



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:25 PM GMT

PDB ID : 3SWR  
Title : Structure of human DNMT1 (601-1600) in complex with Sinefungin  
Authors : Hashimoto, H.; Cheng, X.  
Deposited on : 2011-07-14  
Resolution : 2.49 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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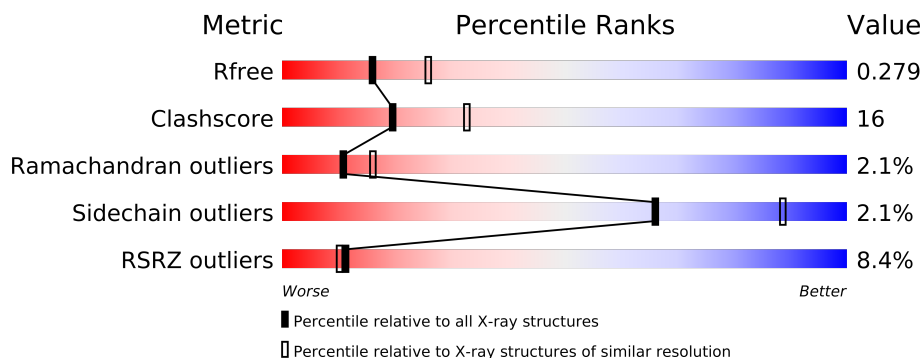
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.49 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1002	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MES	A	4	-	X
5	EDO	A	101	-	X
5	EDO	A	102	-	X
5	EDO	A	104	-	X
5	EDO	A	106	-	X
5	EDO	A	107	-	X
5	EDO	A	109	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	EDO	A	110	-	X
5	EDO	A	113	-	X
5	EDO	A	116	-	X
5	EDO	A	117	-	X
5	EDO	A	119	-	X
5	EDO	A	122	-	X
5	EDO	A	123	-	X
5	EDO	A	124	-	X
5	EDO	A	125	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7924 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

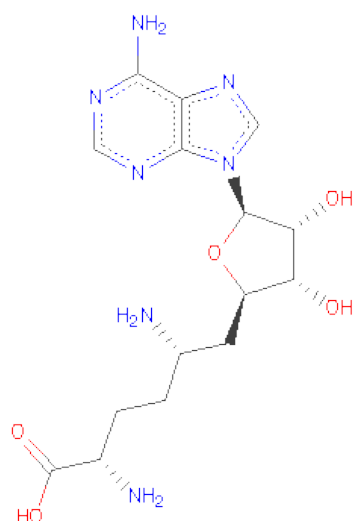
- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	965	7478	4706	1322	1396	54	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	599	HIS	-	EXPRESSION TAG	UNP P26358
A	600	MET	-	EXPRESSION TAG	UNP P26358

- Molecule 2 is SINEFUNGIN (three-letter code: SFG) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>7</sub>O<sub>5</sub>).



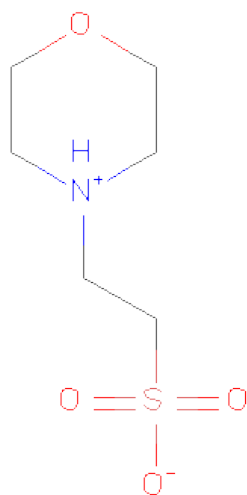
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	27	15	7	5	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



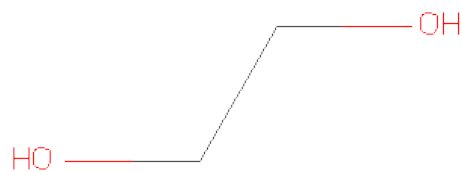
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total Zn 4 4	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	286	Total O 286 286	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.00Å 110.77Å 201.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.49 30.01 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-2.49) 91.9 (30.01-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.220 , 0.272 0.237 , 0.279	Depositor DCC
$R_{free}$ test set	2177 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 31.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 46552 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7924	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SFG, ZN, EDO, MES, SO4

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	0.36	0/7656	0.63	6/10378 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1537	GLY	N-CA-C	6.26	128.74	113.10
1	A	1538	ARG	N-CA-C	-6.00	94.79	111.00
1	A	959	PRO	N-CA-CB	5.73	110.18	103.30
1	A	1130	PRO	N-CA-CB	5.57	109.98	103.30
1	A	955	PRO	N-CA-CB	5.49	109.89	103.30
