



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 20, 2021 – 02:26 PM EDT

PDB ID : 7M8R
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 : 2.22 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 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	:	2.22
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)	:	2.22

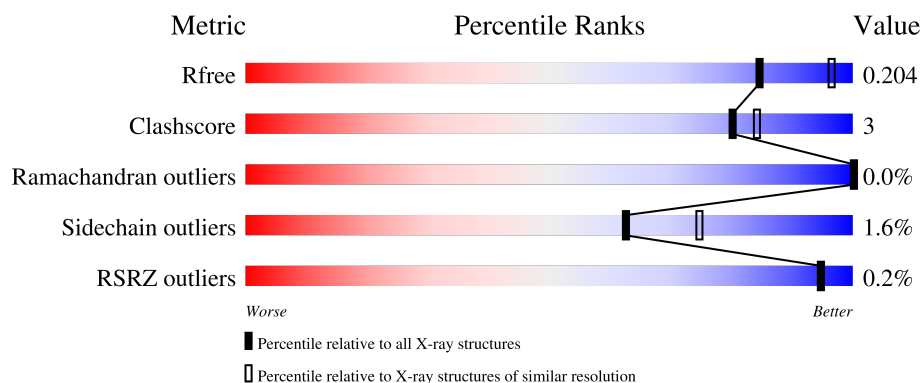
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





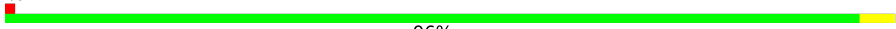
The reported resolution of this entry is 2.22 Å.

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.



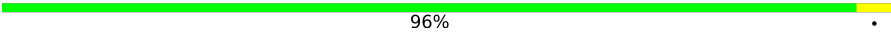


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	515	 91% 9%
1	E	515	 90% 10%
2	B	392	 94% 6%
2	F	392	 93% 6%
3	C	168	 96%

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Mol	Chain	Length	Quality of chain
3	G	168	 96% .
4	D	136	 85% 10% . .
4	H	136	 4% 93% 6% .

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	608	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21512 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	2682	725	765	12			
1	E	515	Total	C	N	O	S	0	7	0
			4235	2709	734	779	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	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	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	130	Total	C	F	N	O	S	0	0	0
			989	630	2	159	194	4			
4	H	136	Total	C	F	N	O	S	0	0	0
			1031	656	2	165	204	4			

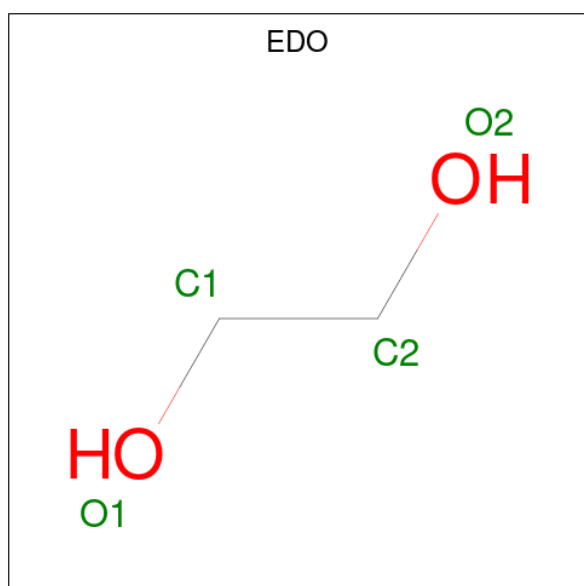
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	15	CYS	LYS	engineered mutation	UNP A0A2D2D0T8
H	15	CYS	LYS	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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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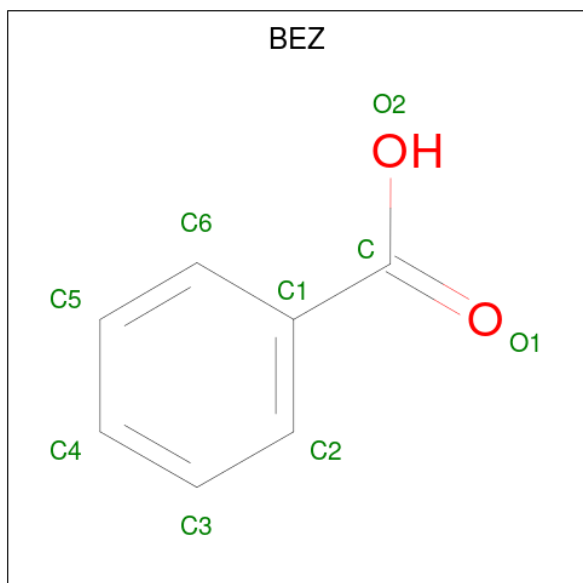
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0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

