



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:57 PM GMT

PDB ID : 1I1E
Title : CRYSTAL STRUCTURE OF CLOSTRIDIUM BOTULINUM NEURO-
TOXIN B COMPLEXED WITH DOXORUBICIN
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Deposited on : 2001-02-01
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

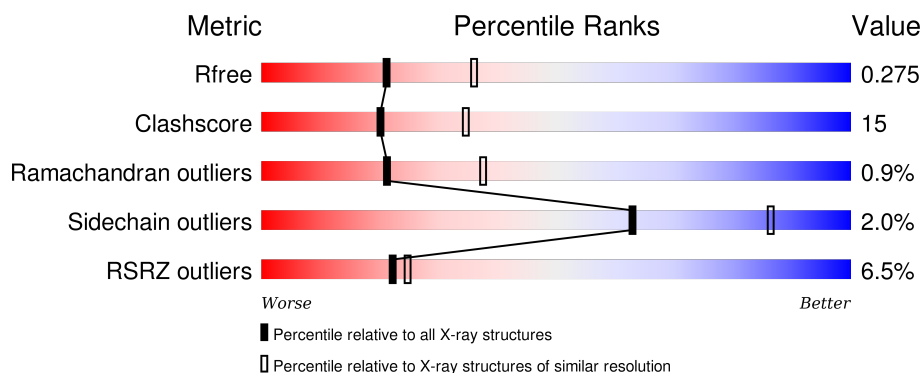
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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 ≥ 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	1290	<div> <div>7%</div> <div>72%</div> <div>27%</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
2	DM2	A	3001	-	-	X	X

2 Entry composition [i](#)

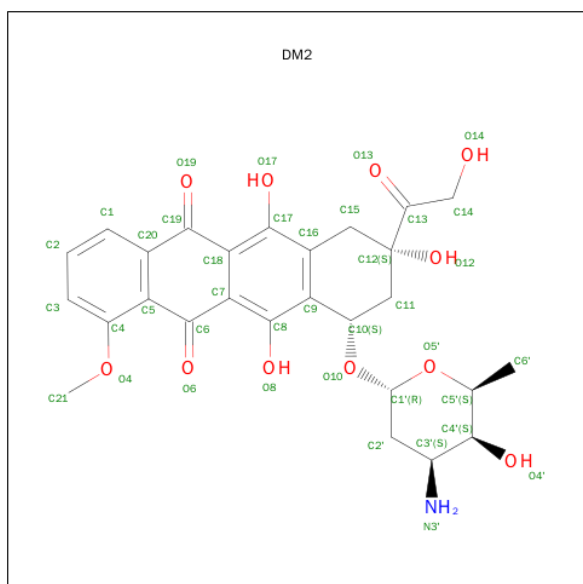
There are 5 unique types of molecules in this entry. The entry contains 11016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BOTULINUM NEUROTOXIN TYPE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1287	Total	C	N	O	S	0	0	0
			10617	6847	1708	2029	33			

- Molecule 2 is DOXORUBICIN (three-letter code: DM2) (formula: $C_{27}H_{29}NO_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			39	27	1	11		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

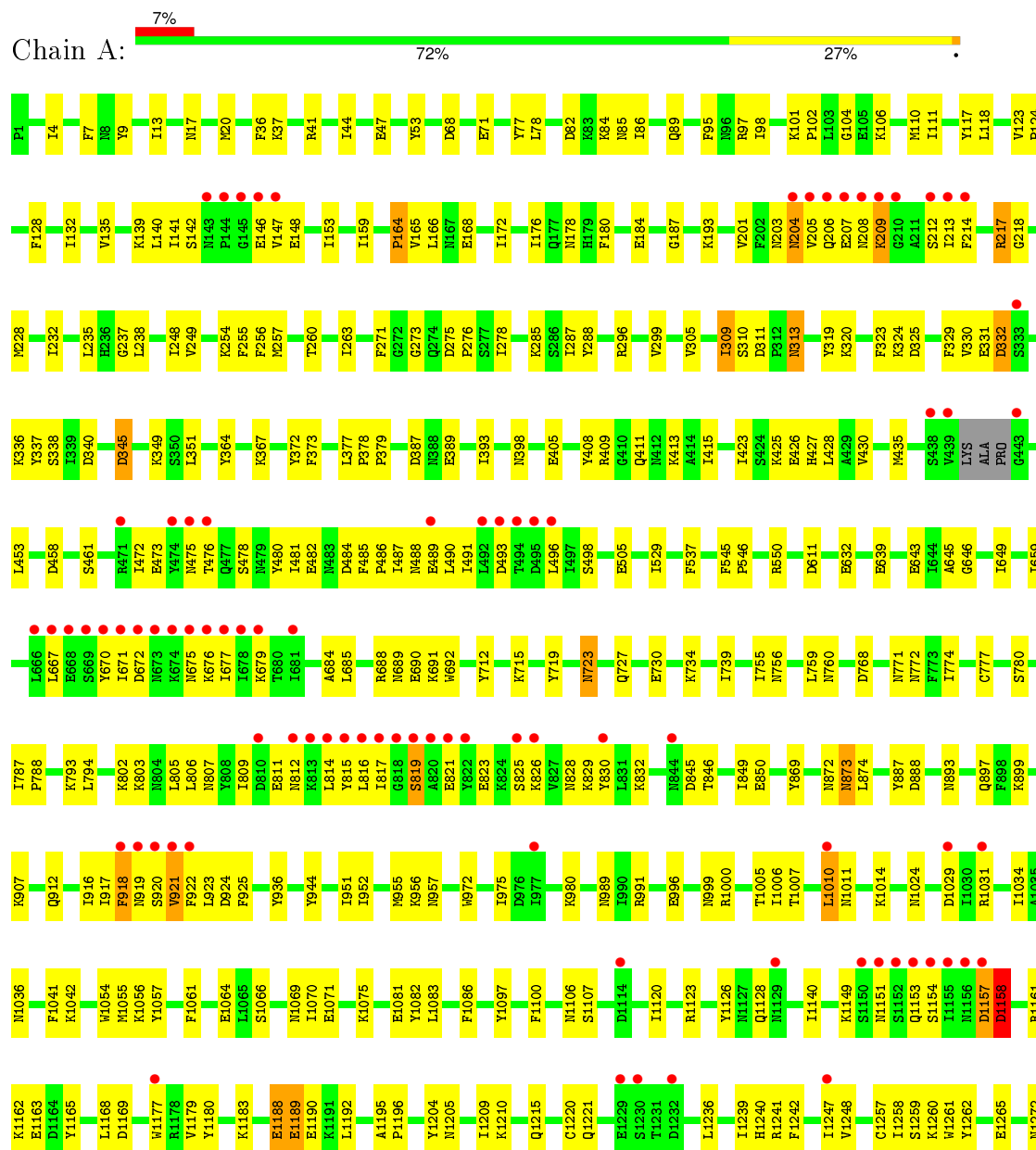
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	354	Total	O	0	0
			354	354		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: BOTULINUM NEUROTOXIN TYPE B



