



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:59 PM UTC

PDB ID : 2G7P / pdb_00002g7p
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 : 2.30 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
Xtriage (Phenix) : 2.0
EDS : 3.0
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

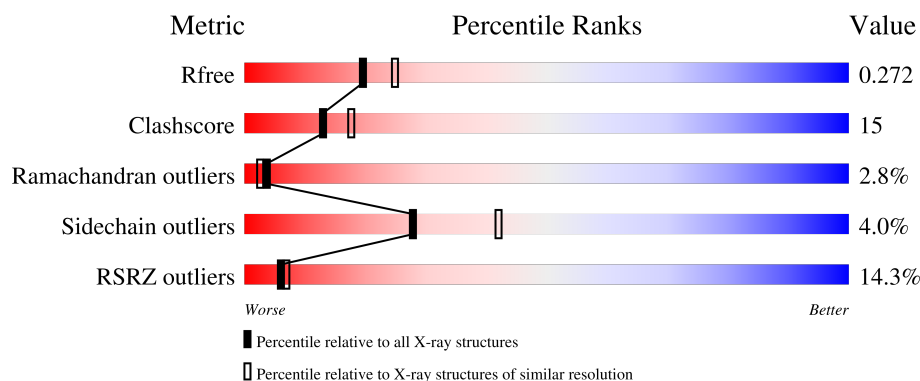
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	10% 71% 21% 5% .
1	B	425	17% 67% 23% 6% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6864 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 (CCD ID: 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	167	Total	O	0	0
			167	167		
3	B	72	Total	O	0	0
			72	72		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.21Å 110.26Å 167.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.19 – 2.30 20.19 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.6 (20.19-2.30) 89.6 (20.19-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.30Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.275 0.230 , 0.272	Depositor DCC
R_{free} test set	5195 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.9	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	0.91	EDS
Total number of atoms	6864	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: 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	0.46	0/3398	0.95	15/4597 (0.3%)
1	B	0.39	0/3373	0.89	14/4561 (0.3%)
All	All	0.43	0/6771	0.92	29/9158 (0.3%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ALA	N-CA-C	-9.55	101.31	113.72
1	A	167	PHE	N-CA-C	9.34	121.54	111.36
1	B	26	ALA	N-CA-C	-7.51	103.85	113.16
1	A	304	GLY	N-CA-C	-6.49	103.72	114.48
1	A	386	LYS	N-CA-C	6.46	118.41	111.36
1	B	229	HIS	N-CA-C	-6.33	104.46	111.36
1	A	249	TYR	N-CA-C	-6.16	106.04	112.93
1	B	114	ILE	N-CA-C	5.98	114.81	108.95
1	A	159	ILE	N-CA-C	5.85	117.29	110.62
1	B	52	ASN	CA-C-N	5.82	125.29	119.24
1	B	52	ASN	C-N-CA	5.82	125.29	119.24
1	A	211	LYS	N-CA-C	5.62	118.38	110.23
1	A	395	ASN	N-CA-C	-5.58	106.33	113.02
1	A	41	ILE	N-CA-C	5.57	116.02	107.77
1	A	174	LEU	N-CA-C	5.56	118.06	111.33
1	B	174	LEU	N-CA-C	5.52	118.82	111.75
1	B	200	GLU	N-CA-C	-5.47	101.94	110.42
1	B	121	THR	N-CA-C	-5.34	106.72	113.18
