Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 12:47 AM EDT

PDB ID	:	7M8Q
Title	:	Complex structure of Methane monooxygenase hydroxylase and regulatory subunit with fluorosubstituted tryptophans
Authors	:	Johns, J.C.; Banerjee, R.; Shi, K.; Semonis, M.M.; Aihara, H.; Pomerantz, W.C.K.; Lipscomb, J.D.
Deposited on	:	2021-03-30
Resolution	:	2.08 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:

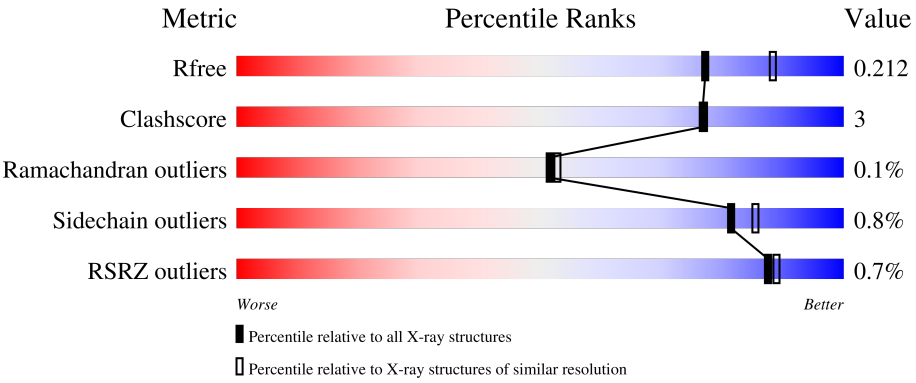
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	90% 10%
1	E	515	91% 9%
2	B	392	94% 5%
2	F	392	92% 7%
3	C	168	95% 5%

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Mol	Chain	Length	Quality of chain
3	G	168	2% 95% 5%
4	D	137	2% 85% 11%
4	H	137	% 84% 12%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 21830 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	1	0
			4181	2679	724	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	0	0
			3185	2033	556	591	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			

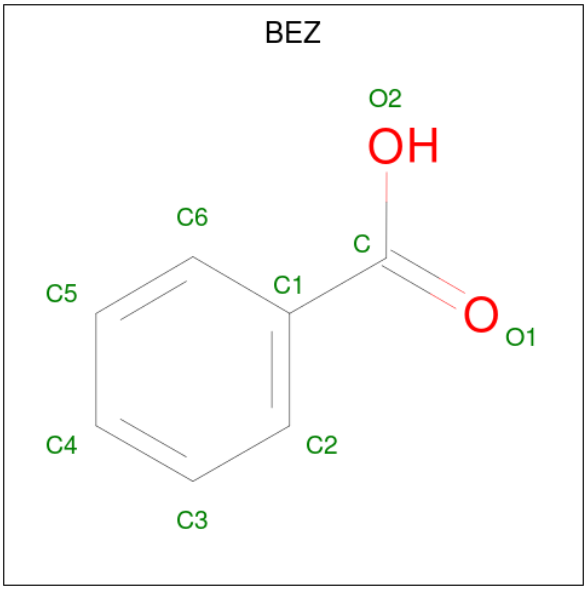
- Molecule 4 is a protein called Methane monooxygenase regulatory protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	132	Total	C	F	N	O	S	0	0	0
			1003	639	2	162	197	3			
4	H	132	Total	C	F	N	O	S	0	0	0
			1004	639	2	162	198	3			

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

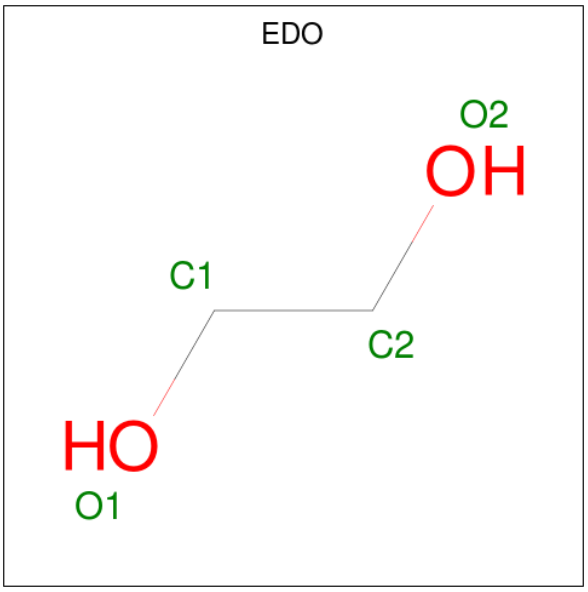
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Fe 2 2	0	0
5	E	2	Total Fe 2 2	0	0

- Molecule 6 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).