L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.27Å 122.93Å 95.42Å 90.00° 112.95° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 37.18 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 95.5 (37.18-2.49)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.276 0.221 , 0.275	Depositor DCC
R_{free} test set	1073 reflections (2.00%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.0	EDS
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53954 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11016	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: DM2, ZN, 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	0.39	0/10848	0.60	0/14652

There are no bond length outliers.

There are no bond angle outliers.

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	10617	0	10473	310	0
2	A	39	0	29	26	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	354	0	0	8	0
All	All	11016	0	10502	310	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 15.

All (310) 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:1241:ARG:H	2:A:3001:DM2:H4'	0.99	1.11
1:A:212:SER:HA	1:A:760:ASN:ND2	1.77	0.99
1:A:1188:GLU:HB3	2:A:3001:DM2:O19	1.64	0.98
1:A:1241:ARG:N	2:A:3001:DM2:H4'	1.81	0.95
1:A:1066:SER:H	1:A:1069:ASN:HD22	1.08	0.91
1:A:1075:LYS:HE2	1:A:1215:GLN:HE22	1.39	0.86
1:A:203:ASN:HD22	1:A:377:LEU:HD11	1.42	0.83
1:A:1071:GLU:OE2	1:A:1075:LYS:HE3	1.81	0.81
1:A:205:VAL:HG21	1:A:712:TYR:HE1	1.45	0.81
1:A:826:LYS:HA	1:A:829:LYS:HE2	1.65	0.78
1:A:85:ASN:ND2	1:A:89:GLN:HE21	1.80	0.78
1:A:639:GLU:O	1:A:643:GLU:HG3	1.85	0.77
1:A:330:VAL:CG1	1:A:340:ASP:HB2	2.14	0.77
1:A:367:LYS:H	1:A:411:GLN:HE22	1.32	0.76
1:A:730:GLU:HG3	1:A:734:LYS:HE3	1.67	0.76
1:A:1241:ARG:H	2:A:3001:DM2:C4'	1.90	0.76
1:A:493:ASP:OD2	1:A:496:LEU:HB2	1.87	0.74
1:A:1236:LEU:HD12	1:A:1262:TYR:HB3	1.71	0.73
1:A:893:ASN:HD21	1:A:897:GLN:HB2	1.53	0.72
1:A:309:ILE:HD13	1:A:309:ILE:H	1.54	0.72
1:A:85:ASN:HD21	1:A:89:GLN:HE21	1.37	0.72
1:A:1075:LYS:HE2	1:A:1215:GLN:NE2	2.04	0.71
1:A:140:LEU:HD11	1:A:147:VAL:HA	1.72	0.71
1:A:209:LYS:HD2	1:A:209:LYS:H	1.56	0.70
1:A:398:ASN:HD21	1:A:411:GLN:HE21	1.38	0.70
1:A:206:GLN:HA	1:A:771:ASN:ND2	2.06	0.70
1:A:1240:HIS:HA	2:A:3001:DM2:H5'	1.72	0.70
1:A:1240:HIS:HB2	2:A:3001:DM2:O13	1.93	0.69
1:A:146:GLU:HG3	1:A:148:GLU:HG2	1.74	0.68
1:A:1262:TYR:CE2	2:A:3001:DM2:C14	2.77	0.67
1:A:212:SER:HA	1:A:760:ASN:HD21	1.59	0.67
1:A:1247:ILE:HG13	1:A:1248:VAL:HG23	1.77	0.66
1:A:1236:LEU:HD12	1:A:1262:TYR:CB	2.25	0.66
1:A:209:LYS:CD	1:A:217:ARG:HB2	2.25	0.66
1:A:180:PHE:O	1:A:184:GLU:HG3	1.95	0.66
1:A:330:VAL:HG11	1:A:340:ASP:HB2	1.78	0.66
1:A:1240:HIS:ND1	2:A:3001:DM2:O12	2.29	0.65
1:A:330:VAL:HG13	1:A:340:ASP:HB2	1.77	0.65
1:A:1221:GLN:HE21	1:A:1278:ASN:HD22	1.42	0.65
1:A:1010:LEU:HD13	1:A:1011:ASN:ND2	2.10	0.65
1:A:1066:SER:H	1:A:1069:ASN:ND2	1.90	0.65
1:A:205:VAL:HG21	1:A:712:TYR:CE1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:921:VAL:O	1:A:921:VAL:HG12	1.97	0.65
1:A:142:SER:CB	1:A:148:GLU:HG3	2.27	0.64
1:A:893:ASN:ND2	1:A:897:GLN:HB2	2.12	0.64
1:A:139:LYS:HG3	1:A:141:ILE:CD1	2.27	0.64
1:A:255:PHE:HB2	1:A:529:ILE:HD13	1.79	0.64
1:A:228:MET:O	1:A:232:ILE:HG13	1.97	0.64
1:A:1189:GLU:HB3	2:A:3001:DM2:O17	1.97	0.64
1:A:172:ILE:HD11	1:A:193:LYS:NZ	2.12	0.64
1:A:670:TYR:CD1	1:A:676:LYS:HB3	2.32	0.64
1:A:1221:GLN:HE21	1:A:1278:ASN:ND2	1.97	0.62
1:A:667:LEU:HD11	1:A:805:LEU:HD23	1.80	0.62
1:A:255:PHE:HB2	1:A:529:ILE:CD1	2.29	0.62
1:A:685:LEU:HB3	1:A:830:TYR:CE2	2.35	0.62
1:A:309:ILE:HD13	1:A:309:ILE:N	2.15	0.61
1:A:1262:TYR:CE2	2:A:3001:DM2:H141	2.36	0.61
1:A:1259:SER:CB	2:A:3001:DM2:H152	2.30	0.61
1:A:675:ASN:O	1:A:679:LYS:HG3	2.00	0.61