1	A	52	ASN	CA-C-N	5.27	124.59	118.85
1	A	52	ASN	C-N-CA	5.27	124.59	118.85
1	B	368	PHE	N-CA-C	5.25	117.90	110.50
1	A	336	LYS	N-CA-C	-5.18	105.71	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	VAL	N-CA-C	-5.15	106.66	111.45
1	B	317	LYS	N-CA-C	-5.15	105.75	111.36
1	B	202	ASP	N-CA-C	5.11	118.55	112.72
1	A	305	THR	N-CA-C	5.09	117.47	110.35
1	A	20	TYR	N-CA-C	-5.08	101.69	109.76
1	B	286	TYR	N-CA-C	-5.04	105.87	111.36
1	B	371	ALA	N-CA-C	5.01	116.45	108.79

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	3323	0	3252	95	0
1	B	3300	0	3241	103	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	167	0	0	5	0
3	B	72	0	0	2	0
All	All	6864	0	6493	197	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 (197) 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:B:416:LYS:HG2	1:B:417:ASN:H	1.14	1.08
1:A:225:ILE:O	1:A:228:GLU:HG3	1.69	0.93
1:A:171:VAL:HG23	1:A:172:LEU:HD13	1.55	0.89
1:A:61:PRO:HB2	1:A:62:PRO:HD2	1.55	0.88
1:B:410:ARG:HB2	1:B:410:ARG:HH11	1.38	0.85
1:B:416:LYS:HG2	1:B:417:ASN:N	1.91	0.85
1:A:199:LEU:HD23	1:A:199:LEU:H	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ASP:OD2	1:B:392:LYS:HG3	1.78	0.84
1:B:204:ASN:ND2	1:B:206:LEU:H	1.77	0.83
1:A:204:ASN:C	1:A:204:ASN:HD22	1.92	0.78
1:A:204:ASN:HD22	1:A:205:PRO:N	1.82	0.77
1:A:417:ASN:ND2	3:A:698:HOH:O	2.21	0.74
1:B:22:LYS:HE2	1:B:31:PRO:HG3	1.73	0.70
1:B:410:ARG:HB2	1:B:410:ARG:NH1	2.05	0.70
1:A:1:MET:SD	1:A:1:MET:N	2.62	0.69
1:B:143:TYR:H	1:B:143:TYR:HD2	1.40	0.69
1:A:387:ASP:OD2	1:A:392:LYS:HG3	1.92	0.69
1:B:138:GLN:HB3	1:B:139:PRO:HD2	1.74	0.68
1:A:391:LEU:O	1:A:397:SER:HB3	1.93	0.67
1:B:122:ILE:HG22	1:B:124:THR:HG22	1.75	0.67
1:B:325:ASP:OD2	1:B:329:LYS:HB3	1.95	0.66
1:A:52:ASN:ND2	1:A:55:GLU:HG3	2.11	0.66
1:B:204:ASN:C	1:B:204:ASN:HD22	2.03	0.66
1:A:52:ASN:HD22	1:A:55:GLU:HG3	1.62	0.65
1:B:300:LYS:O	1:B:309:LEU:HD22	1.97	0.65
1:B:160:ILE:HD13	1:B:372:VAL:HG21	1.79	0.64
1:B:371:ALA:HA	1:B:417:ASN:HB2	1.79	0.64
1:B:48:ASP:OD1	1:B:51:THR:HG22	1.97	0.64
1:A:204:ASN:ND2	1:A:206:LEU:H	1.97	0.62
1:B:117:TRP:CE2	1:B:128:VAL:HB	2.34	0.62
1:B:52:ASN:HD22	1:B:55:GLU:HG3	1.65	0.62
1:A:29:MET:HE3	1:A:30:GLN:O	1.99	0.62
