Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 05:22 AM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

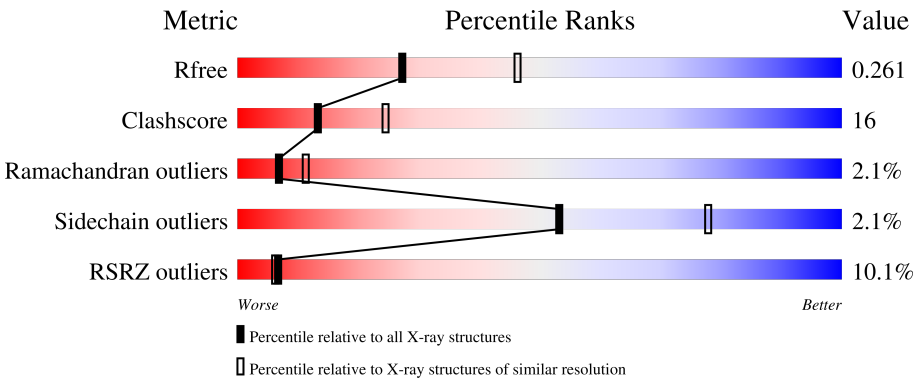
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	10% 66% 28%

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	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.

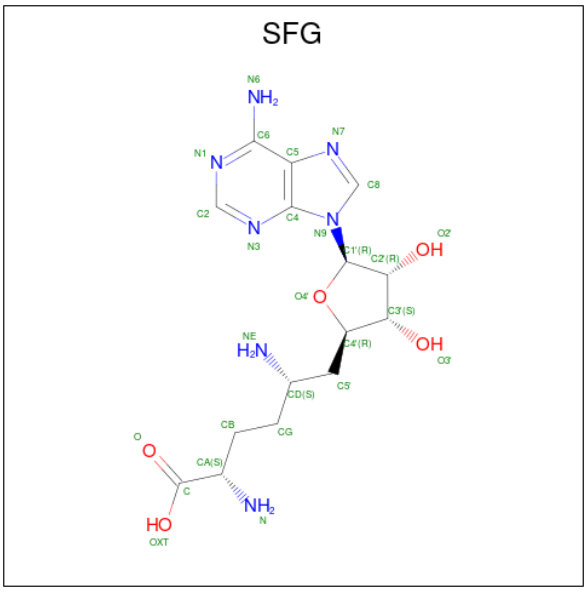
- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 1.

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:

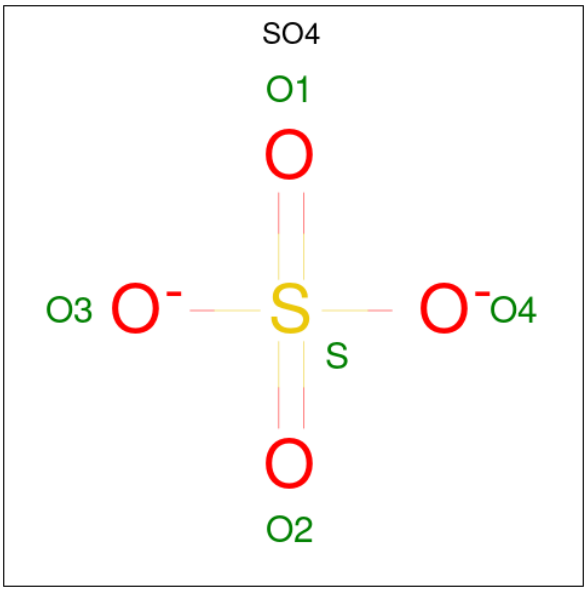
Chain	Residue	Modelled	Actual	Comment	Reference
A	599	HIS	-	expression tag	UNP P26358
A	600	MET	-	expression tag	UNP P26358

- Molecule 2 is SINEFUNGIN (three-letter code: SFG) (formula: $C_{15}H_{23}N_7O_5$).



