



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:35 PM UTC

PDB ID : 3SWR / pdb_00003swr
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

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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

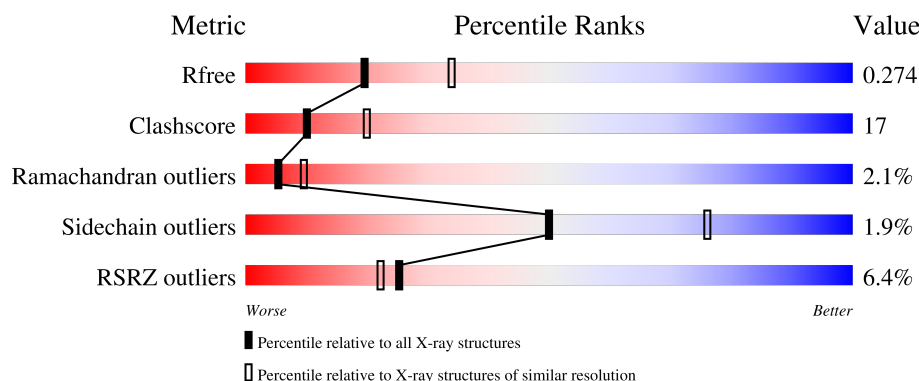
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	1002	

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
5	EDO	A	116	-	-	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.

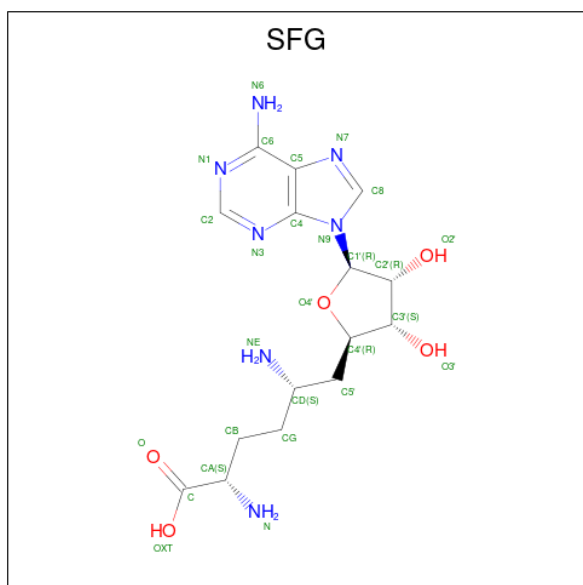
- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			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 (CCD ID: SFG) (formula: C₁₅H₂₃N₇O₅).



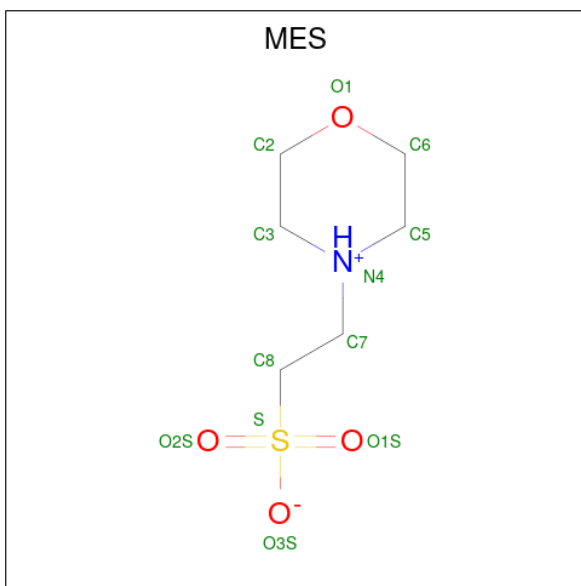
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	27	15	7	5	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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 (CCD ID: EDO) (formula: C₂H₆O₂).



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 (CCD ID: ZN) (formula: Zn).

