Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 09:02 PM EST

PDB ID	:	1DFQ
Title	:	THE HC FRAGMENT OF TETANUS TOXIN COMPLEXED WITH SIALIC ACID
Authors	:	Emsley, P.; Fotinou, C.; Black, I.; Fairweather, N.F.; Charles, I.G.; Watts, C.; Hewitt, E.; Isaacs, N.W.
Deposited on	:	1999-11-20
Resolution	:	2.60 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:

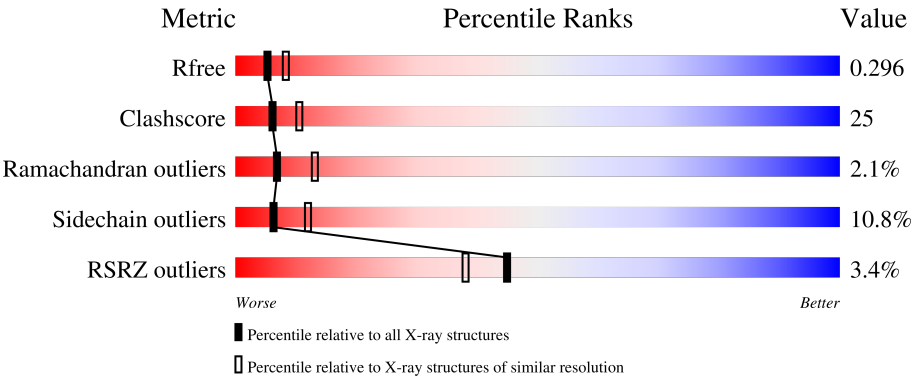
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	444	3% 44% 39% 13%

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	SLB	A	1400	-	-	-	X

2 Entry composition

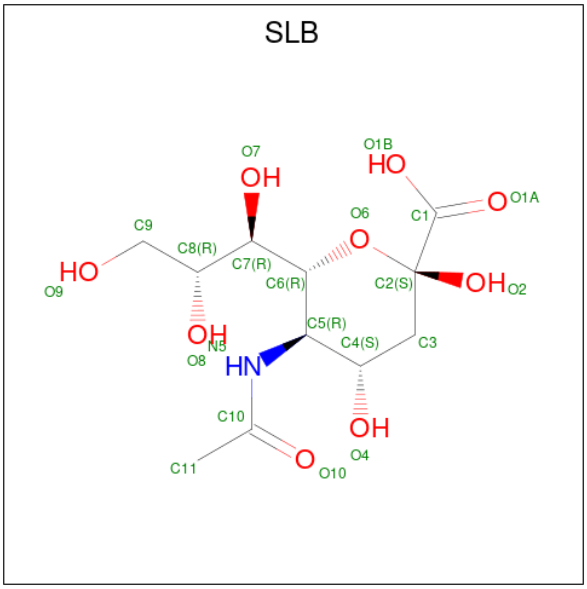
There are 3 unique types of molecules in this entry. The entry contains 3805 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TETANUS TOXIN HC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	441	3563	2282	597	675	9	0	0	0

- Molecule 2 is N-acetyl-beta-neuraminic acid (three-letter code: SLB) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	21	11	1	9	0	0

- Molecule 3 is water.

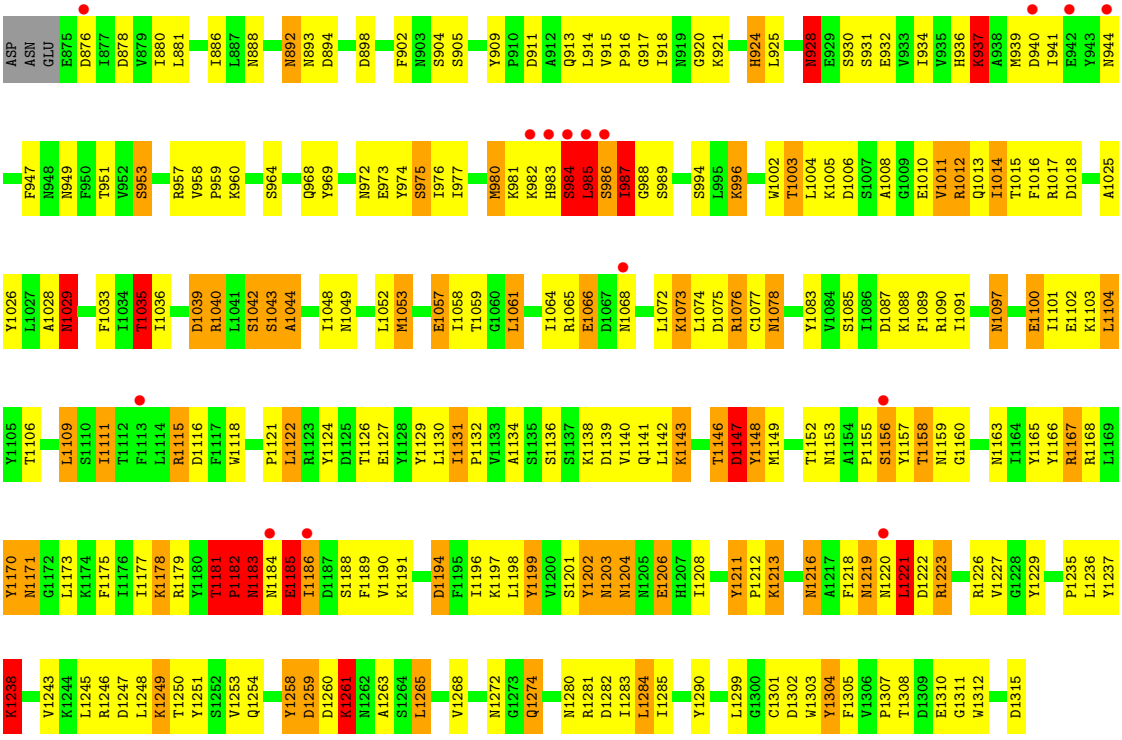
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	221	221	221	0	0