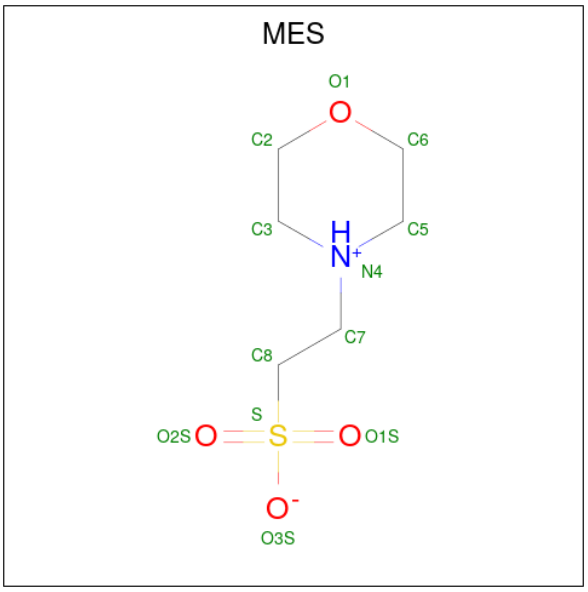
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	27	15	7	5	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



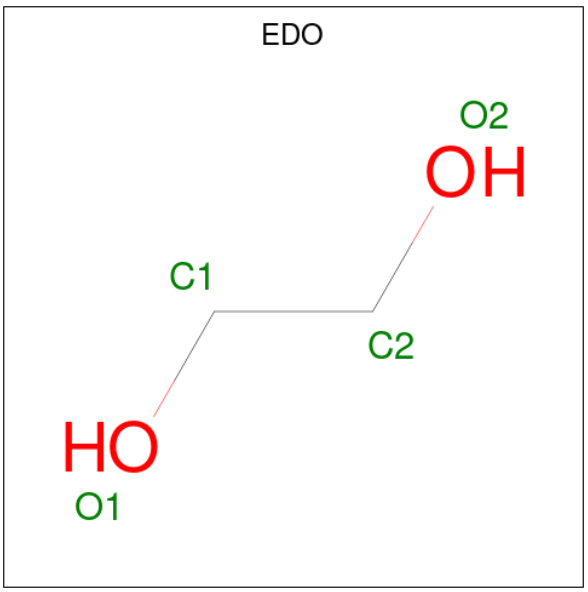
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0

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



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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

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

- Molecule 7 is water.

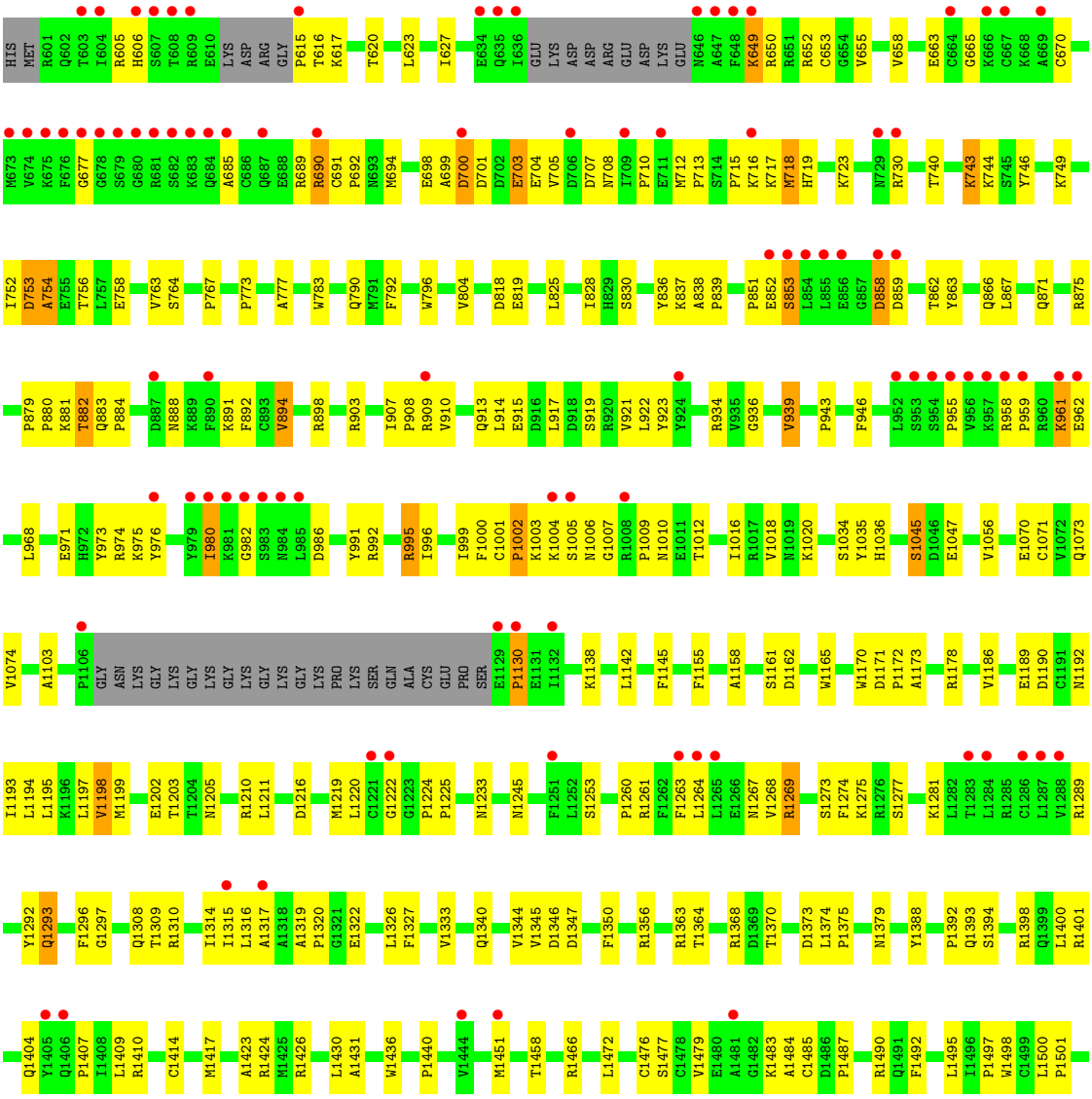
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	286	286	286	0	0