1	A	1293	GLN	N-CA-C	-5.07	97.30	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7478	0	7108	242	0
2	A	27	0	22	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	24	0	26	1	0
5	A	100	0	150	19	0
6	A	4	0	0	0	0
7	A	286	0	0	8	0
All	All	7924	0	7306	242	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (242) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1010:ASN:HD21	1:A:1012:THR:HG22	1.12	1.09
1:A:700:ASP:HA	1:A:1268:VAL:HG11	1.45	0.99
1:A:1010:ASN:ND2	1:A:1012:THR:HG22	1.83	0.94
1:A:1261:ARG:HD2	1:A:1322:GLU:OE1	1.72	0.89
1:A:649:LYS:H	1:A:649:LYS:HD3	1.39	0.86
1:A:1233:ASN:O	1:A:1275:LYS:HE2	1.83	0.79
1:A:1263:PHE:HB3	1:A:1317:ALA:HB3	1.65	0.79
1:A:1379:ASN:HD21	1:A:1417:MET:H	1.29	0.78
1:A:1326:LEU:HD12	5:A:104:EDO:H21	1.65	0.78
1:A:1410:ARG:O	1:A:1551:ARG:HD2	1.86	0.75
1:A:700:ASP:HA	1:A:1268:VAL:CG1	2.18	0.74
1:A:650:ARG:HH21	1:A:694:MET:HB3	1.52	0.74
1:A:1036:HIS:O	1:A:1398:ARG:NH2	2.21	0.74
1:A:1394:SER:HB3	5:A:106:EDO:H12	1.70	0.73
1:A:866:GLN:HG3	1:A:867:LEU:HG	1.70	0.73
1:A:939:VAL:HG22	1:A:1056:VAL:HG13	1.69	0.73
1:A:743:LYS:H	1:A:743:LYS:HD2	1.54	0.73
1:A:763:VAL:CG2	1:A:828:ILE:HG23	2.19	0.73
1:A:1404:GLN:OE1	1:A:1407:PRO:HA	1.88	0.73
1:A:1189:GLU:OE2	1:A:1193:ILE:HD11	1.89	0.73
1:A:649:LYS:N	1:A:649:LYS:HD3	2.03	0.73
1:A:705:VAL:HG12	1:A:708:ASN:HB2	1.72	0.71
1:A:763:VAL:HG22	1:A:764:SER:H	1.56	0.70
1:A:919:SER:O	1:A:1003:LYS:HB2	1.91	0.70
1:A:701:ASP:OD1	1:A:703:GLU:HB2	1.93	0.69
1:A:1195:LEU:O	1:A:1199:MET:HG3	1.93	0.69
1:A:1557:GLN:OE1	1:A:1581:PRO:HG3	1.94	0.67
1:A:1430:LEU:H	5:A:123:EDO:H12	1.60	0.66
1:A:767:PRO:HG2	1:A:773:PRO:O	1.95	0.66
1:A:894:VAL:O	1:A:898:ARG:HG3	1.95	0.66
1:A:1310:ARG:NH2	1:A:1577:GLY:O	2.30	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1190:ASP:OD1	1:A:1192:ASN:HB2	1.95	0.65
1:A:1430:LEU:HD22	1:A:1543:GLU:HA	1.77	0.64
1:A:753:ASP:O	1:A:754:ALA:HB3	1.98	0.64
1:A:652:ARG:HH12	1:A:689:ARG:HD3	1.61	0.64
1:A:652:ARG:HH22	1:A:689:ARG:NH1	1.96	0.64
1:A:716:LYS:HA	7:A:290:HOH:O	1.99	0.63
1:A:907:ILE:HG13	1:A:907:ILE:O	1.97	0.63
1:A:1477:SER:HB2	1:A:1484:ALA:O	1.99	0.63
1:A:1145:PHE:CE2	1:A:1224:PRO:HB3	2.35	0.62
1:A:763:VAL:HG21	1:A:828:ILE:HG23	1.81	0.62
1:A:1035:TYR:HB3	5:A:106:EDO:H21	1.82	0.61
1:A:763:VAL:HG22	1:A:764:SER:N	2.16	0.61
1:A:836:TYR:CE1	1:A:838:ALA:HB2	2.35	0.60
1:A:1210:ARG:NH1	5:A:116:EDO:H11	2.16	0.60
1:A:1314:ILE:HB	1:A:1327:PHE:HE1	1.65	0.60
1:A:1165:TRP:HE1	5:A:116:EDO:H12	1.66	0.60
1:A:652:ARG:HH22	1:A:689:ARG:HH11	1.48	0.59
1:A:1205:ASN:HB3	1:A:1211:LEU:HD11	1.84	0.59
1:A:719:HIS:O	1:A:723:LYS:NZ	2.36	0.59
1:A:1016:ILE:HG22	1:A:1018:VAL:HG13	1.85	0.59
1:A:650:ARG:HH21	1:A:694:MET:CB	2.15	0.58
