



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 23, 2021 – 04:10 PM EST

PDB ID : 7S6Q  
Title : Complex structure of Methane monooxygenase hydroxylase and regulatory subunit DBL2  
Authors : Johns, J.C.; Banerjee, R.; Semonis, M.M.; Shi, K.; Aihara, H.; Lipscomb, J.D.  
Deposited on : 2021-09-14  
Resolution : 1.96 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](mailto: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 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 : 2.25  
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) : 2.25

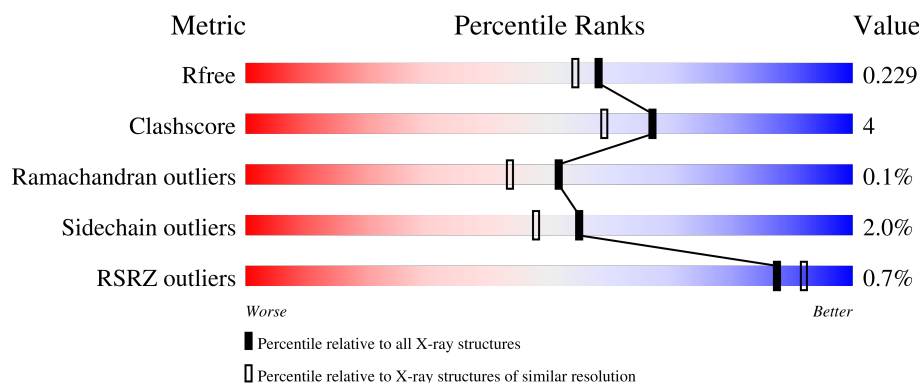
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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  $\geq 3$ , 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	515	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	E	515	<div> <div>%</div> <div>88%</div> <div>12%</div> </div>
2	B	392	<div> <div>%</div> <div>93%</div> <div>7%</div> <div>.</div> </div>
2	F	392	<div> <div>%</div> <div>91%</div> <div>9%</div> <div>.</div> </div>
3	C	168	<div> <div>89%</div> <div>11%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	G	168	 92% 8%
4	D	131	 3% 88% 10% ..
4	H	131	 3% 84% 13% ..

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
7	EDO	F	402	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 21399 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	1	0
			4184	2681	724	767	12			
1	E	515	Total	C	N	O	S	0	1	0
			4183	2680	725	766	12			

- 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	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 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	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	130	Total	C	N	O	S	0	0	0
			987	632	160	192	3			
4	H	130	Total	C	N	O	S	0	1	0
			990	635	158	194	3			

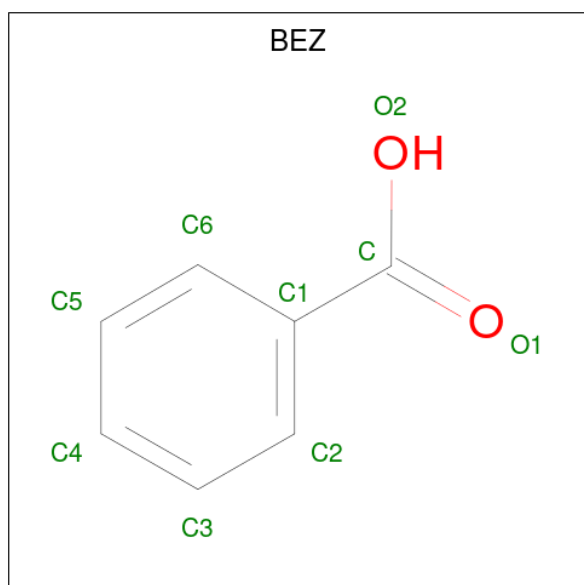
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	109	ALA	SER	engineered mutation	UNP A0A2D2D0T8
D	111	ALA	THR	engineered mutation	UNP A0A2D2D0T8
H	109	ALA	SER	engineered mutation	UNP A0A2D2D0T8
H	111	ALA	THR	engineered mutation	UNP A0A2D2D0T8

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

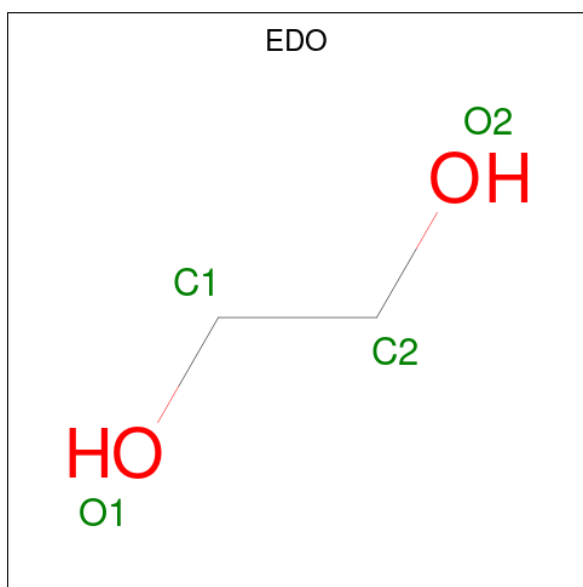
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Fe 2 2	0	0
5	E	2	Total Fe 2 2	0	0