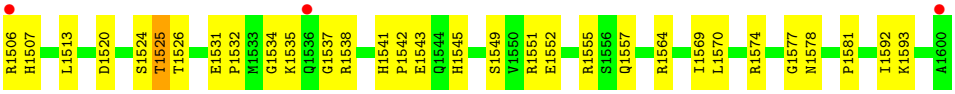
3 Residue-property plots (i)

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

Chain A:




R1506
H1507
L1513
D1520
S1524
T1525
T1526
E1531
P1532
M1533
G1534
K1535
Q1536
G1537
R1538
H1541
P1542
E1543
Q1544
H1545
S1549
V1550
R1551
E1552
R1555
S1556
Q1557
R1564
I1569
L1570
R1574
G1577
N1578
P1581
I1592
K1593
A1600

4 Data and refinement statistics (i)

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 30.01 – 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
$< I/\sigma(I) >$ [1]	2.85 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.220 , 0.272 0.211 , 0.261	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 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: EDO, SFG, ZN, 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(^{o})	Ideal(^{o})
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: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

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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: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
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: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:1219:MET:HE1	1:A:1592:ILE:HG21	1.87	0.55
1:A:999:ILE:HA	1:A:1016:ILE:HD13	1.86	0.55
1:A:1193:ILE:C	1:A:1193:ILE:HD12	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:730:ARG:O	1:A:752:ILE:HA	2.08	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:HH11	1:A:1210:ARG:HG2	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: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:1189:GLU:CD	1:A:1193:ILE:HD11	2.31	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: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: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: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: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: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: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:915:GLU:CD	1:A:917:LEU:HD21	2.35	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:1524:SER:O	1:A:1525:THR:C	2.52	0.47
1:A:1541:HIS:CG	1:A:1542:PRO:HD2	2.50	0.47
1:A:943:PRO:HA	1:A:992:ARG:HG2	1.97	0.47
1:A:606:HIS:C	1:A:685:ALA:HB2	2.34	0.46
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: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: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:881:LYS:O	1:A:882:THR:C	2.54	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: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: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:1392:PRO:HG3	1:A:1401:ARG:HD3	1.99	0.44
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: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:1178:ARG:HG3	1:A:1186:VAL:HG21	2.01	0.43
1:A:980:ILE:C	1:A:982:GLY:N	2.71	0.43
1:A:1368:ARG:NH2	1:A:1520:ASP:OD1	2.52	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
1:A:934:ARG:HH11	1:A:934:ARG:HG3	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: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

