



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:47 AM GMT

PDB ID : 2ISE  
Title : Botulinum Neurotoxin A Light Chain WT Crystal Form A  
Authors : Brunger, A.T.; Stegmann, C.M.  
Deposited on : 2006-10-17  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

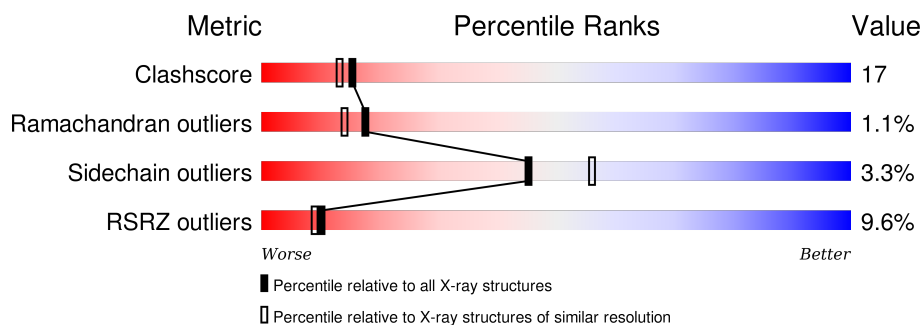
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	421	<p>9% 66% 32% .</p>
1	B	421	<p>10% 66% 32% .</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6915 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 Neurotoxin BoNT/A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	48	0	0
			3404	2194	557	645	8			
1	B	421	Total	C	N	O	S	48	0	0
			3404	2194	557	645	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	PRO	-	CLONING ARTIFACT	UNP Q7B8V4
A	422	GLY	-	CLONING ARTIFACT	UNP Q7B8V4
B	421	PRO	-	CLONING ARTIFACT	UNP Q7B8V4
B	422	GLY	-	CLONING ARTIFACT	UNP Q7B8V4

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

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

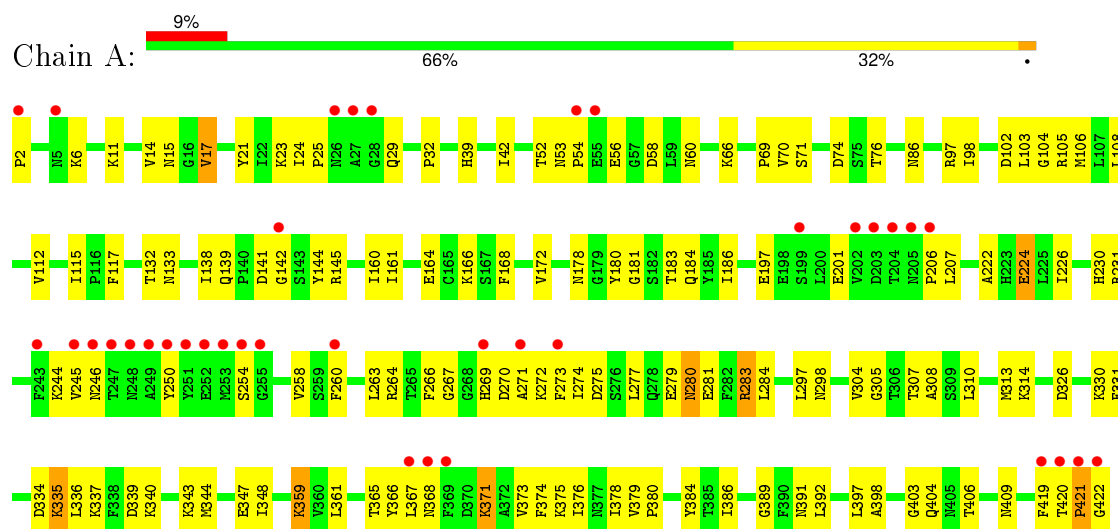
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	B	51	Total	O	0	0
			51	51		