- Molecule 6 is BENZOIC ACID (three-letter code: BEZ) (formula: C<sub>7</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	365	Total O 365 365	0	0
8	B	314	Total O 317 317	0	3
8	C	159	Total O 159 159	0	0
8	D	49	Total O 50 50	0	1
8	E	356	Total O 358 358	0	2

*Continued on next page...*

*Continued from previous page...*

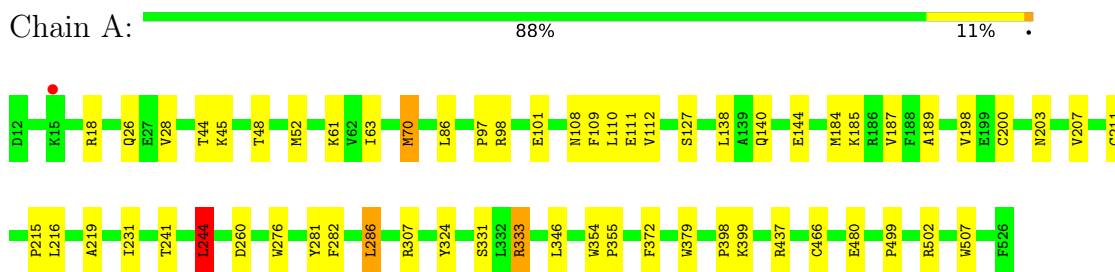
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	346	Total 347	O 347	0	1
8	G	166	Total 166	O 166	0	0
8	H	57	Total 57	O 57	0	0



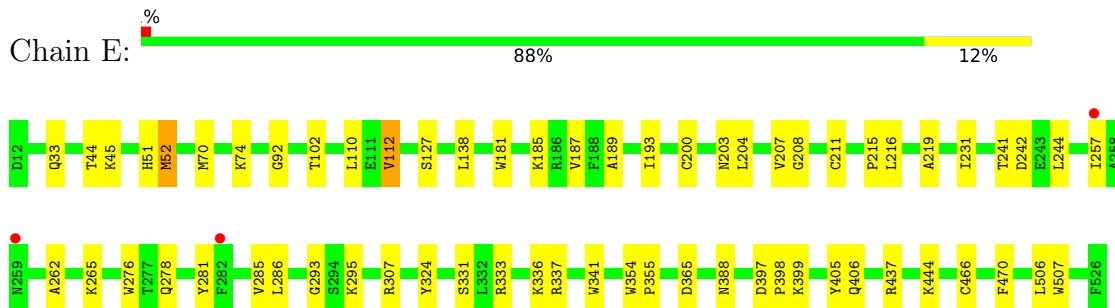
### 3 Residue-property plots [i](#)

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.

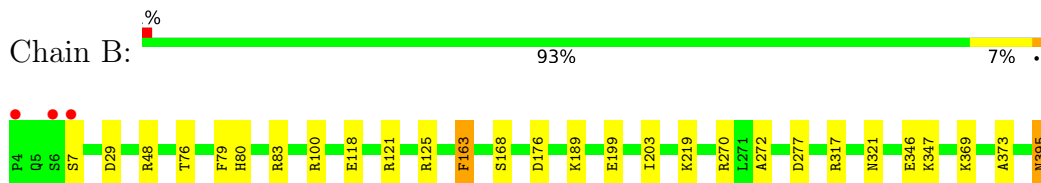
- Molecule 1: Methane monooxygenase component A alpha chain



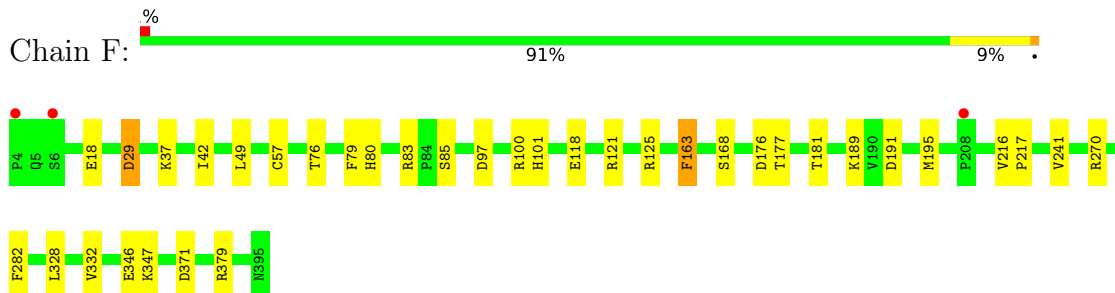
- Molecule 1: Methane monooxygenase component A alpha chain




