



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 01:34 PM EDT

PDB ID : 2G7Q
Title : Structure of the Light Chain of Botulinum Neurotoxin Serotype A Bound to Small Molecule Inhibitors
Authors : Fu, Z.; Baldwin, M.R.; Boldt, G.E.; Janda, K.D.; Barbieri, J.T.; Kim, J.-J.P.
Deposited on : 2006-02-28
Resolution : 2.41 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 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 : 2.23.2
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) : 2.23.2

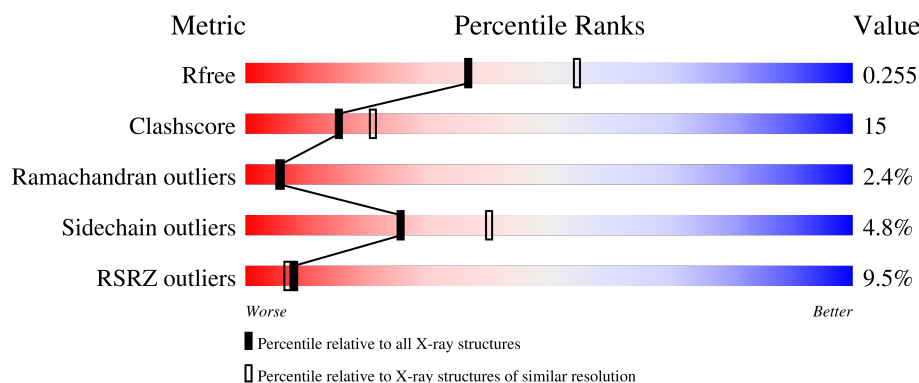
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	425	
1	B	425	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6797 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3323	2135	545	636	7			
1	B	409	Total	C	N	O	S	0	0	0
			3300	2118	544	631	7			

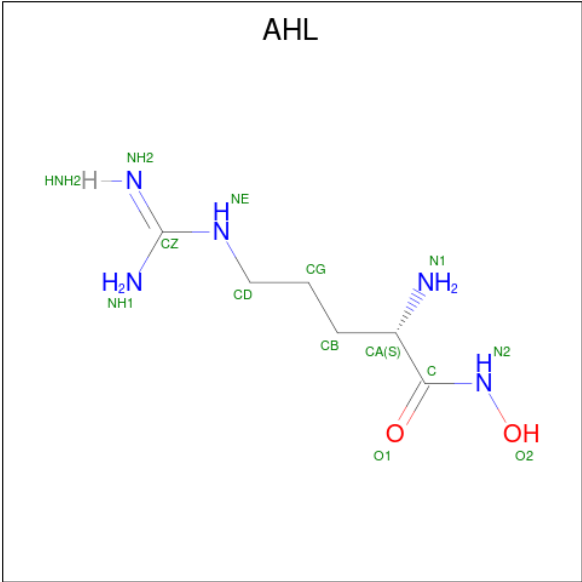
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q45894
A	362	ALA	ARG	engineered mutation	UNP Q45894
A	365	PHE	TYR	engineered mutation	UNP Q45894
B	1	MET	-	initiating methionine	UNP Q45894
B	362	ALA	ARG	engineered mutation	UNP Q45894
B	365	PHE	TYR	engineered mutation	UNP Q45894

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N-HYDROXY-L-ARGININAMIDE (three-letter code: AHL) (formula: C₆H₁₅N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	6	5	2		