1:A:23:ILE:HG23	1:A:24:PRO:HD2	1.80	0.62
1:A:225:ILE:HA	1:A:228:GLU:HG2	1.82	0.61
1:A:278:GLU:HG3	1:B:245:ASN:OD1	2.00	0.61
1:A:237:ASN:CG	1:A:239:ASN:HD22	2.08	0.61
1:A:381:GLU:H	1:A:381:GLU:CD	2.09	0.60
1:A:247:ASN:HB3	1:A:249:TYR:H	1.65	0.60
1:B:171:VAL:O	1:B:172:LEU:HB2	2.01	0.59
1:B:228:GLU:CG	1:B:344:LEU:HD22	2.33	0.59
1:A:61:PRO:HB2	1:A:62:PRO:CD	2.31	0.59
1:A:69:VAL:HG13	1:A:69:VAL:O	2.03	0.58
1:A:169:HIS:CE1	1:A:171:VAL:HG22	2.38	0.58
1:A:197:GLU:HG3	1:A:207:LEU:HD13	1.85	0.58
1:B:116:PHE:HA	1:B:316:PHE:CE1	2.39	0.58
1:A:225:ILE:O	1:A:228:GLU:CG	2.49	0.58
1:B:200:GLU:HB2	1:B:203:THR:HG23	1.86	0.58
1:B:371:ALA:HA	1:B:417:ASN:CB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:VAL:HG11	1:B:20:TYR:CD1	2.39	0.58
1:B:378:VAL:HB	1:B:379:PRO:HD3	1.85	0.58
1:A:54:GLU:HA	3:A:667:HOH:O	2.04	0.57
1:B:228:GLU:OE1	1:B:344:LEU:O	2.23	0.57
1:B:367:ASN:HD21	1:B:370:LYS:HZ1	1.53	0.57
1:A:199:LEU:H	1:A:199:LEU:CD2	2.16	0.57
1:A:271:LYS:HE2	3:A:714:HOH:O	2.06	0.56
1:B:124:THR:HA	1:B:298:LYS:O	2.05	0.56
1:A:302:ILE:HD11	1:A:312:MET:HG3	1.87	0.56
1:B:136:VAL:HG12	1:B:137:ILE:N	2.21	0.56
1:A:398:THR:HG22	1:A:399:ASN:ND2	2.21	0.56
1:B:304:GLY:O	1:B:306:THR:HG22	2.06	0.56
1:A:228:GLU:OE2	1:A:348:TYR:HD2	1.89	0.56
1:B:138:GLN:HB3	1:B:139:PRO:CD	2.35	0.56
1:B:416:LYS:CG	1:B:417:ASN:H	1.99	0.56
1:B:204:ASN:HD22	1:B:205:PRO:N	2.04	0.54
1:A:199:LEU:HD23	1:A:199:LEU:N	2.18	0.54
1:B:204:ASN:ND2	1:B:204:ASN:C	2.66	0.54
1:B:360:ILE:HG22	1:B:403:GLN:CD	2.33	0.54
1:A:171:VAL:HG23	1:A:172:LEU:CD1	2.34	0.54
1:B:96:ARG:HA	1:B:385:ILE:HG23	1.88	0.54
1:A:22:LYS:HA	1:A:29:MET:HE2	1.90	0.53
1:A:158:ASP:OD2	1:A:161:GLN:HB2	2.08	0.53
1:A:204:ASN:C	1:A:204:ASN:ND2	2.64	0.53
1:A:416:LYS:HD2	1:A:417:ASN:OD1	2.09	0.53
1:A:200:GLU:HB2	1:A:203:THR:HG23	1.90	0.53
1:A:197:GLU:HG2	1:A:360:ILE:HD11	1.91	0.53
1:A:201:VAL:O	1:A:202:ASP:CB	2.57	0.53
1:A:52:ASN:HD22	1:A:55:GLU:CG	2.22	0.53
1:A:195:PHE:HZ	1:A:360:ILE:HG23	1.73	0.53
1:B:153:ILE:HG12	1:B:154:GLY:N	2.24	0.52
1:A:24:PRO:O	1:A:25:ASN:C	2.52	0.52
1:A:114:ILE:H	1:A:114:ILE:HD12	1.75	0.52
1:B:110:ILE:HG23	1:B:231:LEU:CD1	2.39	0.52
1:A:237:ASN:CG	1:A:239:ASN:ND2	2.68	0.52