1:A:309:ILE:CD1	1:A:309:ILE:H	2.13	0.61
1:A:139:LYS:HG3	1:A:141:ILE:HD11	1.83	0.60
1:A:485:PHE:HE2	1:A:490:LEU:HB2	1.65	0.60
1:A:1014:LYS:HE2	1:A:1024:ASN:HD21	1.66	0.60
1:A:206:GLN:HA	1:A:771:ASN:HD22	1.67	0.60
1:A:85:ASN:HD21	1:A:89:GLN:NE2	2.00	0.59
1:A:1081:GLU:O	1:A:1162:LYS:HG3	2.02	0.59
1:A:1259:SER:OG	2:A:3001:DM2:H152	2.02	0.59
1:A:1262:TYR:HE2	2:A:3001:DM2:C14	2.16	0.58
1:A:425:LYS:HD3	1:A:428:LEU:HD12	1.85	0.58
1:A:1014:LYS:HE2	1:A:1024:ASN:ND2	2.19	0.58
1:A:209:LYS:HE2	1:A:217:ARG:HD3	1.86	0.58
1:A:263:ILE:HD13	1:A:372:TYR:HE2	1.68	0.58
1:A:1190:GLU:HB2	5:A:1465:HOH:O	2.04	0.58
1:A:330:VAL:HG22	1:A:338:SER:O	2.04	0.57
1:A:819:SER:C	1:A:821:GLU:H	2.07	0.57
1:A:685:LEU:O	1:A:688:ARG:HB3	2.05	0.56
1:A:208:ASN:HD22	1:A:208:ASN:N	2.02	0.56
1:A:805:LEU:O	1:A:809:ILE:HG13	2.05	0.56
1:A:97:ARG:HA	1:A:393:ILE:HG23	1.87	0.56
1:A:153:ILE:HA	1:A:505:GLU:O	2.06	0.56
1:A:47:GLU:HG2	1:A:84:LYS:HE3	1.86	0.56
1:A:309:ILE:HG12	1:A:310:SER:N	2.20	0.56
1:A:204:ASN:N	1:A:204:ASN:OD1	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LEU:HB3	1:A:378:PRO:CD	2.36	0.55
1:A:1262:TYR:OH	2:A:3001:DM2:H141	2.06	0.55
1:A:1157:ASP:O	1:A:1158:ASP:HB2	2.05	0.55
1:A:845:ASP:O	1:A:849:ILE:HG12	2.07	0.55
1:A:923:LEU:HD11	1:A:925:PHE:CE2	2.41	0.55
1:A:1262:TYR:CD2	1:A:1277:CYS:HB3	2.41	0.55
1:A:325:ASP:OD1	1:A:498:SER:HB2	2.06	0.55
1:A:201:VAL:HG12	1:A:377:LEU:HD12	1.90	0.54
1:A:689:ASN:ND2	1:A:830:TYR:OH	2.40	0.54
1:A:1272:ASN:HB3	1:A:1275:LEU:HG	1.89	0.54
1:A:209:LYS:HD3	1:A:217:ARG:HB2	1.88	0.54
1:A:611:ASP:OD2	1:A:643:GLU:OE2	2.25	0.54
1:A:249:VAL:HG23	1:A:458:ASP:HB3	1.89	0.54
1:A:482:GLU:C	1:A:484:ASP:H	2.12	0.54
1:A:117:TYR:HA	1:A:323:PHE:CZ	2.41	0.54
1:A:4:ILE:HD12	1:A:95:PHE:HB3	1.90	0.53
1:A:482:GLU:HG3	1:A:484:ASP:HB3	1.91	0.53
1:A:324:LYS:HE3	1:A:329:PHE:O	2.09	0.53
1:A:1163:GLU:CD	1:A:1210:LYS:HZ2	2.12	0.53
1:A:140:LEU:CD1	1:A:147:VAL:HA	2.39	0.53
1:A:677:ILE:HG21	1:A:816:LEU:HD21	1.90	0.53
1:A:204:ASN:ND2	1:A:207:GLU:OE1	2.37	0.52
1:A:487:ILE:O	1:A:491:ILE:HG13	2.09	0.52
1:A:980:LYS:HE2	1:A:1029:ASP:HB3	1.91	0.52
1:A:505:GLU:HG2	5:A:1622:HOH:O	2.10	0.52
1:A:923:LEU:HD11	1:A:925:PHE:HE2	1.75	0.52
1:A:1192:LEU:HG	1:A:1257:CYS:HA	1.92	0.52
1:A:1240:HIS:HD1	2:A:3001:DM2:HO12	1.49	0.52
1:A:550:ARG:HH11	1:A:550:ARG:HG2	1.74	0.52
1:A:1107:SER:HB3	1:A:1120:ILE:CG2	2.40	0.52
1:A:692:TRP:CD2	1:A:794:LEU:HD13	2.44	0.52
1:A:273:GLY:O	1:A:276:PRO:HD2	2.10	0.52
1:A:956:LYS:HE2	1:A:1034:ILE:HG21	1.90	0.51
1:A:955:MET:CE	1:A:975:ILE:HD12	2.40	0.51
1:A:1007:THR:HB	1:A:1064:GLU:HG3	1.92	0.51
1:A:1005:THR:HG21	1:A:1070:ILE:HG12	1.92	0.51
1:A:1259:SER:HB3	2:A:3001:DM2:H142	1.92	0.51
1:A:922:PHE:CZ	1:A:924:ASP:HB2	2.46	0.51
1:A:379:PRO:HG2	1:A:423:ILE:HD12	1.93	0.51
1:A:1262:TYR:CE2	2:A:3001:DM2:H142	2.44	0.51
1:A:936:TYR:HB3	1:A:944:TYR:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1257:CYS:HB2	2:A:3001:DM2:O13	2.11	0.51
1:A:204:ASN:HB2	1:A:207:GLU:HB2	1.93	0.51
1:A:1126:TYR:CE1	1:A:1128:GLN:HB2	2.46	0.51
1:A:213:ILE:CG2	1:A:723:ASN:HD21	2.24	0.50
1:A:819:SER:C	1:A:821:GLU:N	2.63	0.50
1:A:13:ILE:HD13	1:A:20:MET:HG2	1.92	0.50
1:A:209:LYS:H	1:A:209:LYS:CD	2.22	0.50
1:A:36:PHE:N	1:A:36:PHE:CD1	2.80	0.50
1:A:453:LEU:HD22	1:A:537:PHE:CZ	2.47	0.50
1:A:846:THR:O	1:A:850:GLU:HG3	2.12	0.50
1:A:487:ILE:HD12	1:A:490:LEU:HD23	1.93	0.50
1:A:409:ARG:NH1	1:A:415:ILE:HD13	2.26	0.50
1:A:659:ILE:HG22	1:A:793:LYS:HG3	1.94	0.49
1:A:9:TYR:CZ	1:A:84:LYS:HD3	2.48	0.49
1:A:936:TYR:HB3	1:A:944:TYR:CE1	2.46	0.49
1:A:296:ARG:O	1:A:299:VAL:HG12	2.12	0.49
1:A:1183:LYS:HG2	1:A:1204:TYR:CE2	2.47	0.49
1:A:82:ASP:O	1:A:86:ILE:HG13	2.13	0.49
1:A:645:ALA:HB3	1:A:649:ILE:CG2	2.42	0.49
