



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:09 PM UTC

PDB ID : 7S6R / pdb_00007s6r
Title : Complex structure of Methane monooxygenase hydroxylase and regulatory subunit with H5A mutation
Authors : Johns, J.C.; Banerjee, R.; Semonis, M.M.; Shi, K.; Aihara, H.; Lipscomb, J.D.
Deposited on : 2021-09-14
Resolution : 1.89 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

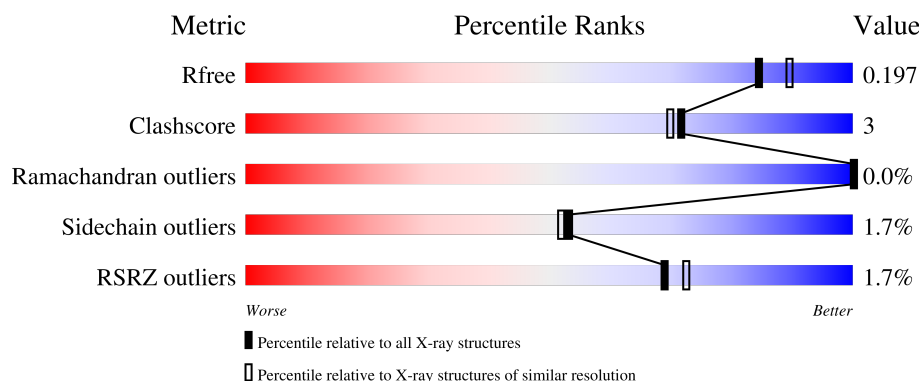
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	2% 91% 9%
1	E	515	3% 89% 10%
2	B	392	94% 5%
2	F	392	% 95% 5%
3	C	168	% 98% %

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Mol	Chain	Length	Quality of chain
3	G	168	% 89% 11%
4	D	132	3% 89% 10%
4	H	132	3% 89% 10%

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	A	612	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 22057 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	2	0
			3197	2038	558	596	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	168	Total	C	N	O	S	0	0	0
			1362	874	234	253	1			
3	G	168	Total	C	N	O	S	0	1	0
			1371	880	236	254	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	132	Total	C	N	O	S	0	0	0
			998	636	160	199	3			
4	H	132	Total	C	N	O	S	0	0	0
			997	636	160	198	3			

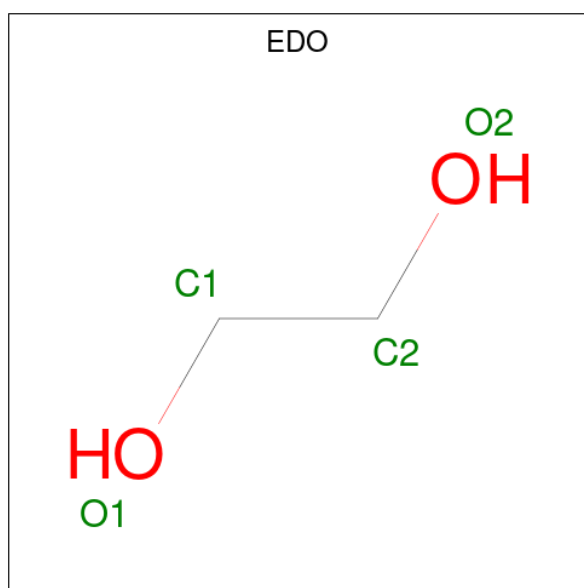
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	5	ALA	HIS	engineered mutation	UNP A0A2D2D0T8
H	5	ALA	HIS	engineered mutation	UNP A0A2D2D0T8

- Molecule 5 is FE (III) ION (CCD ID: 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 (CCD ID: 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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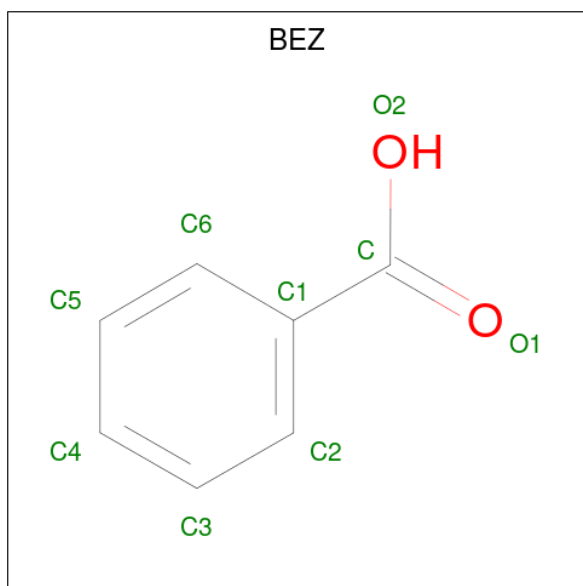
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	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	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	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 (CCD ID: BEZ) (formula: $C_7H_6O_2$).