1:A:22:LYS:HA	1:A:29:MET:CE	2.40	0.52
1:B:113:GLY:HA2	1:B:319:LYS:HE3	1.92	0.52
1:B:302:ILE:HD11	1:B:312:MET:HG3	1.92	0.51
1:A:303:ILE:HG22	1:A:304:GLY:N	2.26	0.51
1:A:161:GLN:HG3	3:A:604:HOH:O	2.11	0.51
1:B:197:GLU:OE2	1:B:360:ILE:HD11	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASN:ND2	1:A:206:LEU:N	2.58	0.51
1:B:51:THR:CG2	1:B:186:ARG:HH21	2.23	0.51
1:A:201:VAL:O	1:A:202:ASP:HB3	2.10	0.50
1:B:325:ASP:OD1	1:B:327:SER:HB3	2.11	0.50
1:A:360:ILE:HG22	1:A:403:GLN:CD	2.36	0.50
1:B:130:ASP:OD1	1:B:131:THR:HG23	2.12	0.50
1:B:117:TRP:CD2	1:B:312:MET:HE2	2.46	0.50
1:B:29:MET:O	1:B:29:MET:HG3	2.11	0.49
1:A:250:TYR:HB3	1:A:254:GLY:N	2.27	0.49
1:B:63:GLU:O	1:B:64:ALA:HB3	2.12	0.49
1:B:228:GLU:HG2	1:B:344:LEU:HD22	1.93	0.49
1:A:26:ALA:CB	1:A:29:MET:HG2	2.43	0.49
1:B:410:ARG:HH11	1:B:410:ARG:CB	2.19	0.48
1:B:392:LYS:C	1:B:394:ALA:H	2.22	0.48
1:A:59:ASN:ND2	1:A:59:ASN:N	2.62	0.48
1:B:6:GLN:HE21	1:B:6:GLN:HA	1.77	0.48
1:A:171:VAL:CG2	1:A:172:LEU:HD13	2.36	0.48
1:B:274:ASP:OD1	1:B:274:ASP:C	2.56	0.48
1:A:274:ASP:OD1	1:A:277:GLN:NE2	2.47	0.48
1:B:166:SER:OG	1:B:183:GLN:NE2	2.46	0.48
1:A:24:PRO:O	1:A:26:ALA:N	2.47	0.48
1:B:392:LYS:O	1:B:394:ALA:N	2.47	0.47
1:A:122:ILE:HG22	1:A:124:THR:HG22	1.96	0.47
1:B:367:ASN:HD21	1:B:370:LYS:NZ	2.11	0.47
1:B:196:GLU:H	1:B:370:LYS:NZ	2.11	0.47
1:B:204:ASN:HD21	1:B:206:LEU:HB2	1.78	0.47
1:A:200:GLU:HB2	1:A:203:THR:CG2	2.43	0.47
1:A:239:ASN:OD1	1:A:239:ASN:C	2.57	0.47
1:B:136:VAL:O	1:B:143:TYR:HA	2.15	0.47
1:B:279:ASN:O	1:B:283:LEU:HD23	2.14	0.47
1:B:325:ASP:O	1:B:327:SER:N	2.43	0.46
1:A:96:ARG:HA	1:A:385:ILE:HG23	1.97	0.46
1:B:24:PRO:O	1:B:26:ALA:N	2.48	0.46
1:B:136:VAL:HG12	1:B:137:ILE:H	1.81	0.46
1:B:225:ILE:O	1:B:228:GLU:OE2	2.32	0.46
1:A:381:GLU:CD	1:A:381:GLU:N	2.74	0.46
1:B:228:GLU:HG3	1:B:344:LEU:HD22	1.98	0.46
1:A:266:GLY:HA2	1:A:270:ALA:HB2	1.98	0.46
1:A:84:ASP:O	1:A:88:LYS:HD3	2.15	0.45
1:A:126:LEU:HD12	1:A:126:LEU:HA	1.76	0.45
1:A:26:ALA:HB1	1:A:29:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASP:OD1	1:B:171:VAL:HG23	2.17	0.45
1:B:13:VAL:HG11	1:B:20:TYR:CE1	2.52	0.44
1:B:203:THR:O	1:B:204:ASN:C	2.61	0.44
1:A:23:ILE:HG23	1:A:24:PRO:CD	2.46	0.44
1:B:363:LYS:HG3	3:B:580:HOH:O	2.16	0.44