1:A:999:ASN:ND2	1:A:1287:GLY:HA3	2.27	0.49
1:A:490:LEU:CD1	1:A:496:LEU:HD22	2.43	0.49
1:A:206:GLN:NE2	1:A:771:ASN:ND2	2.60	0.49
1:A:1239:ILE:O	2:A:3001:DM2:H6'1	2.12	0.49
1:A:989:ASN:ND2	1:A:991:ARG:H	2.10	0.49
1:A:1100:PHE:HD2	1:A:1280:GLN:HB2	1.78	0.49
1:A:425:LYS:C	1:A:427:HIS:H	2.16	0.49
1:A:311:ASP:OD1	1:A:313:ASN:HB2	2.13	0.49
1:A:213:ILE:H	1:A:760:ASN:HD22	1.60	0.49
1:A:9:TYR:H	1:A:85:ASN:ND2	2.11	0.49
1:A:101:LYS:HB2	1:A:364:TYR:CZ	2.48	0.49
1:A:128:PHE:CZ	1:A:305:VAL:HG21	2.48	0.48
1:A:208:ASN:N	1:A:208:ASN:ND2	2.62	0.48
1:A:332:ASP:OD1	1:A:336:LYS:N	2.40	0.48
1:A:1192:LEU:HD21	1:A:1258:ILE:HB	1.95	0.48
1:A:1083:LEU:HD13	1:A:1209:ILE:CD1	2.43	0.48
1:A:248:ILE:HA	1:A:461:SER:HB3	1.95	0.48
1:A:128:PHE:CE1	1:A:305:VAL:HG21	2.49	0.48
1:A:142:SER:HB3	1:A:148:GLU:HG3	1.95	0.48
1:A:209:LYS:HB2	1:A:218:GLY:H	1.77	0.48
1:A:1188:GLU:HG3	1:A:1260:LYS:HB2	1.94	0.48
1:A:1066:SER:OG	1:A:1069:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ILE:HG21	1:A:684:ALA:HB2	1.96	0.48
1:A:254:LYS:HB2	1:A:257:MET:HG3	1.96	0.48
1:A:1082:TYR:HA	1:A:1161:ARG:HA	1.95	0.48
1:A:172:ILE:HD11	1:A:193:LYS:HZ1	1.77	0.47
1:A:1162:LYS:O	1:A:1163:GLU:HB2	2.14	0.47
1:A:213:ILE:HG23	1:A:760:ASN:HD22	1.79	0.47
1:A:873:ASN:ND2	1:A:874:LEU:H	2.12	0.47
1:A:777:CYS:O	1:A:780:SER:HB3	2.13	0.47
1:A:830:TYR:HD1	5:A:1617:HOH:O	1.96	0.47
1:A:956:LYS:HE2	1:A:1034:ILE:CG2	2.45	0.47
1:A:77:TYR:CD2	1:A:78:LEU:HG	2.49	0.47
1:A:367:LYS:HB2	1:A:408:TYR:CG	2.50	0.47
1:A:1149:LYS:HB3	1:A:1165:TYR:O	2.14	0.47
1:A:68:ASP:OD2	1:A:260:THR:HB	2.14	0.46
1:A:178:ASN:N	1:A:178:ASN:ND2	2.62	0.46
1:A:1262:TYR:CZ	2:A:3001:DM2:H141	2.49	0.46
1:A:922:PHE:O	1:A:923:LEU:HB3	2.15	0.46
1:A:723:ASN:OD1	1:A:727:GLN:NE2	2.48	0.46
1:A:41:ARG:HA	5:A:1326:HOH:O	2.15	0.46
1:A:214:PHE:CD1	1:A:756:ASN:HB3	2.50	0.46
1:A:489:GLU:O	1:A:493:ASP:N	2.49	0.46
1:A:1276:GLY:HA3	5:A:1459:HOH:O	2.15	0.46
1:A:187:GLY:HA2	1:A:237:GLY:O	2.15	0.46
1:A:204:ASN:ND2	1:A:207:GLU:HB2	2.30	0.46
1:A:111:ILE:HG23	1:A:238:LEU:CD1	2.46	0.46
1:A:53:TYR:CD2	1:A:164:PRO:HG2	2.50	0.46
1:A:235:LEU:HD21	1:A:351:LEU:CD2	2.46	0.46
1:A:204:ASN:HD22	1:A:207:GLU:CB	2.29	0.46
1:A:1240:HIS:HD2	1:A:1242:PHE:CE1	2.34	0.46
1:A:802:LYS:O	1:A:806:LEU:HG	2.15	0.46
1:A:916:ILE:O	1:A:918:PHE:N	2.49	0.46
1:A:692:TRP:CE2	1:A:794:LEU:HB3	2.51	0.46
1:A:1056:LYS:HE2	1:A:1057:TYR:CE1	2.50	0.46
1:A:823:GLU:HA	1:A:826:LYS:HB3	1.99	0.46
1:A:263:ILE:HD13	1:A:372:TYR:CE2	2.49	0.46
1:A:320:LYS:HE3	1:A:337:TYR:HE1	1.81	0.46
1:A:209:LYS:CE	1:A:217:ARG:HB2	2.46	0.45
1:A:1086:PHE:CG	1:A:1282:ILE:HG12	2.51	0.45
1:A:1083:LEU:HD22	1:A:1220:CYS:CB	2.47	0.45
1:A:887:TYR:CD1	1:A:907:LYS:HG3	2.52	0.45
1:A:1240:HIS:CE1	2:A:3001:DM2:H3'	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:PHE:HB2	1:A:1061:PHE:O	2.15	0.45
1:A:1126:TYR:CZ	1:A:1128:GLN:HB2	2.51	0.45
1:A:1106:ASN:HA	1:A:1123:ARG:HD2	1.97	0.45
1:A:787:ILE:HB	1:A:788:PRO:HD3	1.99	0.45
1:A:271:PHE:CD2	1:A:275:ASP:OD2	2.70	0.45
1:A:1261:TRP:CZ3	1:A:1265:GLU:HG3	2.51	0.45
1:A:1177:TRP:NE1	1:A:1196:PRO:HG3	2.31	0.45
1:A:1010:LEU:CD1	1:A:1011:ASN:ND2	2.76	0.45
1:A:17:ASN:OD1	1:A:37:LYS:HD2	2.16	0.45
1:A:176:ILE:HD12	5:A:1439:HOH:O	2.16	0.45
1:A:912:GLN:NE2	1:A:1036:ASN:HA	2.32	0.45
1:A:1215:GLN:HA	1:A:1215:GLN:NE2	2.31	0.45
1:A:102:PRO:HB2	1:A:491:ILE:HG23	1.99	0.45
1:A:165:VAL:HB	1:A:168:GLU:HB2	1.99	0.45
1:A:819:SER:O	1:A:821:GLU:N	2.50	0.45
1:A:117:TYR:CZ	1:A:128:PHE:HE2	2.35	0.45
1:A:814:LEU:C	1:A:816:LEU:H	2.20	0.45
1:A:480:TYR:OH	1:A:690:GLU:HA	2.16	0.44
1:A:951:ILE:HG13	1:A:952:ILE:HG13	1.99	0.44
1:A:387:ASP:OD1	1:A:389:GLU:HB3	2.18	0.44
1:A:832:LYS:HA	1:A:832:LYS:HD2	1.87	0.44