1:A:1490:ARG:HD3	1:A:1492:PHE:CZ	2.39	0.57
1:A:763:VAL:HG21	1:A:828:ILE:HG12	1.86	0.57
1:A:708:ASN:HA	1:A:1340:GLN:OE1	2.05	0.57
1:A:690:ARG:HD2	1:A:690:ARG:O	2.04	0.57
1:A:913:GLN:HA	1:A:923:TYR:HA	1.86	0.57
1:A:1003:LYS:HE3	1:A:1007:GLY:O	2.05	0.57
1:A:1210:ARG:HH11	5:A:116:EDO:H11	1.70	0.56
1:A:1010:ASN:HD21	1:A:1012:THR:CG2	2.02	0.56
1:A:968:LEU:O	1:A:1440:PRO:HA	2.06	0.56
1:A:699:ALA:O	1:A:701:ASP:N	2.35	0.56
1:A:663:GLU:HB3	1:A:670:CYS:SG	2.45	0.56
1:A:1219:MET:HE1	1:A:1592:ILE:HG21	1.87	0.55
1:A:1193:ILE:HD12	1:A:1193:ILE:C	2.26	0.55
1:A:999:ILE:HA	1:A:1016:ILE:HD13	1.86	0.55
1:A:1520:ASP:HB3	5:A:124:EDO:H11	1.88	0.55
1:A:999:ILE:HG12	1:A:1016:ILE:CD1	2.37	0.55
1:A:1404:GLN:CD	1:A:1407:PRO:HA	2.27	0.55
1:A:1310:ARG:HG3	1:A:1525:THR:HG23	1.88	0.55
1:A:961:LYS:O	1:A:962:GLU:HG2	2.07	0.55
1:A:705:VAL:HG13	5:A:120:EDO:O2	2.08	0.54
1:A:730:ARG:O	1:A:752:ILE:HA	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:665:GLY:HA2	1:A:670:CYS:HB3	1.89	0.54
1:A:704:GLU:HG3	7:A:293:HOH:O	2.07	0.54
1:A:1490:ARG:HD3	1:A:1492:PHE:CE2	2.42	0.54
1:A:818:ASP:OD2	1:A:898:ARG:NH1	2.41	0.54
1:A:1424:ARG:CZ	1:A:1497:PRO:HG3	2.38	0.54
1:A:922:LEU:CD2	1:A:1000:PHE:HB3	2.38	0.53
1:A:716:LYS:O	1:A:718:MET:N	2.41	0.53
1:A:1264:LEU:CD2	1:A:1316:LEU:HD23	2.39	0.53
1:A:910:VAL:HG21	1:A:923:TYR:CZ	2.44	0.53
1:A:980:ILE:C	1:A:982:GLY:H	2.13	0.53
1:A:1346:ASP:H	5:A:113:EDO:H12	1.72	0.53
1:A:914:LEU:O	1:A:915:GLU:HB2	2.08	0.52
1:A:701:ASP:C	1:A:703:GLU:H	2.13	0.52
1:A:903:ARG:O	1:A:907:ILE:HG23	2.09	0.52
1:A:1210:ARG:HG2	1:A:1210:ARG:HH11	1.74	0.52
1:A:1297:GLY:HA2	5:A:102:EDO:H21	1.92	0.52
1:A:884:PRO:HG3	1:A:892:PHE:CD2	2.45	0.51
1:A:1158:ALA:O	1:A:1593:LYS:HE3	2.11	0.51
1:A:1171:ASP:HB3	1:A:1172:PRO:HD3	1.92	0.51
1:A:1315:ILE:N	1:A:1315:ILE:HD12	2.26	0.51
1:A:888:ASN:O	1:A:892:PHE:HB2	2.11	0.51
1:A:1189:GLU:CD	1:A:1193:ILE:HD11	2.31	0.51
1:A:858:ASP:O	1:A:862:THR:HB	2.11	0.51
1:A:1485:CYS:O	1:A:1487:PRO:HD3	2.12	0.50
1:A:653:CYS:O	1:A:653:CYS:SG	2.70	0.50
1:A:907:ILE:HG13	1:A:909:ARG:HD3	1.92	0.50
1:A:1073:GLN:HA	1:A:1073:GLN:HE21	1.76	0.50
1:A:752:ILE:O	1:A:753:ASP:C	2.50	0.49
1:A:1193:ILE:HD12	1:A:1194:LEU:N	2.28	0.49
1:A:971:GLU:HG3	1:A:1436:TRP:HZ3	1.77	0.49
1:A:1513:LEU:HD12	1:A:1513:LEU:N	2.28	0.49
1:A:792:PHE:HB3	1:A:825:LEU:HD21	1.95	0.49
1:A:907:ILE:O	1:A:908:PRO:C	2.51	0.49
1:A:1004:LYS:C	1:A:1006:ASN:H	2.16	0.49
1:A:753:ASP:O	1:A:754:ALA:CB	2.60	0.49
1:A:1426:ARG:HA	1:A:1545:HIS:ND1	2.27	0.49
1:A:1277:SER:O	1:A:1281:LYS:HG3	2.13	0.49
1:A:839:PRO:HG2	1:A:1320:PRO:HB3	1.95	0.48
1:A:1370:THR:O	1:A:1555:ARG:NH1	2.45	0.48
1:A:1165:TRP:CH2	1:A:1216:ASP:HB3	2.49	0.48
