



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:33 PM UTC

PDB ID : 2ZOE / pdb_00002zoe
Title : HA3 subcomponent of Clostridium botulinum type C progenitor toxin, complex with N-acetylneuramic acid
Authors : Nakamura, T.; Kotani, M.; Tono-zuka, T.; Ide, A.; Oguma, K.; Nishikawa, A.
Deposited on : 2008-05-09
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

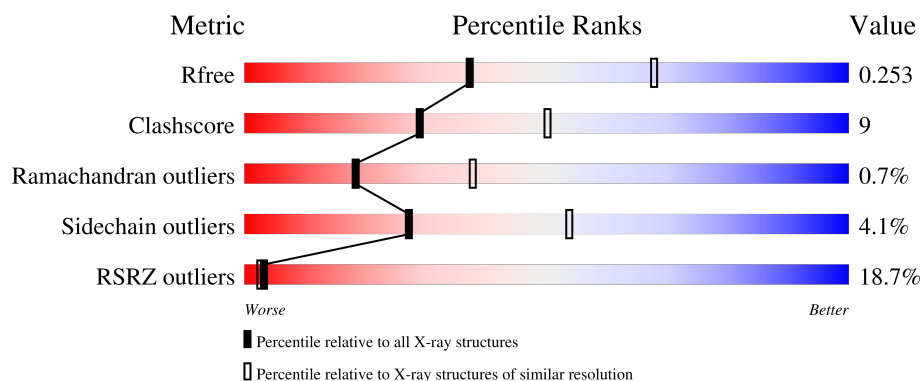
1 Overall quality at a glance

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	205	17% 66% 13% • 18%
2	B	420	18% 82% 15% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4997 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 Hemagglutinin components HA3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	Se	0	0	0
			1368	873	224	268	2	1			

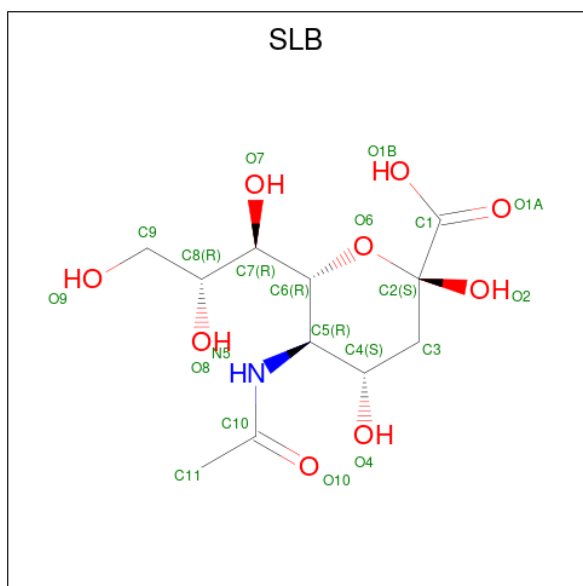
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	ILE	-	expression tag	UNP P46085
A	-19	SER	-	expression tag	UNP P46085
A	-18	GLU	-	expression tag	UNP P46085
A	-17	PHE	-	expression tag	UNP P46085
A	-16	ASP	-	expression tag	UNP P46085
A	-15	TYR	-	expression tag	UNP P46085
A	-14	LYS	-	expression tag	UNP P46085
A	-13	ASP	-	expression tag	UNP P46085
A	-12	HIS	-	expression tag	UNP P46085
A	-11	GLU	-	expression tag	UNP P46085
A	-10	ILE	-	expression tag	UNP P46085
A	-9	ASP	-	expression tag	UNP P46085
A	-8	TYR	-	expression tag	UNP P46085
A	-7	LYS	-	expression tag	UNP P46085
A	-6	ASP	-	expression tag	UNP P46085
A	-5	ASP	-	expression tag	UNP P46085
A	-4	ASP	-	expression tag	UNP P46085
A	-3	ASP	-	expression tag	UNP P46085
A	-2	LYS	-	expression tag	UNP P46085
A	-1	TRP	-	expression tag	UNP P46085
A	0	ILE	-	expression tag	UNP P46085