1:A:1153:GLN:O	1:A:1154:SER:HB2	2.17	0.44
1:A:435:MET:HG2	1:A:529:ILE:HD11	2.00	0.44
1:A:802:LYS:HE2	1:A:828:ASN:OD1	2.17	0.44
1:A:1195:ALA:HB1	1:A:1196:PRO:CD	2.47	0.44
1:A:768:ASP:O	1:A:772:ASN:ND2	2.51	0.44
1:A:204:ASN:ND2	1:A:207:GLU:CB	2.80	0.44
1:A:907:LYS:HD3	1:A:1042:LYS:HD2	2.00	0.44
1:A:1240:HIS:HB2	2:A:3001:DM2:O12	2.18	0.44
1:A:209:LYS:HE2	1:A:217:ARG:CD	2.46	0.44
1:A:473:GLU:C	1:A:475:ASN:N	2.71	0.44
1:A:807:ASN:O	1:A:811:GLU:HG3	2.18	0.44
1:A:213:ILE:HG13	1:A:214:PHE:N	2.33	0.44
1:A:1188:GLU:O	1:A:1189:GLU:HB3	2.18	0.43
1:A:1169:ASP:HB3	1:A:1177:TRP:O	2.18	0.43
1:A:1262:TYR:CE2	1:A:1277:CYS:HB3	2.54	0.43
1:A:1195:ALA:HB1	1:A:1196:PRO:HD2	2.00	0.43
1:A:213:ILE:H	1:A:760:ASN:ND2	2.16	0.43
1:A:1247:ILE:HG13	1:A:1248:VAL:N	2.33	0.43
1:A:44:ILE:HD13	1:A:159:ILE:HB	2.00	0.43
1:A:671:ILE:O	1:A:672:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ASN:HD21	1:A:411:GLN:NE2	2.10	0.43
1:A:475:ASN:HD22	1:A:475:ASN:HA	1.61	0.43
1:A:132:ILE:HD11	1:A:135:VAL:HG23	2.00	0.43
1:A:1241:ARG:CB	2:A:3001:DM2:H4'	2.49	0.43
1:A:646:GLY:O	1:A:649:ILE:HG12	2.17	0.43
1:A:203:ASN:OD1	1:A:203:ASN:O	2.36	0.43
1:A:209:LYS:HG2	1:A:217:ARG:HB2	2.01	0.43
1:A:1240:HIS:ND1	2:A:3001:DM2:H3'	2.33	0.43
1:A:324:LYS:NZ	1:A:331:GLU:HB2	2.34	0.42
1:A:1236:LEU:HD12	1:A:1262:TYR:HB2	2.00	0.42
1:A:1031:ARG:HG2	5:A:1584:HOH:O	2.18	0.42
1:A:209:LYS:HE2	1:A:217:ARG:HB2	2.02	0.42
1:A:1177:TRP:CE2	1:A:1196:PRO:HG3	2.54	0.42
1:A:869:TYR:CE1	1:A:872:ASN:HA	2.54	0.42
1:A:413:LYS:HB3	1:A:413:LYS:HE2	1.83	0.42
1:A:727:GLN:O	1:A:730:GLU:HB3	2.20	0.42
1:A:688:ARG:O	1:A:691:LYS:HB2	2.19	0.42
1:A:166:LEU:N	1:A:166:LEU:HD23	2.35	0.42
1:A:330:VAL:HG23	1:A:330:VAL:O	2.19	0.42
1:A:825:SER:O	1:A:828:ASN:N	2.53	0.42
1:A:907:LYS:HA	1:A:1041:PHE:O	2.19	0.42
1:A:1180:TYR:CE1	1:A:1205:ASN:HB3	2.54	0.42
1:A:123:VAL:HA	1:A:124:PRO:HD3	1.91	0.42
1:A:325:ASP:OD1	1:A:498:SER:CB	2.67	0.42
1:A:20:MET:O	1:A:139:LYS:HA	2.20	0.42
1:A:1240:HIS:HA	2:A:3001:DM2:C5'	2.44	0.42
1:A:309:ILE:CG1	1:A:310:SER:N	2.83	0.42
1:A:204:ASN:HD22	1:A:207:GLU:HB2	1.85	0.42
1:A:1157:ASP:O	1:A:1158:ASP:CB	2.67	0.42
1:A:812:ASN:O	1:A:816:LEU:HG	2.20	0.42
1:A:256:PHE:O	1:A:453:LEU:HB3	2.19	0.42
1:A:1086:PHE:CB	1:A:1282:ILE:HG12	2.50	0.42
1:A:956:LYS:O	1:A:957:ASN:HB2	2.19	0.42
1:A:213:ILE:HB	1:A:723:ASN:HD21	1.85	0.41
1:A:920:SER:O	1:A:921:VAL:HB	2.20	0.41
1:A:972:TRP:CD2	1:A:1006:ILE:HG21	2.55	0.41
1:A:106:LYS:O	1:A:110:MET:HG2	2.20	0.41
1:A:899:LYS:HD2	1:A:1054:TRP:CZ2	2.55	0.41
1:A:278:ILE:HD12	1:A:373:PHE:CE1	2.55	0.41
1:A:1188:GLU:CB	2:A:3001:DM2:O19	2.52	0.41
1:A:71:GLU:HG2	1:A:168:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:MET:HE3	1:A:110:MET:HB3	1.80	0.41
1:A:1168:LEU:O	1:A:1179:VAL:HG23	2.20	0.41
1:A:478:SER:HB3	1:A:480:TYR:HE1	1.85	0.41
1:A:739:ILE:HA	1:A:739:ILE:HD13	1.91	0.41
1:A:545:PHE:HA	1:A:546:PRO:HD3	1.93	0.41
1:A:104:GLY:HA3	1:A:364:TYR:OH	2.20	0.41
1:A:996:GLU:HA	1:A:1000:ARG:HH11	1.85	0.41
1:A:755:ILE:O	1:A:759:LEU:HG	2.20	0.41
1:A:287:ILE:O	1:A:288:TYR:C	2.59	0.41
1:A:285:LYS:HG2	1:A:481:ILE:CD1	2.50	0.41
1:A:719:TYR:O	1:A:723:ASN:HB2	2.21	0.41
1:A:324:LYS:C	1:A:324:LYS:HD3	2.41	0.41
1:A:324:LYS:HZ2	1:A:331:GLU:HB2	1.86	0.41
1:A:980:LYS:HE2	1:A:1029:ASP:CB	2.50	0.41
1:A:98:ILE:O	1:A:104:GLY:HA3	2.21	0.41
1:A:345:ASP:O	1:A:349:LYS:HG3	2.21	0.41
1:A:1140:ILE:HG13	5:A:1609:HOH:O	2.21	0.41
1:A:715:LYS:HG3	1:A:774:ILE:HG21	2.01	0.41
1:A:550:ARG:HG2	1:A:550:ARG:NH1	2.35	0.40
1:A:1097:TYR:CG	1:A:1281:PHE:HB3	2.56	0.40
1:A:999:ASN:HD21	1:A:1287:GLY:HA3	1.85	0.40
1:A:118:LEU:HD11	1:A:319:TYR:CE2	2.57	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	1283/1290 (100%)	1188 (93%)	84 (6%)	11 (1%)	21	37