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

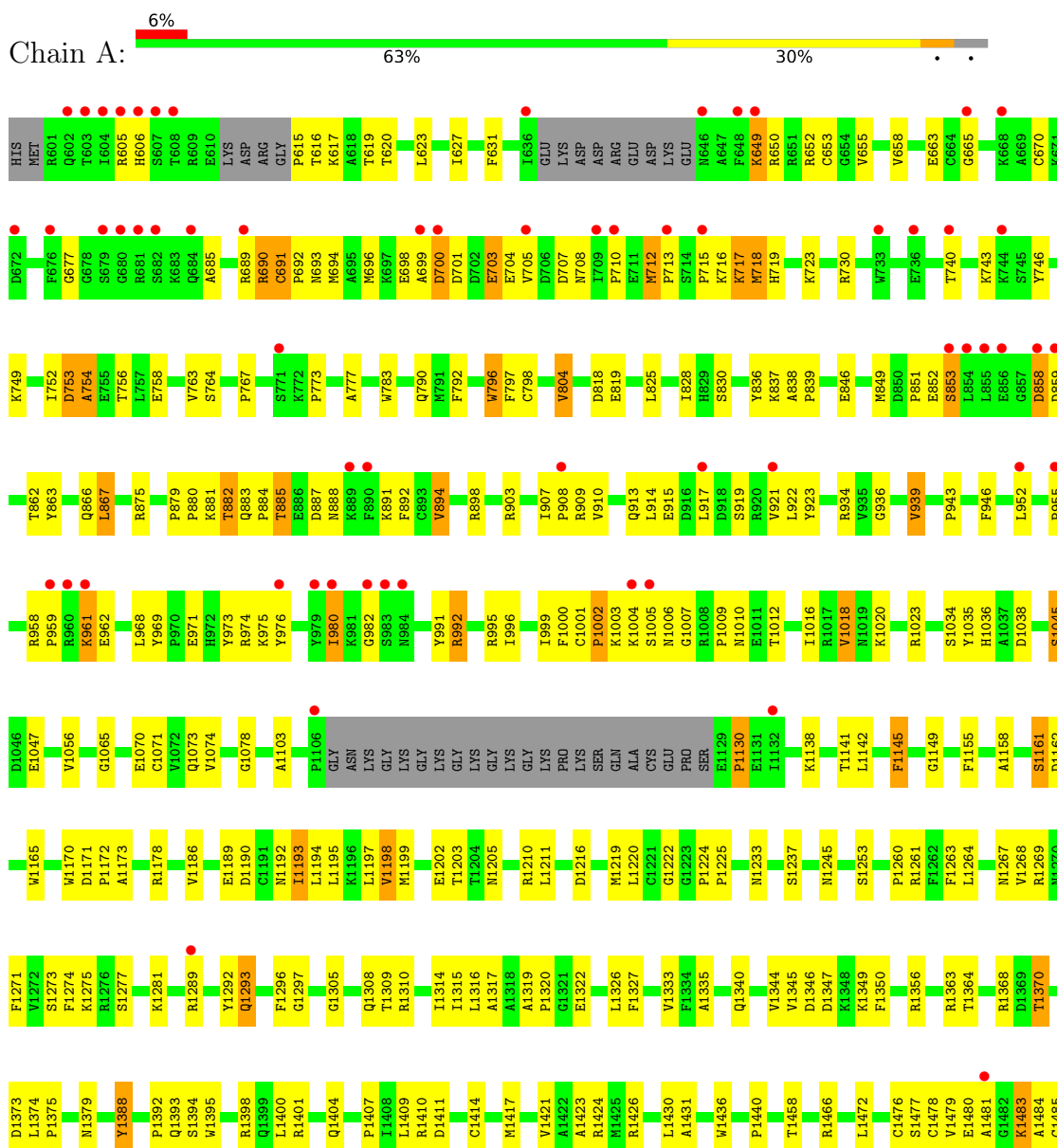
- Molecule 7 is water.

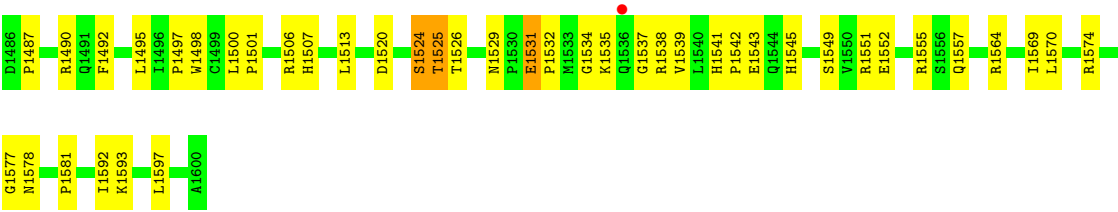
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	286	Total O 286 286	0	0

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: DNA (cytosine-5)-methyltransferase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.00Å 110.77Å 201.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.49 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-2.49) 91.9 (30.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	2317 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7924	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: MES, ZN, EDO, SO4, SFG