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

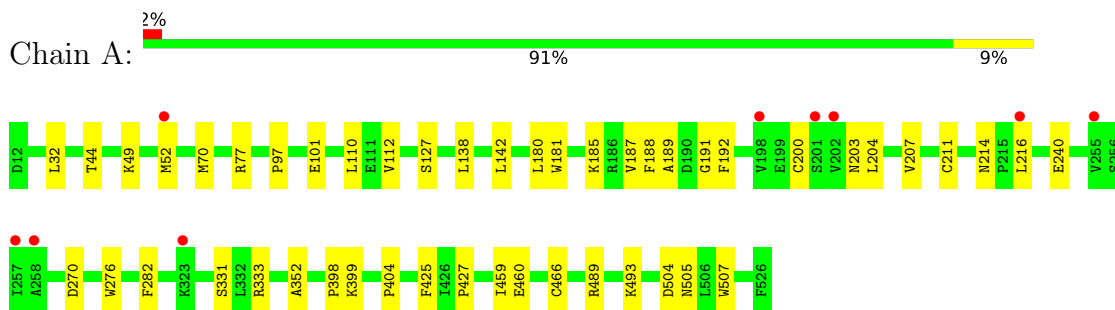
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	459	Total 459	O 459	0	0
8	B	435	Total 437	O 437	0	2
8	C	230	Total 231	O 231	0	1
8	D	72	Total 72	O 72	0	0
8	E	432	Total 434	O 434	0	2
8	F	434	Total 434	O 434	0	0
8	G	221	Total 221	O 221	0	0
8	H	73	Total 73	O 73	0	0

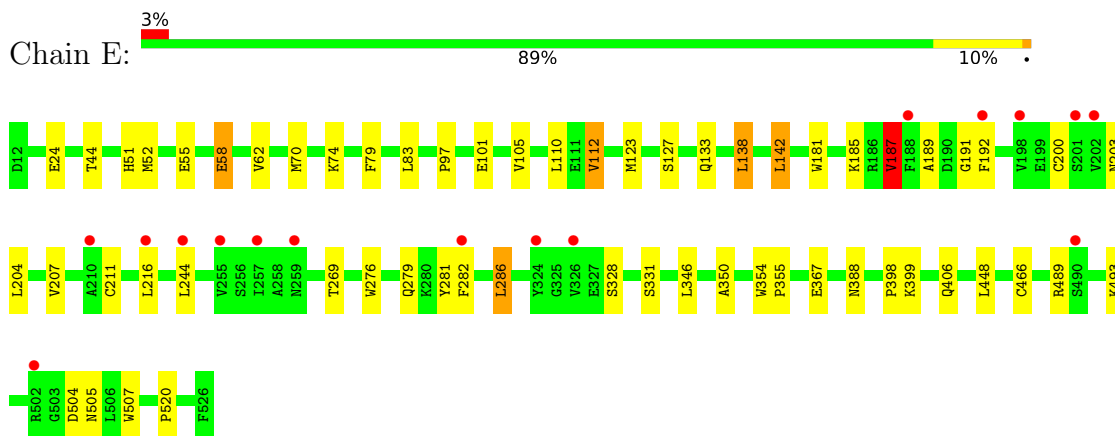
3 Residue-property plots [i](#)

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.

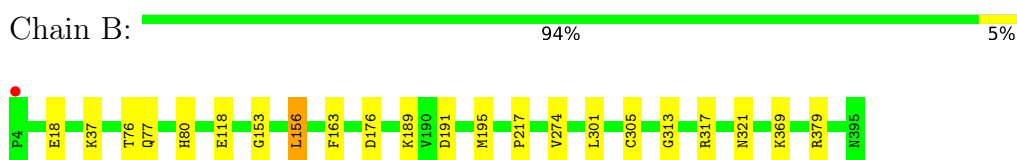
- Molecule 1: Methane monooxygenase component A alpha chain



- Molecule 1: Methane monooxygenase component A alpha chain



- Molecule 2: Methane monooxygenase beta chain



- Molecule 2: Methane monooxygenase beta chain

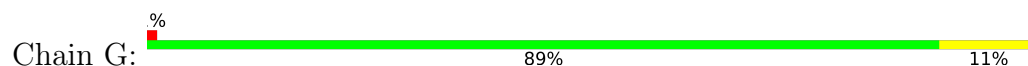




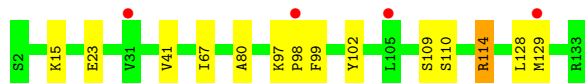
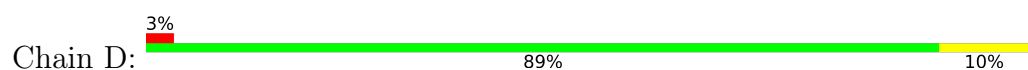
- Molecule 3: Methane monooxygenase gamma chain