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	THR
1	A	1151	ASN
1	A	921	VAL
1	A	1158	ASP
1	A	632	GLU
1	A	815	TYR
1	A	817	ILE
1	A	917	ILE
1	A	426	GLU
1	A	819	SER
1	A	486	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	1185/1189 (100%)	1161 (98%)	24 (2%)	63 86

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	164	PRO
1	A	204	ASN
1	A	209	LYS
1	A	217	ARG
1	A	309	ILE
1	A	313	ASN
1	A	332	ASP
1	A	345	ASP
1	A	405	GLU
1	A	430	VAL
1	A	488	ASN
1	A	723	ASN
1	A	803	LYS
1	A	873	ASN
1	A	888	ASP

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Mol	Chain	Res	Type
1	A	918	PHE
1	A	919	ASN
1	A	1010	LEU
1	A	1055	MET
1	A	1157	ASP
1	A	1158	ASP
1	A	1188	GLU
1	A	1189	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	85	ASN
1	A	178	ASN
1	A	203	ASN
1	A	206	GLN
1	A	208	ASN
1	A	411	GLN
1	A	475	ASN
1	A	523	GLN
1	A	595	GLN
1	A	605	ASN
1	A	683	ASN
1	A	689	ASN
1	A	723	ASN
1	A	727	GLN
1	A	760	ASN
1	A	771	ASN
1	A	772	ASN
1	A	799	ASN
1	A	853	ASN
1	A	862	ASN
1	A	872	ASN
1	A	873	ASN
1	A	978	ASN
1	A	989	ASN
1	A	999	ASN
1	A	1011	ASN
1	A	1069	ASN
1	A	1215	GLN
1	A	1278	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
4	SO4	A	1292	3	4,4,4	0.33	0	6,6,6	0.28	0
2	DM2	A	3001	-	41,43,43	3.30	23 (56%)	55,67,67	1.57	11 (20%)

