



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:43 AM UTC

PDB ID : 1DFQ / pdb_00001dfq
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	:	4-5-2 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

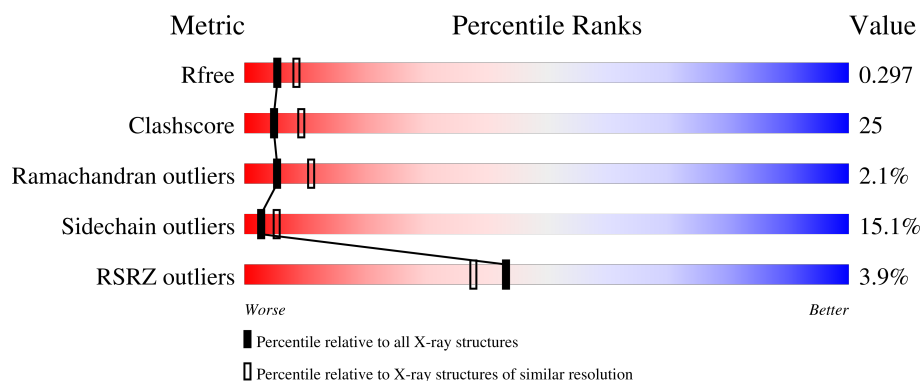
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	444	

2 Entry composition [i](#)

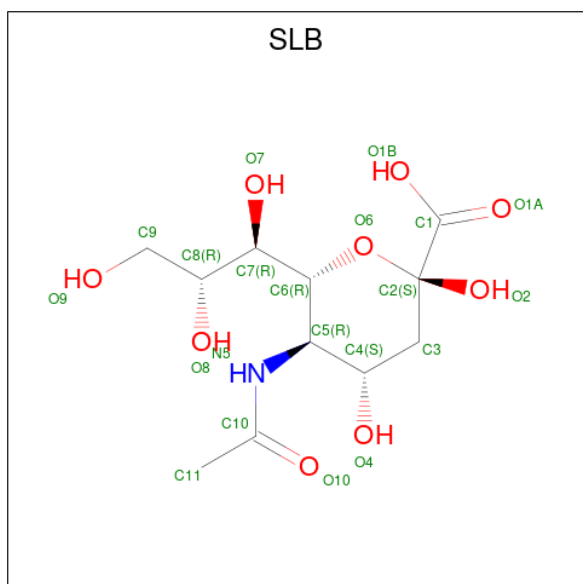
There are 3 unique types of molecules in this entry. The entry contains 3805 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	441	Total	C	N	O	S	0	0	0
			3563	2282	597	675	9			

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



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

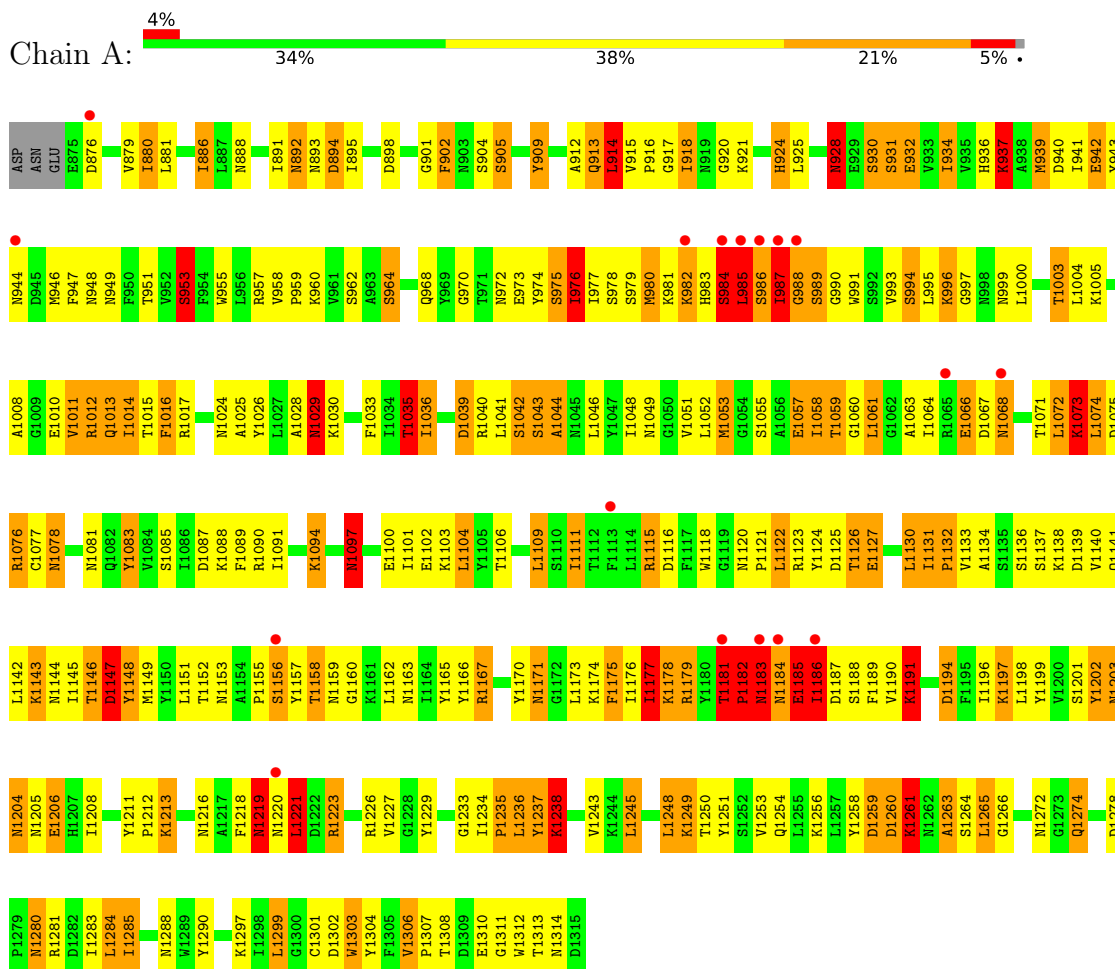
- Molecule 3 is water.