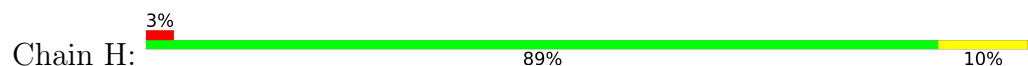
- Molecule 3: Methane monooxygenase gamma chain



- 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	102.66Å 105.91Å 299.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.71 – 1.89 73.71 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.0 (73.71-1.89) 99.9 (73.71-1.89)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.161 , 0.195 0.162 , 0.197	Depositor DCC
R_{free} test set	12941 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.044 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22057	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

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

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: EDO, FE, BEZ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/4314	0.64	0/5861
1	E	0.48	0/4365	0.63	1/5930 (0.0%)
2	B	0.49	0/3283	0.60	0/4464
2	F	0.49	0/3290	0.60	0/4476
3	C	0.48	0/1388	0.57	0/1877
3	G	0.46	0/1397	0.57	0/1888
4	D	0.40	0/1013	0.52	0/1368
4	H	0.38	0/1012	0.48	0/1368
All	All	0.48	0/20062	0.60	1/27232 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	187	VAL	CB-CA-C	-6.88	102.89	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	489	ARG	Sidechain
1	E	489	ARG	Sidechain

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	31	0
1	E	4235	0	4017	42	0
2	B	3190	0	3019	19	0
2	F	3197	0	3023	13	0
3	C	1362	0	1400	4	0
3	G	1371	0	1412	12	0
4	D	998	0	993	11	0
4	H	997	0	993	10	0
5	A	2	0	0	0	0
5	E	2	0	0	0	0
6	A	36	0	54	13	0
6	B	24	0	36	0	0
6	C	8	0	12	0	0
6	D	12	0	18	2	0
6	E	24	0	36	3	0
6	F	24	0	36	0	0
6	G	8	0	12	0	0
6	H	4	0	6	0	0
7	A	9	0	5	0	0
7	E	9	0	5	0	0
8	A	459	0	0	5	0
8	B	437	0	0	5	0
8	C	231	0	0	0	0
8	D	72	0	0	0	0
8	E	434	0	0	12	1
8	F	434	0	0	3	1
8	G	221	0	0	2	0
8	H	73	0	0	2	0
All	All	22057	0	19061	128	1