- Molecule 2 is a protein called Hemagglutinin components HA3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	Se	0	0	0
			3338	2109	553	671	2	3			

- Molecule 3 is N-acetyl-beta-neuraminic acid (CCD ID: SLB) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			21	11	1	9		

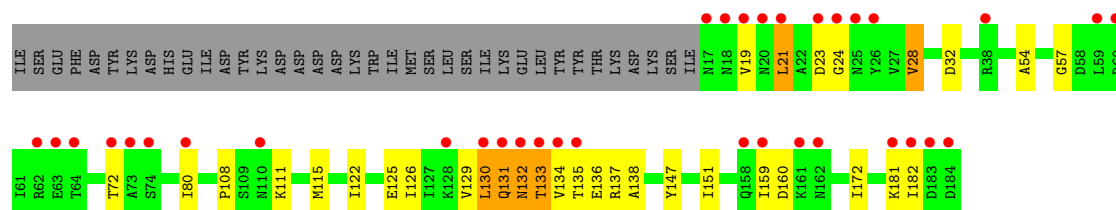
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	70	Total O 70 70	0	0
4	B	200	Total O 200 200	0	0

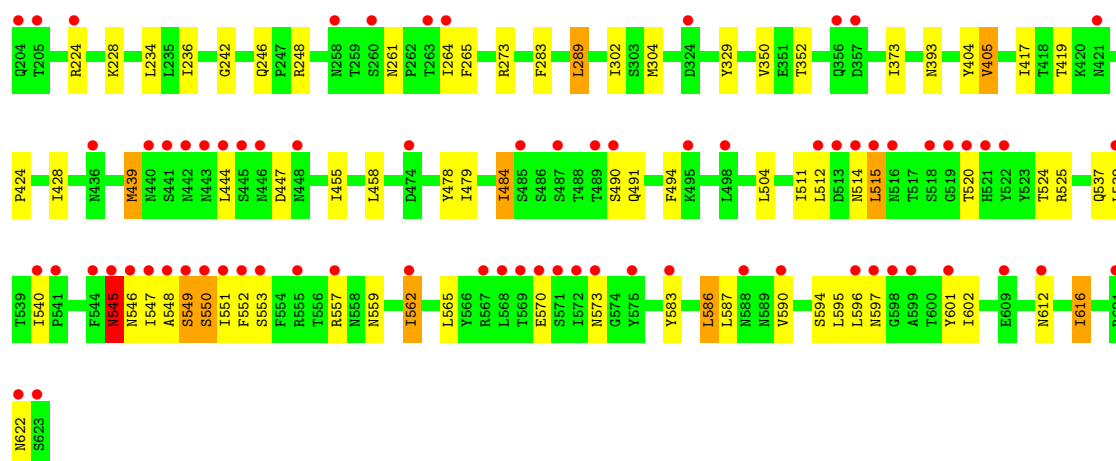
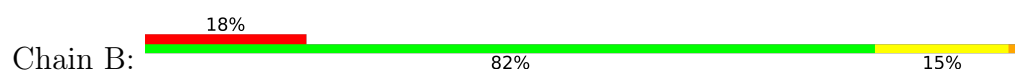
3 Residue-property plots [i](#)

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: Hemagglutinin components HA3



• Molecule 2: Hemagglutinin components HA3



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	177.08 Å 177.08 Å 81.04 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.21 – 2.60 33.21 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.21-2.60) 99.9 (33.21-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.96 (at 2.61 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.253 0.234 , 0.253	Depositor DCC
R_{free} test set	4507 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4997	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.29% 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: 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	0.49	1/1396 (0.1%)	0.75	2/1892 (0.1%)
2	B	0.46	1/3401 (0.0%)	0.68	1/4633 (0.0%)
All	All	0.47	2/4797 (0.0%)	0.70	3/6525 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	GLN	N-CA	7.39	1.55	1.46
2	B	545	ASN	N-CA	5.38	1.53	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	LEU	O-C-N	-6.84	113.50	122.59
1	A	131	GLN	N-CA-C	6.38	124.38	110.80
2	B	573	ASN	N-CA-C	-5.04	100.07	110.80

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	1368	0	1320	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3338	0	3275	61	0
3	B	21	0	18	3	0
4	A	70	0	0	0	0
4	B	200	0	0	1	0
All	All	4997	0	4613	81	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 9.