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
4	SO4	A	1292	3	-	0/0/0/0	0/0/0/0
2	DM2	A	3001	-	-	0/13/60/60	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	DM2	C2'-C3'	2.01	1.58	1.53
2	A	3001	DM2	C3'-N3'	2.10	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	DM2	C20-C5	2.13	1.44	1.41
2	A	3001	DM2	C18-C17	2.38	1.46	1.41
2	A	3001	DM2	C18-C7	2.47	1.46	1.41
2	A	3001	DM2	C2-C1	2.52	1.44	1.38
2	A	3001	DM2	C11-C10	2.58	1.58	1.52
2	A	3001	DM2	C17-C16	2.71	1.44	1.40
2	A	3001	DM2	C2-C3	2.87	1.44	1.38
2	A	3001	DM2	O4-C4	2.90	1.41	1.37
2	A	3001	DM2	O4'-C4'	2.98	1.50	1.43
2	A	3001	DM2	C3-C4	3.12	1.46	1.39
2	A	3001	DM2	O5'-C1'	3.16	1.50	1.42
2	A	3001	DM2	C7-C8	3.28	1.48	1.41
2	A	3001	DM2	C5-C4	3.41	1.46	1.40
2	A	3001	DM2	C8-C9	3.44	1.46	1.40
2	A	3001	DM2	C11-C12	3.49	1.61	1.53
2	A	3001	DM2	O5'-C5'	3.62	1.53	1.44
2	A	3001	DM2	C2'-C1'	3.92	1.59	1.51
2	A	3001	DM2	C1-C20	4.84	1.48	1.39
2	A	3001	DM2	O19-C19	6.38	1.34	1.22
2	A	3001	DM2	O6-C6	8.72	1.38	1.22
2	A	3001	DM2	O13-C13	10.96	1.41	1.21