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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:HG22	1:A:1203:THR:O	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:1273:SER:O	1:A:1274:PHE:C	2.58	0.42
1:A:883:GLN:HA	1:A:884:PRO:HD3	1.73	0.42
1:A:1269:ARG:HD3	1:A:1269:ARG:C	2.40	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:623:LEU:C	1:A:623:LEU:HD23	2.40	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: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:740:THR:O	1:A:740:THR:HG22	2.20	0.41
1:A:744:LYS:HZ2	1:A:783:TRP:HE1	1.65	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:1346:ASP:O	1:A:1347:ASP:HB2	2.21	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: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: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

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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: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%)	7 11

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 (i)

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%)	53 78

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

Sometimes 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 (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 monosaccharides 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	102	-	3,3,3	0.63	0	2,2,2	0.24	0
5	EDO	A	108	-	3,3,3	0.52	0	2,2,2	0.31	0
5	EDO	A	115	-	3,3,3	0.50	0	2,2,2	0.26	0
5	EDO	A	117	-	3,3,3	0.37	0	2,2,2	0.38	0
5	EDO	A	122	-	3,3,3	0.53	0	2,2,2	0.25	0
5	EDO	A	116	-	3,3,3	0.54	0	2,2,2	0.25	0
5	EDO	A	107	-	3,3,3	0.51	0	2,2,2	0.29	0
5	EDO	A	105	-	3,3,3	0.47	0	2,2,2	0.33	0
2	SFG	A	300	-	25,29,29	1.74	4 (16%)	23,42,42	2.30	9 (39%)
5	EDO	A	120	-	3,3,3	0.56	0	2,2,2	0.25	0
5	EDO	A	111	-	3,3,3	0.39	0	2,2,2	0.39	0
5	EDO	A	112	-	3,3,3	0.52	0	2,2,2	0.30	0
5	EDO	A	103	-	3,3,3	0.41	0	2,2,2	0.39	0
5	EDO	A	106	-	3,3,3	0.58	0	2,2,2	0.22	0
5	EDO	A	125	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	114	-	3,3,3	0.56	0	2,2,2	0.25	0
5	EDO	A	104	-	3,3,3	0.58	0	2,2,2	0.25	0
5	EDO	A	124	-	3,3,3	0.49	0	2,2,2	0.29	0
5	EDO	A	101	-	3,3,3	0.55	0	2,2,2	0.27	0
5	EDO	A	123	-	3,3,3	0.49	0	2,2,2	0.30	0
5	EDO	A	118	-	3,3,3	0.48	0	2,2,2	0.30	0
5	EDO	A	121	-	3,3,3	0.46	0	2,2,2	0.33	0
3	SO4	A	1	-	4,4,4	0.28	0	6,6,6	0.10	0
5	EDO	A	110	-	3,3,3	0.52	0	2,2,2	0.28	0
4	MES	A	4	-	12,12,12	1.06	1 (8%)	14,16,16	1.18	2 (14%)
5	EDO	A	119	-	3,3,3	0.49	0	2,2,2	0.30	0
5	EDO	A	109	-	3,3,3	0.49	0	2,2,2	0.31	0
4	MES	A	2	-	12,12,12	1.21	1 (8%)	14,16,16	1.19	2 (14%)
5	EDO	A	113	-	3,3,3	0.47	0	2,2,2	0.30	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	102	-	-	1/1/1/1	-
5	EDO	A	108	-	-	1/1/1/1	-
5	EDO	A	115	-	-	1/1/1/1	-
5	EDO	A	117	-	-	0/1/1/1	-
5	EDO	A	122	-	-	1/1/1/1	-
5	EDO	A	116	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	107	-	-	1/1/1/1	-
5	EDO	A	105	-	-	0/1/1/1	-
2	SFG	A	300	-	-	2/13/33/33	0/3/3/3
5	EDO	A	120	-	-	1/1/1/1	-
5	EDO	A	111	-	-	1/1/1/1	-
5	EDO	A	112	-	-	1/1/1/1	-
5	EDO	A	103	-	-	0/1/1/1	-
5	EDO	A	106	-	-	0/1/1/1	-
5	EDO	A	125	-	-	1/1/1/1	-
5	EDO	A	114	-	-	0/1/1/1	-
5	EDO	A	104	-	-	0/1/1/1	-
5	EDO	A	124	-	-	1/1/1/1	-
5	EDO	A	101	-	-	1/1/1/1	-
5	EDO	A	123	-	-	1/1/1/1	-
5	EDO	A	118	-	-	0/1/1/1	-
5	EDO	A	121	-	-	1/1/1/1	-
5	EDO	A	110	-	-	0/1/1/1	-
4	MES	A	4	-	-	0/6/14/14	0/1/1/1
5	EDO	A	119	-	-	0/1/1/1	-
5	EDO	A	109	-	-	1/1/1/1	-
4	MES	A	2	-	-	0/6/14/14	0/1/1/1
5	EDO	A	113	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	SFG	O4'-C1'	4.77	1.47	1.41
2	A	300	SFG	C5'-C4'	3.96	1.59	1.52
2	A	300	SFG	C2-N3	3.79	1.38	1.32
4	A	2	MES	C8-S	3.06	1.81	1.77
4	A	4	MES	C8-S	2.67	1.81	1.77
2	A	300	SFG	C8-N7	-2.16	1.30	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	300	SFG	O4'-C1'-C2'	-6.96	96.75	106.93
2	A	300	SFG	N3-C2-N1	-4.02	122.39	128.68
2	A	300	SFG	CB-CA-N	3.15	118.44	110.17
2	A	300	SFG	C1'-N9-C4	-3.12	121.17	126.64
2	A	300	SFG	C2-N1-C6	2.74	123.44	118.75
2	A	300	SFG	C3'-C2'-C1'	2.73	105.08	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	300	SFG	C5-C6-N6	2.64	124.37	120.35
4	A	2	MES	O2S-S-C8	2.41	109.81	106.92
4	A	4	MES	O1S-S-C8	2.31	109.70	106.92
4	A	2	MES	O3S-S-C8	2.17	109.28	105.77
4	A	4	MES	O3S-S-C8	2.17	109.27	105.77
2	A	300	SFG	C5-C6-N1	-2.14	115.50	120.35
2	A	300	SFG	CG-CD-NE	2.06	115.01	109.03