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

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



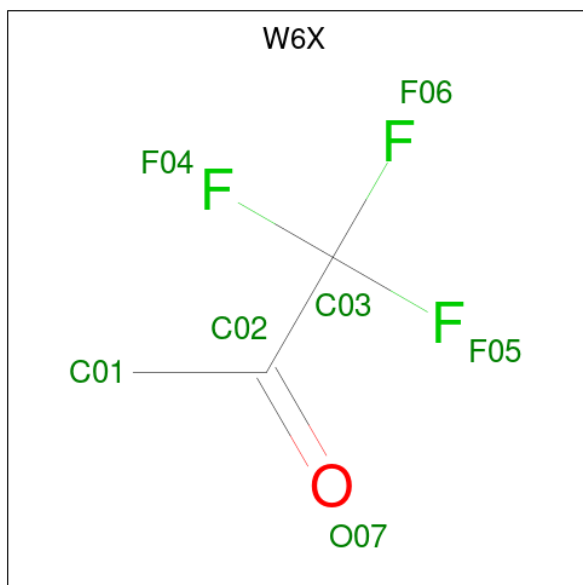
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			9	7	2		

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

- Molecule 8 is 1,1,1-tris(fluoranyl)propan-2-one (three-letter code: W6X) (formula: $C_3H_3F_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	F	O	0	0
			7	3	3	1		
8	H	1	Total	C	F	O	0	0
			7	3	3	1		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Cl	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	372	Total	O	0	0
			372	372		
10	B	313	Total	O	0	2
			315	315		

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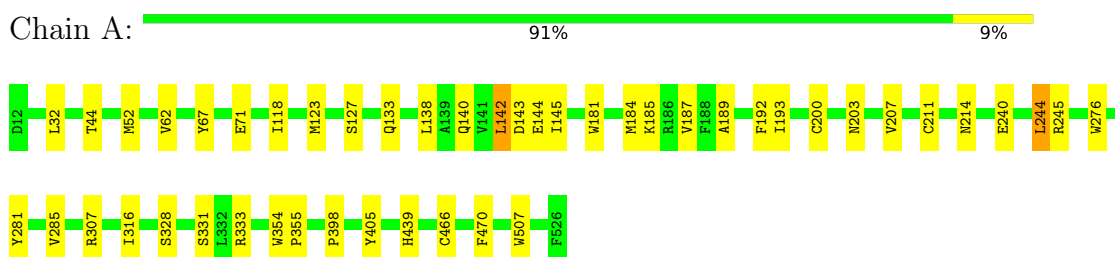
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	161	Total 162	O 162	0	1
10	D	43	Total 43	O 43	0	0
10	E	340	Total 341	O 341	0	3
10	F	336	Total 336	O 336	0	0
10	G	148	Total 148	O 148	0	0
10	H	51	Total 51	O 51	0	0

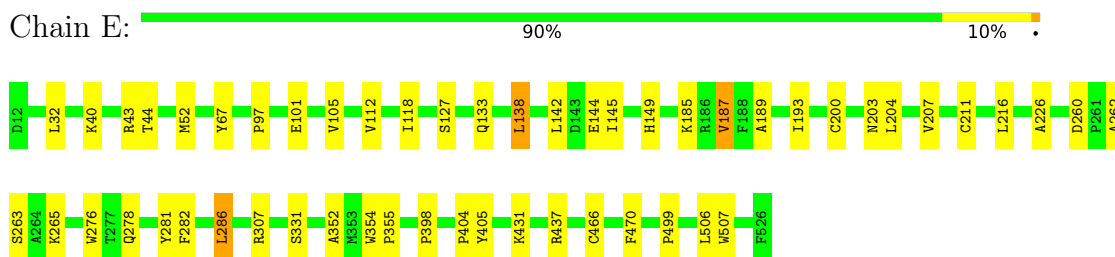
3 Residue-property plots

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.

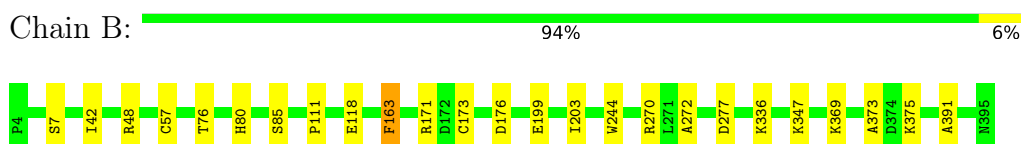
- Molecule 1: Methane monooxygenase component A alpha chain