- Molecule 2: Methane monooxygenase beta chain



- Molecule 2: Methane monooxygenase beta chain



- Molecule 3: Methane monooxygenase gamma chain

Chain C:  89% 11%




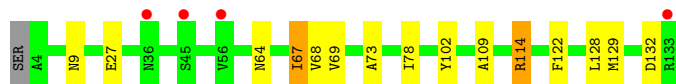
- Molecule 3: Methane monooxygenase gamma chain

Chain G:  92% 8%




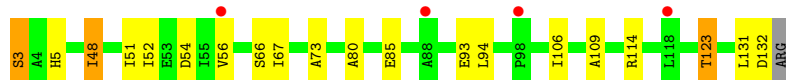
- Molecule 4: Methane monooxygenase regulatory protein B

Chain D:  3% 88% 10% ..



- Molecule 4: Methane monooxygenase regulatory protein B

Chain H:  3% 84% 13% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.18Å 105.36Å 297.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	148.90 – 1.96 148.90 – 1.96	Depositor EDS
% Data completeness (in resolution range)	95.2 (148.90-1.96) 95.3 (148.90-1.96)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.186 , 0.227 0.191 , 0.229	Depositor DCC
$R_{free}$ test set	10695 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.043 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21399	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.39	0/4314	0.59	1/5862 (0.0%)
1	E	0.40	0/4313	0.59	0/5861
2	B	0.39	0/3278	0.58	0/4457
2	F	0.38	0/3286	0.60	0/4468
3	C	0.36	0/1388	0.56	0/1877
3	G	0.37	0/1388	0.56	0/1877
4	D	0.37	0/1003	0.52	0/1356
4	H	0.37	0/1006	0.52	0/1361
All	All	0.39	0/19976	0.58	1/27119 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	LEU	CA-CB-CG	5.70	128.42	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4184	0	3977	38	0
1	E	4183	0	3977	39	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3185	0	3025	22	0
2	F	3193	0	3030	30	1
3	C	1362	0	1400	11	0
3	G	1362	0	1400	9	0
4	D	987	0	983	11	0
4	H	990	0	985	13	0
5	A	2	0	0	0	0
5	E	2	0	0	0	0
6	A	9	0	5	0	0
6	E	9	0	5	0	0
7	A	24	0	36	3	0
7	B	32	0	48	5	0
7	C	12	0	18	0	0
7	D	8	0	12	0	0
7	E	24	0	36	1	0
7	F	8	0	12	5	0
7	G	4	0	6	0	0
8	A	365	0	0	3	0
8	B	317	0	0	2	0
8	C	159	0	0	1	0
8	D	50	0	0	0	0
8	E	358	0	0	6	1
8	F	347	0	0	4	1
8	G	166	0	0	1	0
8	H	57	0	0	3	0
All	All	21399	0	18955	150	2

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 4.