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: TETANUS TOXIN HC

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.86Å 70.24Å 122.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 17.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	82.0 (20.00-2.60) 81.9 (17.99-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.313 0.195 , 0.296	Depositor DCC
R_{free} test set	739 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.865	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3805	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SLB

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	0.79	0/3644	2.09	145/4945 (2.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1090	ARG	NE-CZ-NH2	-20.52	110.04	120.30
1	A	1017	ARG	NE-CZ-NH1	-17.89	111.36	120.30
1	A	1017	ARG	NE-CZ-NH2	15.18	127.89	120.30
1	A	1167	ARG	CD-NE-CZ	13.00	141.80	123.60
1	A	1017	ARG	CD-NE-CZ	12.83	141.56	123.60
1	A	1090	ARG	NE-CZ-NH1	11.72	126.16	120.30
1	A	1152	THR	N-CA-CB	11.34	131.84	110.30
1	A	1259	ASP	CB-CG-OD2	-10.89	108.50	118.30
1	A	1115	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	A	957	ARG	NE-CZ-NH2	10.47	125.54	120.30
1	A	1304	TYR	CB-CG-CD1	10.39	127.23	121.00
1	A	1302	ASP	CB-CG-OD1	-10.02	109.28	118.30
1	A	1018	ASP	CB-CG-OD2	10.01	127.31	118.30
1	A	1226	ARG	NE-CZ-NH2	9.94	125.27	120.30
1	A	1185	GLU	O-C-N	-9.48	107.53	122.70
1	A	1149	MET	CG-SD-CE	9.01	114.61	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1012	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	1223	ARG	NE-CZ-NH1	-8.61	116.00	120.30
1	A	1076	ARG	NE-CZ-NH1	-8.53	116.03	120.30
1	A	1167	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	1258	TYR	CB-CG-CD1	8.35	126.01	121.00
1	A	1199	TYR	CB-CG-CD1	8.32	125.99	121.00
1	A	928	ASN	CA-CB-CG	8.24	131.52	113.40
1	A	940	ASP	CB-CG-OD2	8.21	125.69	118.30
1	A	1006	ASP	CB-CG-OD1	8.01	125.51	118.30
1	A	1223	ARG	CD-NE-CZ	8.00	134.79	123.60
1	A	1129	TYR	CB-CG-CD2	-7.88	116.27	121.00
1	A	1012	ARG	CD-NE-CZ	7.87	134.62	123.60
1	A	953	SER	N-CA-CB	7.85	122.27	110.50
1	A	1136	SER	O-C-N	-7.75	110.30	122.70
1	A	1181	THR	N-CA-CB	7.73	124.98	110.30
1	A	1166	TYR	CA-C-O	-7.54	104.28	120.10
1	A	1134	ALA	CB-CA-C	-7.46	98.92	110.10
1	A	1100	GLU	OE1-CD-OE2	-7.38	114.44	123.30
1	A	1226	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	A	1185	GLU	CA-C-N	7.25	133.16	117.20
1	A	1156	SER	C-N-CA	7.22	139.75	121.70
1	A	1029	ASN	CB-CG-ND2	-7.21	99.40	116.70
1	A	911	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	1261	LYS	CA-CB-CG	7.11	129.04	113.40
1	A	1282	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	1129	TYR	CB-CG-CD1	7.08	125.25	121.00
1	A	1284	LEU	CB-CG-CD2	6.98	122.87	111.00
1	A	1166	TYR	CB-CG-CD1	6.95	125.17	121.00
1	A	1010	GLU	OE1-CD-OE2	-6.93	114.98	123.30
1	A	1284	LEU	CA-CB-CG	6.86	131.08	115.30
1	A	1170	TYR	CB-CG-CD1	6.85	125.11	121.00
1	A	1109	LEU	CA-C-O	6.77	134.32	120.10
1	A	1246	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	1206	GLU	OE1-CD-OE2	-6.72	115.24	123.30
1	A	1061	LEU	N-CA-CB	6.71	123.81	110.40
1	A	1011	VAL	CA-CB-CG2	6.70	120.95	110.90
1	A	1281	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	A	1015	THR	CA-CB-CG2	6.67	121.74	112.40
1	A	980	MET	CA-CB-CG	6.63	124.57	113.30
1	A	1304	TYR	CB-CG-CD2	-6.61	117.03	121.00
1	A	1171	ASN	N-CA-CB	6.52	122.34	110.60
1	A	1064	ILE	CB-CA-C	6.52	124.64	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1182	PRO	CA-C-N	-6.50	102.89	117.20
1	A	937	LYS	CA-CB-CG	6.50	127.70	113.40
1	A	1025	ALA	N-CA-CB	-6.50	101.01	110.10
1	A	1029	ASN	N-CA-C	6.44	128.39	111.00
1	A	1065	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	1285	ILE	CB-CA-C	-6.40	98.81	111.60
1	A	1186	ILE	CA-C-N	-6.36	103.21	117.20
1	A	1124	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	A	1202	TYR	CA-CB-CG	6.23	125.23	113.40
1	A	1115	ARG	NH1-CZ-NH2	6.20	126.22	119.40