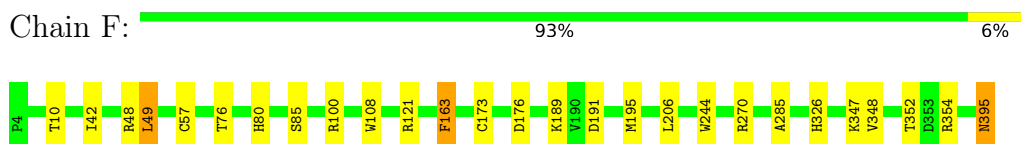
- Molecule 1: Methane monooxygenase component A alpha chain



- Molecule 2: Methane monooxygenase beta chain



- Molecule 2: Methane monooxygenase beta chain



- Molecule 3: Methane monooxygenase gamma chain

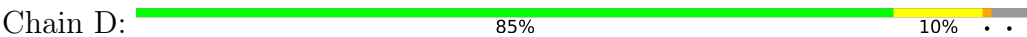




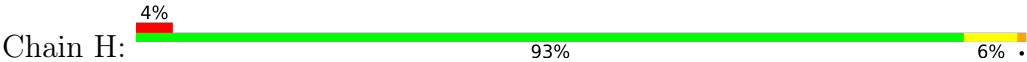
• Molecule 3: Methane monooxygenase gamma chain



• Molecule 4: Methane monooxygenase regulatory protein B



• Molecule 4: Methane monooxygenase regulatory protein B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.39Å 105.47Å 298.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.10 – 2.22 149.09 – 2.22	Depositor EDS
% Data completeness (in resolution range)	98.7 (86.10-2.22) 98.8 (149.09-2.22)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.157 , 0.202 0.164 , 0.204	Depositor DCC
R_{free} test set	7789 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21512	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, FTR, W6X, 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	0.28	0/4314	0.50	0/5861
1	E	0.28	0/4365	0.50	0/5930
2	B	0.28	0/3283	0.51	0/4464
2	F	0.28	0/3286	0.51	0/4468
3	C	0.26	0/1388	0.50	0/1877
3	G	0.27	0/1397	0.50	0/1888
4	D	0.27	0/970	0.47	0/1308
4	H	0.27	0/1012	0.46	0/1366
All	All	0.28	0/20015	0.50	0/27162