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	0.41	0/7656	0.97	38/10378 (0.4%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1539	VAL	N-CA-C	10.90	122.46	112.43
1	A	959	PRO	N-CA-CB	7.85	110.18	103.35
1	A	1023	ARG	N-CA-C	-7.81	100.24	110.39
1	A	992	ARG	N-CA-C	-7.61	99.22	110.48
1	A	1293	GLN	N-CA-C	-7.54	97.30	109.96
1	A	631	PHE	N-CA-C	7.46	121.56	110.52
1	A	1161	SER	N-CA-C	7.36	120.10	109.14
1	A	1524	SER	N-CA-C	-7.28	100.03	110.59
1	A	1145	PHE	N-CA-C	-6.94	101.80	111.52
1	A	797	PHE	N-CA-C	-6.68	100.58	110.46
1	A	1531	GLU	CA-C-N	6.62	126.40	119.05
1	A	1531	GLU	C-N-CA	6.62	126.40	119.05
1	A	1537	GLY	N-CA-C	6.57	128.74	113.18
1	A	1370	THR	N-CA-C	6.56	119.76	111.69
1	A	1130	PRO	N-CA-CB	6.41	109.98	103.25
1	A	955	PRO	N-CA-CB	6.20	109.89	103.38
1	A	1141	THR	N-CA-C	6.17	119.00	109.07
1	A	1538	ARG	N-CA-C	-6.16	94.79	107.67
1	A	1149	GLY	N-CA-C	6.02	123.44	114.95
1	A	969	TYR	CA-C-N	5.96	125.51	119.19
1	A	969	TYR	C-N-CA	5.96	125.51	119.19
1	A	1395	TRP	N-CA-C	-5.85	104.91	111.28
1	A	1335	ALA	CA-C-N	5.79	125.26	119.24
1	A	1335	ALA	C-N-CA	5.79	125.26	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1038	ASP	N-CA-C	-5.68	102.63	110.35
1	A	1078	GLY	N-CA-C	5.64	121.65	114.66
1	A	1065	GLY	N-CA-C	5.63	119.70	112.83
1	A	1271	PHE	N-CA-C	-5.61	105.16	111.28
1	A	712	MET	N-CA-C	5.50	113.17	108.22
1	A	867	LEU	N-CA-C	5.42	117.65	109.41
1	A	1388	TYR	N-CA-C	-5.38	105.98	112.54
1	A	1411	ASP	N-CA-C	5.35	118.96	111.90
1	A	1305	GLY	N-CA-C	5.28	123.49	115.63
1	A	885	THR	N-CA-C	-5.16	103.22	110.50
1	A	691	CYS	CA-C-N	5.10	124.71	119.56
1	A	691	CYS	C-N-CA	5.10	124.71	119.56
1	A	1018	VAL	N-CA-C	5.09	116.18	108.96
1	A	796	TRP	N-CA-C	5.05	117.22	110.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7478	0	7108	259	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
6	A	4	0	0	0	0
7	A	286	0	0	8	0
All	All	7924	0	7306	259	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 17.