1	A	1116	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	1301	CYS	O-C-N	-6.17	112.83	122.70
1	A	1057	GLU	CA-CB-CG	6.17	126.96	113.40
1	A	1222	ASP	CB-CG-OD1	6.08	123.78	118.30
1	A	1194	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	1274	GLN	CA-CB-CG	6.06	126.73	113.40
1	A	1182	PRO	CB-CA-C	-6.02	96.95	112.00
1	A	928	ASN	O-C-N	5.99	132.28	122.70
1	A	958	VAL	CA-CB-CG2	5.96	119.83	110.90
1	A	1147	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	A	1281	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	A	1044	ALA	CA-C-N	5.81	129.99	117.20
1	A	1166	TYR	CA-C-N	5.81	129.99	117.20
1	A	969	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	A	1040	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	A	1014	ILE	O-C-N	-5.74	113.52	122.70
1	A	1305	PHE	CB-CG-CD2	-5.74	116.78	120.80
1	A	1139	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	1029	ASN	CB-CA-C	-5.73	98.94	110.40
1	A	1247	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	1315	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	1158	THR	N-CA-CB	5.68	121.10	110.30
1	A	1186	ILE	CB-CA-C	5.68	122.96	111.60
1	A	1026	TYR	CA-CB-CG	-5.66	102.64	113.40
1	A	1201	SER	N-CA-CB	-5.66	102.00	110.50
1	A	1039	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	1222	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	1199	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	A	1146	THR	N-CA-CB	5.63	120.99	110.30
1	A	968	GLN	CA-CB-CG	5.62	125.75	113.40
1	A	1274	GLN	N-CA-CB	5.60	120.69	110.60
1	A	1290	TYR	CB-CG-CD1	5.55	124.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1078	ASN	CB-CG-ND2	-5.54	103.41	116.70
1	A	1170	TYR	O-C-N	-5.54	113.84	122.70
1	A	985	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	928	ASN	N-CA-CB	-5.51	100.68	110.60
1	A	1246	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	917	GLY	O-C-N	-5.49	113.92	122.70
1	A	1265	LEU	O-C-N	-5.48	113.89	123.20
1	A	892	ASN	N-CA-CB	5.48	120.46	110.60
1	A	1136	SER	CB-CA-C	5.47	120.49	110.10
1	A	1251	TYR	CB-CA-C	5.45	121.29	110.40
1	A	936	HIS	CA-CB-CG	5.44	122.85	113.60
1	A	924	HIS	CG-ND1-CE1	5.42	115.78	108.20
1	A	1301	CYS	CA-C-N	5.40	129.08	117.20
1	A	1221	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	1008	ALA	O-C-N	-5.36	114.09	123.20
1	A	1061	LEU	O-C-N	5.34	132.28	123.20
1	A	1035	THR	CB-CA-C	5.33	125.99	111.60
1	A	1131	ILE	CA-CB-CG1	5.32	121.11	111.00
1	A	1156	SER	CA-C-O	5.28	131.19	120.10
1	A	1148	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	A	1002	TRP	CE3-CZ3-CH2	5.26	126.99	121.20
1	A	1121	PRO	CB-CA-C	5.26	125.16	112.00
1	A	920	GLY	CA-C-O	5.26	130.07	120.60
1	A	1168	ARG	CD-NE-CZ	5.25	130.96	123.60
1	A	1211	TYR	CB-CG-CD2	5.25	124.15	121.00
1	A	1157	TYR	N-CA-CB	5.25	120.04	110.60
1	A	1220	ASN	C-N-CA	5.21	134.74	121.70
1	A	1155	PRO	CA-C-O	5.19	132.66	120.20
1	A	1006	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	957	ARG	CA-C-N	5.18	128.59	117.20
1	A	1182	PRO	CA-C-O	5.17	132.62	120.20
1	A	1250	THR	CA-CB-OG1	-5.17	98.15	109.00
1	A	1238	LYS	CB-CA-C	5.14	120.69	110.40
1	A	1250	THR	CA-CB-CG2	5.14	119.59	112.40
1	A	986	SER	N-CA-CB	5.13	118.19	110.50
1	A	1157	TYR	CB-CA-C	-5.13	100.15	110.40
1	A	892	ASN	CB-CA-C	-5.12	100.16	110.40
1	A	936	HIS	N-CA-CB	5.12	119.81	110.60
1	A	953	SER	O-C-N	5.11	130.88	122.70
1	A	1268	VAL	CA-CB-CG2	-5.11	103.23	110.90
1	A	1259	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	1109	LEU	O-C-N	-5.05	114.62	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	878	ASP	CB-CG-OD1	-5.04	113.77	118.30
1	A	1043	SER	CA-CB-OG	-5.04	97.60	111.20
1	A	1283	ILE	CA-CB-CG2	5.02	120.94	110.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1182	PRO	Peptide
1	A	1183	ASN	Peptide
1	A	1185	GLU	Mainchain

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	3563	0	3516	175	0
2	A	21	0	18	1	0
3	A	221	0	0	29	0
All	All	3805	0	3534	175	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 25.