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	113	EDO	O1-C1-C2-O2
5	A	116	EDO	O1-C1-C2-O2
5	A	120	EDO	O1-C1-C2-O2
5	A	123	EDO	O1-C1-C2-O2
5	A	108	EDO	O1-C1-C2-O2
5	A	121	EDO	O1-C1-C2-O2
5	A	124	EDO	O1-C1-C2-O2
5	A	102	EDO	O1-C1-C2-O2
5	A	109	EDO	O1-C1-C2-O2
5	A	111	EDO	O1-C1-C2-O2
5	A	115	EDO	O1-C1-C2-O2
5	A	107	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
2	A	300	SFG	C4'-C5'-CD-CG

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	115	EDO	1	0
5	A	116	EDO	4	0
5	A	120	EDO	1	0
5	A	106	EDO	3	0
5	A	104	EDO	1	0

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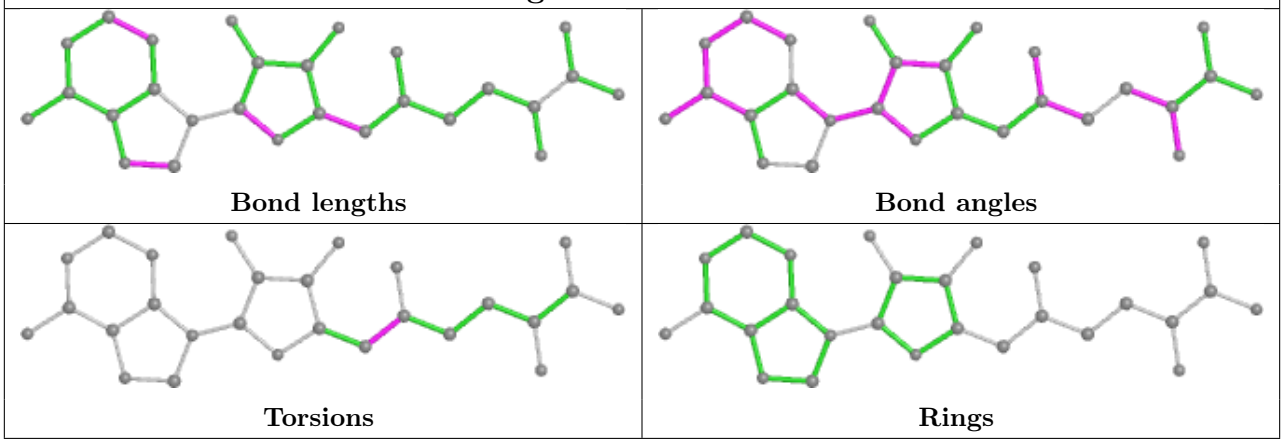
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	124	EDO	1	0
5	A	123	EDO	3	0
4	A	4	MES	1	0
5	A	119	EDO	1	0
5	A	113	EDO	3	0

