



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:05 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 X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

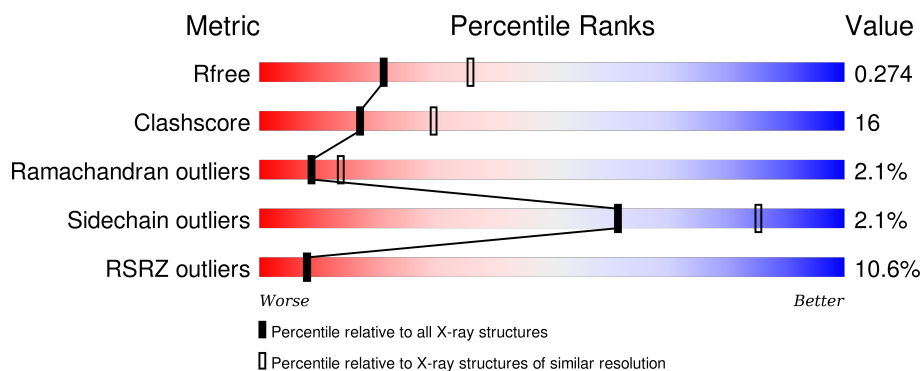
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	1002	<div> <div>10%</div> <div>66%</div> <div>28%</div> <div>••</div> </div>

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
4	MES	A	4	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	101	-	-	-	X
5	EDO	A	102	-	-	-	X
5	EDO	A	103	-	-	-	X
5	EDO	A	106	-	-	-	X
5	EDO	A	109	-	-	-	X
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

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7924 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.

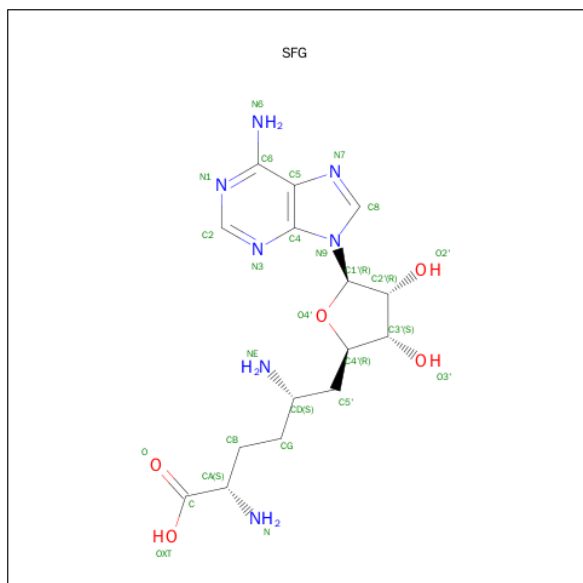
- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 1.

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

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>).



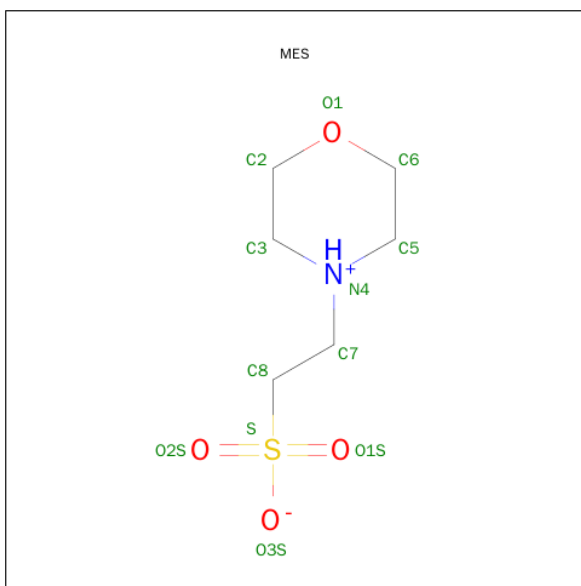
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	15	7	5		