All (175) 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:1182:PRO:HD2	1:A:1183:ASN:HB2	1.21	1.18
1:A:972:ASN:HD21	1:A:1078:ASN:H	1.08	0.96
1:A:1181:THR:HB	1:A:1182:PRO:CD	1.98	0.93
1:A:996:LYS:HG2	3:A:96:HOH:O	1.68	0.92
1:A:1016:PHE:CE1	1:A:1053:MET:HG3	2.04	0.92
1:A:1053:MET:SD	3:A:101:HOH:O	2.29	0.89
1:A:1181:THR:HB	1:A:1182:PRO:HD2	1.52	0.89
1:A:1003:THR:HB	1:A:1013:GLN:HG2	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1198:LEU:HB2	3:A:127:HOH:O	1.76	0.85
1:A:947:PHE:O	1:A:1040:ARG:HG3	1.75	0.85
1:A:915:VAL:HB	1:A:916:PRO:HD2	1.57	0.85
1:A:984:SER:O	1:A:985:LEU:HB3	1.77	0.84
1:A:1141:GLN:HE21	1:A:1142:LEU:H	1.25	0.84
1:A:1005:LYS:HG3	1:A:1011:VAL:HG22	1.60	0.81
1:A:1029:ASN:HB3	1:A:1118:TRP:CE3	2.18	0.79
1:A:1160:GLY:HA3	3:A:64:HOH:O	1.82	0.79
1:A:915:VAL:HB	1:A:916:PRO:CD	2.13	0.78
1:A:972:ASN:ND2	1:A:1078:ASN:H	1.81	0.77
1:A:1182:PRO:CD	1:A:1183:ASN:HB2	2.11	0.77
1:A:977:ILE:HG13	3:A:132:HOH:O	1.82	0.77
1:A:949:ASN:HD21	1:A:1040:ARG:H	1.33	0.76
1:A:1299:LEU:HD12	3:A:202:HOH:O	1.89	0.71
1:A:1106:THR:HA	1:A:1109:LEU:HD12	1.71	0.71
1:A:1284:LEU:HD13	3:A:99:HOH:O	1.90	0.70
1:A:1066:GLU:HG2	3:A:195:HOH:O	1.92	0.70
1:A:973:GLU:HB2	1:A:996:LYS:HG3	1.72	0.69
1:A:1260:ASP:HB3	3:A:115:HOH:O	1.92	0.69
1:A:1216:ASN:HB2	2:A:1400:SLB:H31	1.75	0.69
1:A:1182:PRO:HD2	1:A:1183:ASN:CB	2.14	0.69
1:A:1097:ASN:ND2	1:A:1100:GLU:H	1.91	0.68
1:A:949:ASN:ND2	1:A:1040:ARG:H	1.91	0.68
1:A:1185:GLU:O	1:A:1186:ILE:HD12	1.94	0.68
1:A:982:LYS:HE3	1:A:1076:ARG:NH1	2.08	0.68
1:A:1170:TYR:CE1	1:A:1308:THR:HA	2.29	0.67
1:A:1097:ASN:HD22	1:A:1100:GLU:H	1.40	0.67
1:A:980:MET:HG2	1:A:988:GLY:O	1.95	0.66
1:A:1184:ASN:O	1:A:1185:GLU:HG3	1.96	0.66
1:A:1223:ARG:NH1	3:A:7:HOH:O	2.29	0.65
1:A:1127:GLU:HB3	3:A:119:HOH:O	1.96	0.64
1:A:1143:LYS:HB3	1:A:1147:ASP:HB3	1.79	0.64
1:A:973:GLU:CB	1:A:996:LYS:HG3	2.27	0.64
1:A:928:ASN:OD1	1:A:930:SER:N	2.28	0.64
1:A:1173:LEU:HA	3:A:201:HOH:O	1.97	0.64
1:A:941:ILE:HA	1:A:944:ASN:ND2	2.14	0.63
1:A:1097:ASN:HD21	1:A:1100:GLU:HG3	1.64	0.62
1:A:1182:PRO:CD	1:A:1183:ASN:N	2.62	0.62
1:A:918:ILE:O	1:A:1115:ARG:NH2	2.31	0.61
1:A:1033:PHE:HZ	1:A:1104:LEU:HD13	1.65	0.61
1:A:1130:LEU:HG	1:A:1175:PHE:CD1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1033:PHE:CZ	1:A:1104:LEU:HD13	2.36	0.61
1:A:1212:PRO:HB3	1:A:1229:TYR:CE1	2.36	0.60
1:A:1053:MET:SD	3:A:108:HOH:O	2.56	0.60
1:A:925:LEU:HD13	1:A:1073:LYS:HA	1.83	0.60
1:A:1177:ILE:HG23	1:A:1196:ILE:HD12	1.84	0.60
1:A:1243:VAL:HG23	1:A:1254:GLN:HB2	1.84	0.60
1:A:982:LYS:HE3	1:A:1076:ARG:HH12	1.68	0.59
1:A:1016:PHE:CD1	1:A:1053:MET:HG3	2.38	0.59
1:A:1221:LEU:O	1:A:1223:ARG:NH1	2.36	0.59
1:A:1156:SER:HA	3:A:106:HOH:O	2.02	0.59