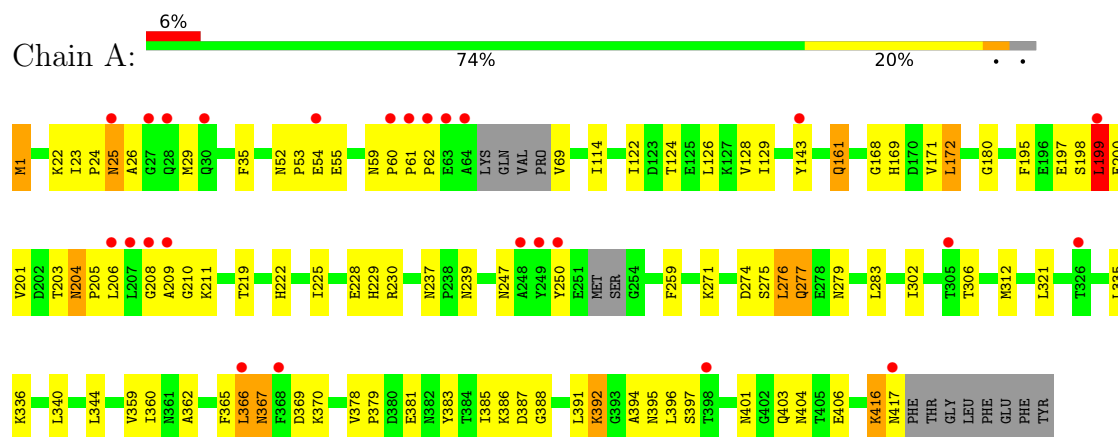
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	104	Total	O	0	0
			104	104		
4	B	55	Total	O	0	0
			55	55		

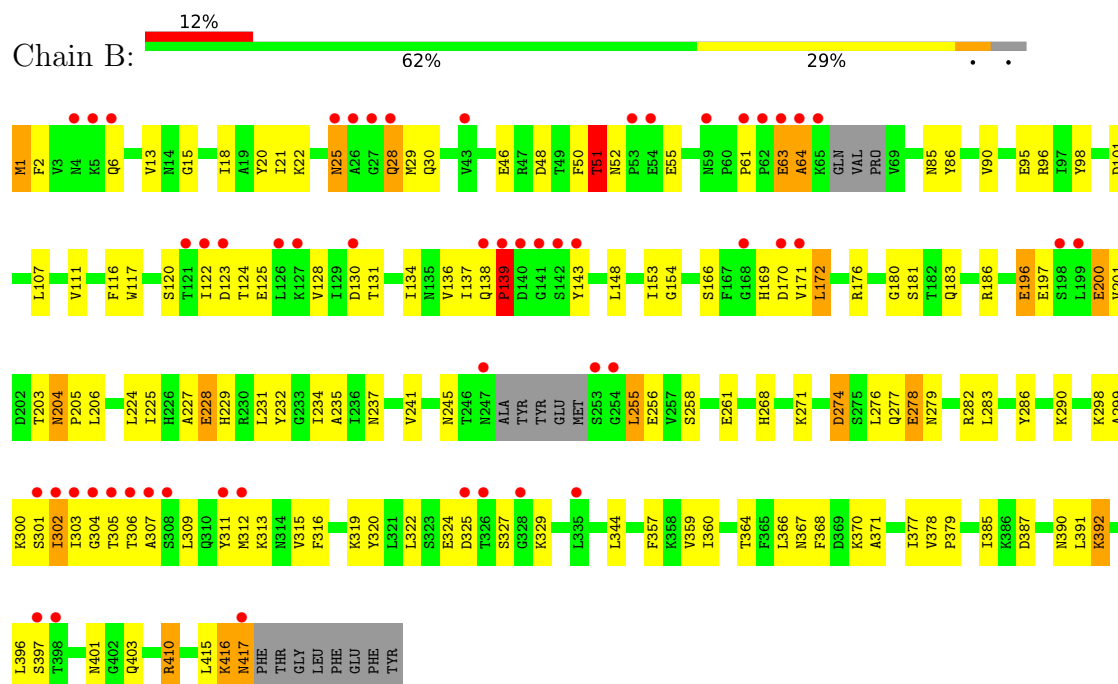
3 Residue-property plots [i](#)

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: Botulinum neurotoxin type A