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



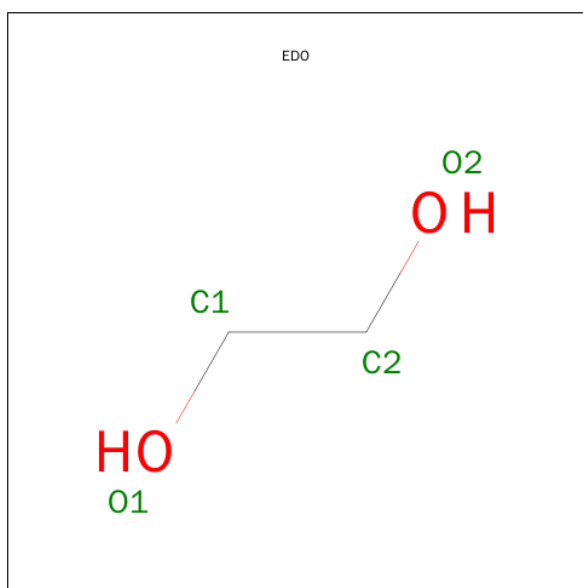
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



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		

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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) 92.0 (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 0.221 , 0.274	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> )	0.28 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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( $^{\circ}$ )	Ideal( $^{\circ}$ )
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 Too-close contacts [i](#)

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	7478	0	7108	242	0
2	A	27	0	22	0	0
3	A	5	0	0	0	0
4	A	24	0	26	1	0
5	A	100	0	150	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	4	0	0	0	0
7	A	286	0	0	8	0
All	All	7924	0	7306	242	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 16.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:ARG:O	1:A:752:ILE:HA	2.08	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:862:THR:HG22	1:A:863:TYR:O	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	959/1002 (96%)	862 (90%)	77 (8%)	20 (2%)	<b>9</b> <b>14</b>

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

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Mol	Chain	Res	Type
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%)	61 85

