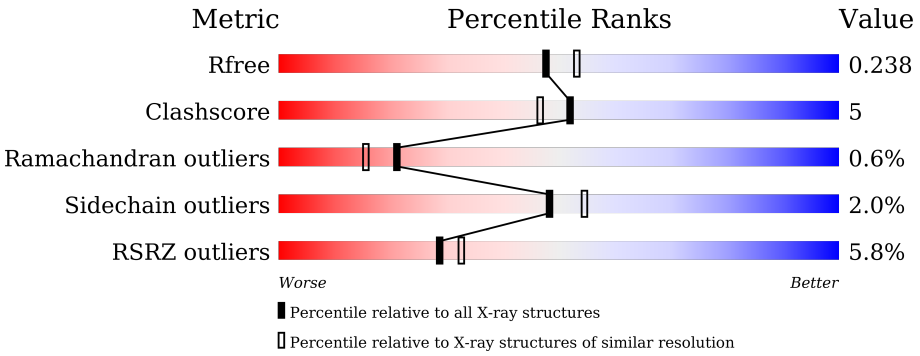
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	4% 81% 19% •
1	B	392	3% 84% 14% ••
1	C	392	4% 86% 12% ••
2	D	115	21% 71% 13% • 15%
2	E	115	12% 86% 7% • 6%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11513 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 Terminal oxygenase component of carbazole.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	389	3146	2010	540	583	13	0	1	0
1	B	389	3162	2024	541	583	14	0	3	0
1	C	388	3128	1999	534	582	13	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	385	LEU	-	expression tag	UNP Q84II6
A	386	GLU	-	expression tag	UNP Q84II6
A	387	HIS	-	expression tag	UNP Q84II6
A	388	HIS	-	expression tag	UNP Q84II6
A	389	HIS	-	expression tag	UNP Q84II6
A	390	HIS	-	expression tag	UNP Q84II6
A	391	HIS	-	expression tag	UNP Q84II6
A	392	HIS	-	expression tag	UNP Q84II6
B	385	LEU	-	expression tag	UNP Q84II6
B	386	GLU	-	expression tag	UNP Q84II6
B	387	HIS	-	expression tag	UNP Q84II6
B	388	HIS	-	expression tag	UNP Q84II6
B	389	HIS	-	expression tag	UNP Q84II6
B	390	HIS	-	expression tag	UNP Q84II6
B	391	HIS	-	expression tag	UNP Q84II6
B	392	HIS	-	expression tag	UNP Q84II6
C	385	LEU	-	expression tag	UNP Q84II6
C	386	GLU	-	expression tag	UNP Q84II6
C	387	HIS	-	expression tag	UNP Q84II6
C	388	HIS	-	expression tag	UNP Q84II6
C	389	HIS	-	expression tag	UNP Q84II6
C	390	HIS	-	expression tag	UNP Q84II6
C	391	HIS	-	expression tag	UNP Q84II6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	392	HIS	-	expression tag	UNP Q84II6

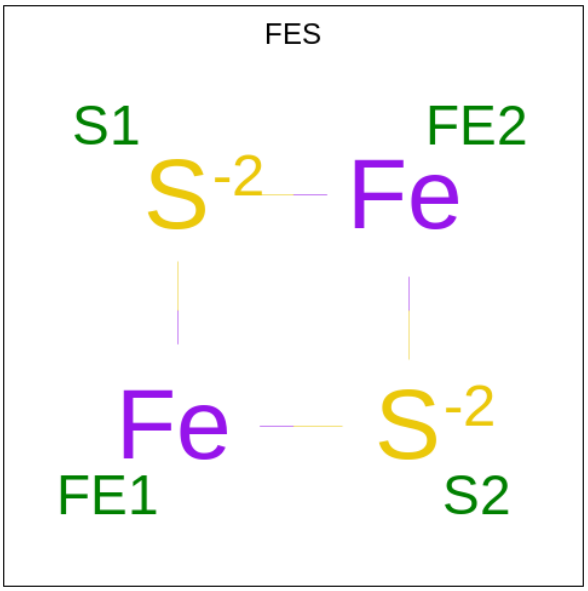
- Molecule 2 is a protein called Ferredoxin CarAc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	98	715	447	120	141	7	0	0	0
			Total	C	N	O	S			
2	E	108	808	507	135	159	7	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	108	LEU	-	expression tag	UNP Q8GI16
D	109	GLU	-	expression tag	UNP Q8GI16
D	110	HIS	-	expression tag	UNP Q8GI16
D	111	HIS	-	expression tag	UNP Q8GI16
D	112	HIS	-	expression tag	UNP Q8GI16
D	113	HIS	-	expression tag	UNP Q8GI16
D	114	HIS	-	expression tag	UNP Q8GI16
D	115	HIS	-	expression tag	UNP Q8GI16
E	108	LEU	-	expression tag	UNP Q8GI16
E	109	GLU	-	expression tag	UNP Q8GI16
E	110	HIS	-	expression tag	UNP Q8GI16
E	111	HIS	-	expression tag	UNP Q8GI16
E	112	HIS	-	expression tag	UNP Q8GI16
E	113	HIS	-	expression tag	UNP Q8GI16
E	114	HIS	-	expression tag	UNP Q8GI16
E	115	HIS	-	expression tag	UNP Q8GI16