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 then 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.

Ligand SFG A 300



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.31	97 (10%) 7 6	26, 50, 108, 137	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	855	LEU	8.6
1	A	980	ILE	7.6
1	A	682	SER	7.3
1	A	956	VAL	6.3
1	A	1130	PRO	6.1
1	A	681	ARG	6.0
1	A	648	PHE	5.8
1	A	678	GLY	5.6
1	A	677	GLY	5.5
1	A	983	SER	5.5
1	A	1005	SER	5.4
1	A	853	SER	5.3
1	A	858	ASP	5.2
1	A	700	ASP	5.1
1	A	955	PRO	4.9
1	A	961	LYS	4.9
1	A	952	LEU	4.8
1	A	679	SER	4.7
1	A	890	PHE	4.7
1	A	676	PHE	4.7
1	A	976	TYR	4.5
1	A	856	GLU	4.5
1	A	982	GLY	4.5
1	A	854	LEU	4.4
1	A	647	ALA	4.4
1	A	684	GLN	4.4
1	A	606	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	954	SER	4.3
1	A	646	ASN	4.1
1	A	984	ASN	4.1
1	A	636	ILE	4.0
1	A	1132	ILE	3.9
1	A	859	ASP	3.9
1	A	690	ARG	3.9
1	A	683	LYS	3.8
1	A	667	CYS	3.8
1	A	958	ARG	3.8
1	A	985	LEU	3.7
1	A	711	GLU	3.7
1	A	1129	GLU	3.6
1	A	979	TYR	3.6
1	A	1444	VAL	3.6
1	A	1004	LYS	3.5
1	A	666	LYS	3.4
1	A	709	ILE	3.4
1	A	959	PRO	3.3
1	A	607	SER	3.3
1	A	729	ASN	3.2
1	A	730	ARG	3.2
1	A	1286	CYS	3.2
1	A	615	PRO	3.2
1	A	953	SER	3.1
1	A	674	VAL	3.1
1	A	685	ALA	3.1
1	A	635	GLN	3.1
1	A	664	CYS	3.1
1	A	1315	ILE	3.1
1	A	1600	ALA	3.1
1	A	673	MET	3.0
1	A	608	THR	3.0
1	A	1287	LEU	3.0
1	A	1264	LEU	2.9
1	A	675	LYS	2.9
1	A	1317	ALA	2.8
1	A	1284	LEU	2.8
1	A	957	LYS	2.8
1	A	1451	MET	2.8
1	A	716	LYS	2.8
1	A	1536	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1265	LEU	2.7
1	A	1283	THR	2.7
1	A	981	LYS	2.6
1	A	603	THR	2.6
1	A	887	ASP	2.6
1	A	604	ILE	2.5
1	A	1008	ARG	2.5
1	A	634	GLU	2.4
1	A	680	GLY	2.4
1	A	1405	TYR	2.4
1	A	1506	ARG	2.4
1	A	669	ALA	2.3
1	A	1222	GLY	2.3
1	A	649	LYS	2.3
1	A	1221	CYS	2.3
1	A	852	GLU	2.3
1	A	706	ASP	2.2
1	A	909	ARG	2.2
1	A	1288	VAL	2.2
1	A	962	GLU	2.2
1	A	687	GLN	2.1
1	A	924	TYR	2.1
1	A	1106	PRO	2.1
1	A	1263	PHE	2.1
1	A	1406	GLN	2.1
1	A	1251	PHE	2.1
1	A	609	ARG	2.1
1	A	1481	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