• Molecule 1: Botulinum neurotoxin type A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.32Å 109.94Å 166.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.55 – 2.41 21.55 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.5 (21.55-2.41) 98.7 (21.55-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.17 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.261 0.216 , 0.255	Depositor DCC
R_{free} test set	4984 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6797	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: AHL, ZN

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	0.42	0/3398	0.64	0/4597
1	B	0.38	0/3373	0.59	1/4561 (0.0%)
All	All	0.40	0/6771	0.62	1/9158 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	GLU	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3323	0	3252	85	0
1	B	3300	0	3241	115	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	13	0	0
4	A	104	0	0	0	0
4	B	55	0	0	3	0
All	All	6797	0	6506	196	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (196) 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:22:LYS:HA	1:A:29:MET:HE1	1.41	0.98
1:B:387:ASP:OD2	1:B:392:LYS:HG3	1.63	0.95
1:A:204:ASN:HD22	1:A:205:PRO:N	1.72	0.87
1:B:228:GLU:HG3	1:B:344:LEU:HD22	1.55	0.86
1:A:171:VAL:HG23	1:A:172:LEU:HD13	1.58	0.85
1:A:52:ASN:HD22	1:A:55:GLU:HG3	1.43	0.83
1:A:209:ALA:H	1:A:404:ASN:HD21	1.27	0.80
1:A:61:PRO:HB2	1:A:62:PRO:HD2	1.65	0.79
1:A:199:LEU:HD23	1:A:199:LEU:H	1.45	0.79
1:A:387:ASP:OD2	1:A:392:LYS:HG3	1.84	0.77
1:B:325:ASP:OD2	1:B:329:LYS:HB3	1.85	0.77
1:B:22:LYS:HE3	1:B:137:ILE:HD11	1.70	0.74
1:A:391:LEU:O	1:A:397:SER:HB3	1.88	0.73
1:B:410:ARG:HB2	1:B:410:ARG:HH11	1.52	0.73
1:A:225:ILE:O	1:A:228:GLU:HG2	1.88	0.73
1:B:325:ASP:OD1	1:B:327:SER:HB3	1.89	0.72
1:B:172:LEU:HD23	1:B:172:LEU:H	1.54	0.70
1:B:6:GLN:HE21	1:B:6:GLN:HA	1.57	0.69
1:B:64:ALA:HB2	4:B:535:HOH:O	1.91	0.69
1:A:204:ASN:ND2	1:A:206:LEU:H	1.90	0.69
1:A:1:MET:SD	1:A:1:MET:N	2.63	0.69
1:B:299:ALA:HB3	1:B:313:LYS:HE2	1.76	0.68
1:A:161:GLN:HE21	1:A:161:GLN:HA	1.57	0.67
1:B:302:ILE:HD11	1:B:312:MET:HG3	1.77	0.67
1:B:52:ASN:HD22	1:B:55:GLU:HG3	1.61	0.66
1:B:304:GLY:O	1:B:306:THR:HG22	1.94	0.66
1:B:196:GLU:H	1:B:370:LYS:NZ	1.92	0.66
1:A:52:ASN:ND2	1:A:55:GLU:HG3	2.10	0.64
1:A:197:GLU:OE1	1:A:360:ILE:HD11	1.97	0.64
1:A:114:ILE:H	1:A:114:ILE:HD12	1.61	0.64
1:A:204:ASN:HD22	1:A:204:ASN:C	1.96	0.64