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

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



4 Data and refinement statistics

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 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	82.0 (20.00-2.60) 81.6 (20.00-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.313 0.195 , 0.297	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)	0.33 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	1.05	1/3644 (0.0%)	2.55	277/4945 (5.6%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1157	TYR	N-CA	-6.00	1.39	1.46

All (277) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	928	ASN	CA-CB-CG	18.92	131.52	112.60
1	A	1185	GLU	O-C-N	-13.12	107.53	122.75
1	A	1167	ARG	CD-NE-CZ	12.43	141.80	124.40
1	A	1017	ARG	CD-NE-CZ	12.26	141.56	124.40
1	A	1156	SER	CA-C-N	11.73	139.75	122.39
1	A	1156	SER	C-N-CA	11.73	139.75	122.39
1	A	1152	THR	N-CA-CB	11.58	131.84	111.69
1	A	918	ILE	N-CA-C	-11.38	99.79	110.82
1	A	1166	TYR	CA-C-O	-11.35	104.28	120.51
1	A	1029	ASN	CB-CG-ND2	-11.34	99.40	116.40
1	A	1219	ASN	CA-CB-CG	11.26	123.86	112.60
1	A	1220	ASN	CA-CB-CG	10.79	123.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1194	ASP	CA-CB-CG	10.74	123.34	112.60
1	A	1121	PRO	CB-CA-C	10.64	125.16	111.64
1	A	1078	ASN	OD1-CG-ND2	10.55	133.15	122.60
1	A	1186	ILE	CB-CA-C	10.53	122.96	111.80
1	A	1109	LEU	CA-C-O	10.39	134.32	122.37
1	A	1064	ILE	CB-CA-C	10.37	124.64	111.15
1	A	1090	ARG	NE-CZ-NH2	-10.18	110.04	119.20
1	A	1017	ARG	NE-CZ-NH1	-10.14	111.36	121.50
1	A	1017	ARG	NE-CZ-NH2	9.65	127.89	119.20
1	A	1035	THR	CB-CA-C	9.53	125.99	109.80
1	A	1016	PHE	CA-CB-CG	-9.37	104.43	113.80
1	A	1248	LEU	N-CA-C	9.15	123.54	112.38
1	A	1000	LEU	CA-C-O	-9.12	110.43	120.38
1	A	936	HIS	CA-CB-CG	9.05	122.85	113.80
1	A	1147	ASP	CA-CB-CG	-9.05	103.55	112.60
1	A	1156	SER	N-CA-C	9.04	124.33	109.95
1	A	1097	ASN	OD1-CG-ND2	-9.03	113.58	122.60
1	A	1013	GLN	OE1-CD-NE2	-8.97	113.63	122.60
1	A	928	ASN	O-C-N	8.90	132.28	123.46
1	A	1156	SER	CA-C-O	8.88	131.19	121.16
1	A	1182	PRO	CB-CA-C	-8.85	96.95	111.56
1	A	1078	ASN	CB-CG-ND2	-8.66	103.41	116.40
1	A	1044	ALA	CA-C-O	-8.48	109.88	120.57
1	A	1302	ASP	CA-CB-CG	-8.44	104.16	112.60
1	A	1029	ASN	OD1-CG-ND2	8.31	130.91	122.60
1	A	1064	ILE	N-CA-C	-8.31	97.92	108.89
1	A	1181	THR	N-CA-CB	8.21	124.98	110.37
1	A	995	LEU	CA-C-O	-8.17	111.27	120.66
1	A	1303	TRP	CA-C-O	8.11	130.60	121.11
1	A	1061	LEU	N-CA-CB	8.06	123.81	110.52
1	A	1144	ASN	CA-CB-CG	8.03	120.63	112.60
1	A	948	ASN	N-CA-C	8.02	120.93	110.43
1	A	1278	ASP	CA-C-O	-7.87	112.06	120.88
1	A	1306	VAL	N-CA-C	7.81	116.52	107.77
1	A	1205	ASN	CA-CB-CG	7.80	120.40	112.60
1	A	993	VAL	CA-C-O	-7.78	112.21	120.53
1	A	1061	LEU	O-C-N	7.77	132.28	123.19
1	A	894	ASP	CA-CB-CG	-7.76	104.84	112.60
1	A	1206	GLU	CA-C-O	-7.72	111.75	120.32
1	A	1043	SER	N-CA-C	7.67	121.41	110.14
1	A	1083	TYR	CA-C-O	-7.64	113.05	121.23
1	A	1185	GLU	CA-C-N	-7.63	110.04	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1185	GLU	C-N-CA	-7.63	110.04	122.33
1	A	1250	THR	CA-CB-OG1	-7.63	98.15	109.60