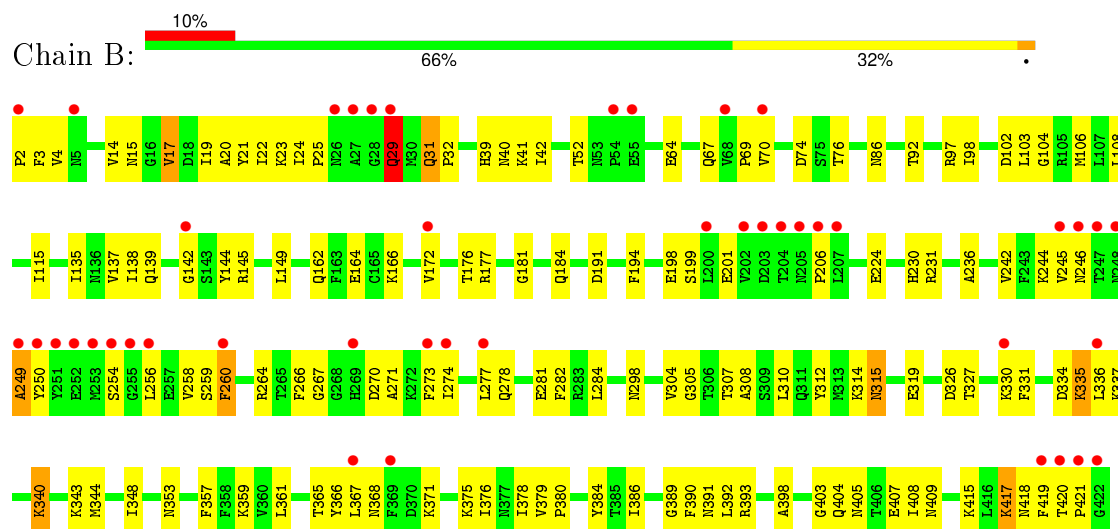
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Neurotoxin BoNT/A



#### • Molecule 1: Neurotoxin BoNT/A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.09Å 189.41Å 39.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.35 – 2.20 42.35 – 2.09	Depositor EDS
% Data completeness (in resolution range)	86.2 (42.35-2.20) 78.5 (42.35-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.242 , 0.299 0.241 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 30.0	EDS
Estimated twinning fraction	0.479 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 38888 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6915	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.39	0/3486	0.57	0/4719
1	B	0.39	0/3486	0.57	0/4719
All	All	0.39	0/6972	0.57	0/9438

There are no bond length outliers.

There are no bond angle outliers.

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	3404	0	3349	104	0
1	B	3404	0	3349	128	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	54	0	0	3	0
3	B	51	0	0	2	0
All	All	6915	0	6698	230	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 17.