1:B:116:PHE:HA	1:B:316:PHE:CE1	2.33	0.63
1:A:225:ILE:O	1:A:228:GLU:CG	2.46	0.63
1:B:415:LEU:O	1:B:416:LYS:HB2	1.99	0.62
1:A:23:ILE:HG23	1:A:24:PRO:HD2	1.79	0.62
1:B:197:GLU:OE2	1:B:360:ILE:HD11	2.00	0.62
1:B:204:ASN:ND2	1:B:206:LEU:H	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:VAL:HG23	1:A:417:ASN:OD1	2.00	0.62
1:B:300:LYS:O	1:B:309:LEU:HD22	1.99	0.61
1:A:211:LYS:HE3	1:A:370:LYS:HB2	1.81	0.61
1:B:232:TYR:O	1:B:234:ILE:HG23	2.01	0.61
1:B:117:TRP:CE2	1:B:128:VAL:HB	2.36	0.61
1:B:196:GLU:HB2	1:B:370:LYS:HE2	1.82	0.60
1:A:209:ALA:N	1:A:404:ASN:HD21	1.98	0.60
1:B:360:ILE:HG22	1:B:403:GLN:CD	2.22	0.60
1:A:69:VAL:HG13	1:A:69:VAL:O	2.00	0.59
1:B:138:GLN:HB3	1:B:139:PRO:HD2	1.84	0.59
1:B:6:GLN:HA	1:B:6:GLN:NE2	2.17	0.59
1:A:228:GLU:HG3	1:A:229:HIS:N	2.16	0.59
1:A:385:ILE:HG22	1:A:386:LYS:HD2	1.86	0.58
1:A:199:LEU:HD23	1:A:199:LEU:N	2.18	0.58
1:B:13:VAL:HA	1:B:18:ILE:HG22	1.85	0.57
1:B:228:GLU:CG	1:B:344:LEU:HD22	2.30	0.57
1:A:200:GLU:HB2	1:A:203:THR:HG23	1.87	0.57
1:A:204:ASN:HD22	1:A:205:PRO:CD	2.17	0.57
1:A:24:PRO:O	1:A:26:ALA:N	2.38	0.56
1:B:169:HIS:CE1	1:B:171:VAL:HG12	2.41	0.55
1:A:169:HIS:CE1	1:A:171:VAL:HG22	2.42	0.55
1:B:51:THR:HG22	1:B:186:ARG:HH21	1.70	0.55
1:B:228:GLU:HG3	1:B:344:LEU:CD2	2.32	0.55
1:B:124:THR:HA	1:B:298:LYS:O	2.05	0.55
1:B:377:ILE:HG12	4:B:520:HOH:O	2.05	0.54
1:B:378:VAL:HB	1:B:379:PRO:HD3	1.90	0.54
1:A:61:PRO:CB	1:A:62:PRO:HD2	2.36	0.54
1:B:21:ILE:HG22	1:B:136:VAL:HA	1.90	0.54
1:B:200:GLU:HB2	1:B:203:THR:HG23	1.90	0.54
1:B:304:GLY:C	1:B:306:THR:H	2.10	0.54
1:B:153:ILE:HG12	1:B:154:GLY:N	2.23	0.53
1:B:371:ALA:HA	1:B:417:ASN:HB3	1.91	0.53
1:A:321:LEU:HD12	1:A:340:LEU:HB2	1.89	0.53
1:B:166:SER:OG	1:B:183:GLN:NE2	2.42	0.53
1:B:225:ILE:O	1:B:228:GLU:OE2	2.27	0.53
1:A:247:ASN:HB2	1:A:250:TYR:HD2	1.74	0.52
1:A:362:ALA:HB1	1:A:367:ASN:HB3	1.91	0.52
1:B:302:ILE:HG23	1:B:302:ILE:O	2.10	0.52
1:B:120:SER:HB3	1:B:125:GLU:O	2.10	0.52
1:B:228:GLU:OE1	1:B:344:LEU:O	2.27	0.52
1:B:387:ASP:HB3	1:B:390:ASN:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:SD	1:B:1:MET:N	2.82	0.52
1:B:107:LEU:O	1:B:111:VAL:HG23	2.10	0.52
1:B:136:VAL:HG12	1:B:137:ILE:N	2.26	0.51
1:B:268:HIS:O	1:B:271:LYS:HB2	2.10	0.51
1:B:416:LYS:CG	1:B:417:ASN:H	2.23	0.51
1:A:396:LEU:HA	1:A:401:ASN:HB2	1.92	0.50
1:A:204:ASN:HD21	1:A:206:LEU:H	1.60	0.50
1:A:228:GLU:OE1	1:A:344:LEU:O	2.29	0.50
1:B:130:ASP:OD1	1:B:131:THR:HG23	2.11	0.50