1:A:1264:LEU:HD22	1:A:1316:LEU:HD23	1.96	0.48
1:A:1374:LEU:HD12	1:A:1552:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1476:CYS:O	1:A:1479:VAL:HG22	2.14	0.48
1:A:991:TYR:OH	1:A:1356:ARG:HG2	2.14	0.48
1:A:1194:LEU:O	1:A:1198:VAL:HG22	2.13	0.48
1:A:1293:GLN:O	1:A:1317:ALA:HA	2.15	0.47
1:A:1345:VAL:HA	5:A:113:EDO:H12	1.95	0.47
1:A:996:ILE:HA	1:A:1018:VAL:HG12	1.97	0.47
1:A:914:LEU:H	1:A:914:LEU:HD23	1.79	0.47
1:A:836:TYR:CE1	4:A:4:MES:H21	2.49	0.47
1:A:777:ALA:HB2	1:A:796:TRP:CE3	2.50	0.47
1:A:698:GLU:HB2	1:A:700:ASP:OD2	2.15	0.47
1:A:1340:GLN:HB3	7:A:42:HOH:O	2.13	0.47
1:A:1309:THR:HG22	1:A:1524:SER:HA	1.95	0.47
1:A:915:GLU:CD	1:A:917:LEU:HD21	2.35	0.47
1:A:1524:SER:O	1:A:1525:THR:C	2.52	0.47
1:A:1165:TRP:NE1	5:A:116:EDO:H12	2.28	0.47
1:A:922:LEU:HD22	1:A:1000:PHE:HB3	1.95	0.47
1:A:1541:HIS:CG	1:A:1542:PRO:HD2	2.50	0.47
1:A:921:VAL:CG2	1:A:1009:PRO:HB3	2.45	0.47
1:A:943:PRO:HA	1:A:992:ARG:HG2	1.97	0.47
1:A:1549:SER:OG	1:A:1552:GLU:HG3	2.15	0.46
1:A:606:HIS:C	1:A:685:ALA:HB2	2.34	0.46
1:A:1267:ASN:HA	5:A:119:EDO:H22	1.98	0.46
1:A:653:CYS:O	1:A:655:VAL:N	2.46	0.46
1:A:1035:TYR:HB3	5:A:106:EDO:C2	2.46	0.46
1:A:1194:LEU:C	1:A:1194:LEU:HD23	2.35	0.46
1:A:1400:LEU:HD23	1:A:1555:ARG:CD	2.46	0.46
1:A:1222:GLY:HA2	7:A:213:HOH:O	2.16	0.46
1:A:743:LYS:HD2	1:A:743:LYS:N	2.26	0.46
1:A:910:VAL:HG21	1:A:923:TYR:CE1	2.51	0.46
1:A:995:ARG:NH2	1:A:1103:ALA:O	2.49	0.46
1:A:707:ASP:O	1:A:710:PRO:HD3	2.16	0.46
1:A:1034:SER:HB2	1:A:1363:ARG:NE	2.31	0.46
1:A:1400:LEU:HD23	1:A:1555:ARG:HD2	1.98	0.45
1:A:1020:LYS:HD2	1:A:1047:GLU:HB3	1.98	0.45
1:A:921:VAL:HG22	1:A:1009:PRO:HB3	1.99	0.45
1:A:875:ARG:HD2	7:A:64:HOH:O	2.16	0.45
1:A:1264:LEU:CD2	1:A:1316:LEU:CD2	2.95	0.45
1:A:1374:LEU:HA	1:A:1375:PRO:HD3	1.81	0.45
1:A:881:LYS:O	1:A:882:THR:C	2.54	0.45
1:A:1210:ARG:HG2	1:A:1210:ARG:NH1	2.32	0.45
1:A:1375:PRO:HG3	1:A:1388:TYR:O	2.17	0.45
1:A:763:VAL:HG23	1:A:830:SER:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1388:TYR:CE1	1:A:1409:LEU:HD13	2.52	0.44
1:A:939:VAL:HG22	1:A:1056:VAL:CG1	2.42	0.44
1:A:1346:ASP:H	5:A:113:EDO:C1	2.29	0.44
1:A:792:PHE:HB3	1:A:825:LEU:CD2	2.48	0.44
1:A:946:PHE:CE2	1:A:992:ARG:HD2	2.52	0.44
1:A:1500:LEU:HB2	1:A:1501:PRO:HD3	1.99	0.44
1:A:790:GLN:HB3	1:A:825:LEU:HD12	1.98	0.44
1:A:1260:PRO:HD2	1:A:1292:TYR:OH	2.18	0.44
1:A:690:ARG:HG3	1:A:690:ARG:HH11	1.83	0.44
1:A:973:TYR:C	1:A:975:LYS:H	2.20	0.44
1:A:1219:MET:CE	1:A:1592:ILE:HG21	2.48	0.44
1:A:1392:PRO:HG3	1:A:1401:ARG:HD3	1.99	0.44
1:A:627:ILE:HD11	1:A:1289[A]:ARG:HG2	2.00	0.44
1:A:1373:ASP:HA	1:A:1393:GLN:NE2	2.33	0.44
1:A:1458:THR:HG21	7:A:207:HOH:O	2.17	0.43