All (259) 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:712:MET:HE3	1:A:1349:LYS:HB2	1.62	0.80
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:650:ARG:HH21	1:A:694:MET:HB3	1.52	0.74
1:A:700:ASP:HA	1:A:1268:VAL:CG1	2.18	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:HD2	1:A:743:LYS:H	1.54	0.73
1:A:763:VAL:CG2	1:A:828:ILE:HG23	2.19	0.73
1:A:1189:GLU:OE2	1:A:1193:ILE:HD11	1.89	0.73
1:A:1404:GLN:OE1	1:A:1407:PRO:HA	1.88	0.73
1:A:649:LYS:HD3	1:A:649:LYS:N	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
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:O	1:A:907:ILE:HG13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1193:ILE:C	1:A:1193:ILE:HD12	2.26	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:846:GLU:HA	1:A:849:MET:HE3	1.85	0.59
1:A:696:MET:HE3	1:A:696:MET:HA	1.84	0.59
1:A:1016:ILE:HG22	1:A:1018:VAL:HG13	1.85	0.59
1:A:1404:GLN:CD	1:A:1407:PRO:HA	2.27	0.58
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:980:ILE:C	1:A:982:GLY:H	2.13	0.57
1:A:701:ASP:C	1:A:703:GLU:H	2.13	0.57
1:A:763:VAL:HG21	1:A:828:ILE:HG12	1.86	0.57
1:A:690:ARG:HD2	1:A:690:ARG:O	2.04	0.57
1:A:708:ASN:HA	1:A:1340:GLN:OE1	2.05	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:663:GLU:HB3	1:A:670:CYS:SG	2.45	0.56
1:A:699:ALA:O	1:A:701:ASP:N	2.35	0.56
1:A:1189:GLU:CD	1:A:1193:ILE:HD11	2.31	0.55
1:A:999:ILE:HA	1:A:1016:ILE:HD13	1.86	0.55
1:A:1219:MET:HE1	1:A:1592:ILE:HG21	1.87	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:961:LYS:O	1:A:962:GLU:HG2	2.07	0.55
1:A:1310:ARG:HG3	1:A:1525:THR:HG23	1.88	0.55
1:A:705:VAL:HG13	5:A:120:EDO:O2	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:730:ARG:O	1:A:752:ILE:HA	2.08	0.54
1:A:752:ILE:O	1:A:753:ASP:C	2.50	0.54
1:A:1490:ARG:HD3	1:A:1492:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ASP:OD2	1:A:898:ARG:NH1	2.41	0.54
1:A:907:ILE:O	1:A:908:PRO:C	2.51	0.54
1:A:1424:ARG:CZ	1:A:1497:PRO:HG3	2.38	0.54
1:A:1004:LYS:C	1:A:1006:ASN:H	2.16	0.53
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: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:903:ARG:O	1:A:907:ILE:HG23	2.09	0.52
1:A:1210:ARG:HH11	1:A:1210:ARG:HG2	1.74	0.52
1:A:915:GLU:CD	1:A:917:LEU:HD21	2.35	0.52
1:A:1297:GLY:HA2	5:A:102:EDO:H21	1.92	0.52
1:A:1524:SER:O	1:A:1525:THR:C	2.52	0.51
1:A:884:PRO:HG3	1:A:892:PHE:CD2	2.45	0.51
1:A:606:HIS:C	1:A:685:ALA:HB2	2.34	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:1194:LEU:C	1:A:1194:LEU:HD23	2.35	0.51
1:A:1315:ILE:HD12	1:A:1315:ILE:N	2.26	0.51
1:A:888:ASN:O	1:A:892:PHE:HB2	2.11	0.51
1:A:858:ASP:O	1:A:862:THR:HB	2.11	0.51
1:A:653:CYS:O	1:A:653:CYS:SG	2.70	0.50
1:A:1485:CYS:O	1:A:1487:PRO:HD3	2.12	0.50
1:A:881:LYS:O	1:A:882:THR:C	2.54	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:971:GLU:HG3	1:A:1436:TRP:HZ3	1.77	0.49
1:A:1193:ILE:HD12	1:A:1194:LEU:N	2.28	0.49
1:A:792:PHE:HB3	1:A:825:LEU:HD21	1.95	0.49
1:A:1513:LEU:N	1:A:1513:LEU:HD12	2.28	0.49
1:A:753:ASP:O	1:A:754:ALA:CB	2.60	0.49
1:A:1277:SER:O	1:A:1281:LYS:HG3	2.13	0.49
1:A:1426:ARG:HA	1:A:1545:HIS:ND1	2.27	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:973:TYR:C	1:A:975:LYS:H	2.20	0.48
1:A:619:THR:CG2	1:A:1199:MET:HE2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:MET:HE1	1:A:1344:VAL:HG13	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:980:ILE:C	1:A:982:GLY:N	2.71	0.47
1:A:1293:GLN:O	1:A:1317:ALA:HA	2.15	0.47
1:A:1534:GLY:O	1:A:1535:LYS:C	2.57	0.47
1:A:1345:VAL:HA	5:A:113:EDO:H12	1.95	0.47
1:A:914:LEU:H	1:A:914:LEU:HD23	1.79	0.47
1:A:996:ILE:HA	1:A:1018:VAL:HG12	1.97	0.47
1:A:777:ALA:HB2	1:A:796:TRP:CE3	2.50	0.47
1:A:836:TYR:CE1	4:A:4:MES:H21	2.49	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:921:VAL:CG2	1:A:1009:PRO:HB3	2.45	0.47
1:A:922:LEU:HD22	1:A:1000:PHE:HB3	1.95	0.47
1:A:1165:TRP:NE1	5:A:116:EDO:H12	2.28	0.47