1:B:176:ARG:HD3	1:B:237:ASN:HA	1.94	0.50
1:A:279:ASN:O	1:A:283:LEU:HD23	2.12	0.50
1:A:114:ILE:HD12	1:A:114:ILE:N	2.26	0.50
1:B:180:GLY:HA3	1:B:231:LEU:O	2.12	0.50
1:A:209:ALA:H	1:A:404:ASN:ND2	2.03	0.49
1:B:181:SER:O	1:B:231:LEU:HD23	2.11	0.49
1:A:199:LEU:H	1:A:199:LEU:CD2	2.19	0.49
1:B:416:LYS:HG2	1:B:417:ASN:H	1.77	0.49
1:B:96:ARG:HA	1:B:385:ILE:HG23	1.95	0.49
1:B:29:MET:O	1:B:29:MET:HG3	2.13	0.48
1:A:204:ASN:ND2	1:A:204:ASN:C	2.64	0.48
1:A:274:ASP:OD2	1:A:276:LEU:HB2	2.13	0.48
1:B:225:ILE:HA	1:B:228:GLU:OE2	2.13	0.48
1:B:279:ASN:ND2	1:B:282:ARG:NH1	2.61	0.48
1:B:25:ASN:HD22	1:B:131:THR:HG22	1.78	0.48
1:A:335:LEU:HD12	1:A:336:LYS:N	2.28	0.48
1:A:259:PHE:HE2	1:A:277:GLN:HG2	1.78	0.48
1:B:304:GLY:O	1:B:306:THR:N	2.43	0.48
1:A:237:ASN:CG	1:A:239:ASN:ND2	2.66	0.48
1:A:195:PHE:HZ	1:A:360:ILE:HG23	1.78	0.48
1:A:171:VAL:HG23	1:A:172:LEU:CD1	2.37	0.47
1:B:278:GLU:OE1	1:B:282:ARG:NH2	2.47	0.47
1:A:198:SER:O	1:A:200:GLU:HG3	2.15	0.47
1:B:134:ILE:HG23	1:B:148:LEU:CD2	2.45	0.47
1:B:368:PHE:O	1:B:370:LYS:NZ	2.46	0.47
1:B:241:VAL:HG12	1:B:258:SER:HA	1.97	0.47
1:A:161:GLN:O	1:A:161:GLN:HG3	2.14	0.47
1:A:416:LYS:CD	1:A:417:ASN:H	2.28	0.47
1:A:225:ILE:HA	1:A:228:GLU:HG2	1.96	0.47
1:B:136:VAL:O	1:B:143:TYR:HA	2.14	0.47
1:B:143:TYR:H	1:B:143:TYR:HD2	1.61	0.46
1:A:274:ASP:OD1	1:A:277:GLN:NE2	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:TYR:O	1:B:315:VAL:HG23	2.15	0.46
1:B:196:GLU:H	1:B:370:LYS:HZ3	1.63	0.46
1:B:48:ASP:OD2	1:B:153:ILE:HD13	2.15	0.46
1:B:229:HIS:NE2	1:B:344:LEU:O	2.48	0.46
1:A:378:VAL:HB	1:A:379:PRO:HD3	1.96	0.46
1:B:274:ASP:OD1	1:B:276:LEU:N	2.49	0.46
1:B:61:PRO:HB2	1:B:63:GLU:OE2	2.15	0.46
1:B:125:GLU:HB2	1:B:301:SER:HB3	1.97	0.46
1:B:6:GLN:NE2	1:B:6:GLN:CA	2.79	0.46
1:B:279:ASN:O	1:B:283:LEU:HD23	2.16	0.46
1:B:13:VAL:HG11	1:B:20:TYR:CD1	2.51	0.45
1:B:360:ILE:HG22	1:B:403:GLN:NE2	2.30	0.45
1:B:2:PHE:HB3	1:B:95:GLU:OE2	2.17	0.45
1:B:15:GLY:O	1:B:138:GLN:NE2	2.49	0.45
1:A:171:VAL:CG2	1:A:172:LEU:HD13	2.39	0.45
1:A:23:ILE:HG23	1:A:24:PRO:CD	2.46	0.45
1:A:381:GLU:N	1:A:381:GLU:CD	2.71	0.45
1:B:86:TYR:CE1	1:B:90:VAL:HG21	2.52	0.44
1:B:312:MET:O	1:B:315:VAL:HB	2.16	0.44
1:B:410:ARG:HB2	1:B:410:ARG:NH1	2.25	0.44
1:A:59:ASN:O	1:A:61:PRO:HD3	2.16	0.44
1:A:237:ASN:CG	1:A:239:ASN:HD22	2.20	0.44
1:B:255:LEU:HD22	1:B:256:GLU:N	2.32	0.44
1:B:416:LYS:CE	1:B:417:ASN:H	2.29	0.44
1:B:30:GLN:HA	1:B:30:GLN:OE1	2.16	0.44