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
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 molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no 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	0.24	0	6,6,6	0.09	0
5	EDO	A	101	-	3,3,3	0.56	0	2,2,2	0.36	0
5	EDO	A	102	-	3,3,3	0.63	0	2,2,2	0.32	0
5	EDO	A	103	-	3,3,3	0.43	0	2,2,2	0.48	0
5	EDO	A	104	-	3,3,3	0.58	0	2,2,2	0.34	0
5	EDO	A	105	-	3,3,3	0.48	0	2,2,2	0.42	0
5	EDO	A	106	-	3,3,3	0.59	0	2,2,2	0.31	0
5	EDO	A	107	-	3,3,3	0.52	0	2,2,2	0.38	0
5	EDO	A	108	-	3,3,3	0.53	0	2,2,2	0.40	0
5	EDO	A	109	-	3,3,3	0.50	0	2,2,2	0.40	0
5	EDO	A	110	-	3,3,3	0.53	0	2,2,2	0.36	0
5	EDO	A	111	-	3,3,3	0.41	0	2,2,2	0.48	0
5	EDO	A	112	-	3,3,3	0.53	0	2,2,2	0.39	0
5	EDO	A	113	-	3,3,3	0.48	0	2,2,2	0.39	0
5	EDO	A	114	-	3,3,3	0.57	0	2,2,2	0.33	0
5	EDO	A	115	-	3,3,3	0.51	0	2,2,2	0.35	0
5	EDO	A	116	-	3,3,3	0.55	0	2,2,2	0.34	0
5	EDO	A	117	-	3,3,3	0.39	0	2,2,2	0.47	0
5	EDO	A	118	-	3,3,3	0.49	0	2,2,2	0.39	0
5	EDO	A	119	-	3,3,3	0.50	0	2,2,2	0.38	0
5	EDO	A	120	-	3,3,3	0.57	0	2,2,2	0.34	0
5	EDO	A	121	-	3,3,3	0.48	0	2,2,2	0.41	0
5	EDO	A	122	-	3,3,3	0.54	0	2,2,2	0.34	0
5	EDO	A	123	-	3,3,3	0.51	0	2,2,2	0.39	0
5	EDO	A	124	-	3,3,3	0.50	0	2,2,2	0.38	0
5	EDO	A	125	-	3,3,3	0.48	0	2,2,2	0.43	0
4	MES	A	2	-	11,12,12	0.82	0	14,16,16	1.35	2 (14%)
2	SFG	A	300	-	21,29,29	1.88	3 (14%)	19,42,42	2.67	6 (31%)
4	MES	A	4	-	11,12,12	0.73	0	14,16,16	1.31	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-	-	0/9/33/33	0/3/3/3
4	MES	A	4	-	-	0/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	SFG	C2-N3	3.40	1.38	1.32
2	A	300	SFG	C5'-C4'	4.11	1.59	1.52
2	A	300	SFG	O4'-C1'	5.17	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	SFG	N3-C2-N1	-8.49	122.39	128.89
2	A	300	SFG	C1'-N9-C4	-3.83	121.17	126.94
2	A	300	SFG	CG-CD-NE	2.01	115.01	109.13
4	A	4	MES	O2S-S-C8	2.39	108.94	106.91
2	A	300	SFG	C2-N1-C6	2.62	123.44	118.77
4	A	2	MES	O1S-S-C8	2.78	109.28	106.91
2	A	300	SFG	CB-CA-N	2.78	118.44	110.52
4	A	4	MES	O1S-S-C8	3.27	109.70	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2	MES	O2S-S-C8	3.41	109.81	106.91
2	A	300	SFG	C4'-O4'-C1'	4.62	114.80	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	102	EDO	1	0
5	A	104	EDO	1	0
5	A	106	EDO	3	0
5	A	113	EDO	3	0
5	A	115	EDO	1	0
5	A	116	EDO	4	0
5	A	119	EDO	1	0
5	A	120	EDO	1	0
5	A	123	EDO	3	0
5	A	124	EDO	1	0
4	A	4	MES	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, 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%)	0.37	102 (10%) 8   8	26, 50, 108, 137	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	855	LEU	8.9
1	A	980	ILE	7.9
1	A	682	SER	7.5
1	A	956	VAL	6.6
1	A	1130	PRO	6.4
1	A	681	ARG	6.2
1	A	648	PHE	6.0
1	A	678	GLY	5.8
1	A	677	GLY	5.8
1	A	983	SER	5.7
1	A	1005	SER	5.6
1	A	853	SER	5.5
1	A	858	ASP	5.4
1	A	700	ASP	5.4
1	A	955	PRO	5.2
1	A	961	LYS	5.1
1	A	952	LEU	5.0
1	A	679	SER	4.9
1	A	890	PHE	4.9
1	A	676	PHE	4.8
1	A	982	GLY	4.7
1	A	976	TYR	4.7
1	A	856	GLU	4.7
1	A	854	LEU	4.6
1	A	647	ALA	4.6
1	A	684	GLN	4.5
1	A	606	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	954	SER	4.4
1	A	646	ASN	4.2
1	A	984	ASN	4.2
1	A	636	ILE	4.2
1	A	1132	ILE	4.1
1	A	859	ASP	4.1
1	A	690	ARG	4.1
1	A	667	CYS	4.0
1	A	683	LYS	4.0
1	A	958	ARG	3.9
1	A	711	GLU	3.9
1	A	985	LEU	3.9
1	A	1129	GLU	3.8
1	A	1444	VAL	3.7
1	A	979	TYR	3.7
1	A	1004	LYS	3.7
1	A	959	PRO	3.5
1	A	709	ILE	3.5
1	A	666	LYS	3.5
1	A	607	SER	3.4
1	A	1286	CYS	3.4
1	A	729	ASN	3.4
1	A	615	PRO	3.3
1	A	730	ARG	3.3
1	A	674	VAL	3.3
1	A	953	SER	3.3
1	A	664	CYS	3.3
1	A	685	ALA	3.3
1	A	1600	ALA	3.3
1	A	673	MET	3.2
1	A	1315	ILE	3.2
1	A	635	GLN	3.2
1	A	608	THR	3.1
1	A	1287	LEU	3.1
1	A	1264	LEU	3.0
1	A	1317	ALA	3.0
1	A	1451	MET	3.0
1	A	1284	LEU	3.0
1	A	675	LYS	3.0
1	A	957	LYS	2.9
1	A	1265	LEU	2.9
1	A	1536	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	716	LYS	2.9
1	A	1283	THR	2.8
1	A	603	THR	2.7
1	A	981	LYS	2.7
1	A	887	ASP	2.7
1	A	604	ILE	2.6
1	A	680	GLY	2.6
1	A	1008	ARG	2.6
1	A	634	GLU	2.6
1	A	1405	TYR	2.5
1	A	1506	ARG	2.5
1	A	669	ALA	2.5
1	A	1222	GLY	2.5
1	A	1221	CYS	2.4
1	A	649	LYS	2.4
1	A	852	GLU	2.4
1	A	706	ASP	2.4
1	A	1288	VAL	2.4
1	A	909	ARG	2.3
1	A	962	GLU	2.3
1	A	687	GLN	2.3
1	A	1106	PRO	2.2
1	A	924	TYR	2.2
1	A	1263	PHE	2.2
1	A	1406	GLN	2.2
1	A	1251	PHE	2.2
1	A	609	ARG	2.2
1	A	1481	ALA	2.2
1	A	734	VAL	2.1
1	A	1482	GLY	2.1
1	A	921	VAL	2.1
1	A	689	ARG	2.0
1	A	1282	LEU	2.0