1:A:1273:SER:O	1:A:1274:PHE:C	2.58	0.47
1:A:1541:HIS:CG	1:A:1542:PRO:HD2	2.50	0.47
1:A:623:LEU:C	1:A:623:LEU:HD23	2.40	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: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:1400:LEU:HD23	1:A:1555:ARG:CD	2.46	0.46
1:A:1269:ARG:HD3	1:A:1269:ARG:C	2.40	0.46
1:A:1222:GLY:HA2	7:A:213:HOH:O	2.16	0.46
1:A:707:ASP:O	1:A:710:PRO:HD3	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:1034:SER:HB2	1:A:1363:ARG:NE	2.31	0.46
1:A:1020:LYS:HD2	1:A:1047:GLU:HB3	1.98	0.45
1:A:1400:LEU:HD23	1:A:1555:ARG:HD2	1.98	0.45
1:A:875:ARG:HD2	7:A:64:HOH:O	2.16	0.45
1:A:921:VAL:HG22	1:A:1009:PRO:HB3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1210:ARG:NH1	1:A:1210:ARG:HG2	2.32	0.45
1:A:1375:PRO:HG3	1:A:1388:TYR:O	2.17	0.45
1:A:885:THR:C	1:A:887:ASP:H	2.24	0.45
1:A:1481:ALA:C	1:A:1483:LYS:H	2.25	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:1219:MET:CE	1:A:1592:ILE:HG21	2.48	0.44
1:A:1525:THR:O	1:A:1526:THR:C	2.60	0.44
1:A:627:ILE:HD11	1:A:1289[A]:ARG:HG2	2.00	0.44
1:A:914:LEU:HD22	1:A:923:TYR:C	2.43	0.44
1:A:1373:ASP:HA	1:A:1393:GLN:NE2	2.33	0.44
1:A:1392:PRO:HG3	1:A:1401:ARG:HD3	1.99	0.44
1:A:701:ASP:CG	1:A:703:GLU:HB2	2.42	0.44
1:A:1417:MET:HE3	1:A:1421:VAL:HG11	1.99	0.43
1:A:1458:THR:HG21	7:A:207:HOH:O	2.17	0.43
1:A:837:LYS:HD2	1:A:859:ASP:OD2	2.18	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:617:LYS:HA	1:A:1245:ASN:OD1	2.18	0.43
1:A:1142:LEU:O	1:A:1220:LEU:HD12	2.19	0.43
1:A:712:MET:HE2	1:A:1344:VAL:HG22	2.00	0.43
1:A:705:VAL:HG12	1:A:705:VAL:O	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:718:MET:HE1	1:A:798:CYS:SG	2.58	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:952:LEU:C	1:A:952:LEU:HD23	2.44	0.43
1:A:615:PRO:HG2	1:A:617:LYS:H	1.83	0.43
1:A:746:TYR:CD1	1:A:783:TRP:HB3	2.54	0.43
1:A:749:LYS:HE2	1:A:758:GLU:CG	2.49	0.43
1:A:804:VAL:HG22	1:A:1350:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:ARG:HH11	1:A:934:ARG:HG3	1.84	0.43
1:A:1478:CYS:C	1:A:1480:GLU:H	2.26	0.43
1:A:1531:GLU:HA	1:A:1532:PRO:HD3	1.87	0.43
1:A:1070:GLU:HB2	7:A:196:HOH:O	2.18	0.42
1:A:1333:VAL:O	1:A:1364:THR:HB	2.19	0.42
1:A:1379:ASN:ND2	1:A:1417:MET:H	2.06	0.42
1:A:719:HIS:ND1	1:A:819:GLU:OE1	2.45	0.42
1:A:693:ASN:CG	1:A:1529:ASN:HD21	2.28	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:971:GLU:OE1	1:A:974:ARG:NH2	2.50	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:HG3	1:A:1436:TRP:CZ3	2.54	0.42
1:A:752:ILE:O	1:A:752:ILE:HG13	2.20	0.42
1:A:1001:CYS:HB3	1:A:1010:ASN:O	2.19	0.42
1:A:883:GLN:HA	1:A:884:PRO:HD3	1.73	0.42
1:A:1314:ILE:C	1:A:1315:ILE:HD12	2.45	0.42
1:A:1524:SER:O	1:A:1526:THR:N	2.52	0.42
1:A:1574:ARG:HG3	1:A:1578:ASN:HD21	1.84	0.42
1:A:1170:TRP:CD1	1:A:1172:PRO:HD2	2.54	0.42
1:A:1430:LEU:H	5:A:123:EDO:C1	2.31	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:740:THR:O	1:A:740:THR:HG22	2.20	0.41
1:A:1020:LYS:O	1:A:1045:SER:HB3	2.19	0.41
1:A:616:THR:HG22	1:A:616:THR:O	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:879:PRO:HA	1:A:880:PRO:HD3	1.81	0.41
1:A:888:ASN:HB2	1:A:891:LYS:HG3	2.03	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:717:LYS:O	1:A:718:MET:C	2.63	0.41
1:A:1296:PHE:HA	1:A:1314:ILE:O	2.20	0.41
1:A:1346:ASP:O	1:A:1347:ASP:HB2	2.21	0.41
1:A:691:CYS:HA	1:A:692:PRO:HD3	1.81	0.41
1:A:852:GLU:O	1:A:853:SER:HB3	2.21	0.41
1:A:1498:TRP:O	1:A:1501:PRO:HD2	2.21	0.41
1:A:649:LYS:C	1:A:696:MET:HE1	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:999:ILE:HG23	1:A:1016:ILE:HD11	2.03	0.40
1:A:1205:ASN:HA	5:A:115:EDO:H12	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:699:ALA:C	1:A:701:ASP:N	2.79	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:1495:LEU:HD12	1:A:1495:LEU:HA	1.91	0.40
1:A:1569:ILE:HG23	1:A:1570:LEU:N	2.36	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%)	5 9

