



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:45 PM UTC

PDB ID : 1I1E / pdb_00001i1e
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

<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

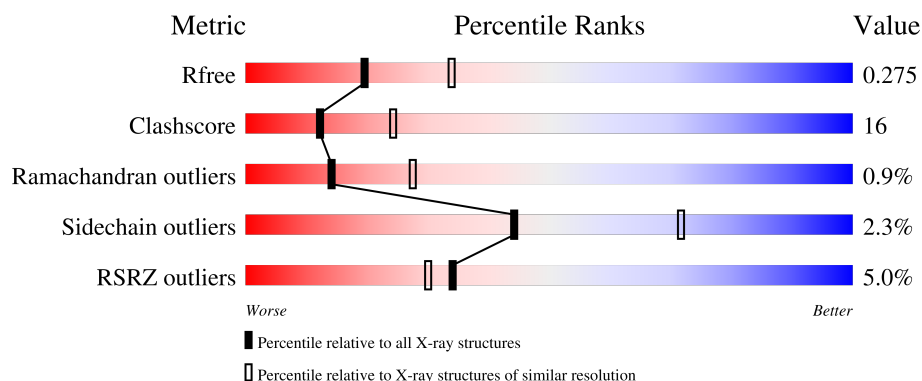
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	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	1290	

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	-

2 Entry composition [i](#)

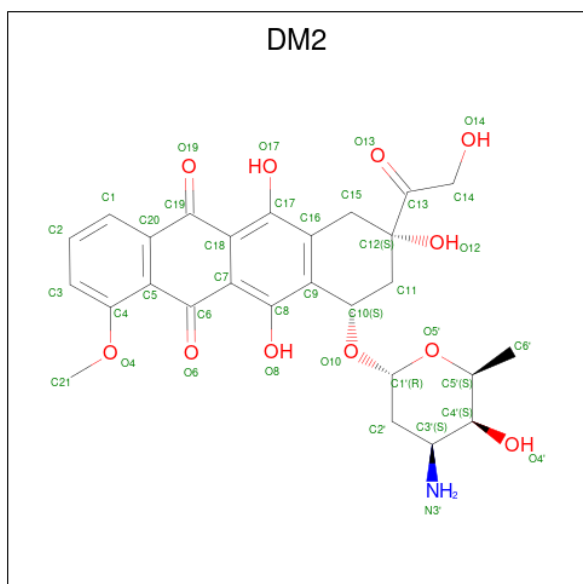
There are 5 unique types of molecules in this entry. The entry contains 11016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: DM2) (formula: $C_{27}H_{29}NO_{11}$).

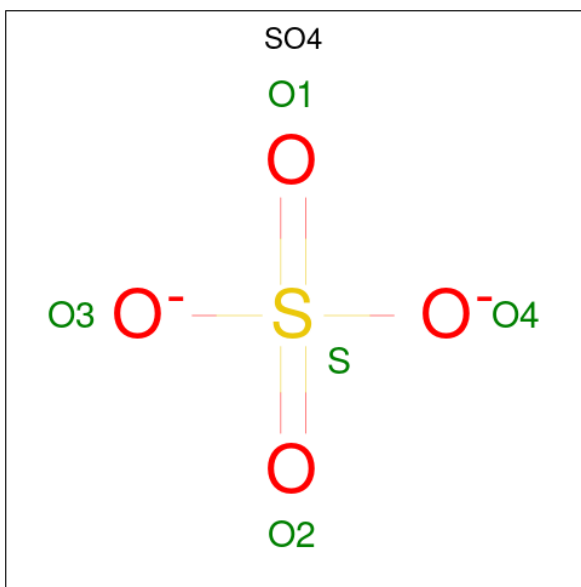


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			39	27	1	11		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