1:A:52:ASN:HD22	1:A:55:GLU:CG	2.22	0.44
1:B:324:GLU:HA	1:B:329:LYS:O	2.17	0.44
1:B:171:VAL:HG13	1:B:172:LEU:N	2.33	0.44
1:B:169:HIS:ND1	1:B:170:ASP:N	2.65	0.44
1:A:209:ALA:HB3	1:A:406:GLU:HG3	2.00	0.43
1:B:396:LEU:HA	1:B:401:ASN:HB2	2.00	0.43
1:B:85:ASN:OD1	1:B:378:VAL:HG21	2.18	0.43
1:A:275:SER:HA	1:B:245:ASN:HB2	2.01	0.43
1:B:224:LEU:O	1:B:227:ALA:HB3	2.19	0.43
1:A:52:ASN:HA	1:A:53:PRO:HD3	1.86	0.43
1:A:60:PRO:HA	1:A:61:PRO:HD2	1.95	0.43
1:B:204:ASN:HD22	1:B:205:PRO:N	2.17	0.43
1:A:23:ILE:HG22	1:A:24:PRO:O	2.19	0.42
1:A:200:GLU:HB2	1:A:203:THR:CG2	2.49	0.42
1:B:98:TYR:HD1	1:B:107:LEU:HD12	1.84	0.42
1:B:138:GLN:HB3	1:B:139:PRO:CD	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LYS:HD3	1:B:320:TYR:CE2	2.53	0.42
1:B:360:ILE:HG22	1:B:403:GLN:OE1	2.19	0.42
1:A:122:ILE:HG22	1:A:124:THR:HG22	2.00	0.42
1:B:258:SER:OG	1:B:261:GLU:HB2	2.19	0.42
1:B:277:GLN:HE21	1:B:277:GLN:HB2	1.67	0.42
1:A:416:LYS:HD2	1:A:417:ASN:OD1	2.18	0.42
1:B:315:VAL:HA	4:B:655:HOH:O	2.18	0.42
1:B:13:VAL:HG11	1:B:20:TYR:HD1	1.84	0.42
1:B:357:PHE:HB3	1:B:359:VAL:HG13	2.02	0.42
1:A:359:VAL:O	1:B:201:VAL:HG21	2.19	0.42
1:A:59:ASN:HA	1:A:60:PRO:HD3	1.83	0.42
1:A:271:LYS:HG3	1:B:366:LEU:HD11	2.01	0.42
1:A:35:PHE:CD1	1:A:35:PHE:N	2.88	0.42
1:B:286:TYR:O	1:B:290:LYS:HG3	2.20	0.42
1:A:381:GLU:CD	1:A:381:GLU:H	2.22	0.41
1:A:161:GLN:HE21	1:A:161:GLN:CA	2.23	0.41
1:A:171:VAL:HG23	1:A:172:LEU:N	2.35	0.41
1:B:274:ASP:OD1	1:B:274:ASP:C	2.59	0.41
1:A:180:GLY:HA2	1:A:230:ARG:O	2.20	0.41
1:A:128:VAL:HG22	1:A:129:ILE:N	2.36	0.41
1:A:365:PHE:CG	1:A:366:LEU:N	2.88	0.41
1:A:383:TYR:HA	1:A:388:GLY:O	2.21	0.41
1:B:51:THR:CG2	1:B:186:ARG:HH21	2.33	0.41
1:B:122:ILE:C	1:B:124:THR:H	2.23	0.41
1:B:125:GLU:OE2	1:B:303:ILE:HG12	2.21	0.41
1:A:271:LYS:HG3	1:B:366:LEU:CD1	2.51	0.41
1:A:302:ILE:HD11	1:A:312:MET:HG3	2.02	0.41
1:A:360:ILE:HG22	1:A:403:GLN:CD	2.41	0.41
1:B:28:GLN:HG2	1:B:28:GLN:O	2.21	0.41
1:B:134:ILE:HG23	1:B:148:LEU:HD22	2.03	0.40
1:B:391:LEU:O	1:B:397:SER:HB3	2.21	0.40
1:B:176:ARG:HG2	1:B:235:ALA:O	2.22	0.40
1:B:204:ASN:HD22	1:B:204:ASN:C	2.25	0.40
1:A:219:THR:O	1:A:222:HIS:HB3	2.22	0.40
1:A:24:PRO:O	1:A:25:ASN:C	2.59	0.40
1:A:416:LYS:HD3	1:A:417:ASN:H	1.86	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	405/425 (95%)	373 (92%)	24 (6%)	8 (2%)	7	8
1	B	403/425 (95%)	363 (90%)	29 (7%)	11 (3%)	5	4
All	All	808/850 (95%)	736 (91%)	53 (7%)	19 (2%)	6	5