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	4184	0	3984	34	0
1	E	4235	0	4017	30	0
2	B	3190	0	3019	18	0
2	F	3193	0	3030	19	0
3	C	1362	0	1400	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1371	0	1412	3	0
4	D	989	0	972	10	0
4	H	1031	0	1015	4	0
5	A	2	0	0	0	0
5	E	2	0	0	0	0
6	A	40	0	60	3	0
6	B	20	0	30	1	0
6	C	8	0	12	0	0
6	D	4	0	6	0	0
6	E	28	0	42	3	0
6	F	36	0	54	2	0
6	G	12	0	18	0	0
6	H	4	0	6	0	0
7	A	9	0	5	0	0
7	E	9	0	5	0	0
8	D	7	0	0	0	0
8	H	7	0	0	0	0
9	D	1	0	0	0	0
10	A	372	0	0	3	0
10	B	315	0	0	1	0
10	C	162	0	0	1	0
10	D	43	0	0	0	0
10	E	341	0	0	3	0
10	F	336	0	0	1	0
10	G	148	0	0	0	0
10	H	51	0	0	0	0
All	All	21512	0	19087	104	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 (104) 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:H:136:THR:HG23	4:H:138:ILE:H	1.54	0.70
1:A:192:PHE:O	10:A:701:HOH:O	2.08	0.70
2:F:100:ARG:NH1	10:F:501:HOH:O	2.27	0.67
3:G:163:LYS:HE3	3:G:165:LEU:HD21	1.77	0.66
1:A:133:GLN:NE2	10:A:703:HOH:O	2.29	0.64
1:E:431:LYS:NZ	10:E:706:HOH:O	2.31	0.63
1:A:466:CYS:HB2	2:B:76:THR:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:VAL:HG12	1:E:278:GLN:HA	1.81	0.61
1:E:187:VAL:HG11	1:E:281:TYR:HB3	1.83	0.60
1:E:187:VAL:CG1	1:E:281:TYR:HB3	2.31	0.60
2:B:111:PRO:HB3	6:B:403:EDO:H11	1.88	0.55
1:A:181:TRP:NE1	1:A:185:LYS:HD2	2.22	0.55
1:A:138:LEU:HD22	2:B:163:PHE:CE1	2.43	0.54
4:D:93:GLU:HB3	2:F:48:ARG:HG3	1.90	0.54
4:D:114:ARG:HD3	4:D:128:LEU:HD23	1.89	0.54
1:E:282:PHE:CE2	1:E:286:LEU:HD22	2.42	0.53
1:E:118:ILE:HD13	1:E:145:ILE:HG12	1.89	0.53
2:B:369:LYS:HA	2:B:373:ALA:HB3	1.91	0.52
2:F:285:ALA:HB2	6:F:401:EDO:H12	1.93	0.51
1:A:71:GLU:OE2	6:A:612:EDO:H11	2.11	0.50
1:A:333:ARG:NH1	4:D:30:GLN:HG3	2.26	0.50
6:E:608:EDO:H21	10:E:778:HOH:O	2.10	0.50
2:F:80:HIS:CD2	3:G:141:MET:HG2	2.47	0.50
2:B:42:ILE:HD13	2:B:57:CYS:HB2	1.94	0.49
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.47	0.49
1:A:185:LYS:O	1:A:189:ALA:HB3	2.12	0.49
1:A:67:TYR:OH	1:A:142:LEU:HB3	2.13	0.49
1:A:316:ILE:O	4:D:114:ARG:NH2	2.41	0.49
1:A:44:THR:HB	1:A:127:SER:HA	1.94	0.48
3:C:116:ARG:O	3:C:120:LYS:HB2	2.12	0.48
2:F:42:ILE:HD13	2:F:57:CYS:HB2	1.95	0.48
3:G:116:ARG:O	3:G:120:LYS:HB2	2.14	0.48
4:H:41:VAL:HG12	4:H:109:SER:HB2	1.96	0.48
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.95	0.47
4:D:41:VAL:HG12	4:D:109:SER:HB2	1.96	0.47
1:E:193:ILE:HD11	2:F:85:SER:HB3	1.95	0.47
1:E:207:VAL:O	1:E:211:CYS:HB3	2.14	0.47
1:E:118:ILE:HG12	1:E:144:GLU:HB2	1.95	0.47
1:A:244:LEU:HD23	1:A:245:ARG:H	1.79	0.47
6:E:607:EDO:O1	10:E:701:HOH:O	2.20	0.47
1:A:200:CYS:HA	1:A:203:ASN:OD1	2.15	0.46
1:E:138:LEU:HG	2:F:163:PHE:HE1	1.80	0.46
1:A:62:VAL:HG11	1:A:245:ARG:HH12	1.79	0.46
2:F:191:ASP:O	2:F:195:MET:HG2	2.16	0.46
1:E:185:LYS:O	1:E:189:ALA:HB3	2.16	0.46
2:B:347:LYS:HA	2:B:347:LYS:HD3	1.74	0.46
1:A:214:ASN:OD1	4:D:110:SER:OG	2.21	0.46
1:E:354:TRP:CH2	1:E:499:PRO:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:HIS:CD2	3:C:141:MET:HG2	2.51	0.45
2:F:354:ARG:HD2	2:F:395:ASN:OD1	2.15	0.45
1:A:244:LEU:HD23	1:A:245:ARG:N	2.31	0.45
1:A:398:PRO:HA	1:A:507:TRP:CE2	2.51	0.45
1:E:354:TRP:CG	1:E:355:PRO:HD3	2.52	0.45
1:E:216:LEU:HD13	1:E:286:LEU:HD11	1.97	0.45