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	DM2	O10-C10-C9	-4.22	97.20	107.92
2	A	3001	DM2	O4'-C4'-C3'	-3.01	104.29	109.87
2	A	3001	DM2	O6-C6-C7	-2.73	116.67	121.49
2	A	3001	DM2	O4-C4-C3	-2.63	119.93	124.35
2	A	3001	DM2	C18-C7-C6	-2.16	116.78	120.00
2	A	3001	DM2	C21-O4-C4	2.22	120.91	117.54
2	A	3001	DM2	C8-C7-C6	2.37	124.80	120.53
2	A	3001	DM2	O4-C4-C5	2.84	120.20	115.78
2	A	3001	DM2	C11-C10-C9	2.87	117.88	111.07
2	A	3001	DM2	C7-C6-C5	2.94	123.46	118.09
2	A	3001	DM2	O12-C12-C11	4.95	119.65	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	DM2	26	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1287/1290 (99%)	0.11	84 (6%)	22 25	11, 27, 53, 63	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1154	SER	10.7
1	A	1152	SER	9.8
1	A	1153	GLN	8.1
1	A	145	GLY	8.0
1	A	1156	ASN	6.9
1	A	1155	ILE	6.6
1	A	921	VAL	6.3
1	A	1151	ASN	6.1
1	A	144	PRO	5.6
1	A	830	TYR	5.4
1	A	147	VAL	5.3
1	A	816	LEU	5.1
1	A	815	TYR	5.0
1	A	814	LEU	4.9
1	A	918	PHE	4.8
1	A	671	ILE	4.7
1	A	208	ASN	4.7
1	A	471	ARG	4.4
1	A	818	GLY	4.4
1	A	677	ILE	4.4
1	A	822	TYR	4.3
1	A	143	ASN	4.2
1	A	146	GLU	4.1
1	A	678	ILE	4.1
1	A	494	THR	3.9
1	A	1157	ASP	3.8
1	A	817	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	672	ASP	3.8
1	A	669	SER	3.8
1	A	820	ALA	3.8
1	A	919	ASN	3.7
1	A	438	SER	3.7
1	A	495	ASP	3.7
1	A	1150	SER	3.5
1	A	922	PHE	3.5
1	A	206	GLN	3.5
1	A	667	LEU	3.5
1	A	670	TYR	3.4
1	A	679	LYS	3.4
1	A	821	GLU	3.3
1	A	213	ILE	3.2
1	A	673	ASN	3.2
1	A	920	SER	3.0
1	A	813	LYS	2.9
1	A	1229	GLU	2.9
1	A	675	ASN	2.9
1	A	209	LYS	2.8
1	A	1232	ASP	2.8
1	A	812	ASN	2.8
1	A	1010	LEU	2.8
1	A	210	GLY	2.7
1	A	439	VAL	2.7
1	A	819	SER	2.7
1	A	1031	ARG	2.7
1	A	676	LYS	2.7
1	A	1129	ASN	2.7
1	A	681	ILE	2.6
1	A	475	ASN	2.6
1	A	496	LEU	2.5
1	A	825	SER	2.5
1	A	214	PHE	2.5
1	A	1029	ASP	2.4
1	A	476	THR	2.4
1	A	212	SER	2.4
1	A	826	LYS	2.4
1	A	1114	ASP	2.4
1	A	443	GLY	2.4
1	A	1247	ILE	2.4
1	A	474	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	977	ILE	2.3
1	A	207	GLU	2.3
1	A	1230	SER	2.3
1	A	492	LEU	2.3
1	A	674	LYS	2.2
1	A	204	ASN	2.1
1	A	666	LEU	2.1
1	A	1177	TRP	2.1
1	A	489	GLU	2.1
1	A	205	VAL	2.1
1	A	810	ASP	2.1
1	A	493	ASP	2.0
1	A	333	SER	2.0
1	A	668	GLU	2.0
1	A	844	ASN	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 carbohydrates 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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	DM2	A	3001	39/39	0.67	0.58	8.49	6,8,10,11	0
4	SO4	A	1292	5/5	0.96	0.12	-2.55	33,36,37,39	0
3	ZN	A	1291	1/1	0.98	0.13	-	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.