All (230) 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:244:LYS:HD2	1:B:254:SER:H	1.22	1.03
1:A:298:ASN:HD21	1:A:331:PHE:H	1.08	1.01
1:A:2:PRO:HA	1:A:108:LEU:HD13	1.48	0.96
1:B:298:ASN:HD21	1:B:331:PHE:H	1.17	0.91
1:B:361:LEU:H	1:B:404:GLN:HE22	1.07	0.90
1:A:361:LEU:H	1:A:404:GLN:HE22	1.20	0.90
1:B:417:LYS:HZ2	1:B:418:ASN:H	1.15	0.90
1:B:334:ASP:HB3	1:B:337:LYS:HB2	1.55	0.88
1:B:31:GLN:NE2	1:B:31:GLN:H	1.72	0.86
1:A:2:PRO:HG3	1:A:108:LEU:HB3	1.57	0.84
1:B:2:PRO:HG3	1:B:108:LEU:HB3	1.60	0.84
1:A:310:LEU:O	1:A:314:LYS:HG3	1.79	0.83
1:B:2:PRO:HA	1:B:108:LEU:HD13	1.60	0.81
1:B:139:GLN:NE2	1:B:145:ARG:HE	1.78	0.80
1:A:2:PRO:HD2	1:A:39:HIS:CG	2.17	0.80
1:A:69:PRO:HG3	1:A:421:PRO:HB2	1.63	0.79
1:B:176:THR:HG21	1:B:231:ARG:NH1	2.00	0.76
1:B:2:PRO:HD2	1:B:39:HIS:CG	2.21	0.75
1:A:371:LYS:HE3	1:A:371:LYS:HA	1.68	0.75
1:B:74:ASP:OD1	1:B:76:THR:HG22	1.86	0.74
1:B:310:LEU:O	1:B:314:LYS:HG3	1.88	0.74
1:A:379:VAL:HB	1:A:380:PRO:HD3	1.70	0.74
1:B:420:THR:HB	1:B:421:PRO:HD3	1.68	0.73
1:B:361:LEU:H	1:B:404:GLN:NE2	1.85	0.72
1:A:69:PRO:HG2	1:A:422:GLY:H	1.54	0.72
1:B:139:GLN:NE2	1:B:145:ARG:HB3	2.04	0.72
1:A:298:ASN:ND2	1:A:331:PHE:H	1.87	0.71
1:B:277:LEU:O	1:B:281:GLU:HG3	1.90	0.70
1:A:244:LYS:HD2	1:A:254:SER:H	1.57	0.70
1:B:361:LEU:N	1:B:404:GLN:HE22	1.88	0.68
1:B:365:THR:HG22	1:B:367:LEU:HG	1.75	0.68
1:B:378:ILE:HG13	1:B:384:TYR:CG	2.30	0.67
1:A:74:ASP:OD1	1:A:76:THR:HG22	1.95	0.66
1:B:199:SER:OG	1:B:201:GLU:HG2	1.96	0.66
1:A:277:LEU:O	1:A:281:GLU:HG3	1.95	0.65
1:B:244:LYS:HD2	1:B:254:SER:N	2.04	0.65
1:A:365:THR:HG22	1:A:367:LEU:HG	1.78	0.65
1:B:97:ARG:HA	1:B:386:ILE:HG23	1.79	0.64
1:B:379:VAL:HB	1:B:380:PRO:HD3	1.80	0.64
1:A:97:ARG:HA	1:A:386:ILE:HG23	1.80	0.63
1:B:14:VAL:HG13	1:B:20:ALA:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ASP:O	1:B:375:LYS:HD2	2.01	0.61
1:B:417:LYS:HZ3	1:B:417:LYS:HA	1.67	0.60
1:A:258:VAL:HG21	1:A:367:LEU:CD2	2.31	0.60
1:A:378:ILE:HG13	1:A:384:TYR:CG	2.37	0.60
1:B:376:ILE:HD12	1:B:378:ILE:HD13	1.84	0.59
1:B:31:GLN:N	1:B:31:GLN:NE2	2.48	0.59
1:B:258:VAL:HG21	1:B:367:LEU:CD2	2.33	0.59
1:A:69:PRO:CG	1:A:421:PRO:HB2	2.33	0.59
1:A:23:LYS:HD2	1:A:144:TYR:OH	2.02	0.59
1:A:361:LEU:H	1:A:404:GLN:NE2	1.97	0.58
1:A:270:ASP:HA	1:A:273:PHE:CE2	2.38	0.58
1:B:24:ILE:HG23	1:B:25:PRO:HD2	1.85	0.58
1:B:86:ASN:ND2	1:B:379:VAL:HG21	2.17	0.58
1:B:139:GLN:HE22	1:B:145:ARG:HE	1.50	0.58
1:A:420:THR:HB	1:A:421:PRO:HD3	1.86	0.58
1:A:384:TYR:HA	1:A:389:GLY:O	2.03	0.58
1:A:230:HIS:CE1	1:A:264:ARG:HD3	2.38	0.58
1:B:384:TYR:HA	1:B:389:GLY:O	2.03	0.58