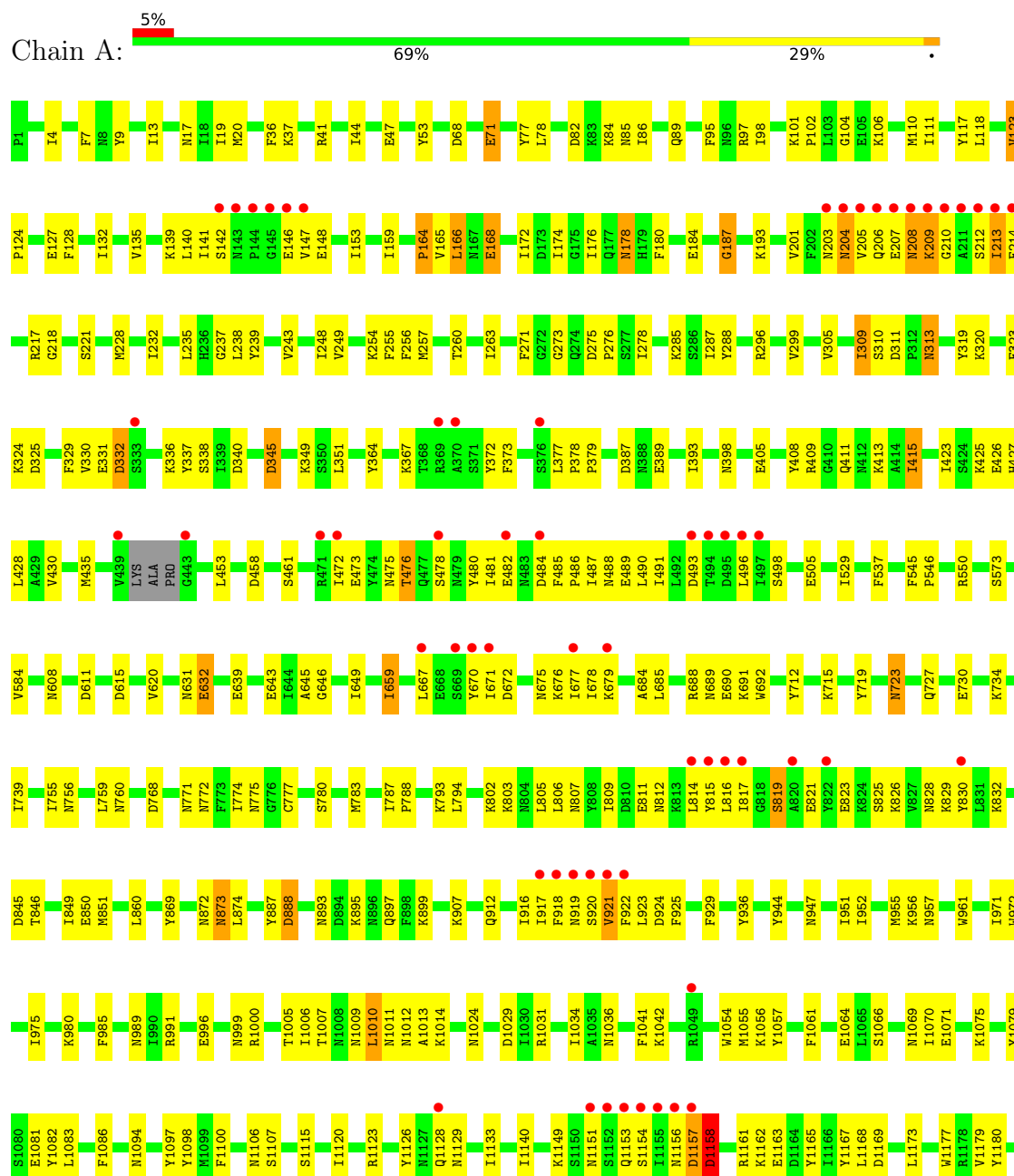
- Molecule 5 is water.

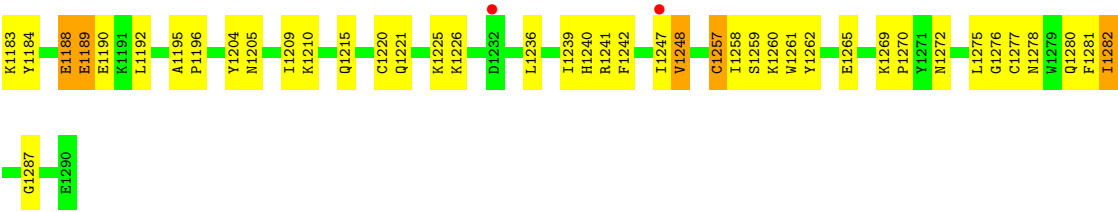
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	354	Total	O	0	0
			354	354		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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: BOTULINUM NEUROTOXIN TYPE B





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 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 95.8 (50.00-2.50)	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 (1.99%)	wwPDB-VP
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 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	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, 0.333 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: SO4, ZN, DM2