2:F:326:HIS:CD2	6:F:407:EDO:H22	2.51	0.45
1:E:466:CYS:HB2	2:F:76:THR:HA	1.99	0.45
2:B:272:ALA:HB1	2:B:277:ASP:HB3	1.98	0.45
1:A:207:VAL:O	1:A:211:CYS:HB3	2.17	0.44
1:E:203:ASN:OD1	1:E:204:LEU:N	2.50	0.44
2:F:189:LYS:HD3	2:F:189:LYS:HA	1.65	0.44
1:E:44:THR:HB	1:E:127:SER:HA	2.00	0.44
1:A:138:LEU:HD22	2:B:163:PHE:HE1	1.82	0.44
1:E:226:ALA:HB2	2:F:10:THR:HG21	1.99	0.44
4:H:69:VAL:HG22	4:H:78:ILE:HG12	1.99	0.44
1:E:200:CYS:HA	1:E:203:ASN:OD1	2.17	0.44
2:B:173:CYS:HA	2:B:244:TRP:CE2	2.53	0.43
2:F:348:VAL:H	2:F:352:THR:HG1	1.60	0.43
2:B:118:GLU:OE2	2:F:121:ARG:HD3	2.17	0.43
1:A:123:MET:HG3	2:B:171:ARG:HD3	2.01	0.43
10:A:908:HOH:O	4:D:12:ILE:HG22	2.18	0.43
1:E:276:TRP:CE3	1:E:331:SER:HB2	2.53	0.43
1:E:262:ALA:O	1:E:265:LYS:NZ	2.42	0.43
1:A:328:SER:HB2	4:D:32:VAL:HG22	2.01	0.43
1:E:97:PRO:O	1:E:101:GLU:HG2	2.18	0.43
1:A:184:MET:HA	1:A:187:VAL:HG12	2.00	0.42
1:E:260:ASP:HB3	1:E:263:SER:OG	2.20	0.42
1:E:352:ALA:HA	1:E:404:PRO:HB2	2.01	0.42
1:A:62:VAL:HG11	1:A:245:ARG:NH1	2.35	0.42
1:A:405:TYR:HH	1:A:470:PHE:HE1	1.64	0.42
2:F:49:LEU:HD23	2:F:49:LEU:HA	1.90	0.42
1:E:405:TYR:HH	1:E:470:PHE:HE1	1.65	0.42
1:E:40:LYS:HE3	1:E:43:ARG:HH12	1.84	0.42
2:B:7:SER:HA	4:D:9:ASN:ND2	2.34	0.42
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.55	0.42
1:A:143:ASP:OD2	6:A:612:EDO:O2	2.35	0.41
1:E:67:TYR:OH	1:E:142:LEU:HB3	2.20	0.41
1:A:245:ARG:NH1	6:A:612:EDO:O1	2.52	0.41
1:A:439:HIS:HB3	3:C:162:VAL:HB	2.02	0.41
1:A:140:GLN:O	1:A:144:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:173:CYS:HA	2:F:244:TRP:CE2	2.55	0.41
2:B:336:LYS:HE3	2:B:391:ALA:HB3	2.03	0.41
1:E:187:VAL:HG13	1:E:281:TYR:HB3	2.02	0.41
1:A:193:ILE:HD11	2:B:85:SER:HB3	2.02	0.41
1:A:276:TRP:CE3	1:A:331:SER:HB2	2.55	0.41
1:E:149:HIS:CE1	2:F:108:TRP:HB2	2.56	0.41
1:E:398:PRO:HA	1:E:507:TRP:CE2	2.55	0.41
2:F:347:LYS:HA	2:F:347:LYS:HD3	1.81	0.41
1:A:240:GLU:HG3	4:D:109:SER:O	2.21	0.41
2:B:48:ARG:HG3	4:H:93:GLU:HB3	2.04	0.40
2:B:375:LYS:NZ	10:B:517:HOH:O	2.55	0.40
3:C:142:GLU:OE1	10:C:301:HOH:O	2.22	0.40
2:B:199:GLU:O	2:B:203:ILE:HG13	2.22	0.40
3:C:41:THR:HG22	3:C:54:TYR:CE1	2.55	0.40
6:E:608:EDO:H22	6:E:610:EDO:O1	2.22	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	514/515 (100%)	494 (96%)	20 (4%)	0	100	100
1	E	520/515 (101%)	506 (97%)	14 (3%)	0	100	100
2	B	391/392 (100%)	380 (97%)	11 (3%)	0	100	100
2	F	391/392 (100%)	383 (98%)	8 (2%)	0	100	100
3	C	166/168 (99%)	163 (98%)	3 (2%)	0	100	100
3	G	167/168 (99%)	165 (99%)	2 (1%)	0	100	100
4	D	126/136 (93%)	122 (97%)	3 (2%)	1 (1%)	19	18
4	H	132/136 (97%)	127 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2407/2422 (99%)	2340 (97%)	66 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	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%)	422 (99%)	5 (1%)	71	82
1	E	433/426 (102%)	422 (98%)	11 (2%)	47	58
2	B	324/324 (100%)	321 (99%)	3 (1%)	78	87
2	F	325/324 (100%)	319 (98%)	6 (2%)	59	71
3	C	145/145 (100%)	145 (100%)	0	100	100
3	G	146/145 (101%)	145 (99%)	1 (1%)	84	91
4	D	101/106 (95%)	99 (98%)	2 (2%)	55	67
4	H	106/106 (100%)	103 (97%)	3 (3%)	43	54
All	All	2007/2002 (100%)	1976 (98%)	31 (2%)	62	76