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

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:321[A]:ASN:ND2	8:F:501:HOH:O	2.02	0.92
6:A:608:EDO:H21	2:B:77:GLN:HE22	1.41	0.85
2:B:369:LYS:NZ	8:B:501:HOH:O	2.08	0.83
1:A:192:PHE:O	8:A:701:HOH:O	1.95	0.82
1:E:406:GLN:NE2	8:E:702:HOH:O	2.10	0.78
6:E:609:EDO:O2	8:E:701:HOH:O	2.01	0.78
3:G:81:LYS:NZ	8:G:301:HOH:O	2.24	0.69
2:B:18:GLU:OE1	8:B:502:HOH:O	2.11	0.68
1:E:216:LEU:HD13	1:E:286:LEU:HD11	1.75	0.68
2:B:321[A]:ASN:ND2	8:B:503:HOH:O	2.26	0.68
2:F:140[B]:ASP:OD2	8:F:502:HOH:O	2.13	0.66
1:E:24[B]:GLU:OE2	8:E:703:HOH:O	2.13	0.65
6:A:608:EDO:H21	2:B:77:GLN:NE2	2.10	0.64
6:A:612:EDO:H21	1:E:83:LEU:HD12	1.78	0.64
1:E:187:VAL:HG13	1:E:281:TYR:HB3	1.78	0.63
1:A:504:ASP:OD2	1:A:505:ASN:ND2	2.33	0.62
1:A:138:LEU:HD22	2:B:163:PHE:CE1	2.35	0.62
6:A:612:EDO:H12	8:E:806:HOH:O	2.00	0.62
4:D:114:ARG:HD3	4:D:128:LEU:HD23	1.83	0.61
1:E:388[A]:ASN:ND2	8:E:714:HOH:O	2.33	0.60
1:A:493[A]:LYS:NZ	8:A:706:HOH:O	2.34	0.60
2:F:80:HIS:CD2	3:G:141:MET:HG2	2.37	0.59
2:F:100:ARG:NH1	8:F:506:HOH:O	2.36	0.59
1:E:493:LYS:NZ	8:E:717:HOH:O	2.35	0.59
2:B:80:HIS:CD2	3:C:141:MET:HG2	2.39	0.57
1:A:333:ARG:HD2	6:A:610:EDO:H22	1.86	0.57
1:E:200:CYS:HA	1:E:203:ASN:OD1	2.06	0.55
1:A:185:LYS:O	1:A:189:ALA:HB3	2.06	0.55
1:E:70[B]:MET:HE2	4:H:102:TYR:HB3	1.88	0.54
1:E:367[A]:GLU:HG3	8:E:1032:HOH:O	2.07	0.54
1:E:520:PRO:HB3	6:E:605:EDO:H12	1.88	0.54
4:D:99:PHE:HE1	6:D:201:EDO:H11	1.73	0.53
1:E:185:LYS:O	1:E:189:ALA:HB3	2.07	0.53
1:A:44:THR:HB	1:A:127:SER:HA	1.91	0.52
1:A:77:ARG:HG2	6:A:612:EDO:H22	1.92	0.52
1:A:200:CYS:HA	1:A:203:ASN:OD1	2.10	0.51
2:B:118:GLU:HG2	2:F:118:GLU:HG2	1.92	0.51
4:H:54:ASP:HB2	4:H:94:LEU:HD21	1.91	0.51
2:B:37:LYS:NZ	8:B:508:HOH:O	2.45	0.50
1:E:133:GLN:NE2	8:E:721:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:504:ASP:OD2	1:E:505:ASN:ND2	2.44	0.50
3:C:56:TYR:OH	3:C:60:LYS:HD2	2.10	0.50
4:D:99:PHE:CE1	6:D:201:EDO:H11	2.46	0.50
6:A:612:EDO:H11	1:E:79:PHE:HB3	1.94	0.50
1:E:44:THR:HB	1:E:127:SER:HA	1.94	0.49
6:A:609:EDO:O2	8:A:702:HOH:O	2.20	0.49
6:A:609:EDO:H11	8:A:898:HOH:O	2.12	0.48
3:C:154:GLU:H	3:C:154:GLU:CD	2.22	0.48
1:E:191:GLY:O	8:E:704:HOH:O	2.19	0.48
1:E:138:LEU:HG	2:F:163:PHE:HE1	1.78	0.48
1:E:276:TRP:CE3	1:E:331:SER:HB2	2.48	0.48
2:F:79:PHE:HB2	2:F:83:ARG:HB3	1.94	0.48
4:D:97:LYS:HB2	4:D:98:PRO:HD2	1.96	0.48
4:H:3:SER:OG	8:H:301:HOH:O	2.20	0.48
2:B:80:HIS:CG	3:C:141:MET:HG2	2.48	0.48
1:E:282:PHE:CD2	1:E:286:LEU:HD13	2.49	0.48
1:E:350:ALA:HA	6:E:607:EDO:H21	1.96	0.48
1:A:214:ASN:OD1	4:D:110:SER:OG	2.29	0.47
1:A:240:GLU:HG3	4:D:109:SER:O	2.15	0.47
4:H:2:SER:N	8:H:307:HOH:O	2.48	0.47
2:F:313:GLY:O	2:F:317:ARG:HG3	2.15	0.47
1:E:138:LEU:HD22	1:E:142:LEU:HD22	1.97	0.47
1:E:269:THR:HG22	3:G:149:TYR:CE2	2.50	0.46
2:F:80:HIS:CG	3:G:141:MET:HG2	2.51	0.46
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.97	0.46
1:E:187:VAL:CG1	1:E:281:TYR:HB3	2.44	0.45
1:E:192:PHE:CE1	1:E:204:LEU:HA	2.52	0.45
1:A:49:LYS:NZ	1:A:270:ASP:OD2	2.49	0.45
1:A:398:PRO:HA	1:A:507:TRP:CE2	2.52	0.45
1:E:58:GLU:OE1	8:E:705:HOH:O	2.21	0.44
4:D:67:ILE:HG12	4:D:80:ALA:HB2	1.99	0.44
1:E:398:PRO:HA	1:E:507:TRP:CE2	2.52	0.44
3:G:163:LYS:HD2	3:G:165:LEU:HD21	1.99	0.44
3:G:166:HIS:HD2	8:G:446:HOH:O	1.99	0.44
4:D:41:VAL:HB	4:D:110:SER:HB3	2.00	0.44
1:E:207:VAL:O	1:E:211:CYS:HB3	2.17	0.44
2:B:189:LYS:HD3	2:B:189:LYS:HA	1.82	0.44
6:A:610:EDO:H11	8:A:962:HOH:O	2.18	0.43
6:A:612:EDO:H11	1:E:79:PHE:CB	2.48	0.43
1:E:110:LEU:HD13	1:E:216:LEU:HD21	2.01	0.43
1:E:216:LEU:HA	1:E:286:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HD13	1:A:216:LEU:HD21	2.00	0.43
1:A:425:PHE:CE2	1:A:427:PRO:HB3	2.54	0.43
1:A:192:PHE:CE1	1:A:204:LEU:HA	2.53	0.43
2:B:313:GLY:O	2:B:317:ARG:HG3	2.18	0.43
3:G:41:THR:HG22	3:G:54:TYR:CD1	2.54	0.43
2:F:347:LYS:HD3	2:F:347:LYS:HA	1.72	0.43
1:E:466:CYS:HB2	2:F:76:THR:HA	2.01	0.42
1:E:123:MET:HG3	2:F:171:ARG:HD3	2.01	0.42
2:B:379:ARG:NH2	8:B:518:HOH:O	2.52	0.42
4:D:129:MET:HE2	4:D:129:MET:HB2	1.99	0.42
3:G:116:ARG:O	3:G:120:LYS:HB2	2.19	0.42
2:B:153:GLY:C	2:B:217:PRO:HB3	2.45	0.42
1:E:97:PRO:O	1:E:101:GLU:HG2	2.20	0.42
1:E:74:LYS:HE2	4:H:106:ILE:HA	2.01	0.42
1:E:399:LYS:HD3	1:E:399:LYS:HA	1.81	0.42
1:A:459:ILE:HG22	1:A:460:GLU:HG3	2.01	0.42
4:H:39:VAL:HB	4:H:112:VAL:HB	2.02	0.42
1:A:97:PRO:O	1:A:101:GLU:HG2	2.20	0.42
1:A:70:MET:HG2	4:D:102:TYR:HB3	2.02	0.42
1:A:181:TRP:NE1	1:A:185:LYS:HD2	2.34	0.42
1:A:187:VAL:HG13	1:A:188:PHE:N	2.35	0.41
4:H:57:LEU:HD12	4:H:57:LEU:HA	1.83	0.41
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.82	0.41
3:G:37:ARG:CZ	3:G:120:LYS:HB3	2.49	0.41
3:G:105:LYS:HE3	3:G:106:TYR:CE2	2.55	0.41
1:E:70[A]:MET:HG2	4:H:102:TYR:HB3	2.01	0.41
1:E:55:GLU:OE1	8:E:706:HOH:O	2.22	0.41
1:A:207:VAL:O	1:A:211:CYS:HB3	2.21	0.41
1:E:354:TRP:CG	1:E:355:PRO:HD3	2.55	0.41
1:A:191:GLY:O	6:A:608:EDO:H11	2.20	0.41
1:A:276:TRP:CE3	1:A:331:SER:HB2	2.54	0.41
2:F:189:LYS:HA	2:F:189:LYS:HD3	1.69	0.41
3:G:121:PRO:HD3	3:G:129:PHE:CG	2.56	0.41
4:D:15:LYS:NZ	4:D:23:GLU:OE1	2.44	0.41
1:A:333:ARG:HD2	6:A:610:EDO:C2	2.52	0.40
1:A:466:CYS:HB2	2:B:76:THR:HA	2.02	0.40
1:A:138:LEU:HD22	2:B:163:PHE:HE1	1.80	0.40
1:A:282:PHE:CD1	1:A:282:PHE:C	2.99	0.40
2:B:156:LEU:C	2:B:156:LEU:HD12	2.46	0.40
1:A:70:MET:HB3	1:A:70:MET:HE2	1.77	0.40
2:B:301:LEU:O	2:B:305:CYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:SER:HB2	4:H:32:VAL:HG22	2.04	0.40
3:G:156:LEU:HD23	3:G:156:LEU:HA	1.91	0.40
2:B:191:ASP:O	2:B:195:MET:HG2	2.22	0.40
1:E:112:VAL:HG21	1:E:181:TRP:HH2	1.87	0.40
4:H:9:ASN:O	4:H:14:GLN:HG2	2.22	0.40
1:E:51:HIS:ND1	8:E:719:HOH:O	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:982:HOH:O	8:F:723:HOH:O[3_555]	2.18	0.02