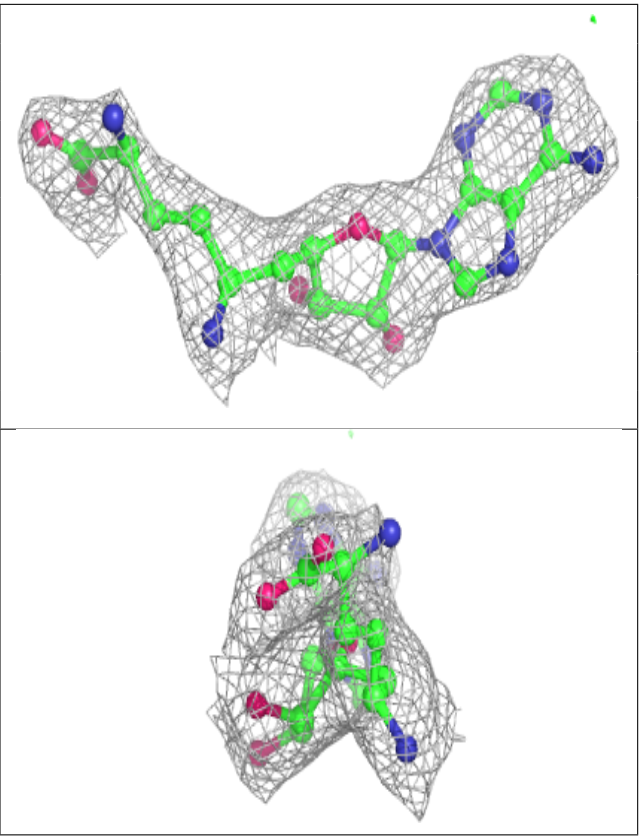
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	116	4/4	0.27	0.55	85,85,86,86	0
5	EDO	A	109	4/4	0.78	0.32	90,91,91,92	0
5	EDO	A	115	4/4	0.82	0.29	68,72,73,74	0
5	EDO	A	122	4/4	0.82	0.30	76,77,78,78	0
5	EDO	A	123	4/4	0.82	0.29	69,69,69,69	0
5	EDO	A	106	4/4	0.83	0.47	60,62,64,64	0
3	SO4	A	1	5/5	0.84	0.20	111,112,112,112	0
5	EDO	A	101	4/4	0.84	0.37	53,53,55,55	0
5	EDO	A	124	4/4	0.84	0.26	68,69,69,69	0
5	EDO	A	125	4/4	0.84	0.32	75,78,79,81	0
5	EDO	A	120	4/4	0.85	0.20	81,83,83,84	0
5	EDO	A	119	4/4	0.86	0.64	87,88,89,89	0
5	EDO	A	110	4/4	0.86	0.37	75,76,76,76	0
5	EDO	A	112	4/4	0.87	0.15	71,72,72,73	0
4	MES	A	4	12/12	0.88	0.25	115,117,119,119	0
5	EDO	A	108	4/4	0.89	0.17	70,71,71,72	0
5	EDO	A	121	4/4	0.89	0.20	76,77,77,79	0
5	EDO	A	105	4/4	0.90	0.16	62,63,65,65	0
5	EDO	A	102	4/4	0.91	0.23	42,46,47,48	0
5	EDO	A	107	4/4	0.91	0.17	63,64,64,65	0
5	EDO	A	114	4/4	0.91	0.19	52,53,54,54	0
2	SFG	A	300	27/27	0.92	0.18	49,55,58,59	0
5	EDO	A	113	4/4	0.92	0.29	57,59,61,64	0
5	EDO	A	104	4/4	0.92	0.15	51,51,51,52	0
6	ZN	A	1602	1/1	0.92	0.04	103,103,103,103	0
4	MES	A	2	12/12	0.95	0.12	67,69,76,77	0
5	EDO	A	103	4/4	0.95	0.17	55,56,56,56	0
5	EDO	A	111	4/4	0.96	0.13	49,51,53,56	0
5	EDO	A	117	4/4	0.97	0.21	53,55,56,56	0
5	EDO	A	118	4/4	0.97	0.17	40,43,43,44	0
6	ZN	A	1601	1/1	0.98	0.10	70,70,70,70	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

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.

Electron density around SFG A 300:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.