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

Mol	Chain	Res	Type
1	A	32	LEU
1	A	52	MET
1	A	142	LEU
1	A	244	LEU
1	A	307	ARG
2	B	163	PHE
2	B	176	ASP
2	B	270	ARG
4	D	114	ARG

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Mol	Chain	Res	Type
4	D	129	MET
1	E	32	LEU
1	E	52	MET
1	E	105	VAL
1	E	112	VAL
1	E	133	GLN
1	E	138	LEU
1	E	187	VAL
1	E	286	LEU
1	E	307	ARG
1	E	437	ARG
1	E	506	LEU
2	F	49	LEU
2	F	163	PHE
2	F	176	ASP
2	F	206	LEU
2	F	270	ARG
2	F	395	ASN
3	G	158	LYS
4	H	57	LEU
4	H	136	THR
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
1	A	505	ASN
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 ⓘ

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	D	77	4	14,16,17	1.48	3 (21%)	14,22,24	1.16	1 (7%)
4	FTR	H	76	4	14,16,17	1.50	3 (21%)	14,22,24	1.30	3 (21%)
4	FTR	H	77	4	14,16,17	1.48	3 (21%)	14,22,24	1.27	3 (21%)
4	FTR	D	76	4	14,16,17	1.48	3 (21%)	14,22,24	1.10	1 (7%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	77	FTR	CH2-CZ3	2.74	1.42	1.37
4	H	76	FTR	CH2-CZ3	2.74	1.42	1.37
4	D	76	FTR	CE3-CZ3	2.68	1.40	1.36
4	D	77	FTR	CH2-CZ3	2.62	1.42	1.37
4	D	77	FTR	CE3-CZ3	2.60	1.40	1.36
4	D	76	FTR	CH2-CZ3	2.53	1.42	1.37
4	H	77	FTR	CE3-CZ3	2.52	1.40	1.36
4	H	76	FTR	CE3-CZ3	2.45	1.40	1.36
4	H	76	FTR	CD1-NE1	2.25	1.41	1.36
4	D	77	FTR	CD1-NE1	2.13	1.41	1.36
4	H	77	FTR	CD1-NE1	2.12	1.41	1.36
4	D	76	FTR	CD1-NE1	2.09	1.40	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	76	FTR	CB-CA-C	-2.27	107.20	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	77	FTR	CH2-CZ2-CE2	-2.26	118.00	120.84
4	H	76	FTR	CH2-CZ2-CE2	-2.20	118.07	120.84
4	H	77	FTR	CG-CB-CA	2.13	117.83	114.53
4	H	76	FTR	CZ2-CH2-CZ3	2.11	121.15	118.74
4	D	76	FTR	CH2-CZ2-CE2	-2.11	118.18	120.84
4	H	77	FTR	CZ2-CH2-CZ3	2.04	121.08	118.74
4	D	77	FTR	CH2-CZ2-CE2	-2.04	118.27	120.84

There are no chirality outliers.

There are no torsion outliers.