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%)	495 (96%)	19 (4%)	0	100	100
1	E	520/515 (101%)	503 (97%)	17 (3%)	0	100	100
2	B	391/392 (100%)	382 (98%)	9 (2%)	0	100	100
2	F	392/392 (100%)	382 (97%)	10 (3%)	0	100	100
3	C	166/168 (99%)	164 (99%)	2 (1%)	0	100	100
3	G	167/168 (99%)	165 (99%)	2 (1%)	0	100	100
4	D	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
4	H	130/132 (98%)	125 (96%)	4 (3%)	1 (1%)	16	8
All	All	2410/2414 (100%)	2340 (97%)	69 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	422 (99%)	5 (1%)	63	63
1	E	433/426 (102%)	420 (97%)	13 (3%)	36	30
2	B	324/324 (100%)	321 (99%)	3 (1%)	70	73
2	F	325/324 (100%)	317 (98%)	8 (2%)	42	37
3	C	145/145 (100%)	145 (100%)	0	100	100
3	G	146/145 (101%)	143 (98%)	3 (2%)	47	44
4	D	104/104 (100%)	103 (99%)	1 (1%)	68	70
4	H	104/104 (100%)	102 (98%)	2 (2%)	50	47
All	All	2008/1998 (100%)	1973 (98%)	35 (2%)	53	52