1	A	957	ARG	CA-C-O	-7.63	110.90	120.28
1	A	1285	ILE	CB-CA-C	-7.61	98.81	111.29
1	A	1029	ASN	N-CA-C	7.55	128.39	113.29
1	A	1171	ASN	N-CA-CB	7.55	122.34	110.56
1	A	1182	PRO	CA-C-N	7.53	133.20	122.05
1	A	1182	PRO	C-N-CA	7.53	133.20	122.05
1	A	1008	ALA	N-CA-C	-7.47	104.16	113.28
1	A	1261	LYS	CA-CB-CG	7.47	129.04	114.10
1	A	1301	CYS	O-C-N	-7.45	112.83	122.37
1	A	1201	SER	N-CA-CB	-7.45	102.00	110.35
1	A	1057	GLU	CA-C-O	-7.44	112.21	120.69
1	A	1223	ARG	CD-NE-CZ	7.42	134.79	124.40
1	A	1256	LYS	CA-C-N	7.42	132.96	122.72
1	A	1256	LYS	C-N-CA	7.42	132.96	122.72
1	A	1012	ARG	CD-NE-CZ	7.30	134.62	124.40
1	A	1265	LEU	CA-C-O	7.29	128.09	119.56
1	A	914	LEU	CA-C-O	-7.27	112.53	120.24
1	A	988	GLY	N-CA-C	-7.26	105.04	115.64
1	A	1155	PRO	CA-C-O	7.19	132.66	122.31
1	A	1014	ILE	O-C-N	-7.16	113.52	122.97
1	A	928	ASN	N-CA-CB	-7.16	100.68	111.56
1	A	1010	GLU	CA-C-O	-7.16	113.99	121.87
1	A	1175	PHE	CA-C-O	-7.15	112.74	121.11
1	A	955	TRP	CA-C-O	-7.14	112.79	121.36
1	A	1274	GLN	CG-CD-NE2	-7.08	105.79	116.40
1	A	1109	LEU	CA-C-N	7.07	130.79	120.82
1	A	1109	LEU	C-N-CA	7.07	130.79	120.82
1	A	1265	LEU	O-C-N	-7.05	113.89	122.34
1	A	957	ARG	NE-CZ-NH2	7.04	125.54	119.20
1	A	1314	ASN	CA-C-O	-7.02	112.74	120.81
1	A	1301	CYS	CA-C-N	7.00	131.75	122.30
1	A	1301	CYS	C-N-CA	7.00	131.75	122.30
1	A	1025	ALA	N-CA-C	6.97	119.96	110.55
1	A	970	GLY	CA-C-O	-6.94	112.91	120.40
1	A	999	ASN	CA-C-O	-6.93	113.36	120.71
1	A	1264	SER	N-CA-C	6.93	120.36	109.96
1	A	928	ASN	CA-C-O	-6.91	113.50	121.10
1	A	1220	ASN	CA-C-N	6.91	134.74	121.54
1	A	1220	ASN	C-N-CA	6.91	134.74	121.54
1	A	937	LYS	CA-CB-CG	6.80	127.70	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1125	ASP	CA-C-O	-6.78	111.87	120.55
1	A	1245	LEU	CA-C-O	6.78	126.22	118.97
1	A	1250	THR	CA-C-O	6.76	129.47	121.36
1	A	917	GLY	O-C-N	-6.75	113.92	122.70
1	A	1043	SER	CA-CB-OG	-6.75	97.60	111.10
1	A	1226	ARG	NE-CZ-NH2	6.75	125.27	119.20
1	A	1299	LEU	CA-C-O	6.70	128.52	120.28
1	A	1251	TYR	CB-CA-C	6.68	121.29	111.88
1	A	1015	THR	CA-CB-CG2	6.61	121.74	110.50
1	A	1182	PRO	CA-C-O	6.60	132.62	120.60
1	A	1109	LEU	O-C-N	-6.59	114.62	122.46
1	A	1136	SER	CA-C-N	6.59	133.41	122.54
1	A	1136	SER	C-N-CA	6.59	133.41	122.54
1	A	924	HIS	ND1-CE1-NE2	-6.56	101.84	108.40
1	A	953	SER	O-C-N	6.56	130.88	123.27
1	A	990	GLY	N-CA-C	6.53	119.24	110.43
1	A	1157	TYR	CB-CA-C	-6.49	100.15	110.14
1	A	1030	LYS	CA-C-O	-6.49	113.75	121.66
1	A	1283	ILE	CA-C-N	-6.46	111.69	120.87
1	A	1283	ILE	C-N-CA	-6.46	111.69	120.87
1	A	1202	TYR	CA-C-O	6.44	127.80	120.84
1	A	1186	ILE	CA-C-O	6.44	129.58	120.89
1	A	1057	GLU	CA-CB-CG	6.43	126.96	114.10
1	A	1029	ASN	CA-CB-CG	-6.42	106.18	112.60
1	A	1237	TYR	CA-C-O	-6.39	113.76	121.05
1	A	1127	GLU	CA-C-N	6.39	133.19	121.94
1	A	1127	GLU	C-N-CA	6.39	133.19	121.94
1	A	1139	ASP	CA-C-O	-6.39	113.87	121.66
1	A	1008	ALA	CA-C-O	6.38	126.78	119.18
1	A	1151	LEU	CA-C-O	-6.38	114.61	121.56
1	A	1035	THR	CA-CB-OG1	6.38	119.17	109.60
1	A	1290	TYR	CA-C-O	-6.38	113.06	120.20
1	A	1251	TYR	CA-C-N	-6.35	112.62	122.59
1	A	1251	TYR	C-N-CA	-6.35	112.62	122.59
1	A	1171	ASN	CA-CB-CG	-6.33	106.27	112.60