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 47 ligands modelled in this entry, 5 are monoatomic - leaving 42 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	BEZ	E	606	5	7,9,9	1.32	1 (14%)	8,11,11	0.50	0
6	EDO	E	608	-	3,3,3	0.47	0	2,2,2	0.26	0
6	EDO	F	409	-	3,3,3	0.47	0	2,2,2	0.28	0
6	EDO	G	201	-	3,3,3	0.50	0	2,2,2	0.34	0
6	EDO	B	403	-	3,3,3	0.47	0	2,2,2	0.34	0
6	EDO	E	607	-	3,3,3	0.51	0	2,2,2	0.21	0
6	EDO	B	402	-	3,3,3	0.46	0	2,2,2	0.38	0
8	W6X	H	202	4	6,6,6	0.58	0	8,9,9	0.73	1 (12%)
6	EDO	G	202	-	3,3,3	0.44	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	W6X	D	202	4	6,6,6	0.60	0	8,9,9	0.77	1 (12%)
6	EDO	A	604	-	3,3,3	0.43	0	2,2,2	0.40	0
6	EDO	A	612	-	3,3,3	0.44	0	2,2,2	0.39	0
6	EDO	E	610	-	3,3,3	0.43	0	2,2,2	0.25	0
6	EDO	F	404	-	3,3,3	0.42	0	2,2,2	0.54	0
6	EDO	E	605	-	3,3,3	0.49	0	2,2,2	0.23	0
6	EDO	F	405	-	3,3,3	0.45	0	2,2,2	0.33	0
6	EDO	C	201	-	3,3,3	0.43	0	2,2,2	0.35	0
6	EDO	A	609	-	3,3,3	0.45	0	2,2,2	0.39	0
6	EDO	B	401	-	3,3,3	0.46	0	2,2,2	0.39	0
6	EDO	F	403	-	3,3,3	0.43	0	2,2,2	0.50	0
6	EDO	H	201	-	3,3,3	0.49	0	2,2,2	0.26	0
6	EDO	E	604	-	3,3,3	0.49	0	2,2,2	0.42	0
6	EDO	A	610	-	3,3,3	0.44	0	2,2,2	0.36	0
6	EDO	A	613	-	3,3,3	0.49	0	2,2,2	0.25	0
6	EDO	B	404	-	3,3,3	0.48	0	2,2,2	0.30	0
6	EDO	F	401	-	3,3,3	0.47	0	2,2,2	0.30	0
6	EDO	G	203	-	3,3,3	0.40	0	2,2,2	0.43	0
6	EDO	F	407	-	3,3,3	0.45	0	2,2,2	0.27	0
6	EDO	A	605	-	3,3,3	0.44	0	2,2,2	0.44	0
6	EDO	F	408	-	3,3,3	0.42	0	2,2,2	0.39	0
6	EDO	C	202	-	3,3,3	0.46	0	2,2,2	0.33	0
6	EDO	E	603	-	3,3,3	0.44	0	2,2,2	0.34	0
6	EDO	F	402	-	3,3,3	0.49	0	2,2,2	0.27	0
6	EDO	B	405	-	3,3,3	0.47	0	2,2,2	0.32	0
6	EDO	D	201	-	3,3,3	0.47	0	2,2,2	0.25	0
7	BEZ	A	607	5	7,9,9	1.28	1 (14%)	8,11,11	0.54	0
6	EDO	A	603	-	3,3,3	0.44	0	2,2,2	0.37	0
6	EDO	E	609	-	3,3,3	0.48	0	2,2,2	0.32	0
6	EDO	A	611	-	3,3,3	0.45	0	2,2,2	0.35	0
6	EDO	A	606	-	3,3,3	0.45	0	2,2,2	0.30	0
6	EDO	F	406	-	3,3,3	0.44	0	2,2,2	0.43	0
6	EDO	A	608	-	3,3,3	0.45	0	2,2,2	0.40	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	BEZ	E	606	5	-	0/0/4/4	0/1/1/1
6	EDO	E	608	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	F	409	-	-	0/1/1/1	-
6	EDO	G	201	-	-	0/1/1/1	-
6	EDO	B	403	-	-	0/1/1/1	-
6	EDO	E	607	-	-	0/1/1/1	-
6	EDO	B	402	-	-	0/1/1/1	-
8	W6X	H	202	4	-	0/6/6/6	-
6	EDO	G	202	-	-	0/1/1/1	-
8	W6X	D	202	4	-	0/6/6/6	-
6	EDO	A	604	-	-	0/1/1/1	-
6	EDO	A	612	-	-	1/1/1/1	-
6	EDO	E	610	-	-	0/1/1/1	-
6	EDO	F	404	-	-	0/1/1/1	-
6	EDO	E	605	-	-	1/1/1/1	-
6	EDO	F	405	-	-	0/1/1/1	-
6	EDO	C	201	-	-	0/1/1/1	-
6	EDO	A	609	-	-	0/1/1/1	-
6	EDO	B	401	-	-	1/1/1/1	-
6	EDO	F	403	-	-	1/1/1/1	-
6	EDO	H	201	-	-	0/1/1/1	-
6	EDO	E	604	-	-	1/1/1/1	-
6	EDO	A	610	-	-	0/1/1/1	-
6	EDO	A	613	-	-	0/1/1/1	-
6	EDO	B	404	-	-	0/1/1/1	-
6	EDO	F	401	-	-	0/1/1/1	-
6	EDO	G	203	-	-	0/1/1/1	-
6	EDO	F	407	-	-	1/1/1/1	-
6	EDO	A	605	-	-	0/1/1/1	-
6	EDO	F	408	-	-	0/1/1/1	-
6	EDO	C	202	-	-	0/1/1/1	-
6	EDO	E	603	-	-	0/1/1/1	-
6	EDO	F	402	-	-	1/1/1/1	-
6	EDO	B	405	-	-	0/1/1/1	-
6	EDO	D	201	-	-	0/1/1/1	-
7	BEZ	A	607	5	-	0/0/4/4	0/1/1/1
6	EDO	A	603	-	-	0/1/1/1	-
6	EDO	E	609	-	-	0/1/1/1	-
6	EDO	A	611	-	-	0/1/1/1	-
6	EDO	A	606	-	-	0/1/1/1	-
6	EDO	F	406	-	-	0/1/1/1	-
6	EDO	A	608	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	606	BEZ	C1-C	3.36	1.50	1.47
7	A	607	BEZ	C1-C	3.24	1.50	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	202	W6X	O07-C02-C03	2.15	121.79	116.37
8	H	202	W6X	O07-C02-C03	2.02	121.47	116.37