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

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Mol	Chain	Res	Type
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%)	765 (98%)	15 (2%)	50	76

All (15) 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	804	VAL
1	A	894	VAL
1	A	939	VAL
1	A	980	ILE
1	A	1045	SER
1	A	1138	LYS
1	A	1162	ASP
1	A	1193	ILE
1	A	1198	VAL
1	A	1237	SER
1	A	1564	ARG
1	A	1597	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	708	ASN
1	A	824	GLN
1	A	888	ASN
1	A	1010	ASN
1	A	1036	HIS
1	A	1073	GLN
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	1529	ASN
1	A	1578	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 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$
5	EDO	A	104	-	3,3,3	0.53	0	2,2,2	0.30	0
5	EDO	A	103	-	3,3,3	0.38	0	2,2,2	0.43	0
5	EDO	A	125	-	3,3,3	0.43	0	2,2,2	0.38	0
4	MES	A	4	-	12,12,12	1.06	1 (8%)	15,16,16	1.02	0
5	EDO	A	121	-	3,3,3	0.42	0	2,2,2	0.37	0
5	EDO	A	110	-	3,3,3	0.48	0	2,2,2	0.32	0
5	EDO	A	101	-	3,3,3	0.51	0	2,2,2	0.32	0
5	EDO	A	105	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	A	109	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	A	112	-	3,3,3	0.48	0	2,2,2	0.35	0
4	MES	A	2	-	12,12,12	1.22	1 (8%)	15,16,16	1.03	1 (6%)
5	EDO	A	117	-	3,3,3	0.34	0	2,2,2	0.42	0
5	EDO	A	120	-	3,3,3	0.52	0	2,2,2	0.30	0
5	EDO	A	115	-	3,3,3	0.47	0	2,2,2	0.31	0
2	SFG	A	300	-	28,29,29	1.71	6 (21%)	34,42,42	1.80	8 (23%)
5	EDO	A	118	-	3,3,3	0.44	0	2,2,2	0.34	0
5	EDO	A	116	-	3,3,3	0.50	0	2,2,2	0.30	0
5	EDO	A	106	-	3,3,3	0.54	0	2,2,2	0.27	0
5	EDO	A	102	-	3,3,3	0.58	0	2,2,2	0.28	0
5	EDO	A	107	-	3,3,3	0.47	0	2,2,2	0.34	0
5	EDO	A	111	-	3,3,3	0.36	0	2,2,2	0.43	0
5	EDO	A	122	-	3,3,3	0.49	0	2,2,2	0.30	0
5	EDO	A	124	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	A	114	-	3,3,3	0.52	0	2,2,2	0.29	0
3	SO4	A	1	-	4,4,4	0.38	0	6,6,6	0.11	0
5	EDO	A	108	-	3,3,3	0.48	0	2,2,2	0.36	0
5	EDO	A	119	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	A	123	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	A	113	-	3,3,3	0.43	0	2,2,2	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	104	-	-	0/1/1/1	-
5	EDO	A	103	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	125	-	-	1/1/1/1	-
4	MES	A	4	-	-	0/6/14/14	0/1/1/1
5	EDO	A	121	-	-	1/1/1/1	-
5	EDO	A	110	-	-	0/1/1/1	-
5	EDO	A	101	-	-	1/1/1/1	-
5	EDO	A	105	-	-	0/1/1/1	-
5	EDO	A	109	-	-	1/1/1/1	-
5	EDO	A	112	-	-	1/1/1/1	-
4	MES	A	2	-	-	0/6/14/14	0/1/1/1
5	EDO	A	117	-	-	0/1/1/1	-
5	EDO	A	120	-	-	1/1/1/1	-
5	EDO	A	115	-	-	1/1/1/1	-
2	SFG	A	300	-	-	2/17/33/33	0/3/3/3
5	EDO	A	118	-	-	0/1/1/1	-
5	EDO	A	116	-	-	1/1/1/1	-
5	EDO	A	106	-	-	0/1/1/1	-
5	EDO	A	102	-	-	1/1/1/1	-
5	EDO	A	107	-	-	1/1/1/1	-
5	EDO	A	111	-	-	1/1/1/1	-
5	EDO	A	122	-	-	1/1/1/1	-
5	EDO	A	124	-	-	1/1/1/1	-
5	EDO	A	114	-	-	0/1/1/1	-
5	EDO	A	108	-	-	1/1/1/1	-
5	EDO	A	119	-	-	0/1/1/1	-
5	EDO	A	123	-	-	1/1/1/1	-
5	EDO	A	113	-	-	1/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	SFG	C1'-N9	-4.41	1.34	1.46
2	A	300	SFG	C5'-C4'	3.87	1.59	1.52
4	A	2	MES	C8-S	3.05	1.81	1.77
2	A	300	SFG	C4-N9	3.05	1.44	1.37
4	A	4	MES	C8-S	2.65	1.81	1.77
2	A	300	SFG	O4'-C1'	2.48	1.47	1.42
2	A	300	SFG	C2-N3	2.40	1.38	1.33
2	A	300	SFG	C5-N7	2.21	1.43	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	SFG	O4'-C1'-C2'	-4.61	96.75	106.62
2	A	300	SFG	N3-C2-N1	-4.09	122.39	128.58
2	A	300	SFG	C1'-N9-C8	3.71	135.32	127.09
2	A	300	SFG	CB-CA-N	3.19	118.44	110.12
2	A	300	SFG	C2-N1-C6	2.87	123.44	118.73
2	A	300	SFG	C4'-O4'-C1'	2.41	114.80	109.47
2	A	300	SFG	C4-N9-C1'	-2.34	121.17	126.63
2	A	300	SFG	C4-N9-C8	-2.12	103.51	105.74
4	A	2	MES	O2S-S-C8	2.04	109.81	106.73

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	101	EDO	O1-C1-C2-O2
5	A	112	EDO	O1-C1-C2-O2
5	A	120	EDO	O1-C1-C2-O2
5	A	113	EDO	O1-C1-C2-O2
5	A	116	EDO	O1-C1-C2-O2
5	A	123	EDO	O1-C1-C2-O2
5	A	108	EDO	O1-C1-C2-O2
2	A	300	SFG	C2'-C1'-N9-C8
5	A	102	EDO	O1-C1-C2-O2
5	A	109	EDO	O1-C1-C2-O2
5	A	121	EDO	O1-C1-C2-O2
5	A	115	EDO	O1-C1-C2-O2
5	A	107	EDO	O1-C1-C2-O2
5	A	111	EDO	O1-C1-C2-O2
5	A	124	EDO	O1-C1-C2-O2
5	A	122	EDO	O1-C1-C2-O2
5	A	125	EDO	O1-C1-C2-O2
2	A	300	SFG	C4'-C5'-CD-NE

There are no ring outliers.