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: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	E	1	Total C O 8 4 4	0	1
7	E	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
7	H	1	Total C O 4 2 2	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total Na 1 1	0	0

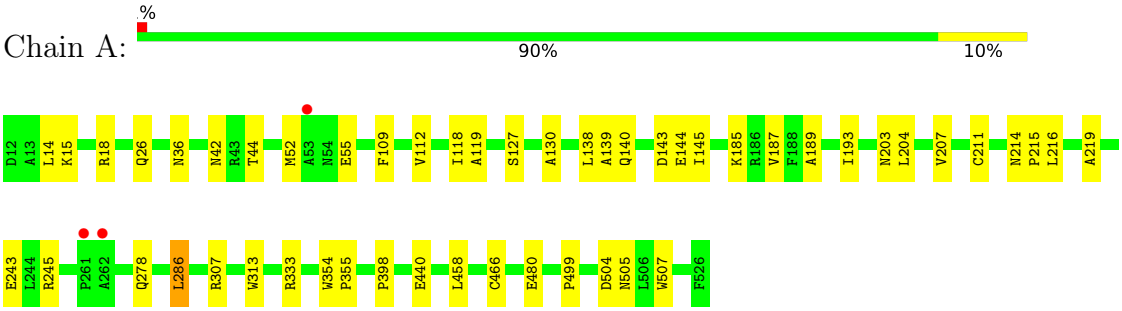
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	438	Total O 439 439	0	1
9	B	414	Total O 414 414	0	0
9	C	216	Total O 216 216	0	0
9	D	102	Total O 102 102	0	0
9	E	436	Total O 436 436	0	0
9	F	378	Total O 378 378	0	0
9	G	204	Total O 204 204	0	0
9	H	93	Total O 93 93	0	0

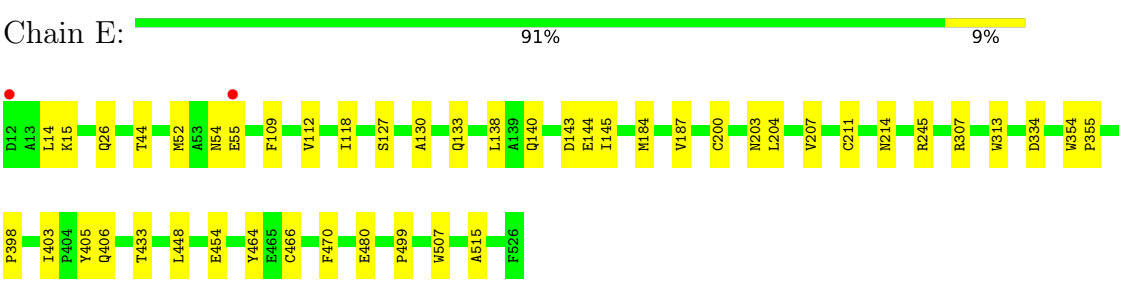
3 Residue-property plots (i)

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.

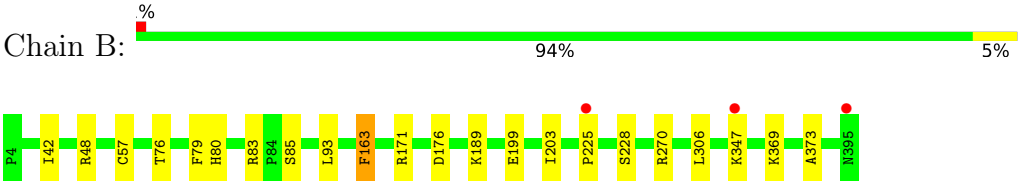
• Molecule 1: Methane monooxygenase component A alpha chain