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

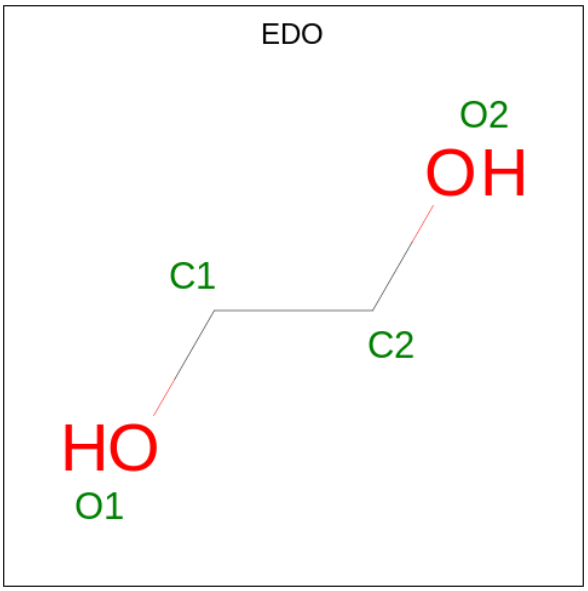


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	D	1	4	2	2	0	0
3	E	1	4	2	2	0	0

- Molecule 4 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

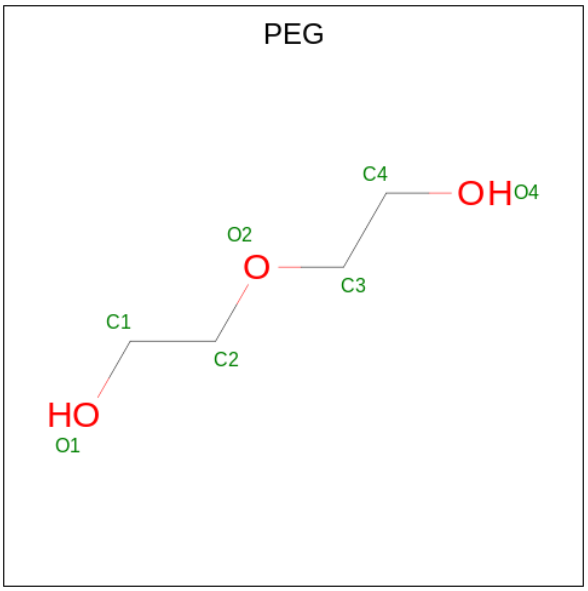
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	7	4	3	0	0
			Total	C	O		
6	E	1	7	4	3	0	0

- Molecule 7 is water.

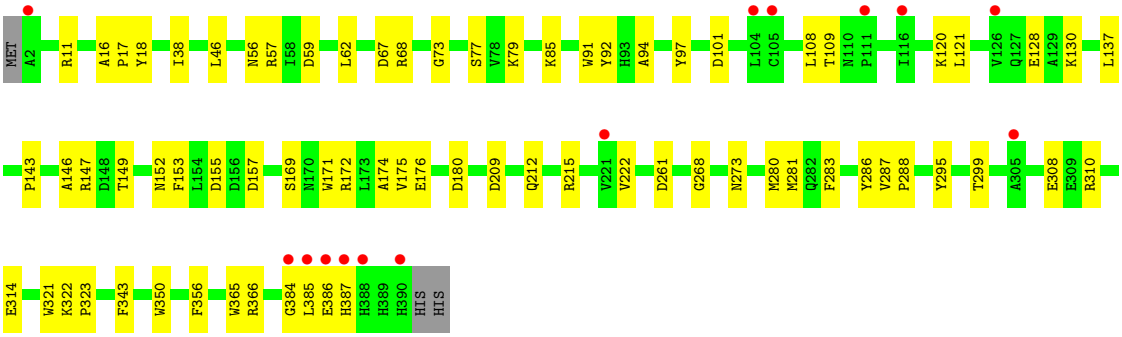
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	104	104	104	0	0
			Total	O		
7	B	214	214	214	0	0
			Total	O		
7	C	129	129	129	0	0
			Total	O		
7	D	9	9	9	0	0
			Total	O		
7	E	21	21	21	0	0

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.

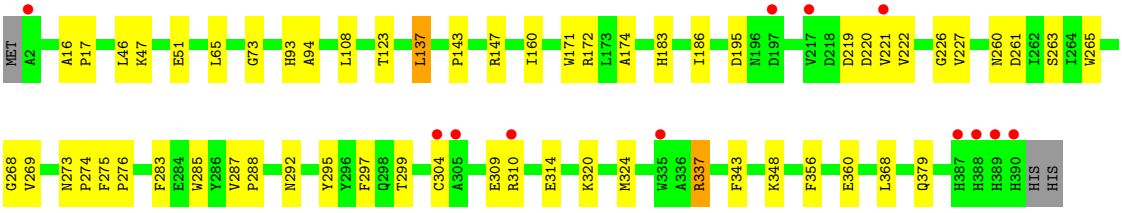
• Molecule 1: Terminal oxygenase component of carbazole

Chain A:



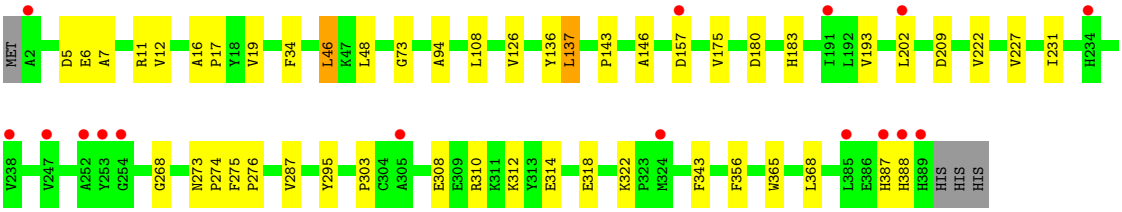
• Molecule 1: Terminal oxygenase component of carbazole