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	0/10848	0.92	33/14652 (0.2%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	GLY	N-CA-C	-8.01	102.58	112.68
1	A	1129	ASN	N-CA-C	7.78	121.59	112.72
1	A	1257	CYS	N-CA-C	7.77	121.22	109.41
1	A	210	GLY	N-CA-C	-7.41	104.82	115.27
1	A	1012	ASN	N-CA-C	7.35	121.46	109.85
1	A	19	ILE	N-CA-C	6.87	116.91	108.53
1	A	1098	TYR	N-CA-C	-6.67	100.65	110.52
1	A	1133	ILE	N-CA-C	6.57	119.57	108.86
1	A	243	VAL	N-CA-C	6.44	117.49	110.21
1	A	584	VAL	N-CA-C	6.42	116.66	108.82
1	A	659	ILE	CA-C-N	6.37	126.34	119.78
1	A	659	ILE	C-N-CA	6.37	126.34	119.78
1	A	1184	TYR	N-CA-C	6.36	120.26	111.55
1	A	71	GLU	N-CA-C	6.33	119.83	109.76
1	A	415	ILE	N-CA-C	6.18	116.91	111.90
1	A	1173	LEU	CB-CA-C	-5.85	109.27	117.23
1	A	783	MET	N-CA-C	5.84	118.59	111.82
1	A	888	ASP	N-CA-C	5.71	119.06	111.75
1	A	895	LYS	N-CA-C	-5.60	105.76	112.59
1	A	123	VAL	N-CA-C	5.41	113.28	108.63
1	A	1282	ILE	N-CA-C	5.38	113.86	107.73
1	A	1248	VAL	CB-CA-C	-5.35	107.16	111.71
1	A	174	ILE	N-CA-C	5.34	115.78	107.99
1	A	573	SER	N-CA-C	5.21	117.02	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1013	ALA	N-CA-C	-5.21	98.91	108.02
1	A	1167	TYR	N-CA-C	-5.18	100.96	109.40
1	A	1079	TYR	N-CA-C	5.17	117.72	110.23
1	A	127	GLU	N-CA-C	5.16	118.13	110.14
1	A	947	ASN	N-CA-C	5.16	117.16	108.96
1	A	221	SER	N-CA-C	5.11	118.04	110.48
1	A	620	VAL	CA-C-N	5.03	125.31	119.47
1	A	620	VAL	C-N-CA	5.03	125.31	119.47
1	A	971	ILE	N-CA-C	5.01	115.70	108.48