1:B:29:GLN:H	1:B:29:GLN:NE2	2.02	0.57
1:A:344:MET:SD	1:A:348:ILE:HD12	2.45	0.57
1:A:260:PHE:CZ	1:A:274:ILE:HD13	2.40	0.56
1:B:31:GLN:HE21	1:B:31:GLN:H	1.50	0.56
1:A:54:PRO:HA	3:A:541:HOH:O	2.04	0.56
1:B:415:LYS:NZ	1:B:418:ASN:HD21	2.04	0.56
1:B:378:ILE:HD11	1:B:390:PHE:CZ	2.40	0.56
1:B:31:GLN:N	1:B:31:GLN:HE21	2.04	0.56
1:A:52:THR:HG21	1:A:166:LYS:HE2	1.87	0.56
1:B:343:LYS:HG2	1:B:348:ILE:CD1	2.35	0.56
1:B:298:ASN:ND2	1:B:331:PHE:H	1.94	0.55
1:A:14:VAL:HG11	1:A:21:TYR:CE1	2.42	0.55
1:A:307:THR:HG22	1:A:308:ALA:N	2.20	0.55
1:A:53:ASN:HB3	1:A:56:GLU:HB2	1.89	0.55
1:A:2:PRO:HD3	1:A:42:ILE:HD12	1.88	0.55
1:B:326:ASP:OD2	1:B:330:LYS:HB3	2.06	0.55
1:A:275:ASP:OD2	1:A:277:LEU:HB2	2.08	0.55
1:A:102:ASP:O	1:A:106:MET:HG3	2.07	0.55
1:B:307:THR:HG22	1:B:308:ALA:N	2.22	0.54
1:A:373:VAL:HG13	1:A:419:PHE:CZ	2.42	0.54
1:A:24:ILE:HG23	1:A:25:PRO:HD2	1.88	0.54
1:B:172:VAL:HG22	1:B:172:VAL:O	2.06	0.54
1:A:142:GLY:O	1:B:32:PRO:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PHE:CG	1:A:366:TYR:HB2	2.43	0.54
1:A:69:PRO:CG	1:A:422:GLY:H	2.19	0.54
1:A:98:ILE:O	1:A:104:GLY:HA3	2.08	0.54
1:A:343:LYS:HG3	1:A:347:GLU:OE1	2.07	0.54
1:B:70:VAL:HA	1:B:419:PHE:CE1	2.43	0.53
1:B:98:ILE:O	1:B:104:GLY:HA3	2.08	0.53
1:B:415:LYS:HD3	1:B:418:ASN:OD1	2.09	0.53
1:B:417:LYS:NZ	1:B:417:LYS:HA	2.23	0.53
1:A:2:PRO:HD2	1:A:39:HIS:ND1	2.24	0.53
1:A:258:VAL:HG21	1:A:367:LEU:HD22	1.90	0.53
1:B:138:ILE:HG23	1:B:142:GLY:O	2.09	0.53
1:A:298:ASN:HD21	1:A:331:PHE:N	1.92	0.53
1:B:392:LEU:O	1:B:398:ALA:HB2	2.09	0.53
1:B:365:THR:CG2	1:B:367:LEU:HG	2.40	0.52
1:A:391:ASN:HD21	1:A:404:GLN:HE21	1.56	0.52
1:A:376:ILE:HD12	1:A:378:ILE:HD13	1.91	0.52
1:B:365:THR:HG22	1:B:367:LEU:H	1.74	0.52
1:A:308:ALA:HB3	1:A:313:MET:HE3	1.90	0.52
1:A:138:ILE:HG23	1:A:142:GLY:O	2.09	0.52
1:A:392:LEU:O	1:A:398:ALA:HB2	2.09	0.52
1:A:52:THR:CG2	1:A:166:LYS:HE2	2.39	0.52
1:B:184:GLN:OE1	1:B:231:ARG:HD3	2.09	0.52
1:A:260:PHE:CZ	1:A:274:ILE:HG21	2.45	0.52
1:A:267:GLY:HA2	1:A:271:ALA:HB2	1.92	0.52
1:B:266:PHE:CG	1:B:366:TYR:HB2	2.45	0.52
1:B:260:PHE:HZ	1:B:274:ILE:HG21	1.75	0.52
1:B:258:VAL:HG21	1:B:367:LEU:HD22	1.92	0.51
1:B:260:PHE:CZ	1:B:274:ILE:HG21	2.45	0.51
1:B:273:PHE:C	1:B:274:ILE:HD12	2.29	0.51
1:B:417:LYS:NZ	1:B:418:ASN:H	1.98	0.51
1:B:267:GLY:HA2	1:B:271:ALA:HB2	1.93	0.51
1:B:2:PRO:HD3	1:B:42:ILE:HD12	1.92	0.51
1:A:326:ASP:OD2	1:A:330:LYS:HB3	2.10	0.50
1:B:135:ILE:HD13	1:B:149:LEU:HD13	1.93	0.50
1:A:115:ILE:H	1:A:115:ILE:HD12	1.77	0.50
1:B:335:LYS:HD3	1:B:335:LYS:N	2.26	0.50
1:B:348:ILE:N	1:B:348:ILE:HD12	2.26	0.50