1:A:221:ALA:O	1:A:225:ILE:HG13	2.17	0.44
1:A:228:GLU:OE2	1:A:348:TYR:HB2	2.18	0.44
1:B:107:LEU:O	1:B:111:VAL:HG23	2.17	0.44
1:A:125:GLU:OE2	1:A:303:ILE:HD11	2.17	0.44
1:A:305:THR:O	1:A:306:THR:OG1	2.32	0.44
1:A:305:THR:C	1:A:306:THR:OG1	2.61	0.44
1:A:180:GLY:HA2	1:A:230:ARG:O	2.18	0.43
1:A:369:ASP:C	1:A:370:LYS:HD2	2.43	0.43
1:B:13:VAL:O	1:B:13:VAL:HG23	2.17	0.43
1:B:130:ASP:OD1	1:B:131:THR:N	2.51	0.43
1:B:59:ASN:HA	1:B:60:PRO:HD3	1.85	0.43
1:B:70:SER:CA	1:B:160:ILE:HD11	2.49	0.43
1:B:101:ASP:OD1	1:B:101:ASP:N	2.49	0.43
1:B:245:ASN:ND2	1:B:245:ASN:C	2.76	0.43
1:B:314:ASN:O	1:B:318:GLU:HG3	2.19	0.43
1:B:360:ILE:HG22	1:B:403:GLN:OE1	2.19	0.43
1:A:197:GLU:CG	1:A:360:ILE:HD11	2.49	0.43
1:A:378:VAL:HB	1:A:379:PRO:HD3	2.00	0.43
1:B:269:ASP:O	1:B:272:PHE:HD2	2.01	0.43
1:B:317:LYS:HD2	1:B:330:PHE:HE1	1.84	0.43
1:A:128:VAL:HG22	1:A:129:ILE:N	2.34	0.42
1:B:114:ILE:HD12	1:B:315:VAL:HG13	2.01	0.42
1:A:52:ASN:HA	1:A:53:PRO:HD3	1.81	0.42
1:A:59:ASN:N	1:A:59:ASN:HD22	2.17	0.42
1:B:13:VAL:HG11	1:B:20:TYR:HD1	1.82	0.42
1:B:211:LYS:H	1:B:211:LYS:HG2	1.68	0.42
1:A:228:GLU:OE2	1:A:348:TYR:CD2	2.71	0.42
1:B:52:ASN:HA	1:B:53:PRO:HD3	1.90	0.42
1:B:368:PHE:O	1:B:370:LYS:NZ	2.51	0.42
1:A:84:ASP:OD1	1:A:88:LYS:HE2	2.19	0.42
1:A:396:LEU:HA	1:A:401:ASN:HB2	2.02	0.42
1:B:70:SER:HA	1:B:160:ILE:HD11	2.00	0.42
1:A:161:GLN:HA	1:A:161:GLN:HE21	1.85	0.42
1:B:143:TYR:CD2	1:B:143:TYR:N	2.85	0.42
1:A:143:TYR:CD1	1:A:143:TYR:N	2.87	0.42
1:A:204:ASN:HD21	1:A:206:LEU:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HG	1:A:199:LEU:O	2.19	0.41
1:A:161:GLN:HA	1:A:161:GLN:NE2	2.35	0.41
1:A:52:ASN:HD22	1:A:55:GLU:CB	2.33	0.41
1:A:365:PHE:CD1	1:A:365:PHE:C	2.98	0.41
1:B:232:TYR:O	1:B:234:ILE:HG23	2.20	0.41
1:B:269:ASP:OD2	1:B:364:THR:HA	2.21	0.41
1:B:416:LYS:O	1:B:417:ASN:HB2	2.19	0.41
1:A:225:ILE:HD13	1:A:349:THR:HA	2.02	0.41
1:B:387:ASP:HB3	1:B:390:ASN:O	2.20	0.41
1:B:22:LYS:HE3	1:B:137:ILE:HD11	2.02	0.41
1:B:410:ARG:HG2	3:B:627:HOH:O	2.20	0.41
1:A:208:GLY:HA3	1:A:404:ASN:ND2	2.36	0.41
1:B:225:ILE:HD13	1:B:349:THR:HA	2.02	0.41
1:B:286:TYR:CE1	1:B:334:LYS:HG2	2.56	0.41
1:A:1:MET:HB2	1:A:4:ASN:OD1	2.21	0.41