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	328	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	9	0
All	All	11016	0	10502	328	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 (328) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:955:MET:HE1	1:A:975:ILE:HD12	1.71	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:140:LEU:HD11	1:A:147:VAL:HA	1.72	0.71
1:A:1075:LYS:HE2	1:A:1215:GLN:NE2	2.04	0.71
1:A:209:LYS:H	1:A:209:LYS:HD2	1.56	0.70
1:A:206:GLN:HA	1:A:771:ASN:ND2	2.06	0.70
1:A:398:ASN:HD21	1:A:411:GLN:HE21	1.38	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
1:A:921:VAL:HG12	1:A:921:VAL:O	1.97	0.65
1:A:142:SER:CB	1:A:148:GLU:HG3	2.27	0.64
1:A:139:LYS:HG3	1:A:141:ILE:CD1	2.27	0.64
1:A:893:ASN:ND2	1:A:897:GLN:HB2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:819:SER:C	1:A:821:GLU:H	2.07	0.62
1:A:309:ILE:HD13	1:A:309:ILE:N	2.15	0.61
1:A:1259:SER:CB	2:A:3001:DM2:H152	2.30	0.61
1:A:1262:TYR:CE2	2:A:3001:DM2:H141	2.36	0.61
1:A:675:ASN:O	1:A:679:LYS:HG3	2.00	0.61
1:A:309:ILE:H	1:A:309:ILE:CD1	2.13	0.61
1:A:139:LYS:HG3	1:A:141:ILE:HD11	1.83	0.60
1:A:1240:HIS:HD1	2:A:3001:DM2:HO12	1.46	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:482:GLU:C	1:A:484:ASP:H	2.12	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:208:ASN:HD22	1:A:208:ASN:N	2.02	0.56
1:A:685:LEU:O	1:A:688:ARG:HB3	2.05	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:OD1	1:A:204:ASN:N	2.30	0.56
1:A:377:LEU:HB3	1:A:378:PRO:CD	2.36	0.55
1:A:1157:ASP:O	1:A:1158:ASP:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1262:TYR:OH	2:A:3001:DM2:H141	2.06	0.55
1:A:845:ASP:O	1:A:849:ILE:HG12	2.07	0.55
1:A:819:SER:C	1:A:821:GLU:N	2.63	0.55
1:A:923:LEU:HD11	1:A:925:PHE:CE2	2.41	0.55
1:A:325:ASP:OD1	1:A:498:SER:HB2	2.06	0.55
1:A:1262:TYR:CD2	1:A:1277:CYS:HB3	2.41	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:117:TYR:HA	1:A:323:PHE:CZ	2.41	0.54
1:A:425:LYS:C	1:A:427:HIS:H	2.16	0.53
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: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:550:ARG:HG2	1:A:550:ARG:HH11	1.74	0.52
1:A:273:GLY:O	1:A:276:PRO:HD2	2.10	0.52
1:A:692:TRP:CD2	1:A:794:LEU:HD13	2.44	0.52
1:A:1107:SER:HB3	1:A:1120:ILE:CG2	2.40	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:1163:GLU:CD	1:A:1210:LYS:HZ2	2.18	0.51
1:A:961:TRP:NE1	5:A:1582:HOH:O	2.43	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:379:PRO:HG2	1:A:423:ILE:HD12	1.93	0.51
1:A:922:PHE:CZ	1:A:924:ASP:HB2	2.46	0.51
1:A:1259:SER:HB3	2:A:3001:DM2:H142	1.92	0.51
1:A:936:TYR:HB3	1:A:944:TYR:CD1	2.46	0.51
1:A:1262:TYR:CE2	2:A:3001:DM2:H142	2.44	0.51
1:A:204:ASN:HB2	1:A:207:GLU:HB2	1.93	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: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:13:ILE:HD13	1:A:20:MET:HG2	1.92	0.50
1:A:36:PHE:CD1	1:A:36:PHE:N	2.80	0.50
1:A:209:LYS:H	1:A:209:LYS:CD	2.22	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:324:LYS:HZ1	1:A:331:GLU:CB	2.25	0.50
1:A:110:MET:HE3	1:A:239:TYR:OH	2.12	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:296:ARG:O	1:A:299:VAL:HG12	2.12	0.49
1:A:936:TYR:HB3	1:A:944:TYR:CE1	2.46	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:206:GLN:NE2	1:A:771:ASN:ND2	2.60	0.49
1:A:490:LEU:CD1	1:A:496:LEU:HD22	2.43	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:311:ASP:OD1	1:A:313:ASN:HB2	2.13	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:213:ILE:H	1:A:760:ASN:HD22	1.60	0.49
1:A:814:LEU:C	1:A:816:LEU:H	2.20	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:248:ILE:HA	1:A:461:SER:HB3	1.95	0.48
1:A:1083:LEU:HD13	1:A:1209:ILE:CD1	2.43	0.48
1:A:1192:LEU:HD21	1:A:1258:ILE:HB	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:212:SER:HA	1:A:760:ASN:CG	2.39	0.48
1:A:254:LYS:HB2	1:A:257:MET:HG3	1.96	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:1066:SER:OG	1:A:1069:ASN:ND2	2.46	0.48
1:A:1188:GLU:HG3	1:A:1260:LYS:HB2	1.94	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:929:PHE:CD1	1:A:1055:MET:HE2	2.50	0.47
1:A:77:TYR:CD2	1:A:78:LEU:HG	2.49	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: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:922:PHE:O	1:A:923:LEU:HB3	2.15	0.46
1:A:1262:TYR:CZ	2:A:3001:DM2:H141	2.49	0.46
1:A:41:ARG:HA	5:A:1326:HOH:O	2.15	0.46
1:A:723:ASN:OD1	1:A:727:GLN:NE2	2.48	0.46
1:A:187:GLY:HA2	1:A:237:GLY: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:53:TYR:CD2	1:A:164:PRO:HG2	2.50	0.46
1:A:111:ILE:HG23	1:A:238:LEU:CD1	2.46	0.46