1:A:186:ILE:HG23	1:A:224:GLU:HG3	1.94	0.50
1:B:340:LYS:NZ	1:B:340:LYS:HB2	2.27	0.50
1:B:70:VAL:HA	1:B:419:PHE:CD1	2.47	0.50
1:B:2:PRO:HD2	1:B:39:HIS:ND1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASN:OD1	1:A:379:VAL:HG21	2.13	0.49
1:B:191:ASP:HB3	1:B:375:LYS:HE3	1.94	0.49
1:B:40:ASN:ND2	1:B:41:LYS:HD3	2.27	0.49
1:A:184:GLN:OE1	1:A:231:ARG:HD3	2.12	0.49
1:B:403:GLY:HA2	1:B:409:ASN:HD22	1.77	0.49
1:B:371:LYS:HG3	3:B:509:HOH:O	2.11	0.49
1:B:417:LYS:HZ2	1:B:418:ASN:N	1.97	0.48
1:A:263:LEU:HD11	1:A:270:ASP:HB3	1.95	0.48
1:A:222:ALA:O	1:A:226:ILE:HG13	2.13	0.48
1:A:260:PHE:CE1	1:A:274:ILE:HD13	2.48	0.48
1:B:344:MET:HA	1:B:348:ILE:HD13	1.95	0.48
1:A:139:GLN:NE2	1:A:145:ARG:HB3	2.29	0.48
1:B:139:GLN:HE22	1:B:145:ARG:NE	2.10	0.48
1:B:246:ASN:HD22	1:B:249:ALA:N	2.12	0.48
1:B:315:ASN:O	1:B:319:GLU:HG3	2.13	0.48
1:A:23:LYS:HD2	1:A:144:TYR:CZ	2.49	0.48
1:A:201:GLU:OE1	1:A:206:PRO:HA	2.14	0.48
1:B:256:LEU:HD12	1:B:256:LEU:H	1.77	0.48
1:A:133:ASN:ND2	1:A:183:THR:H	2.12	0.48
1:A:172:VAL:O	1:A:172:VAL:HG22	2.14	0.47
1:B:335:LYS:HD3	1:B:335:LYS:H	1.79	0.47
1:B:312:TYR:O	1:B:315:ASN:OD1	2.31	0.47
1:B:201:GLU:OE1	1:B:206:PRO:HA	2.13	0.47
1:A:365:THR:HG22	1:A:367:LEU:H	1.77	0.47
1:A:335:LYS:HD3	1:A:335:LYS:H	1.78	0.47
1:B:23:LYS:HE3	1:B:144:TYR:OH	2.15	0.47
1:A:74:ASP:CG	1:A:76:THR:HG22	2.35	0.47
1:B:14:VAL:HG13	1:B:19:ILE:O	2.14	0.47
1:A:207:LEU:N	1:A:207:LEU:HD12	2.30	0.47
1:A:403:GLY:HA2	1:A:409:ASN:HD22	1.80	0.47
1:B:194:PHE:CD1	1:B:194:PHE:N	2.83	0.47
1:A:365:THR:CG2	1:A:367:LEU:HG	2.43	0.47
1:B:343:LYS:HG2	1:B:348:ILE:HD11	1.95	0.47
1:A:334:ASP:HB3	1:A:337:LYS:HB2	1.97	0.47
1:A:70:VAL:HA	1:A:419:PHE:CE1	2.50	0.46
1:B:74:ASP:CG	1:B:76:THR:HG22	2.35	0.46
1:B:102:ASP:O	1:B:106:MET:HG3	2.15	0.46
1:A:335:LYS:HD3	1:A:335:LYS:N	2.31	0.46
1:B:52:THR:CG2	1:B:166:LYS:HZ2	2.29	0.46
1:B:353:ASN:O	1:B:357:PHE:HD1	1.99	0.46
1:B:260:PHE:CE2	1:B:282:PHE:HE2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:HA	1:A:419:PHE:CD1	2.51	0.46
1:B:14:VAL:HG21	1:B:21:TYR:CE1	2.51	0.45
1:A:103:LEU:HD11	1:A:348:ILE:HG22	1.99	0.45
1:B:15:ASN:O	1:B:17:VAL:HG23	2.16	0.45
1:B:103:LEU:HD11	1:B:348:ILE:HG22	1.99	0.45
1:B:198:GLU:HG2	1:B:361:LEU:HD21	1.97	0.45
1:B:64:GLU:O	1:B:67:GLN:HB2	2.17	0.45
1:A:280:ASN:ND2	1:A:283:ARG:HD2	2.31	0.45
1:B:15:ASN:C	1:B:17:VAL:H	2.19	0.45
1:A:132:THR:HB	1:A:168:PHE:HB2	1.99	0.45
1:A:164:GLU:OE2	1:A:166:LYS:HD2	2.16	0.45
1:A:25:PRO:HB3	3:A:512:HOH:O	2.17	0.44
1:B:298:ASN:HD21	1:B:331:PHE:N	2.00	0.44
1:B:391:ASN:HD21	1:B:404:GLN:HE21	1.64	0.44
1:B:270:ASP:HA	1:B:273:PHE:CE2	2.52	0.44