1	A	1274	GLN	CA-CB-CG	6.32	126.73	114.10
1	A	1035	THR	CA-C-O	6.31	128.73	120.21
1	A	1131	ILE	CA-CB-CG1	6.30	121.11	110.40
1	A	1176	ILE	CA-C-O	-6.30	113.68	120.36
1	A	1202	TYR	CA-CB-CG	6.29	125.23	113.90
1	A	1026	TYR	CA-CB-CG	-6.26	102.64	113.90
1	A	892	ASN	CB-CA-C	-6.24	100.16	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1149	MET	CG-SD-CE	6.23	114.61	100.90
1	A	979	SER	CA-C-O	6.22	126.72	119.32
1	A	1146	THR	N-CA-CB	6.21	120.99	110.49
1	A	1025	ALA	N-CA-CB	-6.21	101.01	110.45
1	A	1011	VAL	CA-CB-CG2	6.21	120.95	110.40
1	A	1081	ASN	N-CA-C	6.21	120.69	113.18
1	A	901	GLY	CA-C-O	6.20	125.53	119.27
1	A	892	ASN	N-CA-CB	6.17	120.46	110.77
1	A	1183	ASN	CA-CB-CG	-6.15	106.45	112.60
1	A	1283	ILE	CA-CB-CG2	6.14	120.94	110.50
1	A	976	ILE	N-CA-C	-6.13	107.88	113.71
1	A	1036	ILE	O-C-N	-6.10	116.73	123.20
1	A	1177	ILE	CB-CA-C	-6.08	102.65	110.98
1	A	1197	LYS	CA-C-O	-6.06	113.69	120.66
1	A	991	TRP	CA-C-O	-6.04	114.25	121.56
1	A	1074	LEU	CB-CA-C	-6.04	101.49	110.67
1	A	902	PHE	CA-CB-CG	-6.02	107.78	113.80
1	A	962	SER	CA-C-O	-6.01	114.72	121.81
1	A	1029	ASN	CB-CA-C	-5.97	98.94	110.35
1	A	1260	ASP	CA-CB-CG	-5.96	106.64	112.60
1	A	989	SER	CB-CA-C	5.93	119.16	109.90
1	A	1097	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	1301	CYS	N-CA-CB	-5.93	102.38	110.56
1	A	1266	GLY	CA-C-N	5.92	129.25	120.90
1	A	1266	GLY	C-N-CA	5.92	129.25	120.90
1	A	1280	ASN	CA-C-O	-5.91	114.69	121.19
1	A	912	ALA	O-C-N	-5.88	115.56	122.96
1	A	1008	ALA	O-C-N	-5.86	114.09	122.41
1	A	964	SER	CA-C-O	-5.85	114.31	120.63
1	A	1133	VAL	CA-C-N	5.84	129.94	120.60
1	A	1133	VAL	C-N-CA	5.84	129.94	120.60
1	A	1251	TYR	N-CA-C	-5.84	102.57	110.68
1	A	968	GLN	CA-CB-CG	5.83	125.75	114.10
1	A	1068	ASN	N-CA-C	-5.82	106.18	113.28
1	A	879	VAL	CB-CA-C	-5.81	104.37	111.87
1	A	1187	ASP	N-CA-C	-5.80	99.28	108.73
1	A	953	SER	N-CA-CB	5.77	122.27	111.53
1	A	1120	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	A	936	HIS	N-CA-CB	5.76	119.81	110.42
1	A	987	ILE	N-CA-C	5.76	121.32	109.34
1	A	1263	ALA	O-C-N	5.76	129.93	123.19
1	A	1035	THR	O-C-N	-5.75	116.37	123.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	990	GLY	CA-C-N	-5.74	112.81	122.92
1	A	990	GLY	C-N-CA	-5.74	112.81	122.92
1	A	1259	ASP	CA-CB-CG	5.74	118.33	112.60
1	A	1094	LYS	O-C-N	-5.72	117.79	123.46
1	A	1157	TYR	O-C-N	5.72	130.60	123.28
1	A	1157	TYR	N-CA-CB	5.69	120.04	110.77
1	A	1137	SER	CA-CB-OG	5.67	122.45	111.10
1	A	1183	ASN	N-CA-C	5.67	118.12	109.62
1	A	948	ASN	CA-CB-CG	-5.65	106.95	112.60
1	A	1132	PRO	CB-CA-C	-5.63	106.28	111.40
1	A	1067	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	934	ILE	CB-CA-C	-5.62	102.25	110.62
1	A	1116	ASP	N-CA-CB	5.60	119.06	110.49
1	A	997	GLY	CA-C-N	-5.60	113.66	122.95
1	A	997	GLY	C-N-CA	-5.60	113.66	122.95
1	A	905	SER	CA-C-O	5.57	127.04	120.58
1	A	931	SER	CA-CB-OG	5.57	122.24	111.10
1	A	958	VAL	CA-CB-CG2	5.55	119.83	110.40
1	A	1137	SER	N-CA-C	-5.55	106.18	113.17
1	A	1281	ARG	O-C-N	-5.54	116.47	123.17
1	A	1116	ASP	N-CA-C	-5.54	101.78	110.36
1	A	895	ILE	CB-CG1-CD1	5.52	125.39	113.80
1	A	1223	ARG	NE-CZ-NH1	-5.50	116.00	121.50