1:A:204:ASN:ND2	1:A:207:GLU:HB2	2.30	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: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:929:PHE:CE1	1:A:1055:MET:HE2	2.50	0.46
1:A:1240:HIS:HD2	1:A:1242:PHE:CE1	2.34	0.46
1:A:287:ILE:O	1:A:288:TYR:C	2.59	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: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:823:GLU:HA	1:A:826:LYS:HB3	1.99	0.46
1:A:324:LYS:HD3	1:A:324:LYS:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:887:TYR:CD1	1:A:907:LYS:HG3	2.52	0.45
1:A:1083:LEU:HD22	1:A:1220:CYS:CB	2.47	0.45
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:1240:HIS:CE1	2:A:3001:DM2:H3'	2.52	0.45
1:A:271:PHE:CD2	1:A:275:ASP:OD2	2.70	0.45
1:A:787:ILE:HB	1:A:788:PRO:HD3	1.99	0.45
1:A:1106:ASN:HA	1:A:1123:ARG:HD2	1.97	0.45
1:A:1177:TRP:NE1	1:A:1196:PRO:HG3	2.31	0.45
1:A:1261:TRP:CZ3	1:A:1265:GLU:HG3	2.51	0.45
1:A:17:ASN:OD1	1:A:37:LYS:HD2	2.16	0.45
1:A:1010:LEU:CD1	1:A:1011:ASN:ND2	2.76	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: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:1215:GLN:NE2	1:A:1215:GLN:HA	2.31	0.45
1:A:117:TYR:CZ	1:A:128:PHE:HE2	2.35	0.45
1:A:819:SER:O	1:A:821:GLU:N	2.50	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:HD2	1:A:832:LYS:HA	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:768:ASP:O	1:A:772:ASN:ND2	2.51	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: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:209:LYS:HE2	1:A:217:ARG:CD	2.46	0.44
1:A:807:ASN:O	1:A:811:GLU:HG3	2.18	0.44
1:A:1240:HIS:HB2	2:A:3001:DM2:O12	2.18	0.44
1:A:473:GLU:C	1:A:475:ASN:N	2.71	0.43
1:A:1169:ASP:HB3	1:A:1177:TRP:O	2.18	0.43
1:A:1195:ALA:HB1	1:A:1196:PRO:HD2	2.00	0.43
1:A:1262:TYR:CE2	1:A:1277:CYS:HB3	2.54	0.43
1:A:44:ILE:HD13	1:A:159:ILE:HB	2.00	0.43
1:A:213:ILE:H	1:A:760:ASN:ND2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LYS:HZ1	1:A:331:GLU:HB2	1.83	0.43
1:A:475:ASN:O	1:A:476:THR:C	2.61	0.43
1:A:1247:ILE:HG13	1:A:1248:VAL:N	2.33	0.43
1:A:132:ILE:HD11	1:A:135:VAL:HG23	2.00	0.43
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:671:ILE:O	1:A:672:ASP:HB2	2.18	0.43
1:A:646:GLY:O	1:A:649:ILE:HG12	2.17	0.43
1:A:678:ILE:O	1:A:679:LYS:C	2.61	0.43
1:A:1221:GLN:N	1:A:1221:GLN:CD	2.77	0.43
1:A:1241:ARG:CB	2:A:3001:DM2:H4'	2.49	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:608:ASN:C	1:A:608:ASN:OD1	2.62	0.42
1:A:1031:ARG:HG2	5:A:1584:HOH:O	2.18	0.42
1:A:1236:LEU:HD12	1:A:1262:TYR:HB2	2.00	0.42
1:A:209:LYS:HE2	1:A:217:ARG:HB2	2.02	0.42
1:A:413:LYS:HE2	1:A:413:LYS:HB3	1.83	0.42
1:A:869:TYR:CE1	1:A:872:ASN:HA	2.54	0.42
1:A:1177:TRP:CE2	1:A:1196:PRO:HG3	2.54	0.42
1:A:166:LEU:N	1:A:166:LEU:HD23	2.35	0.42
1:A:615:ASP:C	1:A:860:LEU:HD13	2.44	0.42
1:A:688:ARG:O	1:A:691:LYS:HB2	2.19	0.42
1:A:727:GLN:O	1:A:730:GLU:HB3	2.20	0.42
1:A:775:ASN:HB3	1:A:851:MET:HE3	2.01	0.42
1:A:123:VAL:HA	1:A:124:PRO:HD3	1.91	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: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:204:ASN:HD22	1:A:207:GLU:HB2	1.85	0.42
1:A:256:PHE:O	1:A:453:LEU:HB3	2.19	0.42
1:A:309:ILE:CG1	1:A:310:SER:N	2.83	0.42
1:A:812:ASN:O	1:A:816:LEU:HG	2.20	0.42
1:A:1086:PHE:CB	1:A:1282:ILE:HG12	2.50	0.42
1:A:1157:ASP:O	1:A:1158:ASP:CB	2.67	0.42
1:A:1240:HIS:HA	2:A:3001:DM2:C5'	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:LYS:O	1:A:957:ASN:HB2	2.19	0.42
1:A:1188:GLU:O	1:A:1189:GLU:HB3	2.18	0.42
1:A:213:ILE:HB	1:A:723:ASN:HD21	1.85	0.41
1:A:631:ASN:O	1:A:632:GLU:C	2.63	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:278:ILE:HD12	1:A:373:PHE:CE1	2.55	0.41
1:A:899:LYS:HD2	1:A:1054:TRP:CZ2	2.55	0.41
1:A:71:GLU:HG2	1:A:168:GLU:OE2	2.20	0.41
1:A:1094:ASN:HD22	1:A:1156:ASN:C	2.29	0.41
1:A:1168:LEU:O	1:A:1179:VAL:HG23	2.20	0.41
1:A:1188:GLU:CB	2:A:3001:DM2:O19	2.52	0.41
1:A:478:SER:HB3	1:A:480:TYR:HE1	1.85	0.41
1:A:739:ILE:HD13	1:A:739:ILE:HA	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:755:ILE:O	1:A:759:LEU:HG	2.20	0.41
1:A:920:SER:C	1:A:921:VAL:HG23	2.45	0.41
1:A:996:GLU:HA	1:A:1000:ARG:HH11	1.85	0.41
1:A:285:LYS:HG2	1:A:481:ILE:CD1	2.50	0.41
1:A:1269:LYS:HA	1:A:1270:PRO:C	2.45	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:719:TYR:O	1:A:723:ASN:HB2	2.21	0.41
1:A:980:LYS:HE2	1:A:1029:ASP:CB	2.50	0.41
1:A:1140:ILE:HG13	5:A:1609:HOH:O	2.21	0.41
1:A:1225:LYS:O	1:A:1226:LYS:C	2.64	0.41
1:A:715:LYS:HG3	1:A:774:ILE:HG21	2.01	0.41
1:A:1009:ASN:OD1	1:A:1009:ASN:C	2.63	0.40
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:985:PHE:CD1	1:A:985:PHE:C	2.99	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%)	14	27