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	208	GLY
1	A	392	LYS
1	B	305	THR
1	B	392	LYS
1	B	416	LYS
1	A	199	LEU
1	A	306	THR
1	B	51	THR
1	B	123	ASP
1	B	307	ALA
1	A	210	GLY
1	A	394	ALA
1	B	322	LEU
1	B	64	ALA
1	B	25	ASN
1	B	302	ILE
1	B	139	PRO
1	A	168	GLY

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	367/380 (97%)	351 (96%)	16 (4%)	28	43
1	B	366/380 (96%)	347 (95%)	19 (5%)	23	37
All	All	733/760 (96%)	698 (95%)	35 (5%)	25	40

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	54	GLU
1	A	126	LEU
1	A	143	TYR
1	A	161	GLN
1	A	172	LEU
1	A	199	LEU
1	A	201	VAL
1	A	204	ASN
1	A	276	LEU
1	A	277	GLN
1	A	366	LEU
1	A	367	ASN
1	A	369	ASP
1	A	395	ASN
1	A	416	LYS
1	B	1	MET
1	B	28	GLN
1	B	46	GLU
1	B	50	PHE
1	B	51	THR
1	B	63	GLU
1	B	101	ASP
1	B	139	PRO
1	B	172	LEU
1	B	196	GLU
1	B	204	ASN
1	B	228	GLU
1	B	255	LEU
1	B	274	ASP
1	B	278	GLU
1	B	364	THR
1	B	367	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	410	ARG
1	B	417	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	28	GLN
1	A	30	GLN
1	A	52	ASN
1	A	59	ASN
1	A	135	ASN
1	A	161	GLN
1	A	204	ASN
1	A	367	ASN
1	A	399	ASN
1	B	6	GLN
1	B	25	ASN
1	B	28	GLN
1	B	52	ASN
1	B	59	ASN
1	B	204	ASN
1	B	277	GLN
1	B	279	ASN
1	B	367	ASN
1	B	417	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

