Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 11:37 AM EDT

PDB ID	:	7S6S
Title	:	Complex structure of Methane monooxygenase hydroxylase and regulatory subunit DBL1
Authors	:	Johns, J.C.; Banerjee, R.; Semonis, M.M.; Shi, K.; Aihara, H.; Lipscomb, J.D.
Deposited on	:	2021-09-14
Resolution	:	1.98 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:

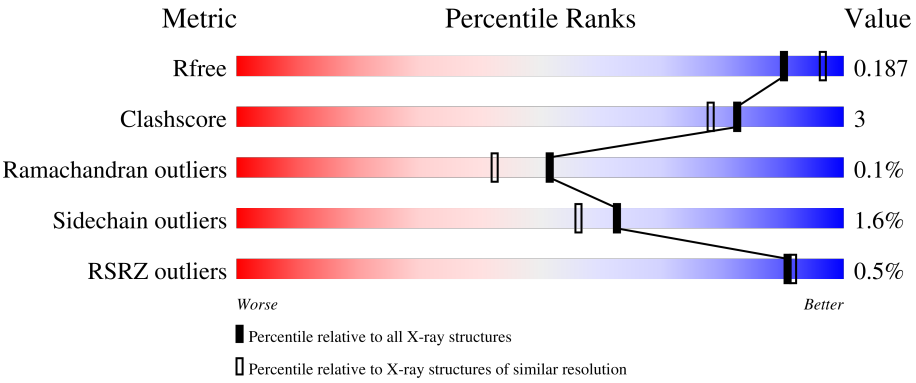
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	515	92% 8%
1	E	515	91% 8%
2	B	392	96%
2	F	392	95% 5%
3	C	168	96%

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Mol	Chain	Length	Quality of chain
3	G	168	97%
4	D	136	% 85% 11%
4	H	136	4% 88% 11%

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
6	EDO	E	611	-	-	-	X
6	EDO	G	203	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 21849 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	2	0
			4195	2688	729	766	12			
1	E	515	Total	C	N	O	S	0	7	0
			4237	2710	737	777	13			

- Molecule 2 is a protein called Methane monooxygenase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	392	Total	C	N	O	S	0	1	0
			3190	2034	557	594	5			
2	F	392	Total	C	N	O	S	0	2	0
			3197	2038	558	596	5			

- Molecule 3 is a protein called Methane monooxygenase gamma chain.

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	1	0
			1371	880	236	254	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	131	Total	C	N	O	S	0	0	0
			991	634	160	194	3			
4	H	136	Total	C	N	O	S	0	0	0
			1027	657	165	202	3			

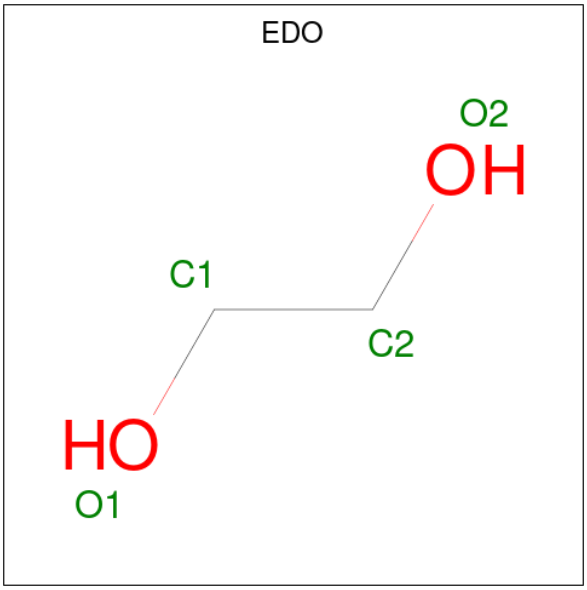
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	107	GLY	ASN	conflict	UNP A0A2D2D0T8
D	110	ALA	SER	conflict	UNP A0A2D2D0T8
H	107	GLY	ASN	conflict	UNP A0A2D2D0T8
H	110	ALA	SER	conflict	UNP A0A2D2D0T8

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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