1:A:171:VAL:HG23	1:A:172:LEU:N	2.36	0.41
1:B:392:LYS:C	1:B:394:ALA:N	2.79	0.41
1:A:208:GLY:HA3	3:A:576:HOH:O	2.21	0.40
1:A:135:ASN:HD22	1:A:135:ASN:HA	1.74	0.40
1:B:398:THR:O	1:B:401:ASN:ND2	2.54	0.40
1:B:30:GLN:OE1	1:B:30:GLN:HA	2.20	0.40
1:B:69:VAL:HA	1:B:417:ASN:HD21	1.86	0.40
1:B:304:GLY:O	1:B:306:THR:N	2.41	0.40
1:B:180:GLY:HA3	1:B:231:LEU:O	2.22	0.40
1:B:367:ASN:ND2	1:B:370:LYS:NZ	2.69	0.40
1:B:381:GLU:H	1:B:381:GLU:CD	2.29	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%)	374 (92%)	19 (5%)	12 (3%)	3	2
1	B	403/425 (95%)	366 (91%)	26 (6%)	11 (3%)	4	3
All	All	808/850 (95%)	740 (92%)	45 (6%)	23 (3%)	4	2

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	MET
1	B	25	ASN
1	B	172	LEU
1	B	305	THR
1	B	392	LYS
1	A	25	ASN
1	A	202	ASP
1	A	208	GLY
1	A	209	ALA
1	A	306	THR
1	B	302	ILE
1	B	393	GLY
1	A	28	GLN
1	A	392	LYS
1	B	123	ASP
1	B	131	THR
1	A	73	ASP
1	A	210	GLY
1	A	394	ALA
1	B	51	THR
1	B	326	THR
1	B	171	VAL
1	A	61	PRO

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	367/380 (97%)	352 (96%)	15 (4%)	27	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	366/380 (96%)	352 (96%)	14 (4%)	29	44
All	All	733/760 (96%)	704 (96%)	29 (4%)	28	42

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	59	ASN
1	A	126	LEU
1	A	143	TYR
1	A	172	LEU
1	A	199	LEU
1	A	228	GLU
1	A	239	ASN
1	A	276	LEU
1	A	277	GLN
1	A	283	LEU
1	A	306	THR
1	A	366	LEU
1	A	414	ARG
1	A	416	LYS
1	B	1	MET
1	B	28	GLN
1	B	46	GLU
1	B	69	VAL
1	B	101	ASP
1	B	139	PRO
1	B	143	TYR
1	B	196	GLU
1	B	204	ASN
1	B	228	GLU
1	B	279	ASN
1	B	363	LYS
1	B	364	THR
1	B	410	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	8	ASN

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Mol	Chain	Res	Type
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	239	ASN
1	A	268	HIS
1	A	361	ASN
1	A	367	ASN
1	A	399	ASN
1	B	6	GLN
1	B	8	ASN
1	B	28	GLN
1	B	52	ASN
1	B	59	ASN
1	B	204	ASN
1	B	277	GLN
1	B	367	ASN
1	B	399	ASN
1	B	417	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	411/425 (96%)	0.41	44 (10%)	11 12	10, 26, 59, 74	0
1	B	409/425 (96%)	1.04	73 (17%)	4 4	18, 38, 68, 79	0
All	All	820/850 (96%)	0.72	117 (14%)	6 7	10, 32, 65, 79	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	THR	8.8