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 [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	1185/1189 (100%)	1158 (98%)	27 (2%)	44	72

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	164	PRO
1	A	166	LEU
1	A	168	GLU
1	A	178	ASN
1	A	204	ASN
1	A	208	ASN
1	A	209	LYS
1	A	213	ILE
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
1	A	919	ASN
1	A	1010	LEU
1	A	1115	SER
1	A	1157	ASP
1	A	1158	ASP
1	A	1188	GLU
1	A	1189	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	15	ASN
1	A	85	ASN
1	A	113	ASN
1	A	178	ASN
1	A	203	ASN
1	A	206	GLN
1	A	208	ASN
1	A	293	GLN
1	A	398	ASN
1	A	411	GLN
1	A	475	ASN

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Mol	Chain	Res	Type
1	A	483	ASN
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	765	GLN
1	A	771	ASN
1	A	772	ASN
1	A	799	ASN
1	A	844	ASN
1	A	853	ASN
1	A	862	ASN
1	A	873	ASN
1	A	914	GLN
1	A	938	ASN
1	A	989	ASN
1	A	999	ASN
1	A	1011	ASN
1	A	1067	GLN
1	A	1069	ASN
1	A	1104	ASN
1	A	1134	ASN
1	A	1215	GLN
1	A	1278	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	0.39	0	6,6,6	0.26	0
2	DM2	A	3001	-	42,43,43	3.49	23 (54%)	56,67,67	1.59	11 (19%)

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
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	O13-C13	12.51	1.41	1.21
2	A	3001	DM2	O6-C6	8.78	1.38	1.22
2	A	3001	DM2	O19-C19	6.43	1.34	1.22
2	A	3001	DM2	C1-C20	5.36	1.48	1.39
2	A	3001	DM2	C8-C9	3.90	1.46	1.40
2	A	3001	DM2	C11-C12	3.88	1.61	1.53
2	A	3001	DM2	O5'-C5'	3.83	1.53	1.44
2	A	3001	DM2	C7-C8	3.57	1.48	1.41
2	A	3001	DM2	C2-C3	3.45	1.44	1.38
2	A	3001	DM2	C2'-C1'	3.44	1.59	1.50
2	A	3001	DM2	C11-C10	3.25	1.58	1.52
2	A	3001	DM2	C3-C4	3.24	1.46	1.39
2	A	3001	DM2	C5-C4	3.23	1.46	1.40
2	A	3001	DM2	O5'-C1'	3.19	1.50	1.42
2	A	3001	DM2	C2-C1	3.03	1.44	1.38
2	A	3001	DM2	O4'-C4'	2.89	1.50	1.43
2	A	3001	DM2	C17-C16	2.87	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	DM2	O4-C4	2.85	1.41	1.37
2	A	3001	DM2	C18-C17	2.58	1.46	1.41
2	A	3001	DM2	O12-C12	2.25	1.47	1.43
2	A	3001	DM2	C18-C7	2.25	1.46	1.41
2	A	3001	DM2	C2'-C3'	2.24	1.58	1.53
2	A	3001	DM2	C20-C5	2.15	1.44	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	DM2	O10-C10-C9	-4.60	97.20	107.54
2	A	3001	DM2	O12-C12-C11	4.51	119.65	109.40
2	A	3001	DM2	C7-C6-C5	3.12	123.46	118.11
2	A	3001	DM2	O4-C4-C5	3.08	120.20	115.84
2	A	3001	DM2	C11-C10-C9	3.06	117.88	110.71
2	A	3001	DM2	O4'-C4'-C3'	-3.00	104.29	109.90
2	A	3001	DM2	O6-C6-C7	-2.85	116.67	121.44
2	A	3001	DM2	C8-C7-C6	2.69	124.80	120.46
2	A	3001	DM2	O4-C4-C3	-2.59	119.93	124.30
2	A	3001	DM2	C18-C7-C6	-2.38	116.78	120.00
2	A	3001	DM2	C21-O4-C4	2.32	120.91	117.51