1:A:1109:LEU:HD22	1:A:1248:LEU:O	2.02	0.59
1:A:1075:ASP:OD1	1:A:1076:ARG:N	2.36	0.58
1:A:1202:TYR:O	1:A:1203:ASN:HB3	2.01	0.58
1:A:1141:GLN:NE2	1:A:1142:LEU:H	1.99	0.58
1:A:1181:THR:CB	1:A:1182:PRO:CD	2.75	0.58
1:A:1223:ARG:CZ	3:A:7:HOH:O	2.52	0.57
1:A:1171:ASN:HB3	3:A:91:HOH:O	2.04	0.57
1:A:1178:LYS:HE3	1:A:1206:GLU:OE1	2.03	0.57
1:A:1223:ARG:NE	3:A:98:HOH:O	2.38	0.57
1:A:1029:ASN:ND2	1:A:1311:GLY:O	2.36	0.56
1:A:1039:ASP:OD2	1:A:1042:SER:OG	2.21	0.56
1:A:1179:ARG:NH2	1:A:1186:ILE:HG13	2.21	0.56
1:A:1182:PRO:HG2	1:A:1183:ASN:HD22	1.71	0.56
1:A:1146:THR:N	1:A:1227:VAL:O	2.33	0.55
1:A:976:ILE:HG13	3:A:132:HOH:O	2.07	0.55
1:A:1188:SER:HB2	3:A:86:HOH:O	2.07	0.55
1:A:915:VAL:CB	1:A:916:PRO:CD	2.81	0.55
1:A:989:SER:O	1:A:1066:GLU:HA	2.07	0.55
1:A:1235:PRO:HA	3:A:167:HOH:O	2.07	0.54
1:A:1197:LYS:HD3	1:A:1208:ILE:CD1	2.39	0.53
1:A:1048:ILE:HD12	1:A:1053:MET:HG2	1.89	0.53
1:A:1253:VAL:HG12	1:A:1254:GLN:N	2.23	0.53
1:A:1141:GLN:HG3	1:A:1142:LEU:N	2.24	0.53
1:A:892:ASN:O	1:A:893:ASN:HB2	2.07	0.53
1:A:1178:LYS:HD3	1:A:1199:TYR:CE1	2.43	0.53
1:A:1028:ALA:O	1:A:1029:ASN:HB2	2.09	0.52
1:A:1075:ASP:OD1	1:A:1076:ARG:HG3	2.09	0.52
1:A:1213:LYS:HG3	1:A:1237:TYR:OH	2.09	0.52
1:A:1048:ILE:O	1:A:1049:ASN:C	2.48	0.52
1:A:1191:LYS:HB2	1:A:1194:ASP:OD1	2.10	0.52
1:A:1237:TYR:HB3	1:A:1258:TYR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:THR:HG22	1:A:1165:TYR:HB3	1.92	0.52
1:A:949:ASN:HD21	1:A:1040:ARG:N	2.06	0.51
1:A:1033:PHE:HZ	1:A:1104:LEU:CD1	2.23	0.51
1:A:1272:ASN:ND2	1:A:1280:ASN:OD1	2.40	0.51
1:A:1040:ARG:HA	1:A:1058:ILE:CD1	2.41	0.51
1:A:977:ILE:HD13	1:A:1089:PHE:CE1	2.46	0.51
1:A:937:LYS:HG3	1:A:941:ILE:CD1	2.41	0.50
1:A:960:LYS:HE3	1:A:1312:TRP:CD2	2.46	0.50
1:A:1131:ILE:HG23	1:A:1138:LYS:O	2.12	0.50
1:A:987:ILE:HG22	1:A:989:SER:N	2.26	0.50
1:A:1083:TYR:OH	1:A:1310:GLU:HG3	2.12	0.49
1:A:1087:ASP:O	1:A:1088:LYS:HB2	2.13	0.49
1:A:1259:ASP:HB3	1:A:1265:LEU:HD11	1.94	0.49
1:A:888:ASN:O	1:A:898:ASP:HA	2.13	0.49
1:A:972:ASN:HD21	1:A:1078:ASN:N	1.92	0.49
1:A:974:TYR:CG	1:A:1077:CYS:HB2	2.48	0.48
1:A:1237:TYR:CD1	1:A:1259:ASP:HA	2.48	0.48
1:A:987:ILE:HG22	1:A:989:SER:H	1.79	0.48
1:A:1182:PRO:HG2	1:A:1183:ASN:ND2	2.29	0.48
1:A:976:ILE:CG1	3:A:132:HOH:O	2.61	0.48
1:A:1211:TYR:CD1	1:A:1223:ARG:HB3	2.49	0.48
1:A:931:SER:O	1:A:932:GLU:HB2	2.13	0.47
1:A:1182:PRO:CG	1:A:1183:ASN:N	2.77	0.47
1:A:924:HIS:HD2	1:A:1085:SER:OG	1.96	0.47
1:A:1035:THR:HG21	1:A:1101:ILE:HG23	1.95	0.47
1:A:1102:GLU:OE2	1:A:1249:LYS:NZ	2.37	0.47
1:A:1004:LEU:O	1:A:1011:VAL:HG13	2.15	0.47
1:A:1181:THR:HG23	3:A:125:HOH:O	2.14	0.47
1:A:977:ILE:HG12	1:A:1072:LEU:HG	1.97	0.47
1:A:1190:VAL:HG12	1:A:1191:LYS:N	2.29	0.47
1:A:886:ILE:HG13	1:A:1091:ILE:O	2.14	0.47