1	A	1081	ASN	CA-CB-CG	-5.50	107.10	112.60
1	A	913	GLN	CA-CB-CG	-5.49	103.11	114.10
1	A	1297	LYS	N-CA-C	-5.49	104.13	112.04
1	A	1236	LEU	CA-C-N	-5.48	113.59	121.42
1	A	1236	LEU	C-N-CA	-5.48	113.59	121.42
1	A	1076	ARG	NE-CZ-NH1	-5.46	116.03	121.50
1	A	1288	ASN	O-C-N	5.46	129.91	122.37
1	A	920	GLY	CA-C-O	5.46	130.07	120.57
1	A	1148	TYR	N-CA-C	5.46	118.54	110.46
1	A	1051	VAL	N-CA-C	5.45	116.32	108.48
1	A	1181	THR	CA-C-O	-5.45	112.70	120.16
1	A	1234	ILE	O-C-N	5.43	126.17	121.12
1	A	1145	ILE	CA-C-O	-5.43	116.15	121.58
1	A	1127	GLU	CB-CG-CD	5.41	121.79	112.60
1	A	1134	ALA	CB-CA-C	-5.41	98.92	110.32
1	A	1278	ASP	O-C-N	5.41	127.58	121.53
1	A	1179	ARG	N-CA-CB	5.40	118.21	110.06
1	A	1017	ARG	CA-C-O	-5.38	114.94	120.54
1	A	1250	THR	CA-CB-CG2	5.35	119.59	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1115	ARG	NH1-CZ-NH2	5.33	126.22	119.30
1	A	1000	LEU	O-C-N	5.32	129.57	123.29
1	A	1174	LYS	CA-C-O	-5.32	114.80	120.92
1	A	978	SER	N-CA-C	5.32	117.34	108.99
1	A	1191	LYS	CA-C-O	-5.30	114.97	120.70
1	A	1060	GLY	N-CA-C	-5.29	107.38	115.00
1	A	1016	PHE	CA-C-O	-5.29	114.70	120.36
1	A	1011	VAL	N-CA-C	5.29	115.51	108.27
1	A	1314	ASN	O-C-N	5.29	129.43	122.93
1	A	1233	GLY	N-CA-C	5.28	122.37	115.40
1	A	1126	THR	CA-C-N	5.27	128.95	121.42
1	A	1126	THR	C-N-CA	5.27	128.95	121.42
1	A	880	ILE	N-CA-CB	5.25	116.14	110.62
1	A	1024	ASN	N-CA-C	5.25	119.65	112.88
1	A	986	SER	CA-C-O	5.24	128.01	120.51
1	A	980	MET	CA-CB-CG	5.24	124.57	114.10
1	A	1221	LEU	O-C-N	-5.23	115.64	122.59
1	A	932	GLU	N-CA-CB	-5.21	101.68	110.49
1	A	1041	LEU	CA-C-O	-5.21	112.97	119.28
1	A	1264	SER	O-C-N	-5.21	116.52	122.93
1	A	1130	LEU	N-CA-CB	5.21	118.76	110.16
1	A	1024	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	A	1179	ARG	CB-CA-C	-5.19	100.75	109.53
1	A	999	ASN	CA-CB-CG	-5.18	107.42	112.60
1	A	918	ILE	CA-C-O	-5.17	114.80	120.96
1	A	1123	ARG	N-CA-CB	-5.17	102.24	111.08
1	A	1055	SER	CA-C-N	5.17	131.03	121.94
1	A	1055	SER	C-N-CA	5.17	131.03	121.94
1	A	943	TYR	N-CA-CB	-5.16	103.79	111.43
1	A	1072	LEU	CA-C-O	-5.16	114.84	120.36
1	A	1238	LYS	CB-CA-C	5.16	120.69	110.42
1	A	993	VAL	O-C-N	5.15	129.13	123.10
1	A	1030	LYS	CB-CG-CD	-5.15	99.45	111.30
1	A	1158	THR	N-CA-CB	5.14	121.10	111.53
1	A	942	GLU	CB-CG-CD	5.14	121.34	112.60
1	A	1136	SER	CB-CA-C	5.14	120.49	110.57
1	A	891	ILE	N-CA-CB	5.14	118.15	111.83
1	A	940	ASP	N-CA-C	5.14	118.33	111.75
1	A	1013	GLN	N-CA-C	5.13	117.77	108.69
1	A	909	TYR	CA-C-N	5.13	126.25	119.84
1	A	909	TYR	C-N-CA	5.13	126.25	119.84
1	A	1201	SER	O-C-N	-5.11	116.14	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1059	THR	N-CA-C	-5.10	102.73	110.28
1	A	1235	PRO	CB-CA-C	5.10	117.66	110.98
1	A	1184	ASN	CA-CB-CG	-5.09	107.51	112.60
1	A	994	SER	O-C-N	-5.09	116.55	122.96
1	A	1073	LYS	CA-C-O	-5.09	113.23	120.51
1	A	1071	THR	N-CA-C	5.08	116.80	108.52
1	A	1265	LEU	N-CA-C	-5.08	106.68	112.92
1	A	1039	ASP	CA-CB-CG	-5.05	107.55	112.60
1	A	1151	LEU	CA-C-N	5.05	130.39	122.21
1	A	1151	LEU	C-N-CA	5.05	130.39	122.21
1	A	1051	VAL	O-C-N	-5.02	117.76	123.18
1	A	1041	LEU	N-CA-C	-5.00	106.95	113.16
1	A	1043	SER	N-CA-CB	-5.00	103.25	110.70