There are no chirality outliers.

There are no torsion outliers.

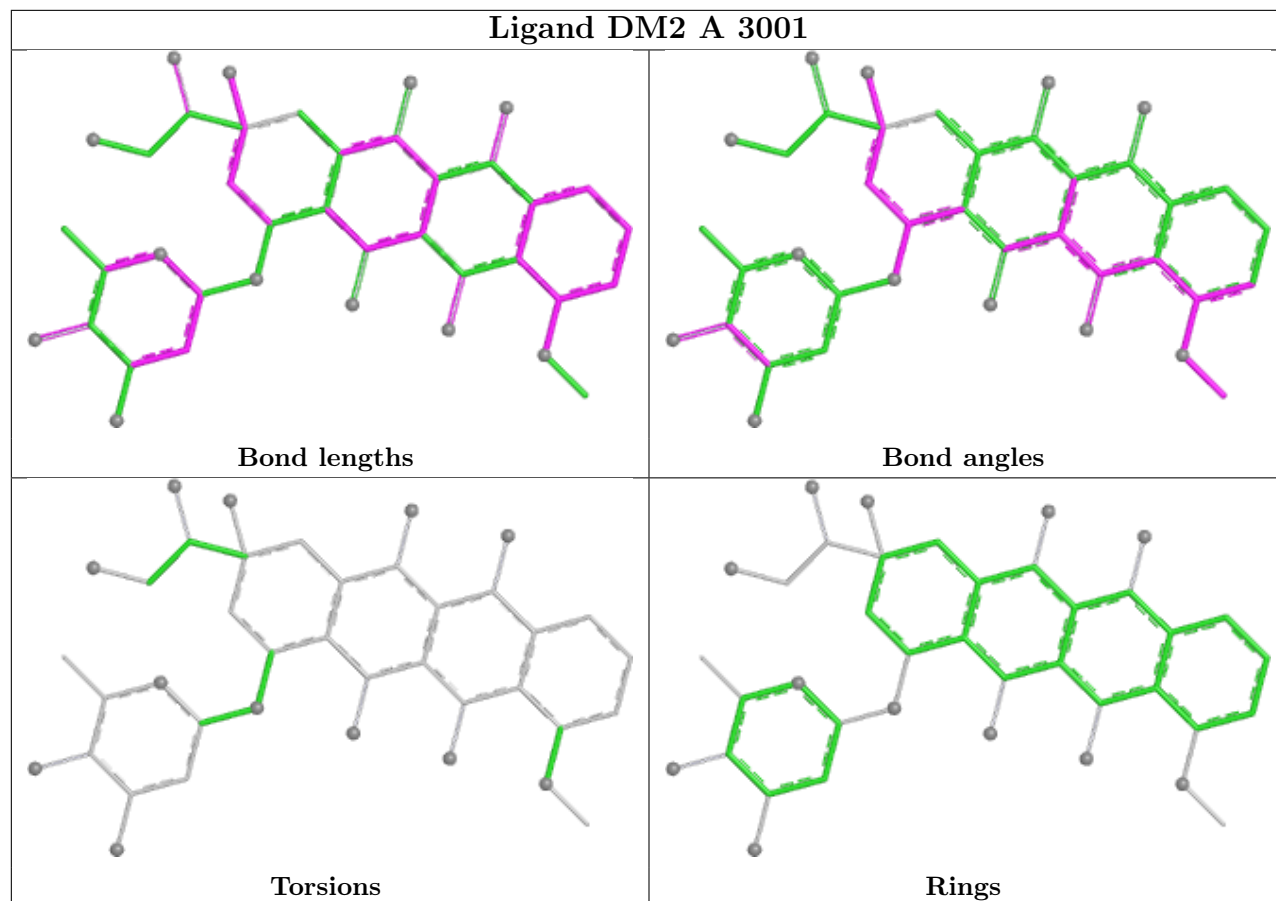
There are no ring outliers.