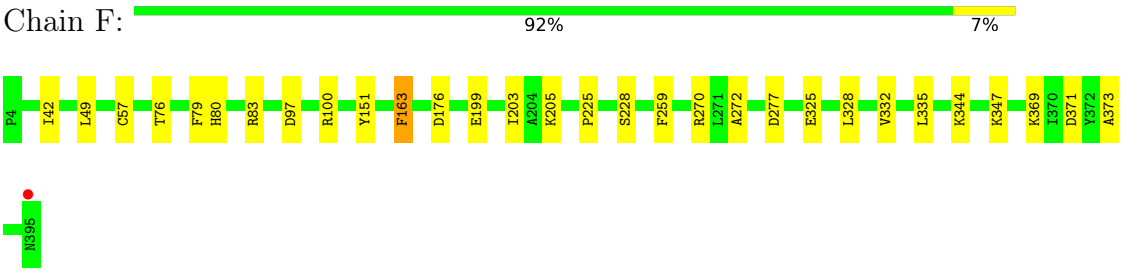
• Molecule 1: Methane monooxygenase component A alpha chain



• Molecule 2: Methane monooxygenase beta chain

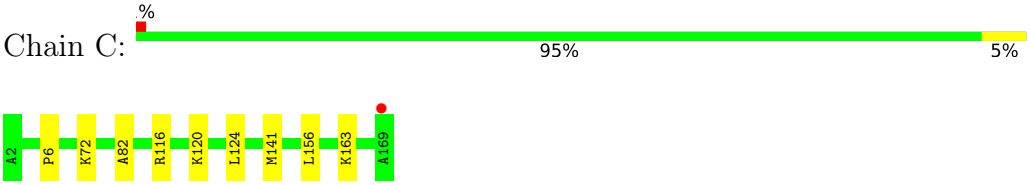


• Molecule 2: Methane monooxygenase beta chain



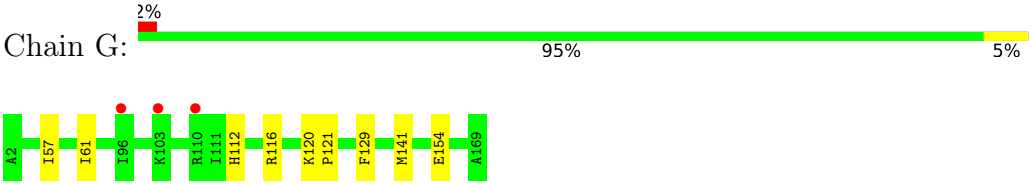
• Molecule 3: Methane monooxygenase gamma chain

Chain C:



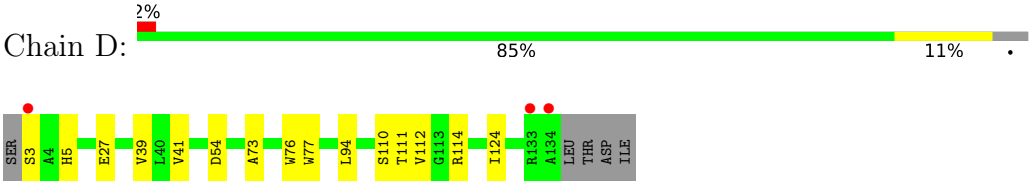
• Molecule 3: Methane monooxygenase gamma chain

Chain G:



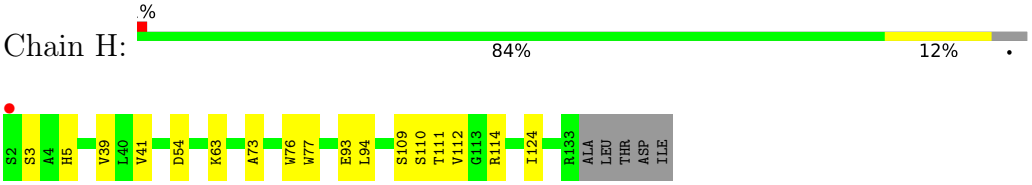
• Molecule 4: Methane monooxygenase regulatory protein B

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	102.49Å 105.62Å 299.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.33 – 2.08 86.33 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.1 (86.33-2.08) 99.1 (86.33-2.08)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.18rc6_3830	Depositor
R, R_{free}	0.182 , 0.212 0.182 , 0.212	Depositor DCC
R_{free} test set	9528 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.047 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21830	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: FE, BEZ, FTR, EDO, NA

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	0.25	0/4325	0.42	0/5875
1	E	0.25	0/4311	0.41	0/5858
2	B	0.24	0/3278	0.41	0/4457
2	F	0.25	0/3278	0.41	0/4457
3	C	0.24	0/1388	0.41	0/1877
3	G	0.23	0/1388	0.41	0/1877
4	D	0.25	0/984	0.44	0/1326
4	H	0.25	0/985	0.43	0/1327
All	All	0.24	0/19937	0.41	0/27054