Chain B:



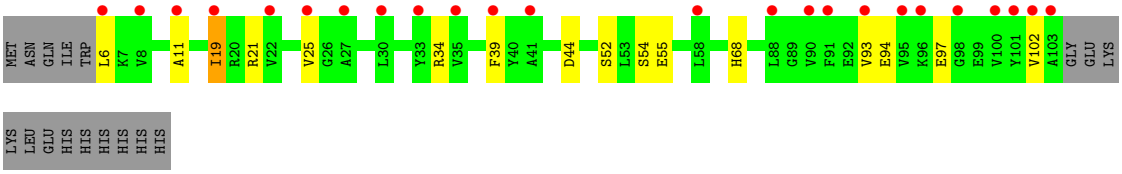
• Molecule 1: Terminal oxygenase component of carbazole

Chain C:



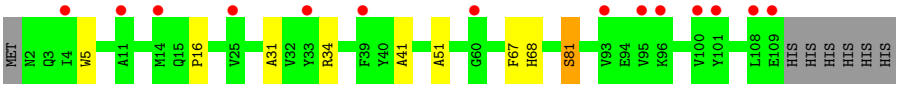
• Molecule 2: Ferredoxin CarAc

Chain D:



- Molecule 2: Ferredoxin CarAc

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.29Å 81.56Å 116.13Å 90.00° 100.12° 90.00°	Depositor
Resolution (Å)	62.17 – 2.15 62.17 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.17-2.15) 99.9 (62.17-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.187 , 0.238 0.194 , 0.238	Depositor DCC
R_{free} test set	4814 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11513	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PEG, FE2, FES

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	1.04	1/3235 (0.0%)	1.30	1/4391 (0.0%)
1	B	1.03	0/3259	1.31	7/4424 (0.2%)
1	C	1.02	0/3213	1.33	2/4362 (0.0%)
2	D	1.16	0/729	1.34	0/993
2	E	1.06	0/827	1.29	0/1124
All	All	1.04	1/11263 (0.0%)	1.31	10/15294 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	TYR	C-O	5.02	1.28	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	337	ARG	CB-CA-C	-7.21	99.55	110.88
1	B	261	ASP	CA-CB-CG	6.15	118.75	112.60
1	C	34	PHE	CA-C-N	5.57	128.02	120.38
1	C	34	PHE	C-N-CA	5.57	128.02	120.38
1	B	261	ASP	CB-CA-C	5.50	119.64	111.17
1	B	260	ASN	CB-CA-C	-5.35	101.76	110.85
1	B	348	LYS	CA-C-N	5.06	126.51	120.13
1	B	348	LYS	C-N-CA	5.06	126.51	120.13
1	B	283	PHE	CA-C-O	-5.06	114.89	120.30
1	A	261	ASP	CA-CB-CG	5.01	117.61	112.60

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	3146	0	3050	38	0
1	B	3162	0	3069	36	0
1	C	3128	0	3030	27	0
2	D	715	0	689	8	0
2	E	808	0	782	7	0
3	A	4	0	0	0	0
3	B	4	0	0	1	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	12	0	18	0	0
5	B	16	0	24	2	0
5	C	12	0	18	0	0
6	B	7	0	10	2	0
6	E	7	0	10	2	0
7	A	104	0	0	1	0
7	B	214	0	0	2	0
7	C	129	0	0	2	0
7	D	9	0	0	0	0
7	E	21	0	0	0	0
All	All	11513	0	10700	111	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 5.