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	52	MET
1	A	112	VAL
1	A	142	LEU
1	A	399	LYS
2	B	156	LEU
2	B	176	ASP
2	B	274	VAL
4	D	114	ARG
1	E	52	MET
1	E	58	GLU
1	E	62	VAL
1	E	105	VAL
1	E	112	VAL
1	E	138	LEU

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Mol	Chain	Res	Type
1	E	142	LEU
1	E	187	VAL
1	E	244	LEU
1	E	279	GLN
1	E	286	LEU
1	E	346	LEU
1	E	448	LEU
2	F	29	ASP
2	F	49	LEU
2	F	176	ASP
2	F	206	LEU
2	F	321[A]	ASN
2	F	321[B]	ASN
2	F	325	GLU
2	F	395	ASN
3	G	99	ILE
3	G	136	LEU
3	G	158	LYS
4	H	57	LEU
4	H	133	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
4	D	33	HIS
1	E	116	ASN
1	E	133	GLN
1	E	205	GLN
1	E	422	GLN
1	E	472	GLN
3	G	166	HIS
4	H	33	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 4 are monoatomic - leaving 37 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	EDO	E	604	-	3,3,3	0.45	0	2,2,2	0.59	0
6	EDO	C	202	-	3,3,3	0.40	0	2,2,2	0.47	0
6	EDO	E	603	-	3,3,3	0.56	0	2,2,2	0.27	0
7	BEZ	E	606	5	9,9,9	0.82	0	11,11,11	0.92	0
6	EDO	A	609	-	3,3,3	0.61	0	2,2,2	0.26	0
6	EDO	B	401	-	3,3,3	0.53	0	2,2,2	0.47	0
6	EDO	F	402	-	3,3,3	0.68	0	2,2,2	0.24	0
6	EDO	G	201	-	3,3,3	0.64	0	2,2,2	0.08	0
6	EDO	A	605	-	3,3,3	0.53	0	2,2,2	0.20	0
6	EDO	D	201	-	3,3,3	0.55	0	2,2,2	0.09	0
6	EDO	B	403	-	3,3,3	0.54	0	2,2,2	0.52	0
6	EDO	A	612	-	3,3,3	0.56	0	2,2,2	0.24	0
6	EDO	G	202	-	3,3,3	0.40	0	2,2,2	0.58	0
6	EDO	A	608	-	3,3,3	0.41	0	2,2,2	0.18	0
6	EDO	H	201	-	3,3,3	0.58	0	2,2,2	0.12	0
6	EDO	B	405	-	3,3,3	0.63	0	2,2,2	0.31	0
6	EDO	A	604	-	3,3,3	0.51	0	2,2,2	0.53	0
6	EDO	E	609	-	3,3,3	0.46	0	2,2,2	1.12	0
6	EDO	F	401	-	3,3,3	0.52	0	2,2,2	0.55	0
6	EDO	E	605	-	3,3,3	0.52	0	2,2,2	0.19	0
6	EDO	A	606	-	3,3,3	0.71	0	2,2,2	0.09	0
6	EDO	D	202	-	3,3,3	0.61	0	2,2,2	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	C	201	-	3,3,3	0.51	0	2,2,2	0.18	0
6	EDO	F	404	-	3,3,3	0.43	0	2,2,2	0.48	0
6	EDO	B	404	-	3,3,3	0.64	0	2,2,2	0.20	0
6	EDO	B	402	-	3,3,3	0.42	0	2,2,2	0.12	0
6	EDO	D	203	-	3,3,3	0.40	0	2,2,2	0.54	0
6	EDO	E	607	-	3,3,3	0.70	0	2,2,2	0.50	0
6	EDO	F	405	-	3,3,3	0.49	0	2,2,2	0.42	0
7	BEZ	A	607	5	9,9,9	0.89	0	11,11,11	1.14	1 (9%)
6	EDO	B	406	-	3,3,3	0.43	0	2,2,2	0.43	0
6	EDO	F	403	-	3,3,3	0.55	0	2,2,2	0.47	0
6	EDO	E	608	-	3,3,3	0.65	0	2,2,2	0.16	0
6	EDO	A	610	-	3,3,3	0.48	0	2,2,2	0.35	0
6	EDO	F	406	-	3,3,3	0.55	0	2,2,2	0.17	0
6	EDO	A	611	-	3,3,3	0.44	0	2,2,2	0.56	0
6	EDO	A	603	-	3,3,3	0.43	0	2,2,2	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	E	604	-	-	0/1/1/1	-
6	EDO	C	202	-	-	1/1/1/1	-
6	EDO	E	603	-	-	0/1/1/1	-
7	BEZ	E	606	5	-	0/4/4/4	0/1/1/1
6	EDO	A	609	-	-	0/1/1/1	-
6	EDO	B	401	-	-	0/1/1/1	-
6	EDO	F	402	-	-	1/1/1/1	-
6	EDO	G	201	-	-	0/1/1/1	-
6	EDO	A	605	-	-	1/1/1/1	-
6	EDO	D	201	-	-	1/1/1/1	-
6	EDO	B	403	-	-	0/1/1/1	-
6	EDO	A	612	-	-	0/1/1/1	-
6	EDO	G	202	-	-	0/1/1/1	-
6	EDO	A	608	-	-	0/1/1/1	-
6	EDO	H	201	-	-	0/1/1/1	-
6	EDO	B	405	-	-	0/1/1/1	-
6	EDO	A	604	-	-	0/1/1/1	-
6	EDO	E	609	-	-	1/1/1/1	-
6	EDO	F	401	-	-	1/1/1/1	-
6	EDO	E	605	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	606	-	-	0/1/1/1	-
6	EDO	D	202	-	-	0/1/1/1	-
6	EDO	C	201	-	-	0/1/1/1	-
6	EDO	F	404	-	-	0/1/1/1	-
6	EDO	B	404	-	-	0/1/1/1	-
6	EDO	B	402	-	-	0/1/1/1	-
6	EDO	D	203	-	-	0/1/1/1	-
6	EDO	E	607	-	-	0/1/1/1	-
6	EDO	F	405	-	-	1/1/1/1	-
7	BEZ	A	607	5	-	0/4/4/4	0/1/1/1
6	EDO	B	406	-	-	0/1/1/1	-
6	EDO	F	403	-	-	0/1/1/1	-
6	EDO	E	608	-	-	1/1/1/1	-
6	EDO	A	610	-	-	1/1/1/1	-
6	EDO	F	406	-	-	0/1/1/1	-
6	EDO	A	611	-	-	0/1/1/1	-
6	EDO	A	603	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	607	BEZ	C6-C1-C2	2.10	121.24	118.57