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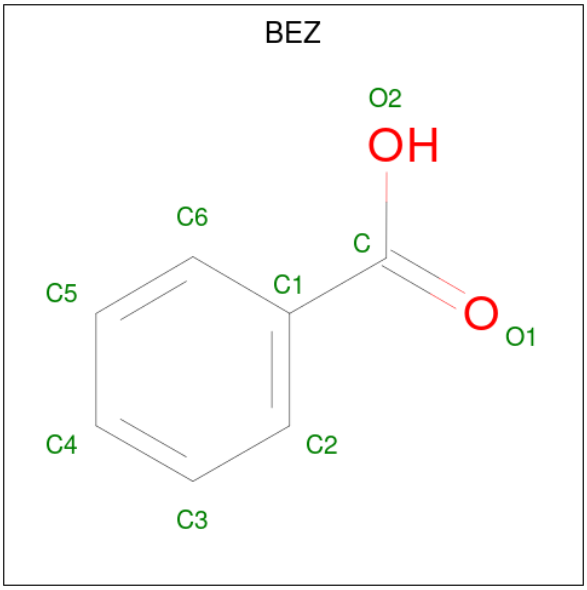
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0

- Molecule 7 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	427	Total O 428 428	0	1
8	B	370	Total O 371 371	0	1
8	C	181	Total O 182 182	0	1
8	D	61	Total O 62 62	0	1

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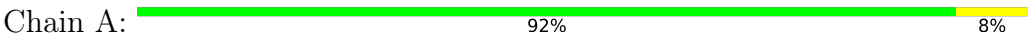
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	395	Total O 397 397	0	4
8	F	373	Total O 373 373	0	0
8	G	185	Total O 185 185	0	0
8	H	59	Total O 59 59	0	0

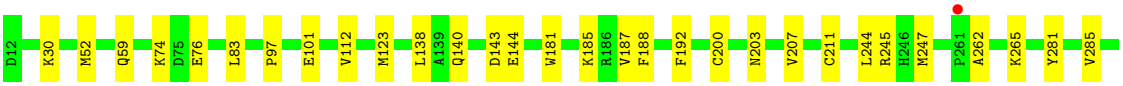
3 Residue-property plots (i)

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

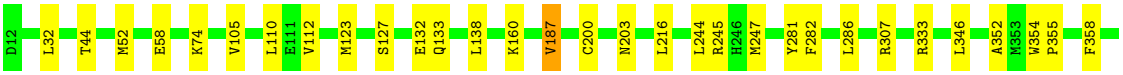
Chain A:





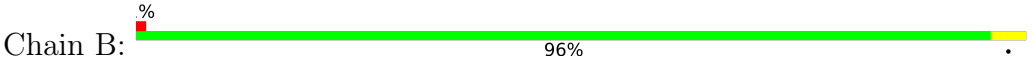
• Molecule 1: Methane monooxygenase component A alpha chain

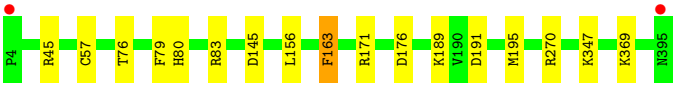
Chain E:



• Molecule 2: Methane monooxygenase beta chain

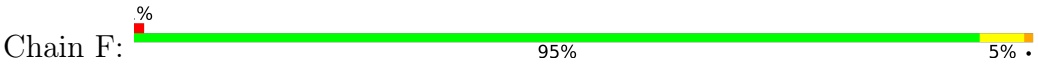
Chain B:

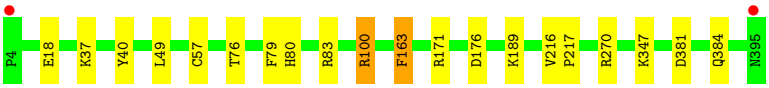




• Molecule 2: Methane monooxygenase beta chain

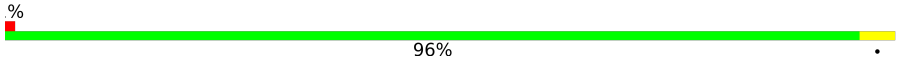
Chain F:





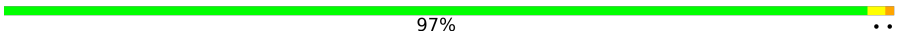
• Molecule 3: Methane monooxygenase gamma chain

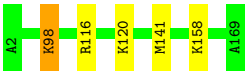
Chain C:



• Molecule 3: Methane monooxygenase gamma chain

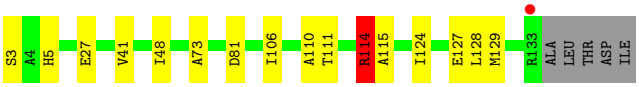
Chain G:





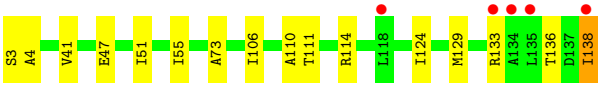
• Molecule 4: Methane monooxygenase regulatory protein B

Chain D:



• Molecule 4: Methane monooxygenase regulatory protein B

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.73Å 105.71Å 299.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.67 – 1.98 73.67 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.3 (73.67-1.98) 98.3 (73.67-1.98)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.154 , 0.189 0.153 , 0.187	Depositor DCC
R_{free} test set	11107 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21849	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.55	0/4325	0.64	0/5875
1	E	0.55	0/4367	0.64	1/5932 (0.0%)
2	B	0.57	0/3283	0.64	0/4464
2	F	0.53	0/3290	0.64	0/4476
3	C	0.49	0/1388	0.62	0/1877
3	G	0.51	0/1397	0.61	0/1888
4	D	0.50	0/1007	0.60	0/1361
4	H	0.48	0/1043	0.56	0/1411
All	All	0.54	0/20100	0.63	1/27284 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
4	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	397	ASP	CB-CG-OD1	5.06	122.85	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	114	ARG	Sidechain
1	E	489	ARG	Sidechain

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	4195	0	3996	27	0
1	E	4237	0	4024	26	0
2	B	3190	0	3019	12	0
2	F	3197	0	3023	13	0
3	C	1362	0	1400	4	0
3	G	1371	0	1412	3	0
4	D	991	0	987	11	0
4	H	1027	0	1025	9	0
5	A	2	0	0	0	0
5	E	2	0	0	0	0
6	A	36	0	54	2	0
6	B	36	0	54	3	0
6	C	8	0	12	0	0
6	D	12	0	18	3	0
6	E	48	0	72	7	0
6	F	28	0	42	0	0
6	G	20	0	30	0	0
6	H	12	0	18	2	0
7	A	9	0	5	1	0
7	E	9	0	5	0	0
8	A	428	0	0	6	0
8	B	371	0	0	2	0
8	C	182	0	0	0	0
8	D	62	0	0	1	0
8	E	397	0	0	7	1
8	F	373	0	0	4	1
8	G	185	0	0	1	0
8	H	59	0	0	0	0
All	All	21849	0	19196	98	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (98) 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)
4:D:3:SER:N	6:D:202:EDO:HO2	1.72	0.86
1:E:463:ARG:HH12	6:E:611:EDO:H12	1.45	0.80
1:A:245[B]:ARG:NH1	8:A:701:HOH:O	2.10	0.79
4:H:136:THR:HG22	4:H:138:ILE:H	1.47	0.78
1:E:187:VAL:HG13	1:E:281:TYR:HB3	1.67	0.77
1:E:480[B]:GLU:OE1	8:E:701:HOH:O	2.04	0.75
4:H:3:SER:N	6:H:203:EDO:HO2	1.88	0.71
4:D:3:SER:N	8:D:301:HOH:O	2.25	0.70
4:H:4:ALA:H	6:H:203:EDO:H21	1.57	0.69
6:A:609:EDO:O2	8:A:702:HOH:O	2.13	0.67
2:F:18:GLU:OE1	8:F:501:HOH:O	2.13	0.65
2:B:80:HIS:CD2	3:C:141:MET:HG2	2.33	0.64
1:E:282:PHE:CE2	1:E:286:LEU:HD22	2.34	0.62
4:D:111:THR:HB	4:D:124:ILE:HD12	1.81	0.62
2:F:80:HIS:CD2	3:G:141:MET:HG2	2.34	0.61
4:D:114:ARG:HD3	4:D:128:LEU:HD23	1.83	0.61
2:B:369:LYS:NZ	8:B:501:HOH:O	2.33	0.59
1:E:406:GLN:NE2	8:E:706:HOH:O	2.35	0.58
3:G:98:LYS:NZ	8:G:302:HOH:O	2.37	0.56
1:A:30:LYS:NZ	8:A:706:HOH:O	2.39	0.56
1:E:187:VAL:CG1	1:E:281:TYR:HB3	2.34	0.54
1:E:138:LEU:HD22	2:F:163:PHE:CE1	2.43	0.54
1:A:247:MET:HE3	8:A:734:HOH:O	2.07	0.53
1:A:504:ASP:OD2	1:A:505:ASN:ND2	2.41	0.53
1:A:466:CYS:HB2	2:B:76:THR:HA	1.91	0.52
2:F:57:CYS:HB3	8:F:811:HOH:O	2.09	0.52
6:E:603:EDO:H21	8:E:866:HOH:O	2.09	0.52
1:E:504:ASP:OD2	1:E:505:ASN:ND2	2.42	0.51
1:A:192:PHE:O	8:A:703:HOH:O	2.18	0.51
1:E:502[A]:ARG:HD2	1:E:504:ASP:OD1	2.10	0.51
6:E:611:EDO:H21	8:F:576:HOH:O	2.10	0.51
6:E:611:EDO:H12	6:E:612:EDO:H11	1.91	0.51
1:A:138:LEU:HD22	2:B:163:PHE:CE1	2.46	0.51
4:D:41:VAL:HB	4:D:110:ALA:HB3	1.91	0.50
2:F:100:ARG:NH1	8:F:506:HOH:O	2.45	0.50
4:H:111:THR:HB	4:H:124:ILE:HD12	1.92	0.50
1:A:262:ALA:O	1:A:265:LYS:HE3	2.12	0.49
1:A:74:LYS:HE2	4:D:106:ILE:HA	1.93	0.49