All (81) 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)
2:B:236:ILE:HD11	2:B:304:MSE:HE2	1.34	1.10
2:B:234:LEU:HD12	2:B:304:MSE:HE3	1.40	1.02
2:B:234:LEU:HD12	2:B:304:MSE:CE	2.02	0.89
1:A:54:ALA:HB3	1:A:115:MSE:HE1	1.66	0.78
2:B:595:LEU:HD12	2:B:601:TYR:CE2	2.21	0.77
2:B:515:LEU:HD23	2:B:515:LEU:H	1.48	0.76
2:B:514:ASN:HD21	3:B:2000:SLB:C11	2.03	0.71
2:B:514:ASN:HD21	3:B:2000:SLB:H112	1.58	0.69
1:A:80:ILE:HD13	1:A:126:ILE:HD12	1.76	0.68
2:B:246:GLN:HE21	2:B:248:ARG:H	1.39	0.68
2:B:557:ARG:HB2	2:B:616:ILE:HB	1.75	0.68
2:B:559:ASN:HD21	2:B:612:ASN:H	1.41	0.66
2:B:540:ILE:HD11	2:B:596:LEU:C	2.21	0.66
1:A:54:ALA:CB	1:A:115:MSE:HE1	2.28	0.63
2:B:562:ILE:O	2:B:583:TYR:O	2.18	0.62
2:B:261:ASN:OD1	2:B:264:ILE:HG22	2.01	0.60
2:B:393:ASN:HD21	2:B:491:GLN:HE21	1.50	0.60
1:A:57:GLY:C	2:B:289:LEU:HD13	2.26	0.59
2:B:236:ILE:HD11	2:B:304:MSE:CE	2.22	0.58
1:A:182:ILE:HD12	1:A:182:ILE:O	2.06	0.56
2:B:417:ILE:HD12	2:B:494:PHE:CD1	2.41	0.55
1:A:19:VAL:HG12	1:A:21:LEU:HG	1.89	0.55
1:A:32:ASP:HA	1:A:122:ILE:HD13	1.87	0.55
2:B:515:LEU:HD23	2:B:515:LEU:N	2.21	0.55
2:B:484:ILE:O	2:B:484:ILE:HG13	2.06	0.54
2:B:547:ILE:CG2	2:B:597:ASN:HD21	2.20	0.54
2:B:234:LEU:CD1	2:B:304:MSE:HE3	2.28	0.54
2:B:549:SER:O	2:B:550:SER:C	2.50	0.53
2:B:540:ILE:HD11	2:B:596:LEU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:504:LEU:HD21	2:B:602:ILE:HG21	1.89	0.53
2:B:562:ILE:O	2:B:586:LEU:HD13	2.09	0.53
2:B:458:LEU:HD11	2:B:525:ARG:HD2	1.91	0.53
1:A:108:PRO:HG2	1:A:111:LYS:HB2	1.90	0.52
1:A:28:VAL:HG13	1:A:125:GLU:HB2	1.93	0.51
2:B:373:ILE:HD11	2:B:478:TYR:CZ	2.45	0.51
1:A:134:VAL:HG21	1:A:137:ARG:HH11	1.76	0.51
2:B:540:ILE:HD12	2:B:549:SER:HB3	1.92	0.50
2:B:547:ILE:HG23	2:B:597:ASN:ND2	2.26	0.50
2:B:242:GLY:C	2:B:304:MSE:HE1	2.36	0.50
2:B:545:ASN:OD1	2:B:547:ILE:HG22	2.13	0.49
1:A:132:ASN:HD22	1:A:133:THR:N	2.11	0.49
2:B:515:LEU:HD13	2:B:538:LEU:CD2	2.41	0.49
1:A:182:ILE:HD12	1:A:182:ILE:C	2.39	0.48
2:B:405:VAL:HG13	2:B:479:ILE:HB	1.96	0.48
2:B:524:THR:OG1	2:B:616:ILE:HD13	2.13	0.47
2:B:540:ILE:HD12	2:B:549:SER:CB	2.44	0.47
2:B:373:ILE:HG23	2:B:404:TYR:CE2	2.49	0.47
2:B:246:GLN:NE2	2:B:248:ARG:H	2.11	0.47
2:B:597:ASN:ND2	4:B:2130:HOH:O	2.47	0.47
1:A:80:ILE:HA	1:A:126:ILE:HD12	1.97	0.46
2:B:548:ALA:HB1	2:B:594:SER:HB2	1.98	0.46
2:B:484:ILE:HD13	2:B:490:SER:OG	2.16	0.46
2:B:512:LEU:HD12	2:B:538:LEU:HG	1.98	0.45
2:B:514:ASN:ND2	3:B:2000:SLB:C11	2.77	0.45
1:A:80:ILE:CD1	1:A:126:ILE:HD12	2.45	0.45
2:B:289:LEU:HD22	2:B:289:LEU:C	2.42	0.45
1:A:136:GLU:HA	2:B:439:MSE:HE3	1.99	0.45
2:B:264:ILE:HG23	2:B:265:PHE:H	1.81	0.44
2:B:540:ILE:HG13	2:B:597:ASN:HA	1.98	0.44
2:B:595:LEU:HD12	2:B:601:TYR:CZ	2.52	0.44
2:B:547:ILE:HG23	2:B:597:ASN:HD21	1.82	0.43
2:B:565:LEU:HD21	2:B:595:LEU:HD11	2.00	0.43
2:B:590:VAL:HG22	2:B:590:VAL:O	2.18	0.43
1:A:54:ALA:HB3	1:A:115:MSE:CE	2.43	0.43
1:A:130:LEU:HD13	1:A:135:THR:OG1	2.18	0.43
1:A:72:THR:HG22	1:A:138:ALA:HB2	2.00	0.42
1:A:23:ASP:OD1	1:A:131:GLN:HB2	2.18	0.42
2:B:428:ILE:HG23	2:B:455:ILE:HB	2.02	0.42
2:B:419:THR:HG21	2:B:424:PRO:HD2	2.00	0.42
1:A:159:ILE:HD12	1:A:160:ASP:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ASN:ND2	2:B:491:GLN:HE21	2.14	0.42
2:B:444:LEU:C	2:B:444:LEU:HD23	2.45	0.42
2:B:283:PHE:HB3	2:B:329:TYR:OH	2.20	0.41
2:B:546:ASN:HA	2:B:596:LEU:HD22	2.02	0.41
2:B:350:VAL:HG12	2:B:352:THR:HG22	2.01	0.41
1:A:147:TYR:CD1	1:A:172:ILE:HD12	2.56	0.41
2:B:224:ARG:HB2	2:B:228:LYS:HB3	2.03	0.41
2:B:559:ASN:HD21	2:B:612:ASN:N	2.12	0.41
1:A:24:GLY:O	1:A:129:VAL:HG22	2.21	0.41
2:B:511:ILE:HD12	2:B:537:GLN:NE2	2.36	0.41
2:B:552:PHE:HB2	2:B:595:LEU:HD23	2.03	0.41