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 ⓘ

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	180	0
2	A	21	0	18	1	0
3	A	221	0	0	29	0
All	All	3805	0	3534	180	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 (180) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:1048:ILE:O	1:A:1049:ASN:C	2.48	0.55
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:1178:LYS:HD3	1:A:1199:TYR:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:ASN:O	1:A:893:ASN:HB2	2.07	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: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
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:1218:PHE:O	1:A:1219:ASN:C	2.54	0.50
1:A:946:MET:HE2	1:A:1063:ALA:HB1	1.93	0.49
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:1103:LYS:O	1:A:1104:LEU:C	2.57	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:939:MET:HE3	1:A:942:GLU:OE2	2.14	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:880:ILE:O	1:A:881:LEU:C	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1039:ASP:OD2	1:A:1042:SER:OG	2.21	0.45
1:A:1143:LYS:HG2	1:A:1148:TYR:CE1	2.51	0.45
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: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:1260:ASP:OD1	1:A:1260:ASP:C	2.60	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: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: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:1124:TYR:OH	1:A:1194:ASP:OD2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:988:GLY:O	1:A:989:SER:C	2.61	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
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%)	5 11

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

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Mol	Chain	Res	Type
1	A	1203	ASN
1	A	1042	SER
1	A	1073	LYS

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	397/400 (99%)	337 (85%)	60 (15%)	3 5

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	876	ASP
1	A	886	ILE
1	A	904	SER
1	A	905	SER
1	A	914	LEU
1	A	928	ASN
1	A	930	SER
1	A	934	ILE
1	A	937	LYS
1	A	939	MET
1	A	953	SER
1	A	964	SER
1	A	975	SER
1	A	976	ILE
1	A	981	LYS
1	A	982	LYS
1	A	984	SER
1	A	985	LEU
1	A	986	SER
1	A	987	ILE
1	A	996	LYS
1	A	1003	THR
1	A	1029	ASN