All (111) 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:11:ALA:O	2:D:34:ARG:NH1	2.09	0.85
1:A:310:ARG:O	1:A:314:GLU:HG3	1.84	0.77
2:D:39:PHE:O	2:D:93:VAL:HG21	1.89	0.71
1:A:215[A]:ARG:NH1	7:A:501:HOH:O	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:403:PEG:H12	6:B:403:PEG:H42	1.80	0.63
1:C:310:ARG:NH2	7:C:502:HOH:O	2.30	0.62
1:B:379:GLN:OE1	5:B:404:EDO:O1	2.17	0.62
1:C:94:ALA:HB1	1:C:108:LEU:HB2	1.82	0.61
1:B:360:GLU:OE2	7:B:501:HOH:O	2.16	0.60
2:D:19:ILE:HG21	2:D:54:SER:HA	1.84	0.59
1:A:171:TRP:CG	1:A:288:PRO:HG3	2.38	0.58
1:C:48:LEU:HD23	1:C:137:LEU:HD23	1.85	0.58
1:B:310:ARG:O	1:B:314:GLU:HG3	2.04	0.56
1:B:287:VAL:HB	1:B:295:TYR:HB2	1.88	0.56
1:B:304:CYS:HB3	1:B:309:GLU:HB2	1.87	0.56
2:D:93:VAL:HG12	2:D:102:VAL:HG12	1.87	0.55
1:B:94:ALA:HB1	1:B:108:LEU:HB2	1.89	0.55
2:E:16:PRO:HA	2:E:34:ARG:HD3	1.89	0.55
1:C:275:PHE:CG	1:C:276:PRO:HA	2.44	0.53
1:A:130:LYS:NZ	1:A:155:ASP:O	2.34	0.53
1:B:16:ALA:HB3	1:B:17:PRO:HD3	1.91	0.53
1:B:174:ALA:HA	1:B:337:ARG:HG2	1.91	0.52
1:A:322:LYS:HB3	1:A:323:PRO:HD3	1.91	0.52
1:B:160:ILE:HG23	1:B:299:THR:HB	1.92	0.52
1:B:47:LYS:NZ	7:B:513:HOH:O	2.43	0.52
2:D:44:ASP:OD2	2:D:52:SER:OG	2.21	0.51
1:B:221:VAL:HG13	1:B:222:VAL:HG13	1.91	0.51
1:B:368:LEU:C	1:B:368:LEU:HD13	2.36	0.50
1:A:209:ASP:OD1	1:A:212:GLN:HG3	2.09	0.50
1:C:227:VAL:HG23	1:C:368:LEU:HD22	1.92	0.50
1:C:388:HIS:HA	2:E:81:SER:HB3	1.93	0.50
1:A:350:TRP:O	2:D:68:HIS:HD2	1.95	0.50
1:C:7:ALA:O	1:C:11:ARG:HG3	2.12	0.50
1:A:97:TYR:CD2	1:A:121:LEU:HB2	2.47	0.49
1:C:146:ALA:CB	1:C:222:VAL:HG21	2.42	0.49
1:B:320:LYS:O	1:B:324[B]:MET:HB2	2.13	0.48
1:A:57:ARG:NH1	1:A:128:GLU:OE1	2.33	0.48
1:B:195:ASP:CB	1:B:324[B]:MET:HE2	2.44	0.47
1:A:18:TYR:CE2	1:A:366:ARG:HG2	2.50	0.47
1:A:56:ASN:O	1:A:62:LEU:HA	2.14	0.47
1:C:94:ALA:CB	1:C:108:LEU:HB2	2.45	0.47
1:C:175:VAL:HG11	1:C:365:TRP:CE2	2.50	0.47
2:E:5:TRP:CE2	6:E:202:PEG:H11	2.50	0.47
1:B:220:ASP:OD1	1:B:222:VAL:HG22	2.15	0.47
1:B:65:LEU:HD23	1:B:123:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ALA:HB1	1:A:286:TYR:CD1	2.50	0.46
2:D:21:ARG:NH2	2:D:55:GLU:OE2	2.48	0.46
1:A:73:GLY:HA3	1:C:343:PHE:CG	2.51	0.46
1:A:68:ARG:HH22	1:A:384:GLY:HA3	1.80	0.46
1:A:273:ASN:OD1	1:A:281:MET:HE2	2.16	0.46
1:C:16:ALA:HB3	1:C:17:PRO:HD3	1.97	0.46
1:B:292:ASN:HB3	5:B:405:EDO:H11	1.97	0.46
1:A:176:GLU:O	1:A:180:ASP:HB2	2.16	0.46
1:C:287:VAL:HB	1:C:295:TYR:HB2	1.98	0.46
1:B:94:ALA:CB	1:B:108:LEU:HB2	2.46	0.45
1:B:183:HIS:O	1:B:186:ILE:HG12	2.17	0.45
1:A:171:TRP:CE2	1:A:172:ARG:HG3	2.51	0.45
1:B:343:PHE:CG	1:C:73:GLY:HA3	2.52	0.45
1:C:5:ASP:OD1	1:C:6:GLU:N	2.50	0.45
1:C:12:VAL:HG21	1:C:19:VAL:HG21	1.99	0.45
1:B:195:ASP:HB3	1:B:324[B]:MET:CE	2.47	0.44
1:C:273:ASN:HA	1:C:274:PRO:HA	1.80	0.44
1:A:67:ASP:OD2	1:A:77:SER:OG	2.28	0.44
1:B:143:PRO:HG3	1:B:147:ARG:CZ	2.47	0.44
1:A:108:LEU:HD12	1:A:108:LEU:N	2.31	0.44
2:E:31:ALA:O	2:E:41:ALA:HA	2.18	0.44
1:B:93:HIS:HB2	3:B:401:FES:S1	2.58	0.44
1:B:174:ALA:HB2	1:B:337:ARG:HD3	1.99	0.44
1:A:343:PHE:CG	1:B:73:GLY:HA3	2.53	0.44
1:A:130:LYS:HE3	1:A:153:PHE:O	2.18	0.44
1:A:385:LEU:N	1:A:385:LEU:HD12	2.33	0.44
1:A:175:VAL:HG11	1:A:365:TRP:CE2	2.54	0.43
1:A:222:VAL:HG12	1:A:222:VAL:O	2.19	0.43
1:A:283:PHE:HB2	1:A:299:THR:OG1	2.18	0.43
2:E:5:TRP:CD2	6:E:202:PEG:H11	2.54	0.43
2:E:68:HIS:HB2	3:E:201:FES:S1	2.58	0.43
1:A:101:ASP:O	1:A:120:LYS:HE2	2.18	0.43
1:A:287:VAL:HB	1:A:295:TYR:HB2	2.01	0.43
1:C:137:LEU:HD22	1:C:137:LEU:HA	1.94	0.43
1:A:16:ALA:HB3	1:A:17:PRO:HD3	2.01	0.42
1:C:46:LEU:CD1	1:C:46:LEU:N	2.82	0.42
1:C:322:LYS:NZ	7:C:514:HOH:O	2.52	0.42
1:C:180:ASP:HB3	1:C:183:HIS:HB3	2.01	0.42
1:B:47:LYS:HA	1:B:51:GLU:O	2.20	0.42
1:B:171:TRP:CE2	1:B:172:ARG:HG3	2.55	0.42
1:B:275:PHE:CG	1:B:276:PRO:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ALA:HB1	1:A:108:LEU:HB2	2.02	0.42
1:B:195:ASP:HB3	1:B:324[B]:MET:HE2	2.01	0.42
1:B:137:LEU:HD22	1:B:137:LEU:HA	1.95	0.42
1:C:136:TYR:CE1	1:C:143:PRO:HD2	2.55	0.42
1:C:308:GLU:O	1:C:312:LYS:HG2	2.20	0.42
1:A:280:MET:HE1	1:A:321:TRP:CE2	2.54	0.41
1:A:11:ARG:HB3	2:D:68:HIS:O	2.20	0.41
1:A:68:ARG:NH2	1:A:384:GLY:HA3	2.35	0.41
1:A:143:PRO:HG3	1:A:147:ARG:CZ	2.50	0.41
1:B:226:GLY:HA3	1:B:265:TRP:CE3	2.54	0.41
1:C:146:ALA:HB3	1:C:222:VAL:HG21	2.03	0.41
1:A:59:ASP:OD1	1:A:85:LYS:NZ	2.48	0.41
1:A:79:LYS:HB3	1:A:91:TRP:HB3	2.02	0.41
1:C:314:GLU:O	1:C:318:GLU:HG2	2.21	0.41
2:E:51:ALA:HB2	2:E:67:PHE:CG	2.56	0.41
1:B:273:ASN:HA	1:B:274:PRO:HA	1.78	0.41
1:B:285:TRP:HB2	1:B:297:PHE:HB3	2.02	0.41
1:A:16:ALA:N	1:A:17:PRO:CD	2.83	0.40
6:B:403:PEG:C1	6:B:403:PEG:C4	2.99	0.40
1:C:157:ASP:OD2	1:C:303:PRO:HB3	2.22	0.40
1:A:109:THR:HG22	1:C:202:LEU:O	2.20	0.40
1:B:287:VAL:HA	1:B:288:PRO:HD3	1.95	0.40
1:A:146:ALA:HA	1:A:149:THR:OG1	2.22	0.40
1:B:227:VAL:O	1:B:263:SER:HA	2.21	0.40
1:B:265:TRP:HB2	1:B:269:VAL:HG13	2.02	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	388/392 (99%)	366 (94%)	20 (5%)	2 (0%)	24 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	390/392 (100%)	367 (94%)	21 (5%)	2 (0%)	24	20
1	C	386/392 (98%)	366 (95%)	17 (4%)	3 (1%)	16	10
2	D	96/115 (84%)	84 (88%)	11 (12%)	1 (1%)	12	8
2	E	107/115 (93%)	100 (94%)	7 (6%)	0	100	100
All	All	1367/1406 (97%)	1283 (94%)	76 (6%)	8 (1%)	21	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	GLY
1	B	219	ASP
1	B	268	GLY
1	C	268	GLY
1	C	387	HIS
2	D	25	VAL
1	A	152	ASN
1	C	193	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/339 (99%)	328 (97%)	9 (3%)	39	41
1	B	339/339 (100%)	336 (99%)	3 (1%)	70	77
1	C	335/339 (99%)	329 (98%)	6 (2%)	51	58
2	D	77/93 (83%)	73 (95%)	4 (5%)	21	17
2	E	87/93 (94%)	86 (99%)	1 (1%)	65	72
All	All	1175/1203 (98%)	1152 (98%)	23 (2%)	48	54