1 monomer is involved in 26 short contacts:

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

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	1287/1290 (99%)	0.16	64 (4%) 34 30	11, 27, 53, 63	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1156	ASN	5.9
1	A	145	GLY	5.6
1	A	921	VAL	5.4
1	A	1155	ILE	5.1
1	A	1154	SER	5.0
1	A	1153	GLN	4.9
1	A	918	PHE	4.8
1	A	208	ASN	4.6
1	A	1152	SER	4.6
1	A	147	VAL	4.5
1	A	919	ASN	4.4
1	A	830	TYR	4.2
1	A	1151	ASN	3.8
1	A	144	PRO	3.7
1	A	817	ILE	3.7
1	A	146	GLU	3.6
1	A	206	GLN	3.6
1	A	210	GLY	3.5
1	A	671	ILE	3.5
1	A	920	SER	3.5
1	A	494	THR	3.4
1	A	204	ASN	3.3
1	A	471	ARG	3.3
1	A	667	LEU	3.3
1	A	496	LEU	3.2
1	A	209	LYS	3.1
1	A	495	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	333	SER	3.0
1	A	922	PHE	3.0
1	A	143	ASN	2.9
1	A	205	VAL	2.9
1	A	669	SER	2.8
1	A	370	ALA	2.8
1	A	213	ILE	2.7
1	A	207	GLU	2.7
1	A	1157	ASP	2.7
1	A	211	ALA	2.7
1	A	212	SER	2.6
1	A	214	PHE	2.6
1	A	439	VAL	2.5
1	A	472	ILE	2.5
1	A	484	ASP	2.4
1	A	917	ILE	2.4
1	A	670	TYR	2.4
1	A	814	LEU	2.4
1	A	820	ALA	2.4
1	A	376	SER	2.3
1	A	816	LEU	2.3
1	A	1232	ASP	2.3
1	A	815	TYR	2.3
1	A	679	LYS	2.3
1	A	478	SER	2.3
1	A	203	ASN	2.2
1	A	1049	ARG	2.3
1	A	1128	GLN	2.2
1	A	142	SER	2.2
1	A	443	GLY	2.2
1	A	482	GLU	2.2
1	A	822	TYR	2.1
1	A	369	ARG	2.1
1	A	497	ILE	2.1
1	A	1247	ILE	2.1
1	A	677	ILE	2.1
1	A	493	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

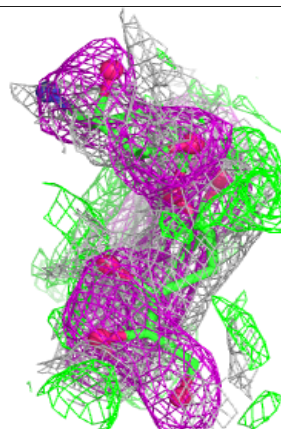
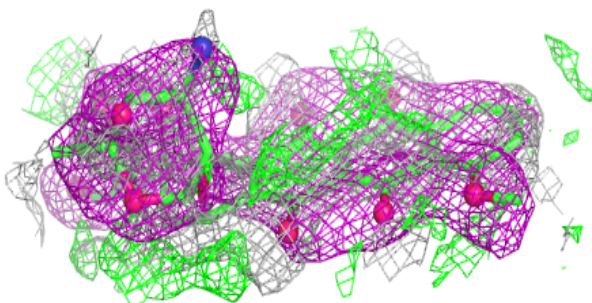
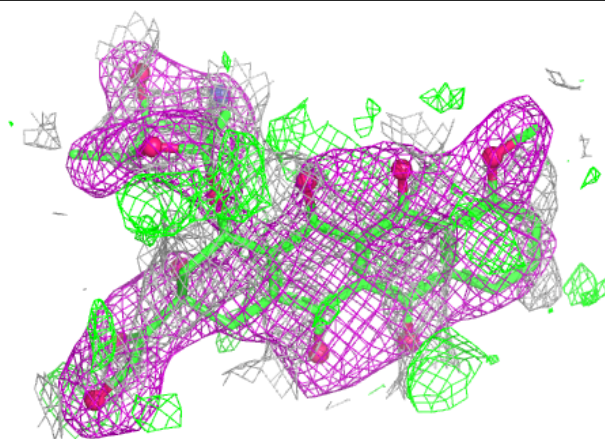
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DM2	A	3001	39/39	0.58	0.17	6,8,10,11	0
4	SO4	A	1292	5/5	0.94	0.15	33,36,37,39	0
3	ZN	A	1291	1/1	1.00	0.05	35,35,35,35	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 DM2 A 3001:

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.