## 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	A	106	4/4	0.83	0.47	12.86	60,62,64,64	0
5	EDO	A	101	4/4	0.84	0.37	8.28	53,53,55,55	0
5	EDO	A	109	4/4	0.78	0.32	6.19	90,91,91,92	0
5	EDO	A	122	4/4	0.82	0.30	6.02	76,77,78,78	0
5	EDO	A	113	4/4	0.92	0.29	6.00	57,59,61,64	0
5	EDO	A	102	4/4	0.91	0.23	5.99	42,46,47,48	0
5	EDO	A	119	4/4	0.86	0.64	3.80	87,88,89,89	0
4	MES	A	4	12/12	0.88	0.25	3.25	115,117,119,119	0
5	EDO	A	110	4/4	0.86	0.36	3.19	75,76,76,76	0
5	EDO	A	117	4/4	0.97	0.21	2.16	53,55,56,56	0
5	EDO	A	103	4/4	0.95	0.17	2.12	55,56,56,56	0
5	EDO	A	105	4/4	0.90	0.16	1.89	62,63,65,65	0
5	EDO	A	108	4/4	0.89	0.17	1.50	70,71,71,72	0
5	EDO	A	118	4/4	0.97	0.17	1.49	40,43,43,44	0
5	EDO	A	121	4/4	0.89	0.20	1.43	76,77,77,79	0
5	EDO	A	115	4/4	0.82	0.29	1.18	68,72,73,74	0
5	EDO	A	114	4/4	0.91	0.19	0.76	52,53,54,54	0
5	EDO	A	112	4/4	0.87	0.15	0.62	71,72,72,73	0
5	EDO	A	120	4/4	0.85	0.20	0.42	81,83,83,84	0
3	SO4	A	1	5/5	0.84	0.20	0.42	111,112,112,112	0
2	SFG	A	300	27/27	0.92	0.18	0.39	49,55,58,59	0
4	MES	A	2	12/12	0.95	0.12	0.30	67,69,76,77	0
6	ZN	A	1601	1/1	0.98	0.10	-1.11	70,70,70,70	0
6	ZN	A	1602	1/1	0.92	0.04	-3.37	103,103,103,103	0
6	ZN	A	3	1/1	0.98	0.12	-	50,50,50,50	0
6	ZN	A	1603	1/1	0.99	0.07	-	62,62,62,62	0
5	EDO	A	104	4/4	0.92	0.15	-	51,51,51,52	0
5	EDO	A	125	4/4	0.84	0.31	-	75,78,79,81	0
5	EDO	A	116	4/4	0.27	0.55	-	85,85,86,86	0
5	EDO	A	124	4/4	0.84	0.26	-	68,69,69,69	0
5	EDO	A	107	4/4	0.91	0.17	-	63,64,64,65	0
5	EDO	A	111	4/4	0.96	0.13	-	49,51,53,56	0
5	EDO	A	123	4/4	0.82	0.29	-	69,69,69,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.