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ILE
1	A	46	LEU
1	A	137	LEU
1	A	157	ASP
1	A	169	SER
1	A	308	GLU
1	A	356	PHE
1	A	386	GLU
1	A	387	HIS
1	B	46	LEU
1	B	137	LEU
1	B	356	PHE
1	C	46	LEU
1	C	126	VAL
1	C	137	LEU
1	C	209	ASP
1	C	231	ILE
1	C	356	PHE
2	D	6	LEU
2	D	19	ILE
2	D	94	GLU
2	D	97	GLU
2	E	81	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	177	ASN
1	B	213	GLN
1	B	260	ASN
1	B	282	GLN
1	B	330	ASN
1	B	388	HIS
1	C	282	GLN
1	C	292	ASN
1	C	330	ASN
1	C	379	GLN
2	D	23	ASN
2	E	2	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 3 are monoatomic - leaving 17 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	PEG	B	403	-	6,6,6	0.46	0	5,5,5	0.08	0
5	EDO	C	403	-	3,3,3	0.16	0	2,2,2	0.25	0
5	EDO	C	405	-	3,3,3	0.20	0	2,2,2	0.40	0
5	EDO	A	404	-	3,3,3	0.19	0	2,2,2	0.20	0
5	EDO	B	404	-	3,3,3	0.22	0	2,2,2	0.06	0
5	EDO	B	406	-	3,3,3	0.07	0	2,2,2	0.26	0
5	EDO	C	404	-	3,3,3	0.41	0	2,2,2	0.51	0
3	FES	E	201	2	0,4,4	-	-	-		
5	EDO	B	405	-	3,3,3	0.39	0	2,2,2	0.73	0
3	FES	A	401	1	0,4,4	-	-	-		
5	EDO	A	403	-	3,3,3	0.17	0	2,2,2	0.21	0
3	FES	D	201	2	0,4,4	-	-	-		
5	EDO	B	407	-	3,3,3	0.11	0	2,2,2	0.08	0
3	FES	C	401	1	0,4,4	-	-	-		
5	EDO	A	405	-	3,3,3	0.09	0	2,2,2	0.18	0
3	FES	B	401	1	0,4,4	-	-	-		
6	PEG	E	202	-	6,6,6	0.17	0	5,5,5	0.13	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	PEG	B	403	-	-	1/4/4/4	-
5	EDO	C	403	-	-	1/1/1/1	-
5	EDO	C	405	-	-	0/1/1/1	-
5	EDO	A	404	-	-	1/1/1/1	-
5	EDO	B	404	-	-	1/1/1/1	-
5	EDO	B	406	-	-	1/1/1/1	-
5	EDO	C	404	-	-	1/1/1/1	-
3	FES	E	201	2	-	-	0/1/1/1
5	EDO	B	405	-	-	0/1/1/1	-
5	EDO	A	403	-	-	1/1/1/1	-
3	FES	A	401	1	-	-	0/1/1/1
3	FES	D	201	2	-	-	0/1/1/1
5	EDO	B	407	-	-	0/1/1/1	-
3	FES	C	401	1	-	-	0/1/1/1
5	EDO	A	405	-	-	1/1/1/1	-
3	FES	B	401	1	-	-	0/1/1/1
6	PEG	E	202	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	404	EDO	O1-C1-C2-O2
6	B	403	PEG	C4-C3-O2-C2
5	A	404	EDO	O1-C1-C2-O2
6	E	202	PEG	O1-C1-C2-O2
5	A	405	EDO	O1-C1-C2-O2
5	B	406	EDO	O1-C1-C2-O2
5	A	403	EDO	O1-C1-C2-O2
5	B	404	EDO	O1-C1-C2-O2
6	E	202	PEG	C4-C3-O2-C2
5	C	403	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	403	PEG	2	0
5	B	404	EDO	1	0
3	E	201	FES	1	0
5	B	405	EDO	1	0
3	B	401	FES	1	0
6	E	202	PEG	2	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 (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	389/392 (99%)	0.48	14 (3%)	46	50	32, 53, 82, 144	1 (0%)
1	B	389/392 (99%)	0.06	12 (3%)	51	55	22, 42, 72, 105	3 (0%)
1	C	388/392 (98%)	0.40	16 (4%)	41	46	29, 52, 83, 118	0
2	D	98/115 (85%)	1.32	24 (24%)	2	2	46, 84, 139, 149	0
2	E	108/115 (93%)	0.84	14 (12%)	7	8	30, 58, 94, 117	1 (0%)
All	All	1372/1406 (97%)	0.43	80 (5%)	29	32	22, 51, 94, 149	5 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	102	VAL	5.5
1	A	385	LEU	4.8
1	C	385	LEU	4.8
2	D	11	ALA	4.0
2	D	6	LEU	4.0
1	A	386	GLU	4.0
1	B	305	ALA	3.6
2	D	91	PHE	3.6
2	D	95	VAL	3.5
2	D	103	ALA	3.4
1	A	387	HIS	3.3
2	D	93	VAL	3.2
2	D	98	GLY	3.2
2	D	25	VAL	3.2
2	D	100	VAL	3.2
1	A	305	ALA	3.1
1	B	388	HIS	3.1
1	C	389	HIS	3.1
1	A	390	HIS	2.9
1	B	387	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	95	VAL	2.9
1	A	384	GLY	2.9
1	B	335[A]	TRP	2.9
1	C	388	HIS	2.8
2	E	100	VAL	2.8
2	D	101	TYR	2.7
1	A	105	CYS	2.7
1	C	191	ILE	2.7
1	C	253	TYR	2.7
1	C	2	ALA	2.6
2	D	39	PHE	2.6
1	C	247	VAL	2.6
1	A	126	VAL	2.6
2	E	11	ALA	2.6
2	D	8	VAL	2.6
1	C	252	ALA	2.5
2	E	39	PHE	2.5
1	C	387	HIS	2.5
1	A	221	VAL	2.5
2	D	19	ILE	2.5
2	D	90	VAL	2.5
2	E	14	MET	2.4
1	A	116	ILE	2.4
2	E	109	GLU	2.4
2	D	96	LYS	2.4
2	D	30	LEU	2.4
1	C	234	HIS	2.4
1	A	2	ALA	2.4
2	E	4	ILE	2.4
1	B	304	CYS	2.4
2	D	41	ALA	2.3
1	A	111	PRO	2.3
1	B	390	HIS	2.3
2	E	93	VAL	2.3
1	B	2	ALA	2.3
1	C	202	LEU	2.3
2	E	101	TYR	2.3
1	C	254	GLY	2.2
2	D	22	VAL	2.2
1	B	310	ARG	2.2
1	B	217	VAL	2.2
2	E	25	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	60	GLY	2.2
2	D	27	ALA	2.2
1	A	388	HIS	2.2
1	B	389	HIS	2.2
2	D	33	TYR	2.2
2	E	33	TYR	2.2
1	A	104	LEU	2.1
1	B	221	VAL	2.1
1	C	324	MET	2.1
2	D	35	VAL	2.1
2	E	96	LYS	2.1
2	D	58	LEU	2.1
2	D	88	LEU	2.1
1	B	197	ASP	2.1
2	E	108	LEU	2.0
1	C	157	ASP	2.0
1	C	238	VAL	2.0
1	C	305	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no 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	EDO	C	405	4/4	0.82	0.14	71,71,72,74	0
6	PEG	B	403	7/7	0.83	0.21	50,65,77,78	0
5	EDO	A	404	4/4	0.84	0.17	69,76,79,79	0
5	EDO	C	404	4/4	0.84	0.18	60,61,66,71	0
5	EDO	A	403	4/4	0.85	0.18	68,69,70,75	0