All (150) 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:341:TRP:HE1	7:E:807:EDO:H12	1.41	0.85
1:A:502:ARG:NH1	8:A:901:HOH:O	2.13	0.80
1:E:406:GLN:NE2	8:E:902:HOH:O	2.16	0.78
2:F:125:ARG:HH11	7:F:402:EDO:H11	1.53	0.74
2:F:101:HIS:NE2	2:F:181:THR:HG21	2.03	0.73
1:E:33:GLN:OE1	8:E:901:HOH:O	2.05	0.72
2:F:18:GLU:OE1	8:F:501:HOH:O	2.12	0.67
4:H:54:ASP:HB2	4:H:94:LEU:HD21	1.77	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:NH2	4:D:27:GLU:OE1	2.31	0.64
1:A:18:ARG:NH2	2:F:371:ASP:OD2	2.30	0.63
1:A:26:GLN:HG2	1:A:61:LYS:HD2	1.81	0.63
2:F:125:ARG:HD3	7:F:402:EDO:H11	1.81	0.62
3:C:153:LEU:O	3:C:157:ARG:HG3	2.01	0.61
4:H:85:GLU:HG3	4:H:123:THR:HG22	1.82	0.61
4:D:114:ARG:HD3	4:D:128:LEU:HD23	1.83	0.60
4:H:132:ASP:O	8:H:201:HOH:O	2.16	0.60
3:C:26:VAL:H	3:C:72:LYS:HZ2	1.49	0.60
1:A:333:ARG:HH22	4:D:27:GLU:CD	2.05	0.59
1:E:52:MET:SD	1:E:257:ILE:HG22	2.44	0.58
2:F:29:ASP:OD1	2:F:29:ASP:N	2.29	0.58
1:E:200:CYS:HA	1:E:203:ASN:OD1	2.03	0.57
2:B:80:HIS:CD2	3:C:141:MET:HG2	2.40	0.56
2:F:121:ARG:NH2	7:F:402:EDO:H12	2.21	0.56
1:E:466:CYS:HB2	2:F:76:THR:HA	1.87	0.56
2:F:328:LEU:O	2:F:332:VAL:HG13	2.06	0.55
2:F:177:THR:O	2:F:181:THR:HG23	2.07	0.55
1:A:184:MET:HA	1:A:187:VAL:HG12	1.87	0.54
1:E:110:LEU:HD13	1:E:216:LEU:HD21	1.90	0.54
1:E:138:LEU:HD22	2:F:163:PHE:CE1	2.43	0.54
1:A:200:CYS:HA	1:A:203:ASN:OD1	2.09	0.53
1:E:92:GLY:HA2	1:E:231:ILE:HD11	1.89	0.53
2:B:395:ASN:OD1	8:B:501:HOH:O	2.19	0.53
2:B:121:ARG:HB3	7:B:403:EDO:H22	1.89	0.53
1:A:241:THR:HA	4:D:109:ALA:HA	1.91	0.52
1:E:208:GLY:HA2	1:E:278:GLN:HE22	1.74	0.52
3:G:154:GLU:H	3:G:154:GLU:CD	2.13	0.52
4:H:3:SER:HB2	4:H:66:SER:HA	1.91	0.52
1:A:466:CYS:HB2	2:B:76:THR:HA	1.92	0.52
1:A:138:LEU:HD22	2:B:163:PHE:CE1	2.45	0.52
1:A:98:ARG:HH21	7:A:809:EDO:H11	1.74	0.51
2:F:121:ARG:CZ	7:F:402:EDO:H12	2.40	0.51
1:E:208:GLY:CA	1:E:278:GLN:HE22	2.24	0.51
1:A:70:MET:HG3	4:D:102:TYR:HB3	1.91	0.51
3:C:154:GLU:H	3:C:154:GLU:CD	2.14	0.50
1:A:480[A]:GLU:OE1	8:A:902:HOH:O	2.18	0.50
1:E:193:ILE:HD11	2:F:85:SER:HB3	1.93	0.50
2:F:37:LYS:NZ	8:F:506:HOH:O	2.34	0.50
1:E:354:TRP:CG	1:E:355:PRO:HD3	2.47	0.50
4:H:48:ILE:HD12	4:H:51:ILE:HD12	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:3:SER:HB3	4:H:5:HIS:CE1	2.48	0.49
1:A:97:PRO:O	1:A:101:GLU:HG2	2.13	0.49
2:F:80:HIS:CD2	3:G:141:MET:HG2	2.48	0.49
1:A:207:VAL:O	1:A:211:CYS:HB3	2.13	0.48
2:B:272:ALA:HB1	2:B:277:ASP:HB3	1.95	0.48
1:E:388[A]:ASN:ND2	8:E:922:HOH:O	2.45	0.48
1:E:295:LYS:NZ	1:E:365:ASP:OD2	2.39	0.48
2:B:79:PHE:HB2	2:B:83:ARG:HB3	1.94	0.48
3:G:110:ARG:NH1	8:G:301:HOH:O	2.23	0.48
4:D:69:VAL:HG22	4:D:78:ILE:HG12	1.96	0.48
2:B:118:GLU:OE2	2:F:121:ARG:HD3	2.14	0.48
4:D:64:ASN:O	4:D:67:ILE:HG23	2.14	0.48
1:E:262:ALA:O	1:E:265:LYS:HG2	2.13	0.47
4:H:52:ILE:HA	4:H:56:VAL:HG13	1.95	0.47
3:C:116:ARG:O	3:C:120:LYS:HB2	2.13	0.47
1:E:185:LYS:O	1:E:189:ALA:HB3	2.14	0.47
3:C:26:VAL:H	3:C:72:LYS:NZ	2.12	0.47
1:E:51:HIS:ND1	8:E:1244[B]:HOH:O	2.35	0.47
1:A:282:PHE:CE2	1:A:286:LEU:HD22	2.49	0.47
1:E:215:PRO:HA	1:E:219:ALA:HB3	1.96	0.47
1:E:276:TRP:CE3	1:E:331:SER:HB2	2.50	0.47
1:A:398:PRO:HA	1:A:507:TRP:CE2	2.49	0.47
2:F:42:ILE:HD13	2:F:57:CYS:HB2	1.96	0.47
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.49	0.47
2:B:347:LYS:HD3	2:B:347:LYS:HA	1.70	0.47
2:B:7:SER:HA	4:D:9:ASN:ND2	2.30	0.46
2:F:125:ARG:HH11	7:F:402:EDO:C1	2.25	0.46
1:E:337:ARG:HD3	8:E:953:HOH:O	2.15	0.46
1:A:399:LYS:NZ	8:A:917:HOH:O	2.49	0.46
2:B:317:ARG:O	2:B:321:ASN:HB2	2.16	0.46
3:C:41:THR:HG22	3:C:54:TYR:CD1	2.50	0.46
2:B:118:GLU:HG2	2:F:118:GLU:HG2	1.96	0.46
2:B:48:ARG:HG3	4:H:93:GLU:HB3	1.98	0.46
2:B:189:LYS:HD3	2:B:189:LYS:HA	1.67	0.46
1:E:44:THR:HB	1:E:127:SER:HA	1.97	0.46
1:A:276:TRP:CE3	1:A:331:SER:HB2	2.51	0.45
1:A:86:LEU:HD13	1:A:231:ILE:HD13	1.97	0.45
2:F:216:VAL:HB	2:F:217:PRO:HD3	1.98	0.45
1:A:185:LYS:O	1:A:189:ALA:HB3	2.16	0.45
1:E:187:VAL:HG23	1:E:278:GLN:HA	1.98	0.45
4:H:123:THR:HG21	8:H:242:HOH:O	2.16	0.45