1:A:1014:ILE:HD11	1:A:1044:ALA:O	2.14	0.47
1:A:913:GLN:O	1:A:914:LEU:HD23	2.14	0.46
1:A:1040:ARG:HH21	1:A:1061:LEU:HB2	1.81	0.46
1:A:1156:SER:CA	3:A:106:HOH:O	2.60	0.46
1:A:1158:THR:HG22	1:A:1165:TYR:CB	2.46	0.46
1:A:894:ASP:OD1	1:A:921:LYS:NZ	2.42	0.46
1:A:976:ILE:HG22	1:A:1074:LEU:HD22	1.97	0.46
1:A:1097:ASN:ND2	1:A:1100:GLU:HG3	2.28	0.46
1:A:1029:ASN:HB3	1:A:1118:TRP:CZ3	2.50	0.45
1:A:1143:LYS:HG2	1:A:1148:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:GLU:HG2	3:A:153:HOH:O	2.15	0.45
1:A:947:PHE:HA	1:A:1040:ARG:HH12	1.80	0.45
1:A:1012:ARG:HG2	1:A:1061:LEU:HD21	1.99	0.45
1:A:1040:ARG:HA	1:A:1058:ILE:HD12	1.99	0.45
1:A:1218:PHE:O	1:A:1219:ASN:C	2.54	0.45
1:A:953:SER:HB3	1:A:1035:THR:HB	2.00	0.44
1:A:932:GLU:HG3	1:A:1073:LYS:HB2	1.99	0.44
1:A:1138:LYS:HE2	1:A:1153:ASN:OD1	2.18	0.44
1:A:1140:VAL:HG12	1:A:1141:GLN:N	2.32	0.44
1:A:1053:MET:CG	3:A:108:HOH:O	2.65	0.44
1:A:1131:ILE:HG23	1:A:1132:PRO:HD2	2.00	0.43
1:A:1259:ASP:OD1	1:A:1263:ALA:HB3	2.18	0.43
1:A:982:LYS:HD2	1:A:982:LYS:HA	1.88	0.43
1:A:1103:LYS:O	1:A:1104:LEU:C	2.57	0.43
1:A:1122:LEU:O	1:A:1189:PHE:HA	2.19	0.43
1:A:937:LYS:HE3	1:A:1068:ASN:O	2.18	0.43
1:A:1261:LYS:HB2	1:A:1261:LYS:HE2	1.44	0.43
1:A:951:THR:HG23	1:A:1036:ILE:O	2.19	0.43
1:A:959:PRO:HA	1:A:1029:ASN:ND2	2.34	0.42
1:A:987:ILE:HA	1:A:987:ILE:HD13	1.81	0.42
1:A:1131:ILE:O	1:A:1304:TYR:HB2	2.19	0.42
1:A:1003:THR:CG2	3:A:200:HOH:O	2.66	0.42
1:A:1208:ILE:HD13	1:A:1238:LYS:HG3	2.01	0.42
1:A:1204:ASN:HD22	1:A:1204:ASN:HA	1.49	0.42
1:A:880:ILE:O	1:A:881:LEU:C	2.55	0.42
1:A:1053:MET:CE	3:A:101:HOH:O	2.66	0.42
1:A:886:ILE:HG22	1:A:902:PHE:CE2	2.55	0.42
1:A:918:ILE:HD12	1:A:918:ILE:HA	1.92	0.42
1:A:941:ILE:HA	1:A:944:ASN:HD21	1.85	0.42
1:A:937:LYS:HG3	1:A:941:ILE:HD11	2.01	0.42
1:A:1115:ARG:HH21	1:A:1115:ARG:HD3	1.46	0.41
1:A:1159:ASN:O	1:A:1163:ASN:N	2.52	0.41
1:A:1208:ILE:HD13	1:A:1238:LYS:CG	2.51	0.41
1:A:909:TYR:HB3	1:A:930:SER:O	2.20	0.41
1:A:1253:VAL:HG12	1:A:1254:GLN:H	1.83	0.41
1:A:1238:LYS:HD2	3:A:137:HOH:O	2.20	0.41
1:A:976:ILE:HG22	1:A:1074:LEU:CD2	2.51	0.40
1:A:982:LYS:HB3	1:A:983:HIS:H	1.63	0.40
1:A:1197:LYS:HD3	1:A:1208:ILE:HD12	2.03	0.40
1:A:1237:TYR:HE1	1:A:1260:ASP:OD2	2.05	0.40
1:A:1048:ILE:HD12	1:A:1053:MET:CG	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1303:TRP:HZ2	3:A:99:HOH:O	2.04	0.40
1:A:1111:ILE:HG23	1:A:1248:LEU:HD11	2.03	0.40
1:A:975:SER:HA	1:A:994:SER:HA	2.02	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	439/444 (99%)	388 (88%)	42 (10%)	9 (2%)	7 13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	984	SER
1	A	985	LEU
1	A	987	ILE
1	A	1219	ASN
1	A	1221	LEU
1	A	1066	GLU
1	A	1203	ASN
1	A	1042	SER
1	A	1073	LYS