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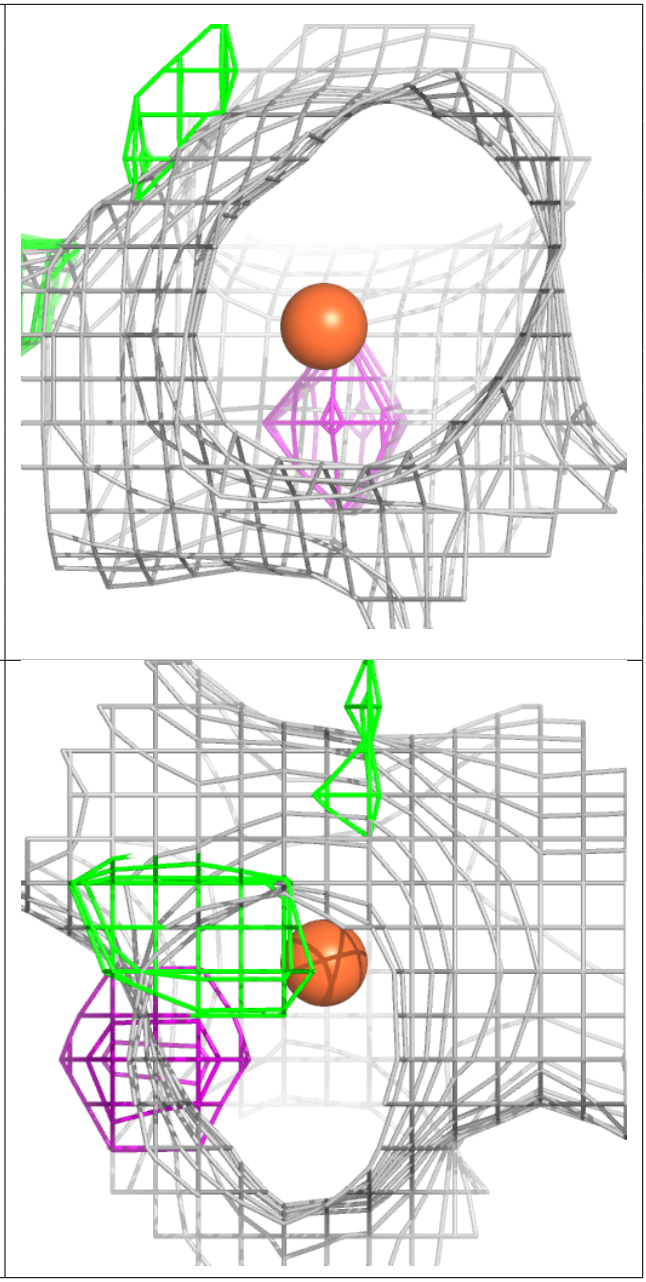
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	C	403	4/4	0.86	0.13	64,67,70,71	0
6	PEG	E	202	7/7	0.87	0.13	67,72,84,87	0
5	EDO	A	405	4/4	0.90	0.14	72,76,76,79	0
5	EDO	B	407	4/4	0.91	0.14	59,66,72,77	0
5	EDO	B	404	4/4	0.91	0.15	55,56,57,63	0
5	EDO	B	405	4/4	0.92	0.18	61,62,63,63	0
5	EDO	B	406	4/4	0.95	0.11	65,69,70,77	0
3	FES	A	401	4/4	0.98	0.05	45,49,50,55	0
4	FE2	C	402	1/1	0.98	0.04	52,52,52,52	0
3	FES	E	201	4/4	0.99	0.03	35,37,37,42	0
4	FE2	A	402	1/1	0.99	0.02	52,52,52,52	0
4	FE2	B	402	1/1	0.99	0.02	43,43,43,43	0
3	FES	D	201	4/4	0.99	0.07	45,46,47,48	0
3	FES	C	401	4/4	1.00	0.02	29,30,32,33	0
3	FES	B	401	4/4	1.00	0.02	32,33,35,36	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.