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	166/205 (81%)	157 (95%)	9 (5%)	0	100	100
2	B	418/420 (100%)	393 (94%)	21 (5%)	4 (1%)	12	28
All	All	584/625 (93%)	550 (94%)	30 (5%)	4 (1%)	18	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	550	SER
2	B	551	ILE
2	B	622	ASN
2	B	562	ILE

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	151/187 (81%)	145 (96%)	6 (4%)	28	55
2	B	385/382 (101%)	369 (96%)	16 (4%)	26	52
All	All	536/569 (94%)	514 (96%)	22 (4%)	27	54

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	28	VAL
1	A	132	ASN
1	A	133	THR
1	A	151	ILE
1	A	181	LYS
2	B	273	ARG
2	B	289	LEU
2	B	302	ILE
2	B	405	VAL
2	B	439	MSE
2	B	447	ASP
2	B	484	ILE
2	B	515	LEU
2	B	520	THR
2	B	545	ASN
2	B	549	SER
2	B	553	SER
2	B	570	GLU
2	B	586	LEU
2	B	587	LEU
2	B	616	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	39	GLN
1	A	41	GLN
1	A	42	ASN
1	A	50	ASN
1	A	83	ASN
1	A	132	ASN
1	A	158	GLN
2	B	246	GLN
2	B	251	ASN
2	B	317	ASN
2	B	319	GLN
2	B	361	GLN
2	B	367	ASN
2	B	393	ASN
2	B	401	ASN
2	B	421	ASN
2	B	436	ASN
2	B	514	ASN
2	B	526	GLN
2	B	558	ASN
2	B	559	ASN
2	B	582	ASN
2	B	612	ASN
2	B	614	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$
3	SLB	B	2000	-	21,21,21	1.02	1 (4%)	24,31,31	1.51	4 (16%)

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
3	SLB	B	2000	-	-	8/20/38/38	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2000	SLB	O2-C2	2.74	1.43	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2000	SLB	C4-C5-N5	-4.36	101.86	110.44
3	B	2000	SLB	C3-C4-C5	2.37	113.38	109.72
3	B	2000	SLB	C6-C5-N5	-2.24	107.33	110.91
3	B	2000	SLB	C3-C2-C1	-2.23	108.69	112.84

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2000	SLB	C5-C6-C7-C8
3	B	2000	SLB	C5-C6-C7-O7
3	B	2000	SLB	O6-C6-C7-C8
3	B	2000	SLB	O6-C6-C7-O7
3	B	2000	SLB	O8-C8-C9-O9
3	B	2000	SLB	C7-C8-C9-O9