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	401	EDO	O1-C1-C2-O2
6	D	201	EDO	O1-C1-C2-O2
6	E	608	EDO	O1-C1-C2-O2
6	F	402	EDO	O1-C1-C2-O2
6	A	610	EDO	O1-C1-C2-O2
6	E	609	EDO	O1-C1-C2-O2
6	A	605	EDO	O1-C1-C2-O2
6	C	202	EDO	O1-C1-C2-O2
6	F	405	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	609	EDO	2	0
6	D	201	EDO	2	0
6	A	612	EDO	5	0
6	A	608	EDO	3	0
6	E	609	EDO	1	0
6	E	605	EDO	1	0
6	E	607	EDO	1	0
6	A	610	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, 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%)	-0.11	9 (1%) 69 72	16, 29, 45, 59	1 (0%)
1	E	515/515 (100%)	-0.02	16 (3%) 51 55	14, 29, 50, 64	7 (1%)
2	B	392/392 (100%)	-0.31	1 (0%) 90 91	15, 28, 40, 71	1 (0%)
2	F	392/392 (100%)	-0.31	2 (0%) 87 89	16, 28, 41, 72	3 (0%)
3	C	168/168 (100%)	-0.15	2 (1%) 76 79	23, 33, 43, 54	0
3	G	168/168 (100%)	-0.02	2 (1%) 76 79	21, 34, 45, 55	1 (0%)
4	D	132/132 (100%)	0.44	4 (3%) 52 56	30, 40, 55, 92	0
4	H	132/132 (100%)	0.59	4 (3%) 52 56	33, 44, 61, 98	0
All	All	2414/2414 (100%)	-0.09	40 (1%) 69 72	14, 30, 48, 98	13 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	2	ALA	4.6
2	F	4	PRO	4.4
2	B	4	PRO	4.1
1	E	202	VAL	4.0
1	E	255	VAL	3.6
1	E	282	PHE	3.6
1	E	188	PHE	3.5
1	E	244	LEU	3.5
4	H	118	LEU	3.5
1	A	201	SER	3.4
1	E	216	LEU	3.0
1	E	259	ASN	3.0
1	E	257	ILE	3.0
1	E	326	VAL	2.8
1	A	255	VAL	2.8
1	E	490[A]	SER	2.7