1:E:358:PHE:CE1	6:E:613:EDO:H11	2.47	0.49
1:A:181:TRP:NE1	1:A:185:LYS:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5:HIS:HE1	4:D:81:ASP:OD1	1.95	0.49
1:E:58:GLU:OE2	1:E:245[B]:ARG:NH2	2.46	0.48
1:E:352:ALA:HA	1:E:404:PRO:HB2	1.96	0.47
1:A:140:GLN:O	1:A:144:GLU:HG2	2.14	0.47
2:F:189:LYS:HA	2:F:189:LYS:HD3	1.63	0.47
4:H:51:ILE:HG23	4:H:55:ILE:HD12	1.96	0.47
4:H:41:VAL:HB	4:H:110:ALA:HB3	1.96	0.47
2:B:189:LYS:HD3	2:B:189:LYS:HA	1.74	0.46
1:E:44:THR:HB	1:E:127:SER:HA	1.96	0.46
4:D:114:ARG:HD2	4:D:127:GLU:O	2.15	0.46
1:A:143:ASP:OD2	1:A:245[A]:ARG:NH1	2.47	0.46
6:E:605:EDO:H22	8:E:1025:HOH:O	2.15	0.46
1:E:74:LYS:HG2	4:H:106:ILE:HG23	1.98	0.46
2:F:37:LYS:HB3	2:F:40:TYR:HB3	1.98	0.46
1:E:132:GLU:OE2	6:E:609:EDO:H12	2.15	0.45
1:E:123:MET:HG3	2:F:171:ARG:HD3	1.98	0.45
4:H:47:GLU:O	4:H:51:ILE:HG13	2.17	0.45
2:F:216:VAL:HB	2:F:217:PRO:HD3	1.99	0.45
2:F:79:PHE:HB2	2:F:83:ARG:HB3	1.97	0.45
2:B:347:LYS:HD3	2:B:347:LYS:HA	1.74	0.45
4:D:115:ALA:H	6:D:203:EDO:H12	1.81	0.45
1:E:354:TRP:CG	1:E:355:PRO:HD3	2.52	0.45
1:A:83:LEU:HD11	6:B:402:EDO:H11	1.99	0.45
1:A:97:PRO:O	1:A:101:GLU:HG2	2.17	0.45
1:E:200:CYS:HA	1:E:203:ASN:OD1	2.17	0.45
3:C:121:PRO:HD3	3:C:129:PHE:CG	2.53	0.44
2:B:79:PHE:HB2	2:B:83:ARG:HB3	1.98	0.44
1:A:188:PHE:CG	7:A:607:BEZ:H4	2.52	0.44
1:A:399:LYS:HD3	1:A:399:LYS:HA	1.72	0.44
1:A:200:CYS:HA	1:A:203:ASN:OD1	2.19	0.43
2:B:191:ASP:O	2:B:195:MET:HG2	2.19	0.43
4:H:136:THR:HG22	4:H:138:ILE:N	2.25	0.43
2:F:381:ASP:HB3	2:F:384:GLN:HB3	2.01	0.43
1:A:207:VAL:O	1:A:211:CYS:HB3	2.19	0.42
1:E:247:MET:HE3	8:E:729:HOH:O	2.18	0.42
1:E:110:LEU:HD13	1:E:216:LEU:HD21	2.02	0.42
1:A:440:GLU:OE2	6:A:611:EDO:O1	2.36	0.42
1:E:216:LEU:CD1	1:E:286:LEU:HD21	2.49	0.42
1:E:398:PRO:HA	1:E:507:TRP:CE2	2.55	0.42
2:F:347:LYS:HA	2:F:347:LYS:HD3	1.75	0.42
2:B:45:ARG:HD3	6:B:404:EDO:H22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:NH2	4:D:27:GLU:OE2	2.33	0.41
3:C:58:GLU:O	3:C:62:GLU:HG3	2.21	0.41
1:A:76:GLU:HG2	8:A:853:HOH:O	2.20	0.41
1:A:123:MET:HG3	2:B:171:ARG:HD3	2.03	0.41
2:B:145:ASP:HB3	6:B:407:EDO:H22	2.03	0.41
1:A:59:GLN:HG3	6:D:203:EDO:O2	2.20	0.41
1:E:466:CYS:HB2	2:F:76:THR:HA	2.03	0.41
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.56	0.41
1:A:440:GLU:HB2	3:C:165:LEU:HD11	2.03	0.41
1:A:187:VAL:HG13	1:A:188:PHE:N	2.36	0.40
1:E:354:TRP:CH2	1:E:499:PRO:HD3	2.56	0.40
1:A:398:PRO:HA	1:A:507:TRP:CE2	2.56	0.40
4:D:48:ILE:HD13	4:D:48:ILE:HA	1.93	0.40
1:E:133:GLN:NE2	8:E:723:HOH:O	2.52	0.40
1:E:160:LYS:HD3	8:E:1046:HOH:O	2.21	0.40
2:B:57:CYS:HB3	8:B:806:HOH:O	2.21	0.40
3:G:116:ARG:O	3:G:120:LYS:HB2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:1016:HOH:O	8:F:759:HOH:O[3_555]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	515/515 (100%)	498 (97%)	17 (3%)	0	100	100
1	E	520/515 (101%)	503 (97%)	17 (3%)	0	100	100
2	B	391/392 (100%)	381 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	F	392/392 (100%)	382 (97%)	10 (3%)	0	100 100
3	C	166/168 (99%)	164 (99%)	2 (1%)	0	100 100
3	G	167/168 (99%)	165 (99%)	2 (1%)	0	100 100
4	D	129/136 (95%)	123 (95%)	5 (4%)	1 (1%)	19 9
4	H	134/136 (98%)	129 (96%)	4 (3%)	1 (1%)	22 11
All	All	2414/2422 (100%)	2345 (97%)	67 (3%)	2 (0%)	51 42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	73	ALA
4	H	73	ALA