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	36	0
1	E	4181	0	3976	31	0
2	B	3185	0	3025	15	0
2	F	3185	0	3025	20	0
3	C	1362	0	1400	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1362	0	1400	5	0
4	D	1003	0	991	7	0
4	H	1004	0	991	8	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	8	0	12	1	0
7	B	12	0	18	0	0
7	C	4	0	6	0	0
7	E	12	0	18	4	0
7	F	4	0	6	0	0
7	G	4	0	6	0	0
7	H	4	0	6	0	0
8	E	1	0	0	0	0
9	A	439	0	0	4	0
9	B	414	0	0	1	0
9	C	216	0	0	1	0
9	D	102	0	0	0	0
9	E	436	0	0	3	0
9	F	378	0	0	4	0
9	G	204	0	0	1	0
9	H	93	0	0	0	0
All	All	21830	0	18886	115	0

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

All (115) 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:406:GLN:HE22	1:E:515:ALA:HB1	1.48	0.78
1:A:36:ASN:HD21	1:A:42:ASN:HD21	1.37	0.72
2:B:93:LEU:HD23	2:B:306:LEU:HD13	1.73	0.69
3:G:154:GLU:OE1	9:G:301:HOH:O	2.12	0.68
2:B:369:LYS:NZ	9:B:502:HOH:O	2.29	0.64
1:E:406:GLN:OE1	9:E:901:HOH:O	2.14	0.64
1:E:480:GLU:OE1	9:E:902:HOH:O	2.15	0.63
1:A:18:ARG:NH2	2:F:371:ASP:OD2	2.31	0.63
1:E:133:GLN:HG3	7:E:805:EDO:H21	1.80	0.63
7:A:805:EDO:H12	3:C:6:PRO:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:805:EDO:O1	9:E:903:HOH:O	2.16	0.61
1:E:214:ASN:OD1	4:H:110:SER:OG	2.15	0.58
1:A:203:ASN:OD1	1:A:204:LEU:N	2.37	0.57
2:F:79:PHE:HB2	2:F:83:ARG:HB3	1.88	0.55
1:E:203:ASN:OD1	1:E:204:LEU:N	2.40	0.54
2:B:79:PHE:HB2	2:B:83:ARG:HB3	1.89	0.53
4:D:54:ASP:HB2	4:D:94:LEU:HD11	1.91	0.52
1:A:26:GLN:NE2	9:A:1213:HOH:O	2.42	0.52
1:A:143:ASP:OD2	1:A:245[A]:ARG:NH1	2.38	0.52
1:A:466:CYS:HB2	2:B:76:THR:HA	1.91	0.52
2:F:328:LEU:O	2:F:332:VAL:HG13	2.09	0.52
1:E:55:GLU:HA	1:E:130:ALA:HB2	1.93	0.51
1:E:403:ILE:HB	1:E:406:GLN:HE21	1.74	0.51
1:A:243:GLU:OE1	9:A:1201:HOH:O	2.19	0.50
2:F:42:ILE:HD13	2:F:57:CYS:HB2	1.93	0.50
4:D:39:VAL:HB	4:D:112:VAL:HB	1.93	0.50
1:A:55:GLU:HA	1:A:130:ALA:HB2	1.94	0.49
1:E:14:LEU:HB3	1:E:15:LYS:HD2	1.94	0.49
4:D:41:VAL:HB	4:D:110:SER:HB3	1.95	0.49
3:G:116:ARG:O	3:G:120:LYS:HB2	2.13	0.49
1:A:139:ALA:HB3	1:A:245[B]:ARG:HH22	1.78	0.49
1:A:398:PRO:HA	1:A:507:TRP:CE2	2.48	0.49
4:D:111:THR:HB	4:D:124:ILE:HD12	1.94	0.48
4:H:41:VAL:HG12	4:H:109:SER:HB2	1.95	0.48
1:E:466:CYS:HB2	2:F:76:THR:HA	1.94	0.48
1:E:207:VAL:O	1:E:211:CYS:HB3	2.13	0.48
1:A:207:VAL:O	1:A:211:CYS:HB3	2.13	0.48
1:A:138:LEU:HD22	2:B:163:PHE:CE1	2.49	0.48
1:E:54:ASN:ND2	7:E:805:EDO:H22	2.28	0.48
2:B:48:ARG:HG3	4:H:93:GLU:HB3	1.96	0.48
2:B:189:LYS:HD3	2:B:189:LYS:HA	1.73	0.47
2:B:347:LYS:HD3	2:B:347:LYS:HA	1.71	0.47
4:H:111:THR:HB	4:H:124:ILE:HD12	1.96	0.47
2:F:347:LYS:HD3	2:F:347:LYS:HA	1.64	0.47
1:A:480:GLU:OE2	9:A:1202:HOH:O	2.20	0.47
1:E:405:TYR:HH	1:E:470:PHE:HE1	1.61	0.47
1:A:214:ASN:OD1	4:D:110:SER:OG	2.30	0.46
2:B:80:HIS:CD2	3:C:141:MET:HG2	2.50	0.46
1:A:26:GLN:HG3	9:A:1526:HOH:O	2.15	0.46
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.50	0.46
1:A:333:ARG:NH2	4:D:27:GLU:OE1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:LYS:HA	2:B:373:ALA:HB3	1.97	0.46
2:F:205:LYS:NZ	9:F:523:HOH:O	2.48	0.46
1:A:14:LEU:HB3	1:A:15:LYS:HD2	1.98	0.45
1:A:119:ALA:HB1	2:B:171:ARG:HD2	1.98	0.45