*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	2.52	0.45
1:E:405:TYR:HH	1:E:470:PHE:HE1	1.60	0.45
1:E:207:VAL:O	1:E:211:CYS:HB3	2.17	0.45
2:F:79:PHE:HB2	2:F:83:ARG:HB3	1.98	0.45
3:G:116:ARG:O	3:G:120:LYS:HB2	2.17	0.45
1:E:281:TYR:CZ	1:E:285:VAL:HG21	2.52	0.45
1:A:28:VAL:HG22	1:A:63:ILE:HG21	2.00	0.44
1:A:140:GLN:O	1:A:144:GLU:HG2	2.17	0.44
1:A:324:TYR:OH	4:D:132:ASP:OD1	2.26	0.44
2:B:125:ARG:HG3	7:B:403:EDO:H21	2.00	0.44
1:A:108:ASN:O	1:A:111:GLU:HB3	2.18	0.44
1:A:215:PRO:HA	1:A:219:ALA:HB3	1.98	0.44
1:A:372:PHE:HB3	1:A:379:TRP:CD2	2.51	0.44
2:F:241:VAL:HG13	3:G:127:ASN:OD1	2.17	0.44
2:B:369:LYS:HA	2:B:373:ALA:HB3	2.00	0.44
1:A:354:TRP:HA	7:A:807:EDO:H11	2.00	0.44
1:A:109:PHE:O	1:A:112:VAL:HG12	2.17	0.43
1:A:187:VAL:HB	1:A:281:TYR:HB3	2.01	0.43
2:F:57:CYS:HB3	8:F:798:HOH:O	2.18	0.43
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.53	0.43
3:C:122:PRO:HA	8:C:365:HOH:O	2.19	0.43
1:E:336:LYS:HE2	1:E:336:LYS:HB3	1.89	0.43
2:B:100:ARG:HE	7:B:408:EDO:C2	2.32	0.43
1:E:112:VAL:HG21	1:E:181:TRP:HH2	1.84	0.43
2:F:189:LYS:HA	2:F:189:LYS:HD3	1.67	0.43
4:H:123:THR:HG23	8:H:245:HOH:O	2.17	0.43
1:A:45:LYS:HD2	2:B:168:SER:HB3	2.01	0.43
1:E:203:ASN:OD1	1:E:204:LEU:N	2.50	0.43
3:G:58:GLU:O	3:G:62:GLU:HG3	2.18	0.43
4:H:67:ILE:HG12	4:H:80:ALA:HB2	2.01	0.42
2:B:219:LYS:HB3	2:B:219:LYS:HE2	1.86	0.42
1:A:110:LEU:HD13	1:A:216:LEU:HD21	2.01	0.42
2:F:97:ASP:HB3	2:F:100:ARG:HG3	2.01	0.42
3:C:23:LEU:HD21	3:C:32:PHE:CD2	2.54	0.42
1:E:74:LYS:NZ	1:E:242:ASP:OD1	2.51	0.42
1:E:241:THR:HA	4:H:109:ALA:HA	2.02	0.42
1:A:44:THR:HB	1:A:127:SER:HA	2.01	0.42
1:E:398:PRO:HA	1:E:507:TRP:CE2	2.54	0.42
1:E:399:LYS:HA	1:E:399:LYS:HD3	1.80	0.42
3:G:121:PRO:HD3	3:G:129:PHE:CG	2.55	0.42
1:A:48:THR:OG1	1:A:198:VAL:HG13	2.20	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:LEU:HD12	1:E:286:LEU:HA	1.81	0.41
2:F:191:ASP:O	2:F:195:MET:HG2	2.20	0.41
1:E:102:THR:OG1	1:E:293:GLY:HA3	2.19	0.41
2:B:199:GLU:O	2:B:203:ILE:HG13	2.20	0.41
2:F:347:LYS:HA	2:F:347:LYS:HD3	1.79	0.41
1:E:45:LYS:HD2	2:F:168:SER:HB3	2.01	0.41
2:B:121:ARG:HD3	2:F:118:GLU:OE2	2.21	0.41
2:F:282:PHE:O	8:F:502:HOH:O	2.21	0.41
1:A:98:ARG:HH21	7:A:809:EDO:C1	2.34	0.41
3:C:5:GLU:OE2	3:C:11:SER:OG	2.33	0.41
3:G:37:ARG:CZ	3:G:120:LYS:HB3	2.50	0.41
1:E:215:PRO:HA	1:E:219:ALA:CB	2.51	0.41
1:A:244:LEU:HD11	4:D:122:PHE:CE2	2.55	0.40
3:G:4:ARG:HA	3:G:4:ARG:NE	2.35	0.40
1:E:444:LYS:NZ	8:E:935:HOH:O	2.50	0.40
1:E:324:TYR:CD2	4:H:131:LEU:HD23	2.56	0.40
2:B:100:ARG:HE	7:B:408:EDO:C1	2.35	0.40
4:D:68:VAL:O	4:D:78:ILE:HA	2.22	0.40
7:B:408:EDO:H22	8:B:511:HOH:O	2.21	0.40