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	428/426 (100%)	423 (99%)	5 (1%)	71 67
1	E	433/426 (102%)	424 (98%)	9 (2%)	53 47
2	B	324/324 (100%)	320 (99%)	4 (1%)	71 67
2	F	325/324 (100%)	320 (98%)	5 (2%)	65 59
3	C	145/145 (100%)	145 (100%)	0	100 100
3	G	146/145 (101%)	144 (99%)	2 (1%)	67 62
4	D	102/106 (96%)	100 (98%)	2 (2%)	55 48
4	H	106/106 (100%)	102 (96%)	4 (4%)	33 21
All	All	2009/2002 (100%)	1978 (98%)	31 (2%)	62 59

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

Mol	Chain	Res	Type
1	A	52	MET

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Mol	Chain	Res	Type
1	A	112	VAL
1	A	244	LEU
1	A	307	ARG
1	A	437	ARG
2	B	156	LEU
2	B	163	PHE
2	B	176	ASP
2	B	270	ARG
4	D	114	ARG
4	D	129	MET
1	E	32	LEU
1	E	52	MET
1	E	105	VAL
1	E	112	VAL
1	E	187	VAL
1	E	244	LEU
1	E	307	ARG
1	E	333	ARG
1	E	346	LEU
2	F	49	LEU
2	F	100	ARG
2	F	163	PHE
2	F	176	ASP
2	F	270	ARG
3	G	98	LYS
3	G	158	LYS
4	H	114	ARG
4	H	129	MET
4	H	133	ARG
4	H	138	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	110	HIS
4	D	5	HIS
4	H	5	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 4 are monoatomic - leaving 52 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	D	203	-	3,3,3	0.43	0	2,2,2	0.38	0
6	EDO	B	405	-	3,3,3	0.50	0	2,2,2	0.31	0
6	EDO	D	202	-	3,3,3	0.40	0	2,2,2	0.73	0
6	EDO	E	613	-	3,3,3	0.42	0	2,2,2	0.46	0
6	EDO	E	612	-	3,3,3	0.53	0	2,2,2	0.27	0
6	EDO	H	203	-	3,3,3	0.46	0	2,2,2	0.31	0
6	EDO	G	205	-	3,3,3	0.46	0	2,2,2	0.39	0
6	EDO	A	605	-	3,3,3	0.43	0	2,2,2	0.70	0
6	EDO	F	403	-	3,3,3	0.45	0	2,2,2	0.93	0
6	EDO	E	611	-	3,3,3	0.50	0	2,2,2	0.37	0
6	EDO	F	401	-	3,3,3	0.60	0	2,2,2	0.18	0
6	EDO	B	408	-	3,3,3	0.47	0	2,2,2	0.52	0
6	EDO	E	604	-	3,3,3	0.54	0	2,2,2	0.27	0
6	EDO	A	608	-	3,3,3	0.41	0	2,2,2	0.59	0
6	EDO	A	606	-	3,3,3	0.58	0	2,2,2	0.15	0
6	EDO	C	201	-	3,3,3	0.46	0	2,2,2	0.26	0
6	EDO	D	201	-	3,3,3	0.57	0	2,2,2	0.11	0
6	EDO	E	608	-	3,3,3	0.62	0	2,2,2	0.15	0
6	EDO	E	615	-	3,3,3	0.44	0	2,2,2	0.49	0
6	EDO	F	405	-	3,3,3	0.41	0	2,2,2	0.74	0
6	EDO	E	605	-	3,3,3	0.54	0	2,2,2	0.18	0
6	EDO	A	609	-	3,3,3	0.68	0	2,2,2	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	F	407	-	3,3,3	0.43	0	2,2,2	0.72	0
6	EDO	E	610	-	3,3,3	0.54	0	2,2,2	0.48	0
6	EDO	E	609	-	3,3,3	0.50	0	2,2,2	0.11	0
6	EDO	E	614	-	3,3,3	0.50	0	2,2,2	0.16	0
6	EDO	A	603	-	3,3,3	0.47	0	2,2,2	0.19	0
6	EDO	G	203	-	3,3,3	0.49	0	2,2,2	0.24	0
6	EDO	B	402	-	3,3,3	0.37	0	2,2,2	0.67	0
6	EDO	H	201	-	3,3,3	0.55	0	2,2,2	0.26	0
6	EDO	F	406	-	3,3,3	0.51	0	2,2,2	0.25	0
6	EDO	E	603	-	3,3,3	0.47	0	2,2,2	0.58	0