1:A:1020:LYS:HD2	1:A:1047:GLU:CB	2.48	0.43
1:A:1197:LEU:HD22	1:A:1202:GLU:HG3	1.99	0.43
1:A:837:LYS:HD2	1:A:859:ASP:OD2	2.18	0.43
1:A:1142:LEU:O	1:A:1220:LEU:HD12	2.19	0.43
1:A:617:LYS:HA	1:A:1245:ASN:OD1	2.18	0.43
1:A:705:VAL:O	1:A:705:VAL:HG12	2.19	0.43
1:A:1224:PRO:HA	1:A:1225:PRO:HD3	1.86	0.43
1:A:1319:ALA:HB3	1:A:1322:GLU:HG2	2.00	0.43
1:A:1431:ALA:H	5:A:123:EDO:H21	1.83	0.43
1:A:1178:ARG:HG3	1:A:1186:VAL:HG21	2.01	0.43
1:A:1368:ARG:NH2	1:A:1520:ASP:OD1	2.52	0.43
1:A:980:ILE:C	1:A:982:GLY:N	2.71	0.43
1:A:615:PRO:HG2	1:A:617:LYS:H	1.83	0.43
1:A:749:LYS:HE2	1:A:758:GLU:CG	2.49	0.43
1:A:934:ARG:HG3	1:A:934:ARG:HH11	1.84	0.43
1:A:1531:GLU:HA	1:A:1532:PRO:HD3	1.87	0.43
1:A:1534:GLY:O	1:A:1535:LYS:C	2.57	0.43
1:A:804:VAL:HG22	1:A:1350:PHE:CZ	2.54	0.43
1:A:746:TYR:CD1	1:A:783:TRP:HB3	2.54	0.43
1:A:1379:ASN:ND2	1:A:1417:MET:H	2.06	0.42
1:A:1333:VAL:O	1:A:1364:THR:HB	2.19	0.42
1:A:1070:GLU:HB2	7:A:196:HOH:O	2.18	0.42
1:A:719:HIS:ND1	1:A:819:GLU:OE1	2.45	0.42
1:A:936:GLY:O	1:A:995:ARG:HD2	2.19	0.42
1:A:1203:THR:O	1:A:1203:THR:HG22	2.19	0.42
1:A:1001:CYS:O	1:A:1002:PRO:O	2.37	0.42
1:A:1170:TRP:CE3	1:A:1173:ALA:HB2	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:971:GLU:OE1	1:A:974:ARG:NH2	2.50	0.42
1:A:971:GLU:HG3	1:A:1436:TRP:CZ3	2.54	0.42
1:A:1001:CYS:HB3	1:A:1010:ASN:O	2.19	0.42
1:A:752:ILE:HG13	1:A:752:ILE:O	2.20	0.42
1:A:1273:SER:O	1:A:1274:PHE:C	2.58	0.42
1:A:1524:SER:O	1:A:1526:THR:N	2.52	0.42
1:A:883:GLN:HA	1:A:884:PRO:HD3	1.73	0.42
1:A:1574:ARG:HG3	1:A:1578:ASN:HD21	1.84	0.42
1:A:1269:ARG:HD3	1:A:1269:ARG:C	2.40	0.42
1:A:1430:LEU:H	5:A:123:EDO:C1	2.31	0.42
1:A:1170:TRP:CD1	1:A:1172:PRO:HD2	2.54	0.42
1:A:623:LEU:HD23	1:A:623:LEU:C	2.40	0.42
1:A:712:MET:HE2	1:A:1344:VAL:HG13	2.02	0.42
1:A:1155:PHE:HB3	1:A:1161:SER:OG	2.20	0.42
1:A:749:LYS:HD3	1:A:756:THR:CG2	2.50	0.41
1:A:1071:CYS:SG	1:A:1074:VAL:HG23	2.60	0.41
1:A:1020:LYS:O	1:A:1045:SER:HB3	2.19	0.41
1:A:744:LYS:HZ2	1:A:783:TRP:HE1	1.65	0.41
1:A:740:THR:O	1:A:740:THR:HG22	2.20	0.41
1:A:616:THR:O	1:A:616:THR:HG22	2.20	0.41
1:A:1506:ARG:O	1:A:1507:HIS:CG	2.74	0.41
1:A:763:VAL:HG21	1:A:828:ILE:CG2	2.49	0.41
1:A:1346:ASP:O	1:A:1347:ASP:HB2	2.21	0.41
1:A:888:ASN:HB2	1:A:891:LYS:HG3	2.03	0.41
1:A:879:PRO:HA	1:A:880:PRO:HD3	1.81	0.41
1:A:1466:ARG:HD3	1:A:1472:LEU:HD23	2.03	0.41
1:A:1308:GLN:OE1	1:A:1310:ARG:HD2	2.20	0.41
1:A:1296:PHE:HA	1:A:1314:ILE:O	2.20	0.41
1:A:1498:TRP:O	1:A:1501:PRO:HD2	2.21	0.41
1:A:852:GLU:O	1:A:853:SER:HB3	2.21	0.41
1:A:691:CYS:HA	1:A:692:PRO:HD3	1.81	0.41
1:A:976:TYR:OH	1:A:980:ILE:HD11	2.21	0.41
1:A:620:THR:HA	1:A:1253:SER:OG	2.20	0.41
1:A:1205:ASN:HA	5:A:115:EDO:H12	2.03	0.40