1:A:71:SER:HA	1:A:161:ILE:HD11	1.99	0.44
1:B:22:ILE:HG22	1:B:137:VAL:HG22	1.99	0.44
1:A:375:LYS:NZ	3:A:536:HOH:O	2.50	0.44
1:B:23:LYS:CE	1:B:32:PRO:HD3	2.47	0.44
1:B:139:GLN:NE2	1:B:145:ARG:NE	2.56	0.44
1:B:304:VAL:HG12	1:B:305:GLY:N	2.32	0.44
1:B:230:HIS:CE1	1:B:264:ARG:HD3	2.52	0.44
1:B:97:ARG:HH11	1:B:97:ARG:HG3	1.82	0.44
1:B:260:PHE:CZ	1:B:274:ILE:HG12	2.52	0.44
1:A:336:LEU:O	1:A:340:LYS:HG2	2.18	0.44
1:B:177:ARG:HG2	1:B:236:ALA:O	2.18	0.44
1:A:15:ASN:C	1:A:17:VAL:H	2.21	0.43
1:B:181:GLY:HA2	1:B:231:ARG:O	2.19	0.43
1:A:58:ASP:CG	1:A:60:ASN:HD22	2.22	0.43
1:B:245:VAL:O	1:B:246:ASN:HB2	2.19	0.43
1:B:115:ILE:HD12	1:B:115:ILE:H	1.84	0.43
1:A:283:ARG:NE	1:A:339:ASP:OD1	2.51	0.42
1:B:242:VAL:HA	1:B:259:SER:HA	2.01	0.42
1:B:417:LYS:HD3	1:B:418:ASN:N	2.34	0.42
1:B:69:PRO:HG2	1:B:421:PRO:HB2	2.01	0.42
1:A:117:PHE:HE1	1:A:297:LEU:HD21	1.85	0.42
1:A:269:HIS:O	1:A:272:LYS:HB2	2.19	0.42
1:A:361:LEU:N	1:A:404:GLN:HE22	2.00	0.42
1:B:327:THR:HG23	3:B:537:HOH:O	2.20	0.42
1:B:162:GLN:NE2	1:B:164:GLU:OE2	2.52	0.42
1:A:181:GLY:HA2	1:A:231:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:PRO:HD3	1:B:42:ILE:CD1	2.50	0.42
1:A:374:PHE:CE1	1:A:406:THR:HG21	2.55	0.42
1:A:2:PRO:HD3	1:A:42:ILE:CD1	2.49	0.41
1:A:105:ARG:NH1	1:A:105:ARG:HB2	2.34	0.41
1:B:246:ASN:HD22	1:B:249:ALA:CA	2.33	0.41
1:A:245:VAL:O	1:A:246:ASN:HB2	2.20	0.41
1:A:74:ASP:HB3	1:A:160:ILE:CD1	2.50	0.41
1:B:274:ILE:N	1:B:274:ILE:HD12	2.35	0.41
1:A:108:LEU:O	1:A:112:VAL:HG23	2.21	0.41
1:B:69:PRO:O	1:B:419:PHE:CD1	2.73	0.41
1:B:405:ASN:OD1	1:B:408:ILE:HG13	2.20	0.41
1:B:393:ARG:HA	1:B:398:ALA:HB2	2.02	0.41
1:A:197:GLU:OE2	1:A:371:LYS:HD2	2.20	0.41
1:A:24:ILE:CG2	1:A:25:PRO:HD2	2.50	0.41
1:A:32:PRO:HG2	1:B:142:GLY:O	2.21	0.41
1:B:278:GLN:HA	1:B:281:GLU:OE2	2.21	0.41
1:B:371:LYS:HE2	1:B:371:LYS:HA	2.03	0.41
1:A:304:VAL:HG12	1:A:305:GLY:N	2.34	0.41
1:B:336:LEU:HD13	1:B:336:LEU:C	2.41	0.41
1:A:376:ILE:HD12	1:A:378:ILE:CD1	2.51	0.40
1:A:359:LYS:HE3	1:A:359:LYS:HB2	1.95	0.40
1:B:139:GLN:CD	1:B:145:ARG:HE	2.21	0.40
1:A:178:ASN:OD1	1:A:180:TYR:HB2	2.20	0.40
1:B:4:VAL:HG21	1:B:92:THR:HG23	2.03	0.40
1:B:3:PHE:O	1:B:39:HIS:HD2	2.05	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	419/421 (100%)	386 (92%)	29 (7%)	4 (1%)	19 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	419/421 (100%)	385 (92%)	29 (7%)	5 (1%)	16	12
All	All	838/842 (100%)	771 (92%)	58 (7%)	9 (1%)	17	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	421	PRO
1	B	17	VAL
1	A	250	TYR
1	B	29	GLN
1	B	249	ALA
1	B	250	TYR
1	A	29	GLN
1	B	368	ASN