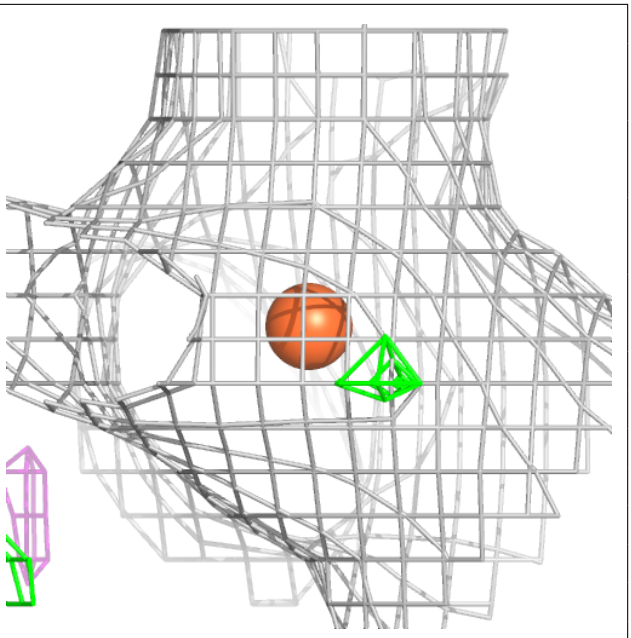
Electron density around FE2 C 402:

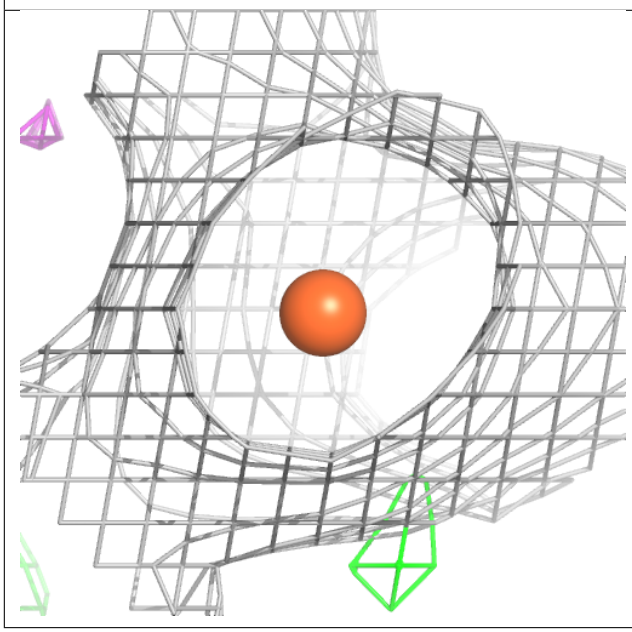
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

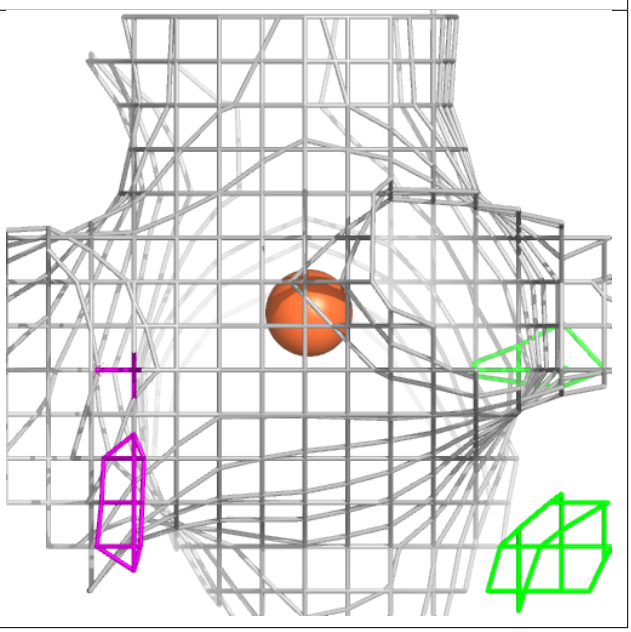


Electron density around FE2 A 402:

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

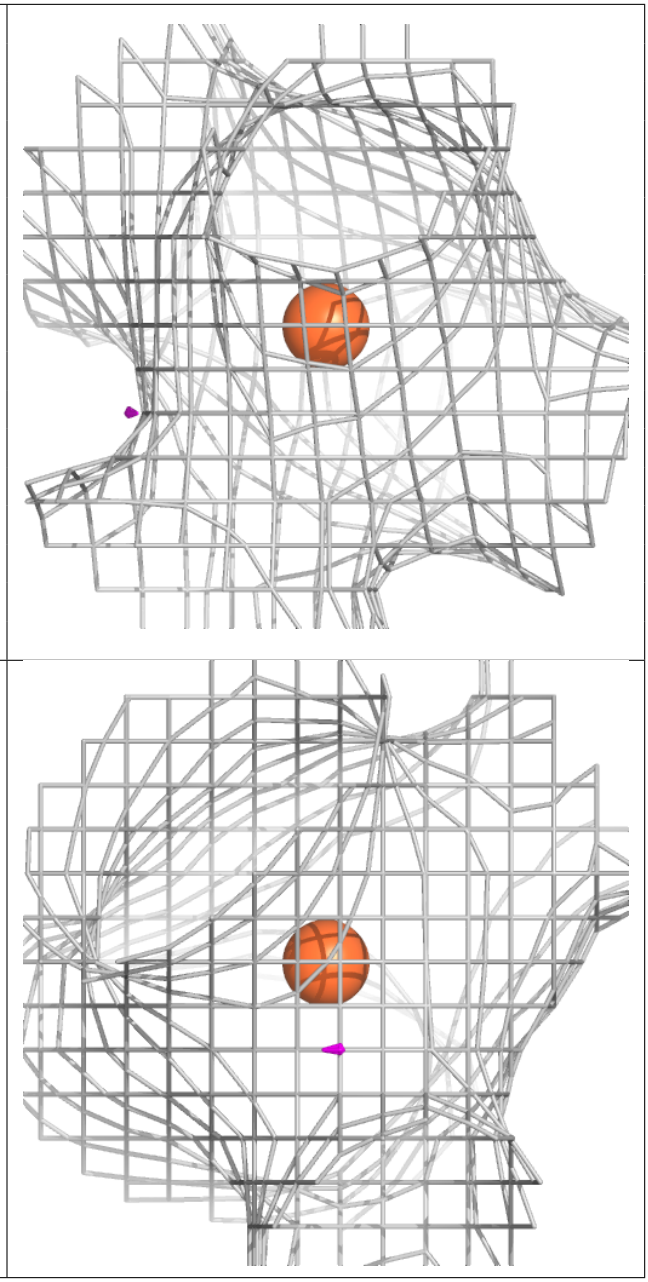






Electron density around FE2 B 402:

$2mF_o$-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.