1:A:999:ILE:HG23	1:A:1016:ILE:HD11	2.03	0.40
1:A:1423:ALA:HA	1:A:1426:ARG:NH1	2.37	0.40
1:A:1532:PRO:HD2	7:A:47:HOH:O	2.20	0.40
1:A:718:MET:HE3	1:A:871:GLN:NE2	2.35	0.40
1:A:658:VAL:HG12	1:A:689:ARG:HA	2.03	0.40
1:A:1414:CYS:HB3	1:A:1549:SER:HA	2.03	0.40
1:A:1569:ILE:HG23	1:A:1570:LEU:N	2.36	0.40
1:A:1495:LEU:HD12	1:A:1495:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:862:THR:HG22	1:A:863:TYR:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	959/1002 (96%)	862 (90%)	77 (8%)	20 (2%)	11 16

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	717	LYS
1	A	718	MET
1	A	961	LYS
1	A	1002	PRO
1	A	1483	LYS
1	A	677	GLY
1	A	753	ASP
1	A	700	ASP
1	A	754	ALA
1	A	853	SER
1	A	882	THR
1	A	1005	SER
1	A	1130	PRO
1	A	605	ARG
1	A	713	PRO
1	A	858	ASP
1	A	958	ARG
1	A	1525	THR
1	A	715	PRO
1	A	851	PRO

### 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	780/867 (90%)	764 (98%)	16 (2%)	66 88

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	649	LYS
1	A	690	ARG
1	A	703	GLU
1	A	743	LYS
1	A	894	VAL
1	A	939	VAL
1	A	980	ILE
1	A	986	ASP
1	A	995	ARG
1	A	1045	SER
1	A	1138	LYS
1	A	1162	ASP
1	A	1198	VAL
1	A	1269	ARG
1	A	1451	MET
1	A	1564	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1010	ASN
1	A	1036	HIS
1	A	1057	GLN
1	A	1073	GLN
1	A	1181	ASN
1	A	1227	GLN
1	A	1379	ASN
1	A	1389	ASN
1	A	1393	GLN
1	A	1427	HIS

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Mol	Chain	Res	Type
1	A	1459	HIS
1	A	1464	ASN
1	A	1505	ASN
1	A	1507	HIS
1	A	1509	HIS
1	A	1578	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 4 are monoatomic - leaving 29 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	$\# Z  > 2$
3	SO4	A	1	-	4,4,4	0.29	0	6,6,6	0.08	0
5	EDO	A	101	-	3,3,3	0.63	0	2,2,2	0.31	0
5	EDO	A	102	-	3,3,3	0.71	0	2,2,2	0.27	0
5	EDO	A	103	-	3,3,3	0.50	0	2,2,2	0.43	0
5	EDO	A	104	-	3,3,3	0.66	0	2,2,2	0.29	0
5	EDO	A	105	-	3,3,3	0.56	0	2,2,2	0.37	0
5	EDO	A	106	-	3,3,3	0.67	0	2,2,2	0.26	0
5	EDO	A	107	-	3,3,3	0.60	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	108	-	3,3,3	0.61	0	2,2,2	0.35	0
5	EDO	A	109	-	3,3,3	0.58	0	2,2,2	0.35	0
5	EDO	A	110	-	3,3,3	0.60	0	2,2,2	0.32	0
5	EDO	A	111	-	3,3,3	0.48	0	2,2,2	0.43	0
5	EDO	A	112	-	3,3,3	0.60	0	2,2,2	0.34	0
5	EDO	A	113	-	3,3,3	0.56	0	2,2,2	0.34	0
5	EDO	A	114	-	3,3,3	0.64	0	2,2,2	0.28	0
5	EDO	A	115	-	3,3,3	0.59	0	2,2,2	0.30	0
5	EDO	A	116	-	3,3,3	0.62	0	2,2,2	0.29	0
5	EDO	A	117	-	3,3,3	0.46	0	2,2,2	0.42	0
5	EDO	A	118	-	3,3,3	0.56	0	2,2,2	0.34	0
5	EDO	A	119	-	3,3,3	0.58	0	2,2,2	0.34	0
5	EDO	A	120	-	3,3,3	0.64	0	2,2,2	0.29	0
5	EDO	A	121	-	3,3,3	0.55	0	2,2,2	0.37	0
5	EDO	A	122	-	3,3,3	0.61	0	2,2,2	0.29	0
5	EDO	A	123	-	3,3,3	0.58	0	2,2,2	0.34	0