1:A:440:GLU:HB3	3:C:163:LYS:HB3	1.98	0.45
2:F:100:ARG:NH1	9:F:510:HOH:O	2.42	0.45
1:E:448:LEU:HD22	1:E:454:GLU:HA	1.98	0.45
3:C:116:ARG:O	3:C:120:LYS:HB2	2.16	0.45
1:A:44:THR:HB	1:A:127:SER:HA	1.98	0.45
4:H:3:SER:HB3	4:H:5:HIS:CE1	2.51	0.44
1:E:334:ASP:HB3	1:E:433:THR:HG21	1.99	0.44
1:A:216:LEU:HA	1:A:286:LEU:HD11	1.99	0.44
3:C:82:ALA:HB2	3:C:124:LEU:HD23	1.98	0.44
1:A:109:PHE:O	1:A:112:VAL:HG12	2.17	0.44
1:A:139:ALA:HB3	1:A:245[B]:ARG:NH2	2.32	0.44
2:F:80:HIS:CD2	3:G:141:MET:HG2	2.53	0.44
1:A:504:ASP:OD2	1:A:505:ASN:ND2	2.50	0.44
2:B:225:PRO:HA	2:B:228:SER:HB2	1.98	0.44
1:E:26:GLN:CD	1:E:26:GLN:H	2.21	0.44
4:D:3:SER:HB3	4:D:5:HIS:CE1	2.53	0.44
1:E:406:GLN:NE2	1:E:515:ALA:HB1	2.24	0.44
1:A:458:LEU:HD13	3:C:156:LEU:HB3	2.00	0.44
1:E:398:PRO:HA	1:E:507:TRP:CE2	2.52	0.44
4:H:54:ASP:HB2	4:H:94:LEU:HD21	1.99	0.44
1:E:138:LEU:HD22	2:F:163:PHE:CE1	2.52	0.43
1:E:354:TRP:CH2	1:E:499:PRO:HD3	2.53	0.43
2:F:225:PRO:HA	2:F:228:SER:HB2	1.99	0.43
2:F:259:PHE:HA	2:F:335:LEU:HD21	2.00	0.43
1:E:354:TRP:CG	1:E:355:PRO:HD3	2.54	0.43
2:F:325:GLU:OE1	9:F:501:HOH:O	2.22	0.43
1:A:193:ILE:HD11	2:B:85:SER:HB3	2.01	0.43
1:E:200:CYS:HA	1:E:203:ASN:OD1	2.18	0.43
1:E:211:CYS:HB2	1:E:313:TRP:CD1	2.53	0.43
1:A:215:PRO:HA	1:A:219:ALA:HB3	2.01	0.43
1:A:118:ILE:HD13	1:A:145:ILE:HG12	2.00	0.42
1:E:109:PHE:O	1:E:112:VAL:HG12	2.20	0.42
2:F:57:CYS:HB3	9:F:817:HOH:O	2.19	0.42
4:H:39:VAL:HB	4:H:112:VAL:HB	2.01	0.42
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.54	0.42
1:A:211:CYS:HB2	1:A:313:TRP:CE2	2.54	0.42
1:E:143:ASP:OD2	1:E:245:ARG:NH1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:63:LYS:HE2	4:H:63:LYS:HB3	1.90	0.41
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.55	0.41
3:C:72:LYS:NZ	9:C:309:HOH:O	2.53	0.41
2:F:199:GLU:O	2:F:203:ILE:HG13	2.20	0.41
1:E:211:CYS:HB2	1:E:313:TRP:CE2	2.56	0.41
2:F:151:TYR:OH	2:F:344:LYS:NZ	2.48	0.41
2:F:272:ALA:HB1	2:F:277:ASP:HB3	2.01	0.41
3:G:57:ILE:O	3:G:61:ILE:HG13	2.21	0.41
2:B:42:ILE:HD13	2:B:57:CYS:HB2	2.02	0.41
2:B:199:GLU:O	2:B:203:ILE:HG13	2.21	0.41
1:E:44:THR:HB	1:E:127:SER:HA	2.01	0.41
1:A:140:GLN:O	1:A:144:GLU:HG2	2.20	0.41
1:A:187:VAL:HG23	1:A:278:GLN:HA	2.02	0.41
1:E:464:TYR:HH	7:E:804[A]:EDO:HO1	1.67	0.41
1:E:118:ILE:HD13	1:E:145:ILE:HG12	2.01	0.41
1:E:184:MET:HA	1:E:187:VAL:HG12	2.02	0.41
2:F:97:ASP:HB3	2:F:100:ARG:HG3	2.02	0.41
3:C:156:LEU:HD12	3:C:156:LEU:HA	1.92	0.41
2:F:369:LYS:HA	2:F:373:ALA:HB3	2.03	0.41
1:A:18:ARG:HH22	2:F:371:ASP:CG	2.24	0.40
1:A:185:LYS:O	1:A:189:ALA:HB3	2.21	0.40
1:E:140:GLN:O	1:E:144:GLU:HG2	2.21	0.40
3:G:121:PRO:HD3	3:G:129:PHE:CG	2.57	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	515/515 (100%)	501 (97%)	14 (3%)	0	100	100
1	E	514/515 (100%)	499 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	390/392 (100%)	381 (98%)	9 (2%)	0	100	100
2	F	390/392 (100%)	382 (98%)	8 (2%)	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	128/137 (93%)	124 (97%)	3 (2%)	1 (1%)	19	14
4	H	128/137 (93%)	124 (97%)	3 (2%)	1 (1%)	19	14
All	All	2397/2424 (99%)	2339 (98%)	56 (2%)	2 (0%)	51	53