### 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	376/376 (100%)	362 (96%)	14 (4%)	41	50
1	B	376/376 (100%)	365 (97%)	11 (3%)	50	62
All	All	752/752 (100%)	727 (97%)	25 (3%)	45	56

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	11	LYS
1	A	66	LYS
1	A	141	ASP
1	A	224	GLU
1	A	279	GLU
1	A	280	ASN

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Mol	Chain	Res	Type
1	A	283	ARG
1	A	284	LEU
1	A	335	LYS
1	A	359	LYS
1	A	368	ASN
1	A	371	LYS
1	A	397	LEU
1	B	29	GLN
1	B	31	GLN
1	B	224	GLU
1	B	260	PHE
1	B	284	LEU
1	B	315	ASN
1	B	335	LYS
1	B	340	LYS
1	B	359	LYS
1	B	407	GLU
1	B	417	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	40	ASN
1	A	60	ASN
1	A	67	GLN
1	A	133	ASN
1	A	280	ASN
1	A	298	ASN
1	A	368	ASN
1	A	404	GLN
1	A	418	ASN
1	B	7	GLN
1	B	29	GLN
1	B	31	GLN
1	B	40	ASN
1	B	60	ASN
1	B	82	ASN
1	B	86	ASN
1	B	133	ASN
1	B	139	GLN
1	B	162	GLN