1	B	25	ASN	7.8
1	B	168	GLY	7.1
1	A	199	LEU	6.2
1	B	305	THR	5.7
1	B	304	GLY	5.7
1	A	208	GLY	5.5
1	B	126	LEU	5.3
1	A	25	ASN	5.2
1	A	64	ALA	5.2
1	A	62	PRO	5.0
1	A	248	ALA	5.0
1	B	417	ASN	4.9
1	B	62	PRO	4.8
1	A	61	PRO	4.7
1	A	209	ALA	4.6
1	A	207	LEU	4.5
1	B	143	TYR	4.4
1	B	139	PRO	4.3
1	A	398	THR	4.2
1	B	65	LYS	4.2
1	B	381	GLU	4.1
1	B	398	THR	4.0
1	B	130	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	138	GLN	4.0
1	A	397	SER	4.0
1	B	397	SER	3.9
1	B	137	ILE	3.9
1	A	26	ALA	3.9
1	B	198	SER	3.9
1	A	228	GLU	3.9
1	A	417	ASN	3.8
1	A	369	ASP	3.7
1	A	381	GLU	3.7
1	A	250	TYR	3.7
1	B	228	GLU	3.6
1	A	368	PHE	3.6
1	A	143	TYR	3.5
1	B	307	ALA	3.4
1	B	311	TYR	3.4
1	B	61	PRO	3.4
1	B	301	SER	3.4
1	A	60	PRO	3.4
1	A	249	TYR	3.4
1	B	393	GLY	3.3
1	A	254	GLY	3.2
1	B	60	PRO	3.2
1	B	303	ILE	3.2
1	B	140	ASP	3.1
1	B	199	LEU	3.1
1	B	122	ILE	3.1
1	A	27	GLY	3.1
1	B	306	THR	3.0
1	A	393	GLY	3.0
1	B	302	ILE	3.0
1	A	28	GLN	3.0
1	B	123	ASP	3.0
1	B	325	ASP	3.0
1	B	323	SER	3.0
1	B	142	SER	2.9
1	A	63	GLU	2.9
1	B	253	SER	2.9
1	B	28	GLN	2.9
1	B	180	GLY	2.8
1	B	64	ALA	2.8
1	A	210	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	251	GLU	2.8
1	A	57	ASP	2.7
1	A	206	LEU	2.7
1	B	332	VAL	2.7
1	B	335	LEU	2.7
1	B	312	MET	2.6
1	A	365	PHE	2.6
1	B	291	ASP	2.6
1	A	69	VAL	2.6
1	B	309	LEU	2.5
1	B	314	ASN	2.5
1	B	69	VAL	2.5
1	B	292	VAL	2.5
1	B	19	ALA	2.5
1	B	59	ASN	2.5
1	B	144	ARG	2.4
1	B	13	VAL	2.4
1	B	331	SER	2.4
1	A	366	LEU	2.4
1	B	330	PHE	2.4
1	B	201	VAL	2.4
1	A	255	LEU	2.4
1	A	168	GLY	2.3
1	B	23	ILE	2.3
1	B	51	THR	2.3
1	B	16	VAL	2.3
1	B	58	LEU	2.3
1	A	58	LEU	2.2
1	A	306	THR	2.2
1	B	63	GLU	2.2
1	B	121	THR	2.2
1	B	53	PRO	2.2
1	B	328	GLY	2.2
1	A	6	GLN	2.2
1	A	101	ASP	2.2
1	B	141	GLY	2.2
1	B	254	GLY	2.2
1	B	308	SER	2.2
1	B	18	ILE	2.2
1	B	327	SER	2.2
1	A	53	PRO	2.1
1	A	1	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	201	VAL	2.1
1	B	54	GLU	2.1
1	B	246	THR	2.1
1	B	4	ASN	2.1
1	B	247	ASN	2.1
1	B	3	VAL	2.1
1	B	6	GLN	2.0
1	A	59	ASN	2.0
1	B	104	ARG	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
2	ZN	B	451	1/1	0.98	0.03	31,31,31,31	0
2	ZN	A	452	1/1	0.99	0.03	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.