5	EDO	A	124	-	3,3,3	0.57	0	2,2,2	0.33	0
5	EDO	A	125	-	3,3,3	0.55	0	2,2,2	0.38	0
4	MES	A	2	-	12,12,12	1.03	1 (8%)	16,16,16	0.94	1 (6%)
2	SFG	A	300	-	29,29,29	1.95	6 (20%)	42,42,42	2.34	12 (28%)
4	MES	A	4	-	12,12,12	0.89	0	16,16,16	0.98	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
3	SO4	A	1	-	-	0/0/0/0	0/0/0/0
5	EDO	A	101	-	-	0/1/1/1	0/0/0/0
5	EDO	A	102	-	-	0/1/1/1	0/0/0/0
5	EDO	A	103	-	-	0/1/1/1	0/0/0/0
5	EDO	A	104	-	-	0/1/1/1	0/0/0/0
5	EDO	A	105	-	-	0/1/1/1	0/0/0/0
5	EDO	A	106	-	-	0/1/1/1	0/0/0/0
5	EDO	A	107	-	-	0/1/1/1	0/0/0/0
5	EDO	A	108	-	-	0/1/1/1	0/0/0/0
5	EDO	A	109	-	-	0/1/1/1	0/0/0/0
5	EDO	A	110	-	-	0/1/1/1	0/0/0/0
5	EDO	A	111	-	-	0/1/1/1	0/0/0/0
5	EDO	A	112	-	-	0/1/1/1	0/0/0/0
5	EDO	A	113	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	114	-	-	0/1/1/1	0/0/0/0
5	EDO	A	115	-	-	0/1/1/1	0/0/0/0
5	EDO	A	116	-	-	0/1/1/1	0/0/0/0
5	EDO	A	117	-	-	0/1/1/1	0/0/0/0
5	EDO	A	118	-	-	0/1/1/1	0/0/0/0
5	EDO	A	119	-	-	0/1/1/1	0/0/0/0
5	EDO	A	120	-	-	0/1/1/1	0/0/0/0
5	EDO	A	121	-	-	0/1/1/1	0/0/0/0
5	EDO	A	122	-	-	0/1/1/1	0/0/0/0
5	EDO	A	123	-	-	0/1/1/1	0/0/0/0
5	EDO	A	124	-	-	0/1/1/1	0/0/0/0
5	EDO	A	125	-	-	0/1/1/1	0/0/0/0
4	MES	A	2	-	-	0/6/14/14	0/1/1/1
2	SFG	A	300	-	-	0/17/33/33	0/1/3/3
4	MES	A	4	-	-	0/6/14/14	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	SFG	C1'-N9	-4.65	1.34	1.48
2	A	300	SFG	C4-N9	4.31	1.44	1.37
2	A	300	SFG	O4'-C1'	4.15	1.47	1.41
2	A	300	SFG	C5'-C4'	4.02	1.59	1.52
2	A	300	SFG	C2-N3	3.05	1.38	1.32
2	A	300	SFG	CA-C	2.08	1.60	1.53
4	A	2	MES	C8-S	2.03	1.81	1.78

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	SFG	N3-C2-N1	-7.55	122.39	128.71
2	A	300	SFG	O4'-C1'-C2'	-6.54	96.75	106.77
2	A	300	SFG	C4'-O4'-C1'	4.65	114.80	109.75
2	A	300	SFG	C8-N9-C1'	4.54	135.32	126.38
2	A	300	SFG	C8-N9-C4	-4.44	103.51	106.90
2	A	300	SFG	CB-CA-N	3.39	118.44	110.14
2	A	300	SFG	C1'-N9-C4	-3.17	121.17	126.64
2	A	300	SFG	C3'-C2'-C1'	2.67	105.08	100.91
2	A	300	SFG	C2-N1-C6	2.59	123.44	118.77
2	A	300	SFG	CG-CD-NE	2.39	115.01	108.68
2	A	300	SFG	O4'-C1'-N9	2.31	110.59	108.44
2	A	300	SFG	CB-CG-CD	2.06	118.04	114.70

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	2	MES	O2S-S-O1S	-2.01	108.56	112.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	965/1002 (96%)	0.28	81 (8%)	11 10	26, 50, 108, 137	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	855	LEU	8.3
1	A	980	ILE	7.3
1	A	682	SER	7.3
1	A	648	PHE	5.8
1	A	853	SER	5.6
1	A	1130	PRO	5.5
1	A	681	ARG	5.4
1	A	983	SER	5.2
1	A	956	VAL	5.2
1	A	700	ASP	5.1
1	A	1005	SER	4.8
1	A	890	PHE	4.8
1	A	854	LEU	4.8
1	A	858	ASP	4.8
1	A	679	SER	4.7
1	A	678	GLY	4.7
1	A	961	LYS	4.6