6	EDO	B	409	-	3,3,3	0.60	0	2,2,2	0.46	0
6	EDO	E	607	-	3,3,3	0.59	0	2,2,2	0.07	0
6	EDO	F	402	-	3,3,3	0.51	0	2,2,2	0.37	0
6	EDO	B	406	-	3,3,3	0.29	0	2,2,2	0.84	0
7	BEZ	A	607	5	9,9,9	0.98	0	11,11,11	1.08	1 (9%)
6	EDO	F	404	-	3,3,3	0.44	0	2,2,2	0.44	0
6	EDO	H	202	-	3,3,3	0.51	0	2,2,2	0.13	0
6	EDO	A	612	-	3,3,3	0.65	0	2,2,2	0.12	0
6	EDO	A	611	-	3,3,3	0.55	0	2,2,2	0.34	0
6	EDO	B	404	-	3,3,3	0.50	0	2,2,2	0.40	0
6	EDO	C	202	-	3,3,3	0.41	0	2,2,2	0.76	0
6	EDO	B	401	-	3,3,3	0.59	0	2,2,2	0.28	0
6	EDO	G	201	-	3,3,3	0.57	0	2,2,2	0.24	0
6	EDO	B	403	-	3,3,3	0.41	0	2,2,2	0.61	0
6	EDO	A	610	-	3,3,3	0.55	0	2,2,2	0.17	0
6	EDO	G	202	-	3,3,3	0.43	0	2,2,2	0.51	0
7	BEZ	E	606	5	9,9,9	0.81	0	11,11,11	1.10	2 (18%)
6	EDO	B	407	-	3,3,3	0.52	0	2,2,2	0.24	0
6	EDO	A	604	-	3,3,3	0.48	0	2,2,2	0.59	0
6	EDO	G	204	-	3,3,3	0.52	0	2,2,2	0.17	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	D	203	-	-	0/1/1/1	-
6	EDO	B	405	-	-	0/1/1/1	-
6	EDO	D	202	-	-	0/1/1/1	-
6	EDO	E	613	-	-	0/1/1/1	-
6	EDO	E	612	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	H	203	-	-	0/1/1/1	-
6	EDO	G	205	-	-	0/1/1/1	-
6	EDO	A	605	-	-	0/1/1/1	-
6	EDO	F	403	-	-	0/1/1/1	-
6	EDO	E	611	-	-	1/1/1/1	-
6	EDO	F	401	-	-	1/1/1/1	-
6	EDO	B	408	-	-	0/1/1/1	-
6	EDO	E	604	-	-	1/1/1/1	-
6	EDO	A	608	-	-	0/1/1/1	-
6	EDO	A	606	-	-	0/1/1/1	-
6	EDO	C	201	-	-	0/1/1/1	-
6	EDO	D	201	-	-	0/1/1/1	-
6	EDO	E	608	-	-	1/1/1/1	-
6	EDO	E	615	-	-	1/1/1/1	-
6	EDO	F	405	-	-	0/1/1/1	-
6	EDO	E	605	-	-	1/1/1/1	-
6	EDO	A	609	-	-	0/1/1/1	-
6	EDO	F	407	-	-	1/1/1/1	-
6	EDO	E	610	-	-	1/1/1/1	-
6	EDO	E	609	-	-	0/1/1/1	-
6	EDO	E	614	-	-	0/1/1/1	-
6	EDO	A	603	-	-	0/1/1/1	-
6	EDO	G	203	-	-	0/1/1/1	-
6	EDO	B	402	-	-	0/1/1/1	-
6	EDO	H	201	-	-	0/1/1/1	-
6	EDO	F	406	-	-	1/1/1/1	-
6	EDO	E	603	-	-	0/1/1/1	-
6	EDO	B	409	-	-	0/1/1/1	-
6	EDO	E	607	-	-	1/1/1/1	-
6	EDO	F	402	-	-	1/1/1/1	-
6	EDO	B	406	-	-	0/1/1/1	-
7	BEZ	A	607	5	-	0/4/4/4	0/1/1/1
6	EDO	F	404	-	-	0/1/1/1	-
6	EDO	H	202	-	-	0/1/1/1	-
6	EDO	A	612	-	-	0/1/1/1	-
6	EDO	A	611	-	-	1/1/1/1	-
6	EDO	B	404	-	-	0/1/1/1	-
6	EDO	C	202	-	-	0/1/1/1	-
6	EDO	B	401	-	-	0/1/1/1	-
6	EDO	G	201	-	-	0/1/1/1	-
6	EDO	B	403	-	-	0/1/1/1	-
6	EDO	A	610	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	G	202	-	-	0/1/1/1	-
7	BEZ	E	606	5	-	0/4/4/4	0/1/1/1
6	EDO	B	407	-	-	0/1/1/1	-
6	EDO	A	604	-	-	0/1/1/1	-
6	EDO	G	204	-	-	1/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	606	BEZ	O2-C-O1	-2.34	118.15	123.35
7	A	607	BEZ	O2-C-O1	-2.11	118.66	123.35
7	E	606	BEZ	O2-C-C1	2.01	120.06	114.85