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AHL	A	500	2	12,12,12	3.58	2 (16%)	12,14,14	0.92	0

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	AHL	A	500	2	-	1/13/13/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	AHL	C-N2	-11.99	1.17	1.33
3	A	500	AHL	O2-N2	-2.46	1.33	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	AHL	NH1-CZ-NE-CD

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	411/425 (96%)	0.01	25 (6%) 21 19	10, 26, 57, 65	0
1	B	409/425 (96%)	0.51	53 (12%) 3 2	15, 39, 61, 69	0
All	All	820/850 (96%)	0.26	78 (9%) 8 7	10, 32, 59, 69	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	ASN	7.8
1	A	27	GLY	6.3
1	B	253	SER	6.2
1	B	303	ILE	6.0
1	B	307	ALA	5.7
1	B	64	ALA	5.5
1	A	61	PRO	5.4
1	A	208	GLY	5.4
1	B	305	THR	5.4
1	A	62	PRO	5.3
1	B	62	PRO	5.0
1	B	311	TYR	5.0
1	B	65	LYS	4.9
1	A	28	GLN	4.9
1	B	304	GLY	4.8
1	B	28	GLN	4.7
1	B	199	LEU	4.5
1	A	209	ALA	4.4
1	B	143	TYR	4.3
1	B	59	ASN	4.2
1	A	305	THR	4.2
1	A	366	LEU	4.0
1	B	168	GLY	4.0
1	A	199	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	170	ASP	3.8
1	A	248	ALA	3.8
1	A	63	GLU	3.7
1	B	312	MET	3.7
1	B	254	GLY	3.6
1	B	6	GLN	3.6
1	B	63	GLU	3.6
1	A	398	THR	3.5
1	B	121	THR	3.5
1	B	247	ASN	3.5
1	B	308	SER	3.5
1	A	25	ASN	3.5
1	B	5	LYS	3.4
1	B	140	ASP	3.3
1	B	4	ASN	3.1
1	B	325	ASP	3.1
1	B	417	ASN	3.1
1	B	122	ILE	3.1
1	B	302	ILE	3.1
1	B	306	THR	3.1
1	B	138	GLN	3.0
1	B	335	LEU	3.0
1	B	139	PRO	3.0
1	B	171	VAL	3.0
1	B	142	SER	3.0
1	B	53	PRO	2.9
1	A	368	PHE	2.9
1	A	60	PRO	2.9
1	B	301	SER	2.9
1	B	27	GLY	2.9
1	B	54	GLU	2.8
1	A	417	ASN	2.8
1	B	130	ASP	2.8
1	B	126	LEU	2.7
1	A	249	TYR	2.7
1	A	250	TYR	2.7
1	B	397	SER	2.6
1	A	207	LEU	2.5
1	B	141	GLY	2.4
1	A	30	GLN	2.3
1	B	326	THR	2.3
1	B	123	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	328	GLY	2.3
1	B	198	SER	2.2
1	B	26	ALA	2.2
1	A	54	GLU	2.2
1	B	127	LYS	2.2
1	B	43	VAL	2.1
1	B	61	PRO	2.1
1	A	143	TYR	2.1
1	A	64	ALA	2.1
1	A	326	THR	2.0
1	A	206	LEU	2.0
1	B	398	THR	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 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, 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(Å ²)	Q<0.9
3	AHL	A	500	13/13	0.81	0.30	37,38,42,42	0
2	ZN	A	452	1/1	0.96	0.07	22,22,22,22	0
2	ZN	B	451	1/1	0.97	0.06	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.