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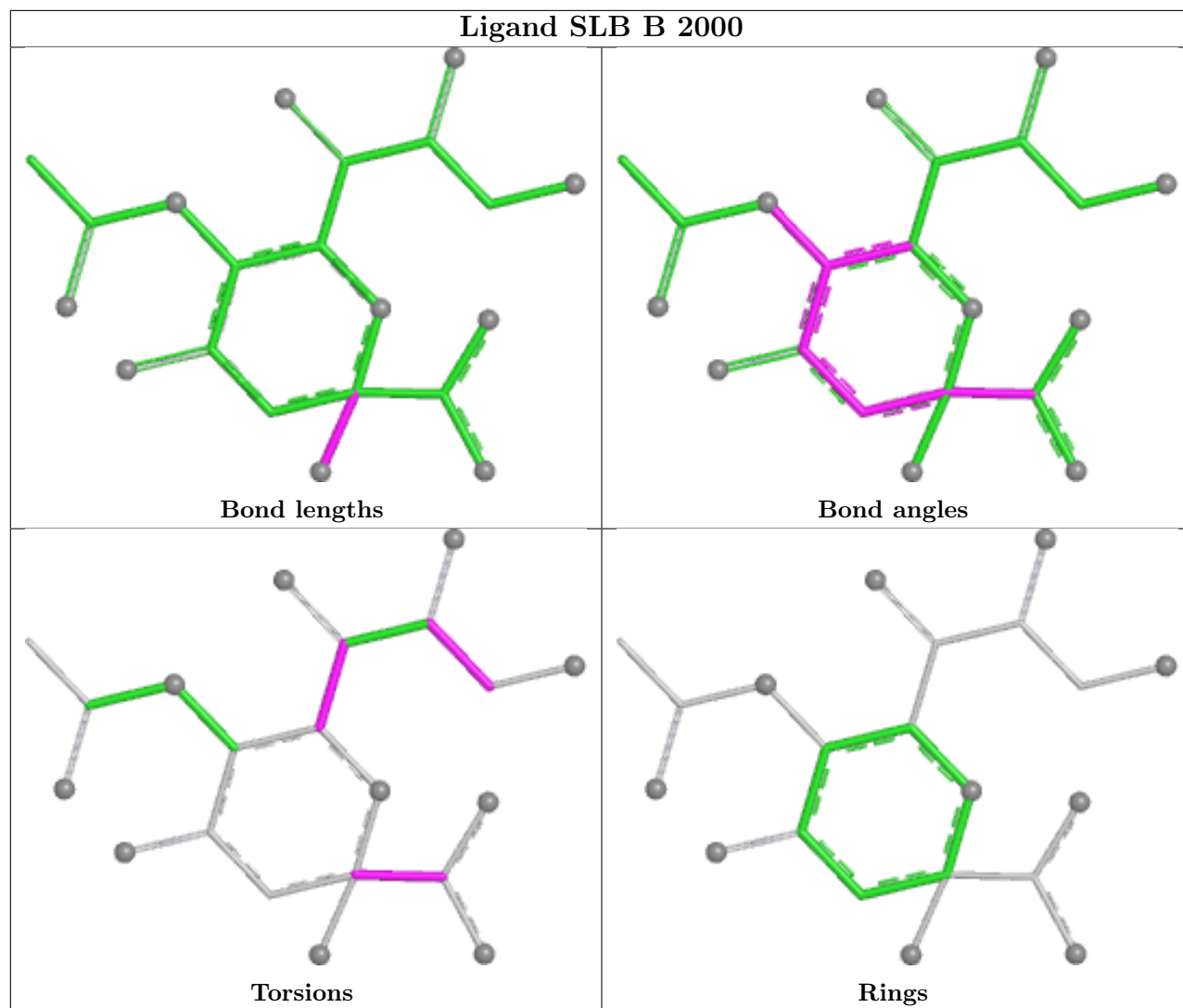
Mol	Chain	Res	Type	Atoms
3	B	2000	SLB	O1A-C1-C2-O2
3	B	2000	SLB	O1B-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2000	SLB	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	167/205 (81%)	0.86	35 (20%) 2 2	31, 55, 84, 100	0
2	B	417/420 (99%)	0.97	74 (17%) 4 3	34, 55, 84, 96	0
All	All	584/625 (93%)	0.94	109 (18%) 3 2	31, 55, 84, 100	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	572	ILE	7.2
2	B	571	SER	6.5
2	B	623	SER	6.3
1	A	131	GLN	6.2
1	A	132	ASN	6.2
2	B	550	SER	5.8
2	B	515	LEU	5.7
1	A	159	ILE	4.7
1	A	184	ASP	4.5
1	A	59	LEU	4.3
2	B	622	ASN	4.2
2	B	204	GLN	4.2
2	B	547	ILE	4.2
2	B	549	SER	4.2
2	B	514	ASN	4.1
2	B	436	ASN	4.1
1	A	133	THR	4.1
2	B	441	SER	3.9
1	A	17	ASN	3.8
1	A	62	ARG	3.8
2	B	440	ASN	3.8
2	B	599	ALA	3.7
1	A	182	ILE	3.7
2	B	570	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	183	ASP	3.7
2	B	569	THR	3.7
2	B	551	ILE	3.7
2	B	609	GLU	3.7
1	A	73	ALA	3.6
2	B	442	ASN	3.6
2	B	516	ASN	3.6
2	B	597	ASN	3.5
1	A	181	LYS	3.5
2	B	224	ARG	3.5
2	B	562	ILE	3.4
2	B	446	ASN	3.3
1	A	63	GLU	3.3
2	B	540	ILE	3.2
1	A	60	ARG	3.2
2	B	555	ARG	3.1
2	B	548	ALA	3.1
1	A	38	ARG	3.0