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Mol	Chain	Res	Type
1	B	174	ASN
1	B	246	ASN
1	B	278	GLN
1	B	288	ASN
1	B	298	ASN
1	B	315	ASN
1	B	404	GLN
1	B	418	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 carbohydrates 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 ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	421/421 (100%)	0.47	37 (8%)	12 11	20, 42, 89, 102	12 (2%)
1	B	421/421 (100%)	0.58	44 (10%)	8 7	20, 42, 89, 102	12 (2%)
All	All	842/842 (100%)	0.53	81 (9%)	10 9	20, 42, 89, 102	24 (2%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	TYR	24.6
1	B	251	TYR	21.6
1	B	202	VAL	15.8
1	B	204	THR	12.8
1	A	202	VAL	11.8
1	B	249	ALA	11.3
1	A	252	GLU	10.6
1	B	250	TYR	10.5
1	B	421	PRO	10.3
1	B	422	GLY	9.9
1	B	255	GLY	9.1
1	B	253	MET	8.8
1	B	203	ASP	7.9
1	A	205	ASN	7.7
1	A	253	MET	7.7
1	A	255	GLY	7.2
1	A	206	PRO	6.8
1	A	421	PRO	6.7
1	A	248	ASN	6.7
1	A	367	LEU	6.1
1	A	250	TYR	6.0
1	B	252	GLU	6.0
1	B	254	SER	5.9
1	B	248	ASN	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	204	THR	5.8
1	A	203	ASP	5.8
1	B	205	ASN	5.7
1	B	27	ALA	5.6
1	A	419	PHE	5.5
1	A	249	ALA	5.5
1	B	419	PHE	5.3
1	A	2	PRO	5.0
1	B	256	LEU	4.7
1	A	26	ASN	4.6
1	A	254	SER	4.5
1	A	422	GLY	4.3
1	A	420	THR	4.3
1	B	260	PHE	4.2
1	B	369	PHE	3.9
1	B	269	HIS	3.8
1	A	27	ALA	3.7
1	B	2	PRO	3.7
1	A	245	VAL	3.6
1	B	420	THR	3.3
1	A	369	PHE	3.3
1	B	68	VAL	3.3
1	B	247	THR	3.3
1	A	28	GLY	3.3
1	B	206	PRO	3.2
1	B	200	LEU	3.2
1	B	245	VAL	3.2
1	B	29	GLN	3.1
1	A	269	HIS	3.1
1	B	246	ASN	3.1
1	A	199	SER	3.1
1	B	5	ASN	3.1
1	B	28	GLY	3.1
1	B	207	LEU	2.9
1	B	277	LEU	2.9
1	A	260	PHE	2.8
1	A	273	PHE	2.8
1	A	5	ASN	2.7
1	A	55	GLU	2.6
1	B	55	GLU	2.6
1	A	368	ASN	2.6
1	B	70	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	271	ALA	2.5
1	B	367	LEU	2.5
1	B	54	PRO	2.5
1	B	172	VAL	2.5
1	B	142	GLY	2.5
1	A	243	PHE	2.4
1	B	26	ASN	2.3
1	A	247	THR	2.3
1	A	142	GLY	2.2
1	A	246	ASN	2.2
1	B	274	ILE	2.1
1	B	273	PHE	2.1
1	B	336	LEU	2.1
1	A	54	PRO	2.1
1	B	330	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	B	501	1/1	1.00	0.09	-1.02	37,37,37,37	0
2	ZN	A	500	1/1	0.99	0.07	-1.91	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.