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%)	425 (99%)	3 (1%)	84	87
1	E	427/426 (100%)	425 (100%)	2 (0%)	88	92
2	B	324/324 (100%)	321 (99%)	3 (1%)	78	83
2	F	324/324 (100%)	320 (99%)	4 (1%)	71	76
3	C	145/145 (100%)	145 (100%)	0	100	100
3	G	145/145 (100%)	144 (99%)	1 (1%)	84	87
4	D	102/107 (95%)	101 (99%)	1 (1%)	76	81
4	H	103/107 (96%)	102 (99%)	1 (1%)	76	81
All	All	1998/2004 (100%)	1983 (99%)	15 (1%)	81	85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	MET
1	A	286	LEU
1	A	307	ARG
2	B	163	PHE
2	B	176	ASP
2	B	270	ARG
4	D	114	ARG
1	E	52	MET
1	E	307	ARG
2	F	49	LEU
2	F	163	PHE
2	F	176	ASP
2	F	270	ARG
3	G	112	HIS
4	H	114	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	133	GLN
1	A	205	GLN
1	A	406	GLN
1	A	505	ASN
2	B	8	GLN
1	E	26	GLN
1	E	205	GLN
1	E	406	GLN
2	F	321	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
4	FTR	H	77	4	14,16,17	2.45	5 (35%)	14,22,24	1.54	2 (14%)
4	FTR	H	76	4	14,16,17	2.44	6 (42%)	14,22,24	1.52	3 (21%)
4	FTR	D	76	4	14,16,17	2.46	5 (35%)	14,22,24	1.49	2 (14%)
4	FTR	D	77	4	14,16,17	2.47	5 (35%)	14,22,24	1.56	2 (14%)