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	611	EDO	O1-C1-C2-O2
6	F	401	EDO	O1-C1-C2-O2
6	F	402	EDO	O1-C1-C2-O2
6	G	204	EDO	O1-C1-C2-O2
6	E	605	EDO	O1-C1-C2-O2
6	A	611	EDO	O1-C1-C2-O2
6	E	610	EDO	O1-C1-C2-O2
6	F	406	EDO	O1-C1-C2-O2
6	E	604	EDO	O1-C1-C2-O2
6	E	615	EDO	O1-C1-C2-O2
6	F	407	EDO	O1-C1-C2-O2
6	E	608	EDO	O1-C1-C2-O2
6	E	607	EDO	O1-C1-C2-O2

There are no ring outliers.

15 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	203	EDO	2	0
6	D	202	EDO	1	0
6	E	613	EDO	1	0
6	E	612	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	203	EDO	2	0
6	E	611	EDO	3	0
6	E	605	EDO	1	0
6	A	609	EDO	1	0
6	E	609	EDO	1	0
6	B	402	EDO	1	0
6	E	603	EDO	1	0
7	A	607	BEZ	1	0
6	A	611	EDO	1	0
6	B	404	EDO	1	0
6	B	407	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	515/515 (100%)	-0.24	1 (0%) 95 95	19, 26, 40, 62	0
1	E	515/515 (100%)	-0.26	0 100 100	19, 27, 41, 59	0
2	B	392/392 (100%)	-0.24	2 (0%) 91 91	21, 27, 38, 66	1 (0%)
2	F	392/392 (100%)	-0.25	2 (0%) 91 91	20, 26, 38, 68	1 (0%)
3	C	168/168 (100%)	-0.10	2 (1%) 79 80	24, 31, 44, 56	0
3	G	168/168 (100%)	-0.05	0 100 100	24, 31, 45, 55	0
4	D	131/136 (96%)	-0.17	1 (0%) 86 87	25, 34, 51, 76	0
4	H	136/136 (100%)	0.08	5 (3%) 41 44	27, 37, 56, 72	0
All	All	2417/2422 (99%)	-0.20	13 (0%) 91 91	19, 28, 44, 76	2 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	135	LEU	5.1
4	H	133	ARG	4.3
4	D	133	ARG	3.8
4	H	138	ILE	3.7
2	B	395	ASN	3.4
2	F	395	ASN	2.9
1	A	261	PRO	2.8
4	H	134	ALA	2.6
3	C	103	LYS	2.6
2	B	4	PRO	2.5
3	C	75	VAL	2.2
2	F	4	PRO	2.2
4	H	118	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	E	611	4/4	0.65	0.43	57,58,60,60	0
6	EDO	A	609	4/4	0.72	0.28	52,54,55,56	0
6	EDO	E	614	4/4	0.72	0.22	75,75,75,75	0
6	EDO	F	404	4/4	0.74	0.17	62,62,65,67	0
6	EDO	F	402	4/4	0.75	0.37	67,67,68,69	0
6	EDO	A	611	4/4	0.78	0.15	58,59,61,62	0
6	EDO	D	201	4/4	0.80	0.26	55,56,56,56	0
6	EDO	G	203	4/4	0.80	0.45	71,72,73,75	0
6	EDO	B	401	4/4	0.81	0.17	42,44,47,49	0