All (2) 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:1228:HOH:O	8:F:762:HOH:O[3_555]	2.07	0.13
1:E:397:ASP:OD2	2:F:379:ARG:NH2[3_555]	2.15	0.05

## 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	514/515 (100%)	496 (96%)	18 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	514/515 (100%)	500 (97%)	14 (3%)	0	100	100
2	B	390/392 (100%)	379 (97%)	11 (3%)	0	100	100
2	F	391/392 (100%)	379 (97%)	12 (3%)	0	100	100
3	C	166/168 (99%)	164 (99%)	2 (1%)	0	100	100
3	G	166/168 (99%)	164 (99%)	2 (1%)	0	100	100
4	D	128/131 (98%)	123 (96%)	4 (3%)	1 (1%)	19	9
4	H	129/131 (98%)	123 (95%)	5 (4%)	1 (1%)	19	9
All	All	2398/2412 (99%)	2328 (97%)	68 (3%)	2 (0%)	51	43

All (2) Ramachandran outliers are listed below:

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

### 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	427/426 (100%)	418 (98%)	9 (2%)	53	46
1	E	427/426 (100%)	419 (98%)	8 (2%)	57	50
2	B	324/324 (100%)	318 (98%)	6 (2%)	57	50
2	F	325/324 (100%)	319 (98%)	6 (2%)	59	53
3	C	145/145 (100%)	144 (99%)	1 (1%)	84	82
3	G	145/145 (100%)	144 (99%)	1 (1%)	84	82
4	D	101/102 (99%)	98 (97%)	3 (3%)	41	30
4	H	102/102 (100%)	96 (94%)	6 (6%)	19	8
All	All	1996/1994 (100%)	1956 (98%)	40 (2%)	55	48