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
4	FTR	H	77	4	-	0/4/6/8	0/2/2/2
4	FTR	H	76	4	-	1/4/6/8	0/2/2/2
4	FTR	D	76	4	-	1/4/6/8	0/2/2/2
4	FTR	D	77	4	-	0/4/6/8	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	76	FTR	CZ2-CE2	-4.64	1.33	1.41
4	D	76	FTR	CZ2-CE2	-4.59	1.33	1.41
4	D	77	FTR	CZ2-CE2	-4.57	1.33	1.41
4	H	77	FTR	CZ2-CE2	-4.51	1.34	1.41
4	D	76	FTR	CE3-CD2	-4.29	1.33	1.42
4	H	77	FTR	CE3-CD2	-4.28	1.33	1.42
4	H	76	FTR	CE3-CD2	-4.27	1.33	1.42
4	D	77	FTR	CE3-CD2	-4.20	1.33	1.42
4	D	77	FTR	CB-CA	-3.67	1.45	1.53
4	H	77	FTR	CB-CA	-3.64	1.45	1.53
4	D	76	FTR	CB-CA	-3.57	1.46	1.53
4	H	76	FTR	CB-CA	-3.33	1.46	1.53
4	H	77	FTR	CD2-CE2	-3.18	1.34	1.42
4	D	76	FTR	CD2-CE2	-3.16	1.34	1.42
4	D	77	FTR	CD2-CE2	-3.16	1.34	1.42
4	H	76	FTR	CD2-CE2	-3.12	1.34	1.42
4	D	76	FTR	CA-N	-2.41	1.40	1.48
4	H	76	FTR	CA-N	-2.39	1.40	1.48
4	H	77	FTR	CA-N	-2.37	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	77	FTR	CA-N	-2.34	1.41	1.48
4	H	76	FTR	CE3-CZ3	2.03	1.39	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	77	FTR	CH2-CZ3-CE3	-4.03	118.78	123.23
4	H	77	FTR	CH2-CZ3-CE3	-3.89	118.94	123.23
4	D	76	FTR	CH2-CZ3-CE3	-3.88	118.95	123.23
4	H	76	FTR	CH2-CZ3-CE3	-3.75	119.09	123.23
4	H	76	FTR	CB-CG-CD1	-2.77	124.54	127.97
4	D	76	FTR	CE3-CD2-CE2	2.30	121.41	118.26
4	H	77	FTR	CE3-CD2-CE2	2.26	121.35	118.26
4	D	77	FTR	CE3-CD2-CE2	2.24	121.31	118.26
4	H	76	FTR	CE3-CD2-CE2	2.16	121.21	118.26

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	76	FTR	O-C-CA-CB
4	H	76	FTR	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	BEZ	E	803	5	9,9,9	1.73	1 (11%)	11,11,11	0.83	0
7	EDO	B	402	-	3,3,3	0.45	0	2,2,2	0.26	0
7	EDO	G	201	-	3,3,3	0.47	0	2,2,2	0.30	0
7	EDO	A	804	-	3,3,3	0.50	0	2,2,2	0.20	0
7	EDO	E	804[A]	-	3,3,3	0.45	0	2,2,2	0.35	0
7	EDO	A	805	-	3,3,3	0.45	0	2,2,2	0.26	0
7	EDO	E	805	-	3,3,3	0.45	0	2,2,2	0.29	0
7	EDO	B	401	-	3,3,3	0.45	0	2,2,2	0.39	0
7	EDO	B	403	-	3,3,3	0.46	0	2,2,2	0.31	0
7	EDO	F	401	-	3,3,3	0.46	0	2,2,2	0.33	0
7	EDO	H	201	-	3,3,3	0.44	0	2,2,2	0.37	0
7	EDO	E	804[B]	-	3,3,3	0.46	0	2,2,2	0.34	0
6	BEZ	A	803	5	9,9,9	1.70	1 (11%)	11,11,11	0.92	1 (9%)
7	EDO	C	201	-	3,3,3	0.45	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
6	BEZ	E	803	5	-	0/4/4/4	0/1/1/1
7	EDO	B	402	-	-	0/1/1/1	-
7	EDO	G	201	-	-	0/1/1/1	-
7	EDO	A	804	-	-	1/1/1/1	-
7	EDO	E	804[A]	-	-	0/1/1/1	-
7	EDO	A	805	-	-	0/1/1/1	-
7	EDO	E	805	-	-	1/1/1/1	-
7	EDO	B	401	-	-	0/1/1/1	-
7	EDO	B	403	-	-	0/1/1/1	-
7	EDO	F	401	-	-	0/1/1/1	-
7	EDO	H	201	-	-	0/1/1/1	-
7	EDO	E	804[B]	-	-	0/1/1/1	-
6	BEZ	A	803	5	-	0/4/4/4	0/1/1/1
7	EDO	C	201	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	803	BEZ	C1-C	-4.72	1.39	1.49
6	A	803	BEZ	C1-C	-4.66	1.39	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	803	BEZ	O2-C-C1	2.12	120.36	114.85