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	397/400 (99%)	354 (89%)	43 (11%)	6 12

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	876	ASP
1	A	904	SER
1	A	905	SER
1	A	928	ASN
1	A	934	ILE
1	A	937	LYS
1	A	939	MET
1	A	964	SER
1	A	975	SER
1	A	981	LYS
1	A	984	SER
1	A	986	SER
1	A	987	ILE
1	A	996	LYS
1	A	1003	THR
1	A	1029	ASN
1	A	1035	THR
1	A	1043	SER
1	A	1052	LEU
1	A	1053	MET
1	A	1059	THR
1	A	1097	ASN
1	A	1104	LEU
1	A	1111	ILE
1	A	1122	LEU
1	A	1126	THR
1	A	1143	LYS
1	A	1147	ASP
1	A	1167	ARG
1	A	1178	LYS
1	A	1181	THR
1	A	1183	ASN
1	A	1204	ASN
1	A	1213	LYS
1	A	1216	ASN
1	A	1221	LEU
1	A	1236	LEU
1	A	1238	LYS

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Mol	Chain	Res	Type
1	A	1245	LEU
1	A	1249	LYS
1	A	1261	LYS
1	A	1274	GLN
1	A	1307	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	924	HIS
1	A	936	HIS
1	A	944	ASN
1	A	949	ASN
1	A	972	ASN
1	A	983	HIS
1	A	1069	ASN
1	A	1097	ASN
1	A	1141	GLN
1	A	1183	ASN
1	A	1204	ASN
1	A	1207	HIS
1	A	1216	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 monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
2	SLB	A	1400	-	21,21,21	1.07	2 (9%)	25,31,31	2.41	6 (24%)

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	SLB	A	1400	-	-	2/20/38/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1400	SLB	O1B-C1	-2.77	1.19	1.30
2	A	1400	SLB	O1A-C1	2.76	1.31	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1400	SLB	O1A-C1-C2	-7.99	111.48	123.59
2	A	1400	SLB	O6-C6-C5	-5.15	104.75	109.78
2	A	1400	SLB	C3-C4-C5	3.91	115.99	109.98
2	A	1400	SLB	C3-C2-C1	2.63	117.90	113.00
2	A	1400	SLB	O7-C7-C6	2.51	114.93	109.50
2	A	1400	SLB	O10-C10-C11	-2.20	117.98	122.06

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1400	SLB	C6-C5-N5-C10
2	A	1400	SLB	C4-C5-N5-C10

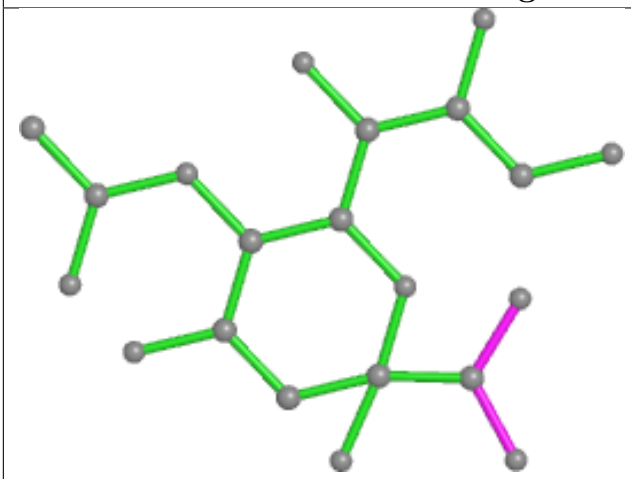
There are no ring outliers.

1 monomer is involved in 1 short contact:

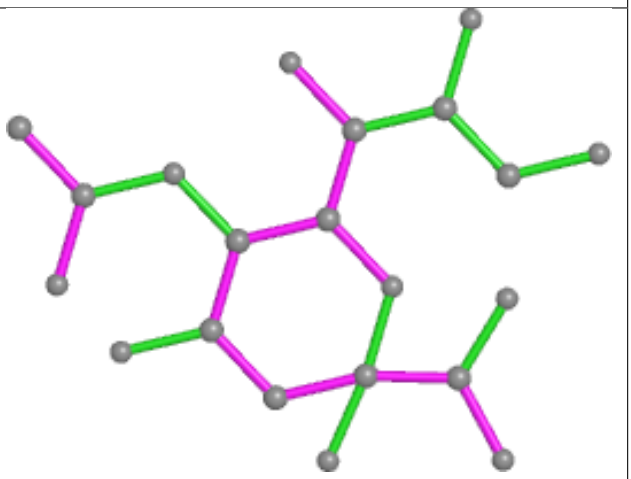
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1400	SLB	1	0

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.