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	MET
1	A	70	MET
1	A	244	LEU
1	A	260	ASP
1	A	286	LEU
1	A	307	ARG
1	A	333	ARG
1	A	346	LEU
1	A	437	ARG
2	B	29	ASP
2	B	163	PHE
2	B	176	ASP
2	B	270	ARG
2	B	346	GLU
2	B	395	ASN
3	C	42	SER
4	D	67	ILE
4	D	114	ARG
4	D	129	MET
1	E	52	MET
1	E	70	MET
1	E	112	VAL
1	E	244	LEU
1	E	307	ARG
1	E	333	ARG
1	E	437	ARG
1	E	506	LEU
2	F	29	ASP
2	F	49	LEU
2	F	163	PHE
2	F	176	ASP
2	F	270	ARG
2	F	346	GLU
3	G	112	HIS
4	H	3	SER
4	H	48	ILE
4	H	106[A]	ILE
4	H	106[B]	ILE
4	H	114	ARG
4	H	123	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	278	GLN
1	E	406	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 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	D	202	-	3,3,3	0.54	0	2,2,2	0.14	0
7	EDO	E	809	-	3,3,3	0.53	0	2,2,2	0.23	0
7	EDO	G	201	-	3,3,3	0.44	0	2,2,2	0.45	0
7	EDO	A	807	-	3,3,3	0.60	0	2,2,2	0.12	0
7	EDO	A	805	-	3,3,3	0.45	0	2,2,2	0.33	0
7	EDO	D	201	-	3,3,3	0.53	0	2,2,2	0.25	0
7	EDO	C	202	-	3,3,3	0.44	0	2,2,2	0.32	0
6	BEZ	A	803	5	7,9,9	0.90	1 (14%)	8,11,11	0.77	0
7	EDO	B	406	-	3,3,3	0.43	0	2,2,2	0.62	0
7	EDO	E	808	-	3,3,3	0.52	0	2,2,2	0.22	0
7	EDO	A	804	-	3,3,3	0.47	0	2,2,2	0.24	0
7	EDO	C	203	-	3,3,3	0.48	0	2,2,2	0.29	0
7	EDO	A	806	-	3,3,3	0.53	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	C	201	-	3,3,3	0.46	0	2,2,2	0.29	0
7	EDO	B	401	-	3,3,3	0.46	0	2,2,2	0.24	0
7	EDO	E	805	-	3,3,3	0.53	0	2,2,2	0.11	0
7	EDO	B	405	-	3,3,3	0.47	0	2,2,2	0.36	0
7	EDO	B	403	-	3,3,3	0.51	0	2,2,2	0.18	0
7	EDO	B	407	-	3,3,3	0.49	0	2,2,2	0.16	0
7	EDO	E	806	-	3,3,3	0.54	0	2,2,2	0.30	0
7	EDO	E	807	-	3,3,3	0.58	0	2,2,2	0.19	0
7	EDO	F	401	-	3,3,3	0.52	0	2,2,2	0.24	0
7	EDO	E	804	-	3,3,3	0.40	0	2,2,2	0.50	0
6	BEZ	E	803	5	7,9,9	1.11	1 (14%)	8,11,11	0.73	0
7	EDO	B	402	-	3,3,3	0.49	0	2,2,2	0.25	0
7	EDO	B	408	-	3,3,3	0.46	0	2,2,2	0.34	0
7	EDO	A	808	-	3,3,3	0.44	0	2,2,2	0.40	0
7	EDO	B	404	-	3,3,3	0.46	0	2,2,2	0.37	0
7	EDO	F	402	-	3,3,3	0.54	0	2,2,2	0.26	0
7	EDO	A	809	-	3,3,3	0.46	0	2,2,2	0.35	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	D	202	-	-	0/1/1/1	-
7	EDO	E	809	-	-	0/1/1/1	-
7	EDO	G	201	-	-	1/1/1/1	-
7	EDO	A	807	-	-	1/1/1/1	-
7	EDO	A	805	-	-	0/1/1/1	-
7	EDO	D	201	-	-	1/1/1/1	-
7	EDO	C	202	-	-	0/1/1/1	-
6	BEZ	A	803	5	-	0/0/4/4	0/1/1/1
7	EDO	B	406	-	-	0/1/1/1	-
7	EDO	E	808	-	-	0/1/1/1	-
7	EDO	A	804	-	-	0/1/1/1	-
7	EDO	C	203	-	-	1/1/1/1	-
7	EDO	A	806	-	-	1/1/1/1	-
7	EDO	C	201	-	-	0/1/1/1	-
7	EDO	B	401	-	-	0/1/1/1	-
7	EDO	E	805	-	-	0/1/1/1	-
7	EDO	B	405	-	-	0/1/1/1	-
7	EDO	B	403	-	-	0/1/1/1	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	407	-	-	1/1/1/1	-
7	EDO	E	806	-	-	0/1/1/1	-
7	EDO	E	807	-	-	1/1/1/1	-
7	EDO	F	401	-	-	0/1/1/1	-
7	EDO	E	804	-	-	0/1/1/1	-
6	BEZ	E	803	5	-	0/0/4/4	0/1/1/1
7	EDO	B	402	-	-	1/1/1/1	-
7	EDO	B	408	-	-	0/1/1/1	-
7	EDO	A	808	-	-	1/1/1/1	-
7	EDO	B	404	-	-	0/1/1/1	-
7	EDO	F	402	-	-	1/1/1/1	-
7	EDO	A	809	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	803	BEZ	C1-C	2.74	1.50	1.47
6	A	803	BEZ	C1-C	2.07	1.49	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	809	EDO	O1-C1-C2-O2