11 monomers are involved in 20 short contacts:

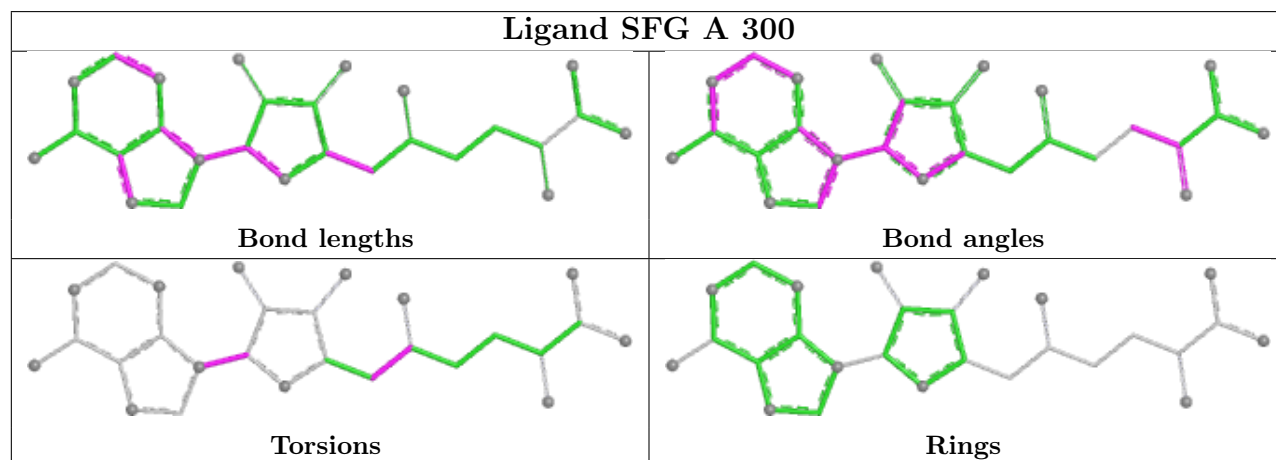
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	104	EDO	1	0
4	A	4	MES	1	0
5	A	120	EDO	1	0
5	A	115	EDO	1	0
5	A	116	EDO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	106	EDO	3	0
5	A	102	EDO	1	0
5	A	124	EDO	1	0
5	A	119	EDO	1	0
5	A	123	EDO	3	0
5	A	113	EDO	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	965/1002 (96%)	0.26	62 (6%)	25 22	20, 50, 108, 137	2 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	684	GLN	5.3
1	A	700	ASP	5.2
1	A	705	VAL	4.8
1	A	682	SER	4.8
1	A	890	PHE	4.5
1	A	604	ILE	4.4
1	A	606	HIS	4.2
1	A	608	THR	3.9
1	A	648	PHE	3.8
1	A	1005	SER	3.5
1	A	855	LEU	3.4
1	A	984	ASN	3.3
1	A	983	SER	3.3
1	A	607	SER	3.2
1	A	856	GLU	3.2
1	A	980	ILE	3.2
1	A	602	GLN	3.1
1	A	681	ARG	3.1
1	A	1536	GLN	2.9
1	A	713	PRO	2.9
1	A	854	LEU	2.9
1	A	636	ILE	2.8
1	A	710	PRO	2.8
1	A	917	LEU	2.8
1	A	699	ALA	2.8
1	A	709	ILE	2.7
1	A	603	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1481	ALA	2.7
1	A	668	LYS	2.7
1	A	858	ASP	2.6
1	A	921	VAL	2.6
1	A	889	LYS	2.6
1	A	908	PRO	2.6
1	A	1132	ILE	2.6
1	A	736	GLU	2.6
1	A	676	PHE	2.6
1	A	672	ASP	2.5
1	A	959	PRO	2.5
1	A	646	ASN	2.5
1	A	605	ARG	2.5
1	A	680	GLY	2.4
1	A	649	LYS	2.4
1	A	976	TYR	2.4
1	A	689	ARG	2.4
1	A	715	PRO	2.3
1	A	1289[A]	ARG	2.3
1	A	982	GLY	2.3
1	A	960	ARG	2.3
1	A	679	SER	2.3
1	A	952	LEU	2.3
1	A	740	THR	2.2
1	A	665	GLY	2.2
1	A	1106	PRO	2.2
1	A	733	TRP	2.2
1	A	955	PRO	2.2
1	A	853	SER	2.1
1	A	961	LYS	2.1
1	A	744	LYS	2.0
1	A	1004	LYS	2.0
1	A	859	ASP	2.0
1	A	771	SER	2.0
1	A	979	TYR	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 oligosaccharides 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. 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.