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	612	EDO	O1-C1-C2-O2
6	F	407	EDO	O1-C1-C2-O2
6	B	401	EDO	O1-C1-C2-O2
6	E	604	EDO	O1-C1-C2-O2
6	E	605	EDO	O1-C1-C2-O2
6	F	402	EDO	O1-C1-C2-O2
6	F	403	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	608	EDO	2	0
6	B	403	EDO	1	0
6	E	607	EDO	1	0
6	A	612	EDO	3	0
6	E	610	EDO	1	0
6	F	401	EDO	1	0
6	F	407	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	515/515 (100%)	-0.37	0	100	100	24, 34, 54, 88	0
1	E	515/515 (100%)	-0.39	0	100	100	25, 35, 53, 85	0
2	B	392/392 (100%)	-0.50	0	100	100	26, 34, 49, 80	1 (0%)
2	F	392/392 (100%)	-0.50	0	100	100	26, 34, 48, 78	1 (0%)
3	C	168/168 (100%)	-0.47	1 (0%)	89	88	29, 39, 52, 61	0
3	G	168/168 (100%)	-0.53	0	100	100	31, 39, 52, 62	0
4	D	128/136 (94%)	-0.25	0	100	100	37, 48, 61, 95	0
4	H	134/136 (98%)	-0.03	5 (3%)	41	39	37, 48, 69, 93	0
All	All	2412/2422 (99%)	-0.41	6 (0%)	95	95	24, 36, 56, 95	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	135	LEU	5.5
4	H	138	ILE	3.9
4	H	133	ARG	3.2
4	H	134	ALA	2.6
4	H	136	THR	2.4
3	C	2	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FTR	H	76	15/16	0.91	0.14	38,43,46,49	0
4	FTR	H	77	15/16	0.93	0.13	36,43,45,48	0
4	FTR	D	76	15/16	0.95	0.11	42,43,48,52	0
4	FTR	D	77	15/16	0.97	0.11	38,41,48,48	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	E	607	4/4	0.54	0.36	67,71,73,73	0
6	EDO	A	610	4/4	0.69	0.37	98,98,99,100	0
6	EDO	E	605	4/4	0.70	0.30	54,54,54,55	0
6	EDO	F	405	4/4	0.71	0.15	70,70,73,75	0
6	EDO	E	608	4/4	0.76	0.44	67,67,68,70	0
9	CL	D	203	1/1	0.82	0.15	94,94,94,94	0
8	W6X	D	202	7/7	0.83	0.16	72,79,88,88	0
6	EDO	F	402	4/4	0.83	0.28	67,68,68,69	0
6	EDO	H	201	4/4	0.86	0.26	64,65,67,68	0
6	EDO	B	405	4/4	0.86	0.17	71,71,73,73	0
8	W6X	H	202	7/7	0.86	0.11	69,79,84,84	0
6	EDO	E	609	4/4	0.86	0.12	60,62,63,63	0
6	EDO	F	403	4/4	0.87	0.31	70,71,71,71	0
6	EDO	A	611	4/4	0.87	0.21	54,59,62,63	0
6	EDO	A	609	4/4	0.88	0.43	57,58,58,62	0
6	EDO	F	409	4/4	0.88	0.14	66,66,67,68	0
6	EDO	C	202	4/4	0.88	0.16	68,68,69,70	0
6	EDO	A	608	4/4	0.89	0.20	68,69,71,73	0
6	EDO	F	406	4/4	0.89	0.23	68,70,71,73	0
6	EDO	B	404	4/4	0.89	0.15	50,52,52,55	0
6	EDO	G	202	4/4	0.89	0.17	72,72,72,72	0
6	EDO	A	612	4/4	0.90	0.17	44,48,53,53	0
6	EDO	E	604	4/4	0.90	0.17	45,46,46,46	0
6	EDO	A	613	4/4	0.91	0.17	53,57,62,64	0
6	EDO	F	407	4/4	0.91	0.15	60,61,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	E	610	4/4	0.92	0.22	42,45,50,53	0
6	EDO	F	408	4/4	0.92	0.11	61,61,62,62	0
6	EDO	F	401	4/4	0.93	0.14	53,53,55,56	0
6	EDO	E	603	4/4	0.94	0.21	63,63,63,63	0
6	EDO	B	401	4/4	0.94	0.13	45,47,49,53	0
6	EDO	A	606	4/4	0.94	0.15	55,56,57,58	0
6	EDO	D	201	4/4	0.94	0.21	62,64,66,69	0
6	EDO	B	403	4/4	0.95	0.16	75,75,76,76	0
6	EDO	G	203	4/4	0.95	0.19	61,62,63,63	0
6	EDO	A	604	4/4	0.95	0.17	49,50,52,55	0
6	EDO	G	201	4/4	0.96	0.13	33,36,38,38	0
6	EDO	B	402	4/4	0.97	0.16	37,38,40,41	0
6	EDO	C	201	4/4	0.97	0.18	36,38,38,39	0
7	BEZ	A	607	9/9	0.97	0.18	37,40,42,43	0
6	EDO	F	404	4/4	0.97	0.15	39,40,40,42	0
6	EDO	A	603	4/4	0.97	0.14	48,48,49,50	0
6	EDO	A	605	4/4	0.97	0.20	43,44,47,51	0
7	BEZ	E	606	9/9	0.98	0.15	39,40,43,44	0
5	FE	E	602	1/1	0.99	0.10	38,38,38,38	0
5	FE	A	602	1/1	0.99	0.12	38,38,38,38	0
5	FE	A	601	1/1	1.00	0.14	34,34,34,34	0
5	FE	E	601	1/1	1.00	0.13	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.