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Mol	Chain	Res	Type	RSRZ
4	H	94	LEU	2.6
3	C	169	ALA	2.6
4	H	105	LEU	2.6
1	A	202	VAL	2.5
1	E	201	SER	2.4
1	E	192	PHE	2.4
3	G	2	ALA	2.4
1	E	198	VAL	2.3
1	E	324	TYR	2.3
2	F	395	ASN	2.3
4	D	98	PRO	2.2
1	A	198	VAL	2.2
4	D	31	VAL	2.2
1	A	216	LEU	2.2
4	H	65	PRO	2.2
1	E	502[A]	ARG	2.2
1	E	210	ALA	2.2
3	G	169	ALA	2.2
1	A	323	LYS	2.1
4	D	129	MET	2.1
1	A	257	ILE	2.1
1	A	52	MET	2.1
4	D	105	LEU	2.0
1	A	258	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	610	4/4	0.60	0.17	50,57,60,68	0
6	EDO	A	612	4/4	0.81	0.21	32,40,42,52	0
6	EDO	A	609	4/4	0.83	0.21	46,46,50,58	0
6	EDO	F	405	4/4	0.83	0.18	43,44,50,60	0
6	EDO	F	403	4/4	0.85	0.17	39,39,47,57	0
6	EDO	E	603	4/4	0.86	0.13	34,38,40,62	0
6	EDO	F	402	4/4	0.87	0.14	39,43,44,54	0
6	EDO	E	607	4/4	0.87	0.19	33,40,40,42	0
6	EDO	E	608	4/4	0.87	0.13	36,38,41,47	0
6	EDO	E	609	4/4	0.88	0.17	41,42,45,51	0
6	EDO	E	605	4/4	0.88	0.17	45,45,48,52	0
6	EDO	C	202	4/4	0.88	0.13	50,50,54,73	0
6	EDO	B	406	4/4	0.88	0.11	50,54,58,62	0
6	EDO	A	608	4/4	0.89	0.17	36,37,48,50	0
6	EDO	E	604	4/4	0.89	0.12	42,43,44,44	0
6	EDO	D	201	4/4	0.89	0.15	48,49,52,56	0
6	EDO	B	401	4/4	0.90	0.17	39,41,44,52	0
6	EDO	B	403	4/4	0.90	0.12	40,42,44,56	0
6	EDO	D	202	4/4	0.90	0.12	41,43,46,47	0
6	EDO	A	605	4/4	0.90	0.20	29,33,37,49	0
6	EDO	F	401	4/4	0.92	0.14	33,35,36,48	0
6	EDO	B	405	4/4	0.92	0.12	34,40,41,42	0
6	EDO	B	402	4/4	0.93	0.10	34,36,46,47	0
6	EDO	A	611	4/4	0.93	0.13	30,41,42,42	0
6	EDO	F	404	4/4	0.93	0.09	48,51,54,62	0
6	EDO	B	404	4/4	0.93	0.13	42,45,52,53	0
6	EDO	A	603	4/4	0.94	0.16	36,45,47,48	0
6	EDO	H	201	4/4	0.94	0.11	40,41,42,48	0
6	EDO	A	604	4/4	0.95	0.09	31,35,38,43	0
6	EDO	F	406	4/4	0.95	0.08	37,38,43,46	0
6	EDO	G	202	4/4	0.95	0.07	42,45,49,54	0
6	EDO	A	606	4/4	0.95	0.09	41,42,42,47	0
7	BEZ	A	607	9/9	0.95	0.07	29,33,33,33	0
7	BEZ	E	606	9/9	0.95	0.09	32,35,39,40	0
6	EDO	D	203	4/4	0.96	0.07	30,34,39,46	0
6	EDO	G	201	4/4	0.96	0.06	30,31,31,32	0
6	EDO	C	201	4/4	0.98	0.06	28,29,30,31	0
5	FE	A	602	1/1	0.99	0.03	34,34,34,34	0
5	FE	A	601	1/1	0.99	0.02	31,31,31,31	0
5	FE	E	602	1/1	1.00	0.02	35,35,35,35	0
5	FE	E	601	1/1	1.00	0.01	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.