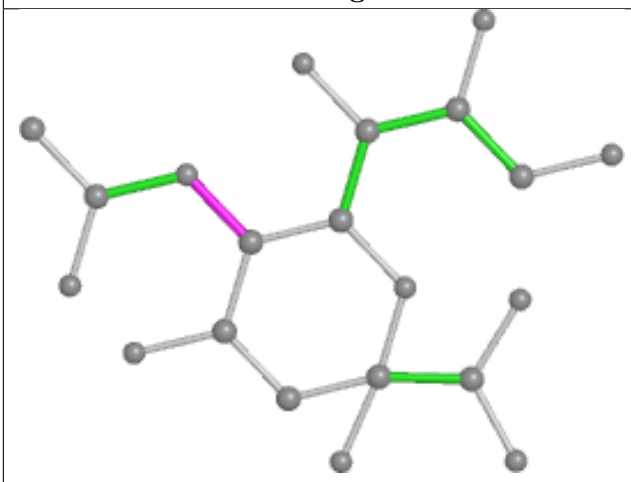
Ligand SLB A 1400



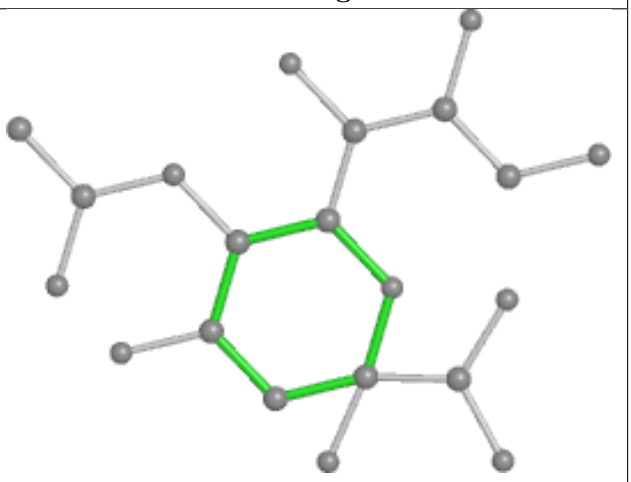
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	441/444 (99%)	-0.57	15 (3%) 45 38	17, 37, 79, 101	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	985	LEU	6.8
1	A	1186	ILE	5.0
1	A	986	SER	4.9
1	A	984	SER	4.4
1	A	983	HIS	3.5
1	A	982	LYS	3.1
1	A	1184	ASN	3.0
1	A	944	ASN	3.0
1	A	1220	ASN	2.6
1	A	942	GLU	2.4
1	A	1156	SER	2.1
1	A	940	ASP	2.1
1	A	876	ASP	2.1
1	A	1068	ASN	2.1
1	A	1113	PHE	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

There are no monosaccharides in this entry.

6.4 Ligands (i)

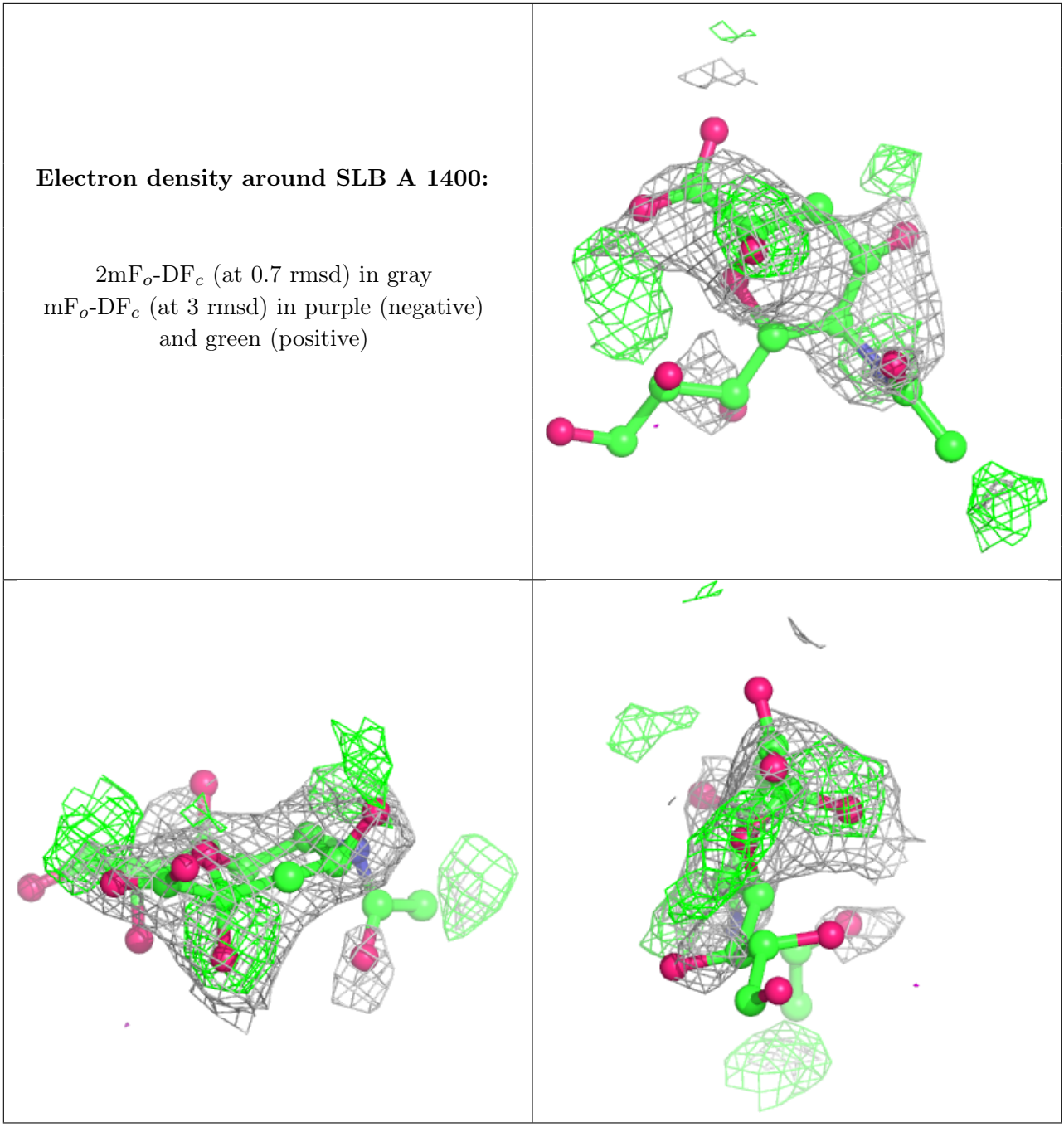
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	SLB	A	1400	21/21	0.58	0.40	64,67,69,69	21

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 SLB A 1400:

$2mF_o$-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.