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Mol	Chain	Res	Type
1	A	1035	THR
1	A	1043	SER
1	A	1046	LEU
1	A	1052	LEU
1	A	1053	MET
1	A	1058	ILE
1	A	1059	THR
1	A	1073	LYS
1	A	1094	LYS
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	1162	LEU
1	A	1167	ARG
1	A	1177	ILE
1	A	1178	LYS
1	A	1181	THR
1	A	1183	ASN
1	A	1186	ILE
1	A	1191	LYS
1	A	1204	ASN
1	A	1213	LYS
1	A	1236	LEU
1	A	1238	LYS
1	A	1245	LEU
1	A	1249	LYS
1	A	1261	LYS
1	A	1274	GLN
1	A	1284	LEU
1	A	1285	ILE
1	A	1306	VAL
1	A	1307	PRO
1	A	1313	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	924	HIS

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Mol	Chain	Res	Type
1	A	936	HIS
1	A	944	ASN
1	A	949	ASN
1	A	968	GLN
1	A	972	ASN
1	A	983	HIS
1	A	1078	ASN
1	A	1082	GLN
1	A	1097	ASN
1	A	1141	GLN
1	A	1183	ASN
1	A	1204	ASN
1	A	1205	ASN
1	A	1207	HIS
1	A	1216	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1.10	2 (9%)	24,31,31	2.45	6 (25%)

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	-2.92	1.19	1.30
2	A	1400	SLB	O1A-C1	2.86	1.31	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1400	SLB	O1A-C1-C2	-7.41	111.48	123.85
2	A	1400	SLB	O6-C6-C5	-5.56	104.75	109.84
2	A	1400	SLB	C3-C4-C5	4.06	115.99	109.72
2	A	1400	SLB	C3-C2-C1	2.73	117.90	112.84
2	A	1400	SLB	O7-C7-C6	2.54	114.93	109.44
2	A	1400	SLB	O10-C10-C11	-2.29	117.98	122.05

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

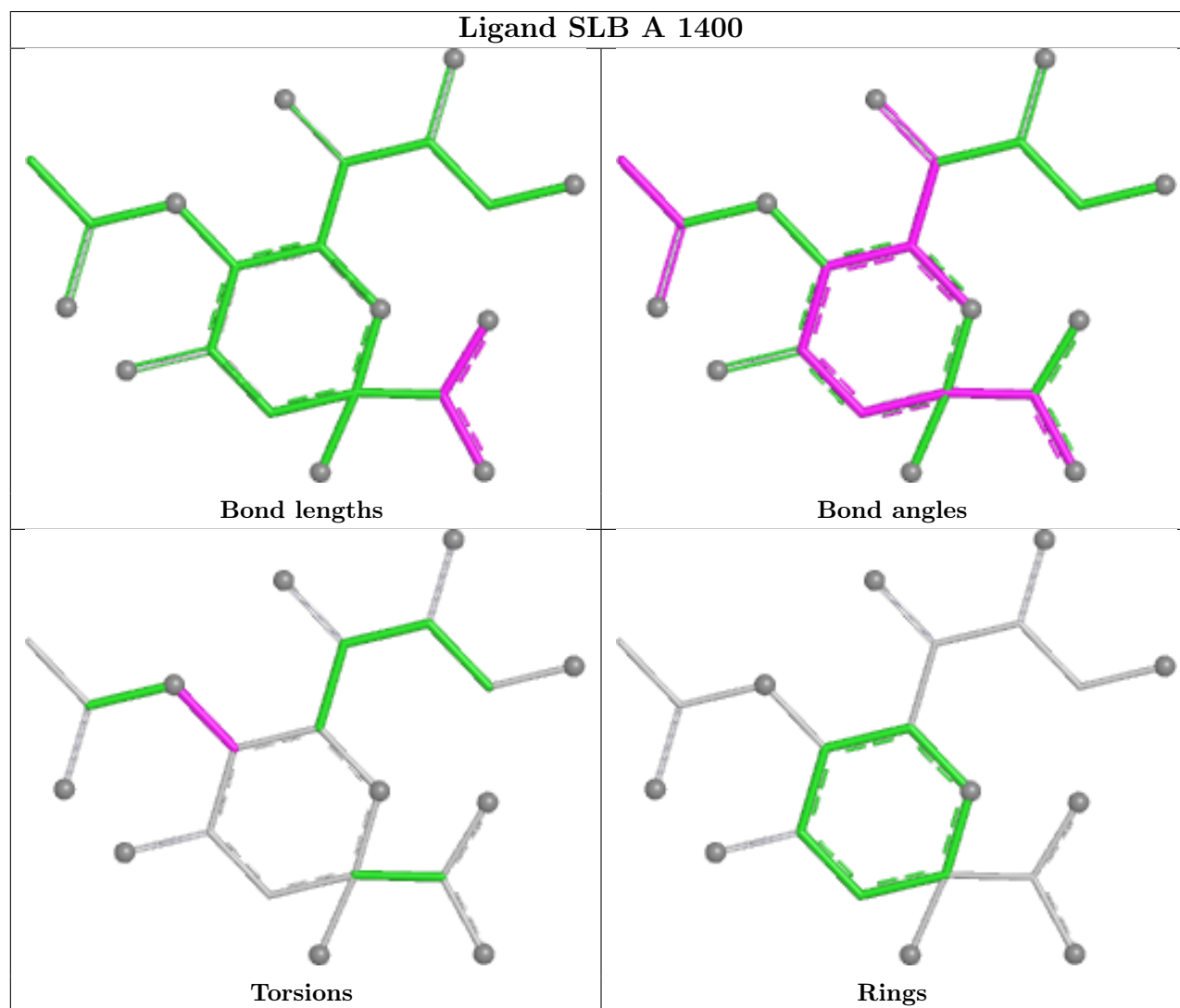
There are no ring outliers.