1	A	135	THR	2.9
1	A	130	LEU	2.9
2	B	490	SER	2.9
2	B	567	ARG	2.8
2	B	552	PHE	2.8
2	B	260	SER	2.8
2	B	487	SER	2.8
1	A	134	VAL	2.7
2	B	513	ASP	2.7
2	B	546	ASN	2.7
2	B	557	ARG	2.7
1	A	161	LYS	2.7
1	A	20	ASN	2.7
1	A	72	THR	2.7
2	B	518	SER	2.7
2	B	445	SER	2.6
2	B	544	PHE	2.6
2	B	356	GLN	2.6
1	A	158	GLN	2.6
2	B	357	ASP	2.5
1	A	128	LYS	2.5
2	B	573	ASN	2.5
1	A	74	SER	2.5
2	B	485	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	596	LEU	2.5
2	B	598	GLY	2.5
2	B	612	ASN	2.4
2	B	601	TYR	2.4
2	B	498	LEU	2.4
1	A	110	ASN	2.4
2	B	519	GLY	2.4
2	B	545	ASN	2.3
2	B	522	TYR	2.3
1	A	25	ASN	2.3
2	B	474	ASP	2.3
2	B	324	ASP	2.3
2	B	520	THR	2.3
2	B	538	LEU	2.3
2	B	583	TYR	2.2
2	B	521	HIS	2.2
2	B	443	ASN	2.2
2	B	621	ARG	2.2
2	B	541	PRO	2.2
2	B	205	THR	2.2
1	A	19	VAL	2.2
1	A	64	THR	2.2
2	B	489	THR	2.2
1	A	26	TYR	2.2
2	B	263	THR	2.1
2	B	495	LYS	2.1
2	B	258	ASN	2.1
2	B	590	VAL	2.1
2	B	568	LEU	2.1
1	A	23	ASP	2.1
1	A	21	LEU	2.1
2	B	444	LEU	2.1
2	B	512	LEU	2.1
2	B	421	ASN	2.1
2	B	588	ASN	2.1
1	A	24	GLY	2.1
2	B	553	SER	2.0
1	A	18	ASN	2.0
1	A	80	ILE	2.0
1	A	162	ASN	2.0
2	B	264	ILE	2.0
2	B	448	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	575	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