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	805	EDO	O1-C1-C2-O2
7	A	804	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	804[A]	EDO	1	0
7	A	805	EDO	1	0
7	E	805	EDO	3	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^{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%)	-0.23	3 (0%)	89	91	19, 26, 42, 71	0
1	E	515/515 (100%)	-0.25	2 (0%)	92	93	19, 28, 44, 87	0
2	B	392/392 (100%)	-0.27	3 (0%)	86	87	20, 27, 41, 68	0
2	F	392/392 (100%)	-0.27	1 (0%)	94	94	20, 28, 41, 72	0
3	C	168/168 (100%)	-0.17	1 (0%)	89	91	25, 33, 45, 56	0
3	G	168/168 (100%)	-0.20	3 (1%)	68	71	25, 34, 46, 61	0
4	D	130/137 (94%)	-0.08	3 (2%)	60	64	26, 36, 53, 86	0
4	H	130/137 (94%)	0.11	1 (0%)	86	87	28, 40, 67, 110	0
All	All	2410/2424 (99%)	-0.21	17 (0%)	87	89	19, 29, 47, 110	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	2	SER	6.2
4	D	134	ALA	5.6
3	C	169	ALA	2.9
4	D	133	ARG	2.9
1	E	55	GLU	2.7
1	A	262	ALA	2.6
2	F	395	ASN	2.5
2	B	225	PRO	2.2
4	D	3	SER	2.2
2	B	395	ASN	2.2
1	A	53	ALA	2.2
2	B	347	LYS	2.1
3	G	110	ARG	2.1
1	E	12	ASP	2.1
1	A	261	PRO	2.1
3	G	103	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	G	96	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
4	FTR	H	76	15/16	0.90	0.13	32,36,39,40	0
4	FTR	H	77	15/16	0.90	0.11	28,30,32,34	0
4	FTR	D	76	15/16	0.92	0.10	29,34,42,42	0
4	FTR	D	77	15/16	0.93	0.11	26,28,30,30	0

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
7	EDO	A	804	4/4	0.73	0.24	31,32,33,34	0
7	EDO	E	805	4/4	0.75	0.20	42,43,45,46	0
7	EDO	E	804[B]	4/4	0.79	0.24	34,35,35,36	4
7	EDO	E	804[A]	4/4	0.79	0.24	34,35,35,36	4
7	EDO	A	805	4/4	0.82	0.21	49,51,51,53	0
8	NA	E	806	1/1	0.82	0.10	63,63,63,63	0
7	EDO	H	201	4/4	0.84	0.17	49,49,49,50	0
7	EDO	F	401	4/4	0.84	0.18	37,37,38,38	0
7	EDO	B	402	4/4	0.86	0.24	37,39,42,44	0
6	BEZ	A	803	9/9	0.94	0.10	26,27,29,29	0
7	EDO	B	403	4/4	0.94	0.17	40,41,41,42	0
6	BEZ	E	803	9/9	0.95	0.11	27,28,29,29	0
7	EDO	B	401	4/4	0.95	0.17	34,34,35,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	C	201	4/4	0.96	0.16	31,32,32,33	0
7	EDO	G	201	4/4	0.97	0.09	31,31,32,32	0
5	FE	E	802	1/1	0.99	0.06	28,28,28,28	0
5	FE	A	801	1/1	0.99	0.10	25,25,25,25	0
5	FE	A	802	1/1	0.99	0.07	25,25,25,25	0
5	FE	E	801	1/1	0.99	0.09	26,26,26,26	0

6.5 Other polymers

There are no such residues in this entry.