7	C	203	EDO	O1-C1-C2-O2
7	A	808	EDO	O1-C1-C2-O2
7	B	402	EDO	O1-C1-C2-O2
7	A	807	EDO	O1-C1-C2-O2
7	E	807	EDO	O1-C1-C2-O2
7	F	402	EDO	O1-C1-C2-O2
7	A	806	EDO	O1-C1-C2-O2
7	B	407	EDO	O1-C1-C2-O2
7	D	201	EDO	O1-C1-C2-O2
7	G	201	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	807	EDO	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	403	EDO	2	0
7	E	807	EDO	1	0
7	B	408	EDO	3	0
7	F	402	EDO	5	0
7	A	809	EDO	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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	515/515 (100%)	0.18	1 (0%) 95 97	22, 32, 47, 58	0
1	E	515/515 (100%)	0.19	3 (0%) 89 93	23, 33, 49, 63	0
2	B	392/392 (100%)	0.14	3 (0%) 86 90	23, 31, 45, 85	0
2	F	392/392 (100%)	0.15	3 (0%) 86 90	24, 32, 44, 89	0
3	C	168/168 (100%)	0.06	0 100 100	25, 35, 47, 58	0
3	G	168/168 (100%)	0.15	0 100 100	26, 38, 49, 56	0
4	D	130/131 (99%)	0.50	4 (3%) 49 58	30, 41, 55, 81	0
4	H	130/131 (99%)	0.52	4 (3%) 49 58	32, 43, 58, 64	0
All	All	2410/2412 (99%)	0.20	18 (0%) 87 92	22, 34, 49, 89	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	4	PRO	5.6
2	B	4	PRO	5.2
4	D	133	ARG	4.8
1	E	282	PHE	3.5
4	D	36	ASN	3.5
1	E	257	ILE	3.5
2	B	6	SER	3.4
2	B	7	SER	3.2
4	H	88	ALA	2.8
4	D	56	VAL	2.7
4	H	118	LEU	2.6
4	H	56	VAL	2.6
4	D	45	SER	2.4
1	A	15	LYS	2.3
2	F	208	PRO	2.1
4	H	98	PRO	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	259	ASN	2.0
2	F	6	SER	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 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
7	EDO	A	807	4/4	0.61	0.31	46,50,52,55	0
7	EDO	B	407	4/4	0.67	0.23	65,67,69,69	0
7	EDO	E	805	4/4	0.71	0.28	57,63,64,66	0
7	EDO	A	806	4/4	0.78	0.13	50,50,51,54	0
7	EDO	B	406	4/4	0.79	0.26	47,50,53,56	0
7	EDO	E	809	4/4	0.80	0.16	50,54,57,58	0
7	EDO	F	402	4/4	0.80	0.21	44,44,48,49	0
7	EDO	B	405	4/4	0.82	0.20	46,52,56,56	0
7	EDO	E	807	4/4	0.82	0.17	40,42,42,46	0
7	EDO	C	203	4/4	0.83	0.32	52,52,53,56	0
7	EDO	B	402	4/4	0.84	0.12	59,59,60,62	0
7	EDO	E	808	4/4	0.85	0.17	62,65,67,69	0
7	EDO	E	806	4/4	0.87	0.17	42,43,43,43	0
7	EDO	D	202	4/4	0.88	0.13	47,50,50,51	0
7	EDO	A	805	4/4	0.89	0.15	39,40,42,45	0
7	EDO	A	808	4/4	0.89	0.15	56,61,63,66	0
7	EDO	B	401	4/4	0.89	0.16	44,44,46,46	0
7	EDO	G	201	4/4	0.89	0.15	58,59,60,64	0
7	EDO	F	401	4/4	0.90	0.13	52,54,55,56	0
7	EDO	B	408	4/4	0.90	0.16	49,54,56,56	0
7	EDO	A	804	4/4	0.90	0.15	41,42,44,49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	C	202	4/4	0.93	0.19	54,55,57,58	0
7	EDO	B	403	4/4	0.93	0.14	38,42,49,55	0
7	EDO	C	201	4/4	0.93	0.15	35,35,36,36	0
7	EDO	E	804	4/4	0.93	0.15	34,37,37,43	0
7	EDO	A	809	4/4	0.94	0.23	47,53,61,67	0
6	BEZ	E	803	9/9	0.95	0.12	28,32,37,37	0
7	EDO	D	201	4/4	0.95	0.09	42,42,42,45	0
7	EDO	B	404	4/4	0.95	0.14	43,43,44,47	0
6	BEZ	A	803	9/9	0.97	0.15	31,32,35,39	0
5	FE	A	802	1/1	0.98	0.09	35,35,35,35	0
5	FE	E	801	1/1	0.98	0.12	34,34,34,34	0
5	FE	A	801	1/1	0.99	0.14	35,35,35,35	0
5	FE	E	802	1/1	0.99	0.09	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.