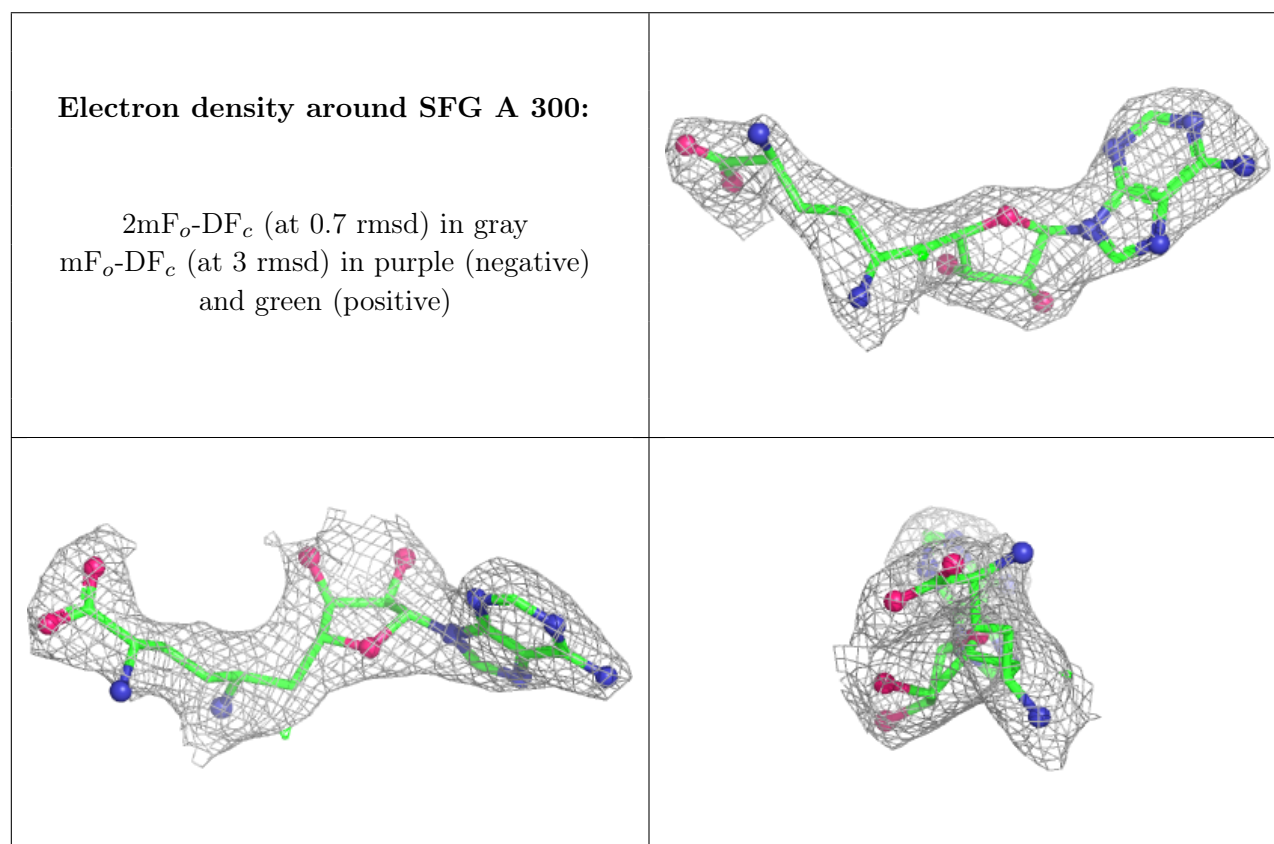
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	116	4/4	0.65	0.22	85,85,86,86	0
5	EDO	A	120	4/4	0.69	0.26	81,83,83,84	0
3	SO4	A	1	5/5	0.76	0.21	111,112,112,112	0
5	EDO	A	123	4/4	0.79	0.15	69,69,69,69	0
5	EDO	A	125	4/4	0.80	0.23	75,78,79,81	0
5	EDO	A	101	4/4	0.82	0.20	53,53,55,55	0
5	EDO	A	106	4/4	0.82	0.32	60,62,64,64	0
5	EDO	A	115	4/4	0.83	0.13	68,72,73,74	0
5	EDO	A	121	4/4	0.84	0.17	76,77,77,79	0
5	EDO	A	119	4/4	0.85	0.28	87,88,89,89	0
4	MES	A	4	12/12	0.86	0.21	115,117,119,119	0
5	EDO	A	110	4/4	0.86	0.18	75,76,76,76	0
5	EDO	A	105	4/4	0.86	0.14	62,63,65,65	0
5	EDO	A	124	4/4	0.87	0.17	68,69,69,69	0
5	EDO	A	122	4/4	0.87	0.19	76,77,78,78	0
5	EDO	A	108	4/4	0.88	0.16	70,71,71,72	0
4	MES	A	2	12/12	0.89	0.12	67,69,76,77	0
5	EDO	A	109	4/4	0.89	0.17	90,91,91,92	0
5	EDO	A	107	4/4	0.89	0.15	63,64,64,65	0
5	EDO	A	102	4/4	0.90	0.17	42,46,47,48	0
2	SFG	A	300	27/27	0.90	0.12	49,55,58,59	0
5	EDO	A	104	4/4	0.91	0.10	51,51,51,52	0
5	EDO	A	112	4/4	0.91	0.14	71,72,72,73	0
5	EDO	A	113	4/4	0.91	0.18	57,59,61,64	0
5	EDO	A	111	4/4	0.92	0.11	49,51,53,56	0
5	EDO	A	103	4/4	0.92	0.11	55,56,56,56	0
5	EDO	A	114	4/4	0.93	0.15	52,53,54,54	0
5	EDO	A	117	4/4	0.94	0.11	53,55,56,56	0
5	EDO	A	118	4/4	0.96	0.07	40,43,43,44	0
6	ZN	A	1602	1/1	0.96	0.05	103,103,103,103	0
6	ZN	A	1601	1/1	0.99	0.04	70,70,70,70	0
6	ZN	A	1603	1/1	0.99	0.03	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ZN	A	3	1/1	1.00	0.05	50,50,50,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.