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 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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	441/444 (99%)	-0.35	17 (3%) 43 38	17, 37, 79, 101	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	985	LEU	4.6
1	A	1186	ILE	4.2
1	A	986	SER	3.9
1	A	982	LYS	3.0
1	A	1156	SER	3.0
1	A	944	ASN	2.9
1	A	1113	PHE	2.6
1	A	1184	ASN	2.6
1	A	1065	ARG	2.5
1	A	987	ILE	2.5
1	A	876	ASP	2.4
1	A	1068	ASN	2.4
1	A	988	GLY	2.2
1	A	984	SER	2.2
1	A	1220	ASN	2.2
1	A	1181	THR	2.1
1	A	1183	ASN	2.1

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 oligosaccharides in this entry.

6.4 Ligands

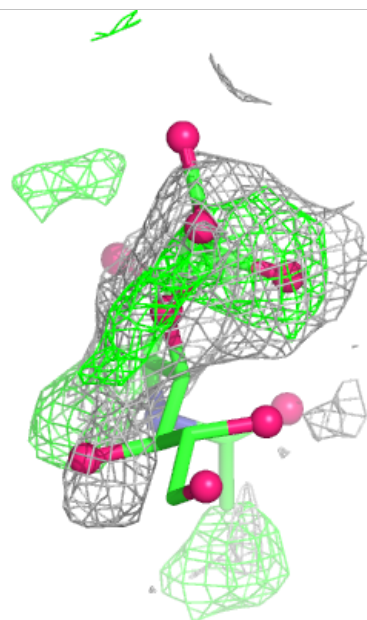
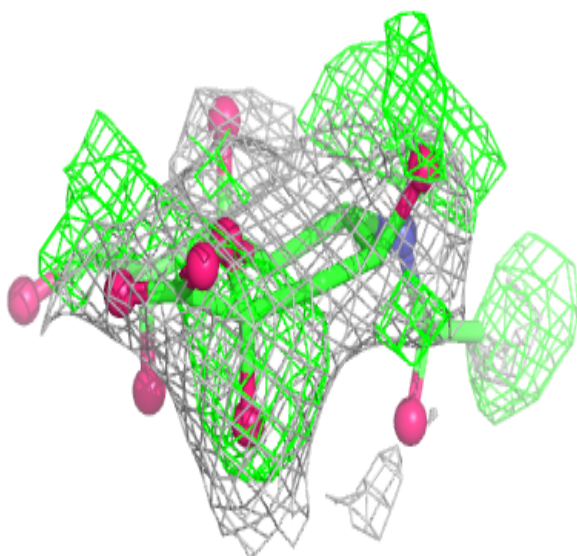
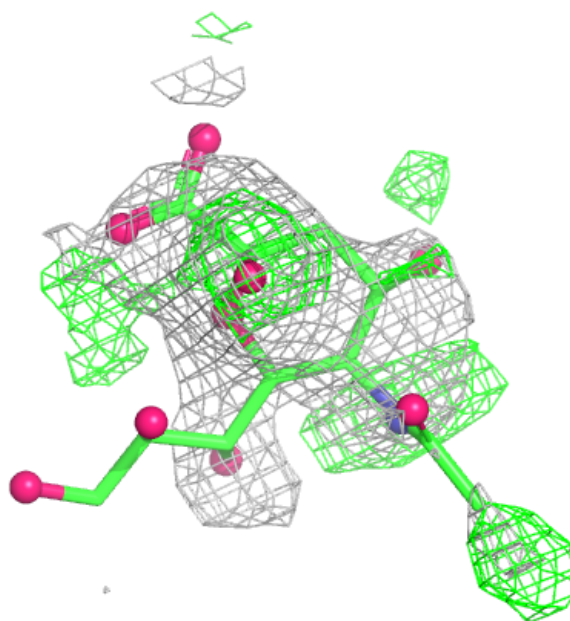
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SLB	A	1400	21/21	0.69	0.27	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.