1	A	952	LEU	4.5
1	A	677	GLY	4.5
1	A	856	GLU	4.5
1	A	636	ILE	4.5
1	A	955	PRO	4.5
1	A	684	GLN	4.3
1	A	954	SER	4.3
1	A	976	TYR	4.3
1	A	606	HIS	4.1
1	A	984	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	683	LYS	4.0
1	A	1132	ILE	4.0
1	A	982	GLY	3.8
1	A	646	ASN	3.8
1	A	711	GLU	3.8
1	A	859	ASP	3.7
1	A	676	PHE	3.7
1	A	647	ALA	3.5
1	A	985	LEU	3.5
1	A	690	ARG	3.4
1	A	615	PRO	3.4
1	A	1286	CYS	3.3
1	A	953	SER	3.3
1	A	958	ARG	3.3
1	A	635	GLN	3.2
1	A	979	TYR	3.2
1	A	1129	GLU	3.1
1	A	667	CYS	3.1
1	A	709	ILE	3.1
1	A	1004	LYS	3.1
1	A	959	PRO	3.0
1	A	1444	VAL	3.0
1	A	608	THR	2.9
1	A	634	GLU	2.9
1	A	1008	ARG	2.8
1	A	1405	TYR	2.8
1	A	664	CYS	2.8
1	A	1287	LEU	2.8
1	A	1315	ILE	2.7
1	A	924	TYR	2.7
1	A	852	GLU	2.7
1	A	607	SER	2.6
1	A	729	ASN	2.6
1	A	887	ASP	2.6
1	A	1600	ALA	2.6
1	A	730	ARG	2.5
1	A	1536	GLN	2.5
1	A	1284	LEU	2.5
1	A	603	THR	2.5
1	A	1317	ALA	2.4
1	A	1406	GLN	2.4
1	A	1283	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1264	LEU	2.4
1	A	1106	PRO	2.4
1	A	685	ALA	2.3
1	A	957	LYS	2.3
1	A	1506	ARG	2.3
1	A	666	LYS	2.3
1	A	1481	ALA	2.2
1	A	981	LYS	2.2
1	A	1288	VAL	2.1
1	A	680	GLY	2.1
1	A	1451	MET	2.1
1	A	1265	LEU	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	A	116	4/4	0.55	51.07	85,85,86,86	0
5	EDO	A	123	4/4	0.34	21.21	69,69,69,69	0
5	EDO	A	106	4/4	0.44	10.88	60,62,64,64	0
5	EDO	A	101	4/4	0.36	9.70	53,53,55,55	0
5	EDO	A	104	4/4	0.15	9.62	51,51,51,52	0
5	EDO	A	125	4/4	0.33	6.03	75,78,79,81	0
5	EDO	A	109	4/4	0.30	5.94	90,91,91,92	0
5	EDO	A	113	4/4	0.31	5.70	57,59,61,64	0
5	EDO	A	122	4/4	0.29	5.66	76,77,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	102	4/4	0.22	5.03	42,46,47,48	0
5	EDO	A	124	4/4	0.29	4.98	68,69,69,69	0
5	EDO	A	110	4/4	0.36	3.84	75,76,76,76	0
4	MES	A	4	12/12	0.27	3.80	115,117,119,119	0
5	EDO	A	119	4/4	0.58	3.27	87,88,89,89	0
5	EDO	A	117	4/4	0.20	2.82	53,55,56,56	0
5	EDO	A	107	4/4	0.17	2.53	63,64,64,65	0
5	EDO	A	121	4/4	0.21	1.99	76,77,77,79	0
5	EDO	A	103	4/4	0.16	1.99	55,56,56,56	0
5	EDO	A	108	4/4	0.18	1.81	70,71,71,72	0
5	EDO	A	105	4/4	0.17	1.76	62,63,65,65	0
5	EDO	A	118	4/4	0.14	1.04	40,43,43,44	0
5	EDO	A	115	4/4	0.23	0.94	68,72,73,74	0
5	EDO	A	120	4/4	0.21	0.75	81,83,83,84	0
5	EDO	A	114	4/4	0.19	0.69	52,53,54,54	0
5	EDO	A	111	4/4	0.13	0.64	49,51,53,56	0
3	SO4	A	1	5/5	0.21	0.53	111,112,112,112	0
6	ZN	A	3	1/1	0.12	0.45	50,50,50,50	0
4	MES	A	2	12/12	0.12	0.44	67,69,76,77	0
2	SFG	A	300	27/27	0.17	0.41	49,55,58,59	0
5	EDO	A	112	4/4	0.14	0.32	71,72,72,73	0
6	ZN	A	1601	1/1	0.10	-0.82	70,70,70,70	0
6	ZN	A	1603	1/1	0.06	-2.33	62,62,62,62	0
6	ZN	A	1602	1/1	0.03	-3.69	103,103,103,103	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.