6	EDO	E	605	4/4	0.87	0.18	49,50,51,51	0
6	EDO	E	608	4/4	0.87	0.13	52,53,54,55	0
6	EDO	E	610	4/4	0.87	0.29	51,52,52,53	0
6	EDO	A	606	4/4	0.87	0.17	43,46,46,48	0
6	EDO	H	203	4/4	0.87	0.10	67,67,68,69	0
6	EDO	E	607	4/4	0.88	0.24	49,55,58,60	0
6	EDO	B	405	4/4	0.89	0.16	64,65,66,66	0
6	EDO	F	405	4/4	0.89	0.26	61,62,65,67	0
6	EDO	E	603	4/4	0.90	0.13	50,52,53,54	0
6	EDO	G	204	4/4	0.91	0.35	60,60,61,63	0
6	EDO	B	403	4/4	0.91	0.22	55,55,57,57	0
6	EDO	B	407	4/4	0.92	0.24	42,42,44,44	0
6	EDO	B	408	4/4	0.92	0.16	51,54,57,60	0
6	EDO	B	404	4/4	0.92	0.17	36,42,46,49	0
6	EDO	A	604	4/4	0.92	0.13	38,40,41,41	0
6	EDO	E	612	4/4	0.92	0.27	43,45,49,51	0
6	EDO	G	205	4/4	0.92	0.35	60,60,62,63	0
6	EDO	H	202	4/4	0.92	0.23	54,55,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	B	406	4/4	0.92	0.29	38,39,49,55	0
6	EDO	C	202	4/4	0.93	0.24	55,55,56,58	0
6	EDO	F	406	4/4	0.93	0.17	45,48,52,54	0
6	EDO	G	202	4/4	0.93	0.32	58,60,61,62	0
6	EDO	E	604	4/4	0.93	0.17	40,40,40,41	0
6	EDO	A	608	4/4	0.93	0.14	56,56,57,57	0
6	EDO	D	202	4/4	0.93	0.14	65,66,67,69	0
6	EDO	D	203	4/4	0.93	0.12	53,54,55,55	0
6	EDO	E	609	4/4	0.93	0.13	39,43,45,48	0
6	EDO	F	407	4/4	0.94	0.13	59,59,60,61	0
6	EDO	F	401	4/4	0.94	0.13	42,44,45,51	0
6	EDO	A	610	4/4	0.94	0.18	34,39,39,40	0
6	EDO	F	403	4/4	0.94	0.20	34,35,38,44	0
6	EDO	B	409	4/4	0.94	0.17	39,41,41,43	0
6	EDO	H	201	4/4	0.94	0.16	50,51,52,53	0
6	EDO	A	605	4/4	0.94	0.11	34,34,36,39	0
6	EDO	A	612	4/4	0.94	0.14	34,39,43,46	0
6	EDO	B	402	4/4	0.95	0.20	38,38,43,44	0
6	EDO	E	615	4/4	0.95	0.13	47,47,51,54	0
6	EDO	G	201	4/4	0.96	0.08	28,30,32,32	0
6	EDO	E	613	4/4	0.96	0.14	29,36,44,48	0
6	EDO	A	603	4/4	0.97	0.11	37,39,39,40	0
7	BEZ	A	607	9/9	0.97	0.09	29,30,31,32	0
7	BEZ	E	606	9/9	0.97	0.10	29,30,32,33	0
6	EDO	C	201	4/4	0.98	0.10	32,33,33,35	0
5	FE	A	602	1/1	0.99	0.08	28,28,28,28	0
5	FE	E	601	1/1	1.00	0.10	27,27,27,27	0
5	FE	E	602	1/1	1.00	0.09	30,30,30,30	0
5	FE	A	601	1/1	1.00	0.10	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.