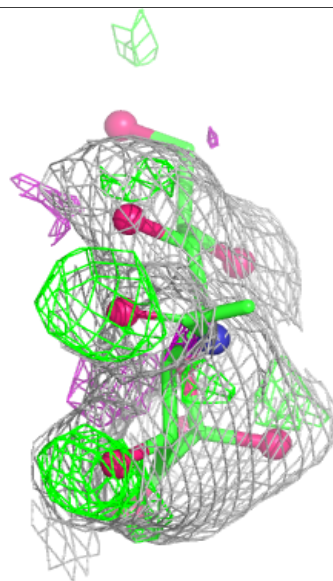
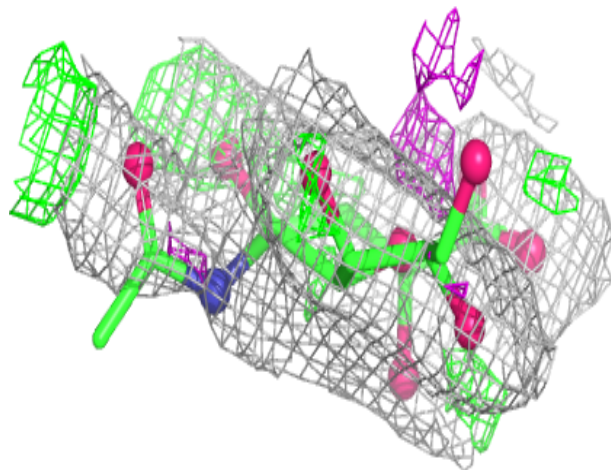
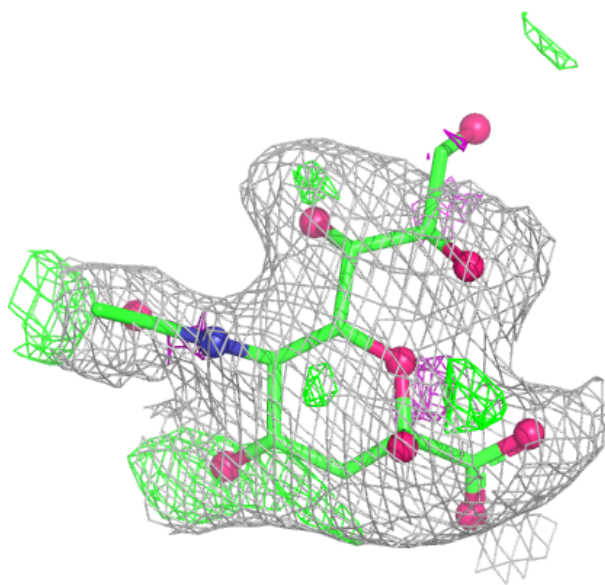
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	SLB	B	2000	21/21	0.76	0.23	73,77,82,83	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 SLB B 2000:

$2mF_o-DF_c$ (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.