



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:58 PM GMT

PDB ID : 2A97  
Title : Crystal structure of catalytic domain of Clostridium botulinum neurotoxin serotype F  
Authors : Agarwal, R.; Binz, T.; Swaminathan, S.  
Deposited on : 2005-07-11  
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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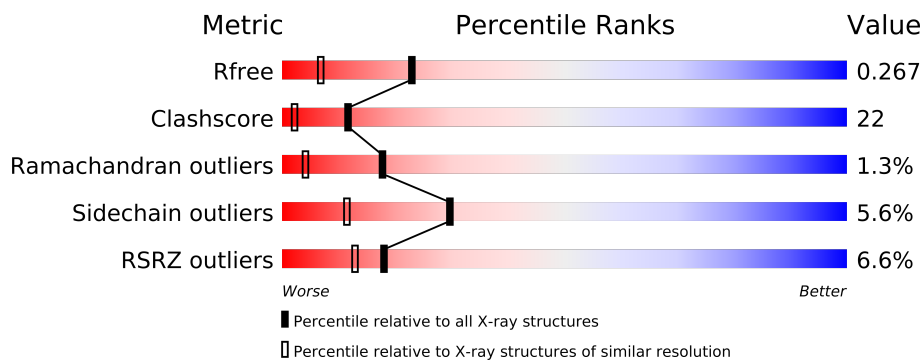
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
$R_{free}$	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	439	
1	B	439	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6586 atoms, of which 0 are hydrogen and 0 are deuterium.

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 F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3168	2038	505	618	7			
1	B	392	Total	C	N	O	S	0	0	0
			3168	2038	505	618	7			

- 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 CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cd	0	0
			2	2		
3	A	5	Total	Cd	0	0
			5	5		

- Molecule 4 is water.

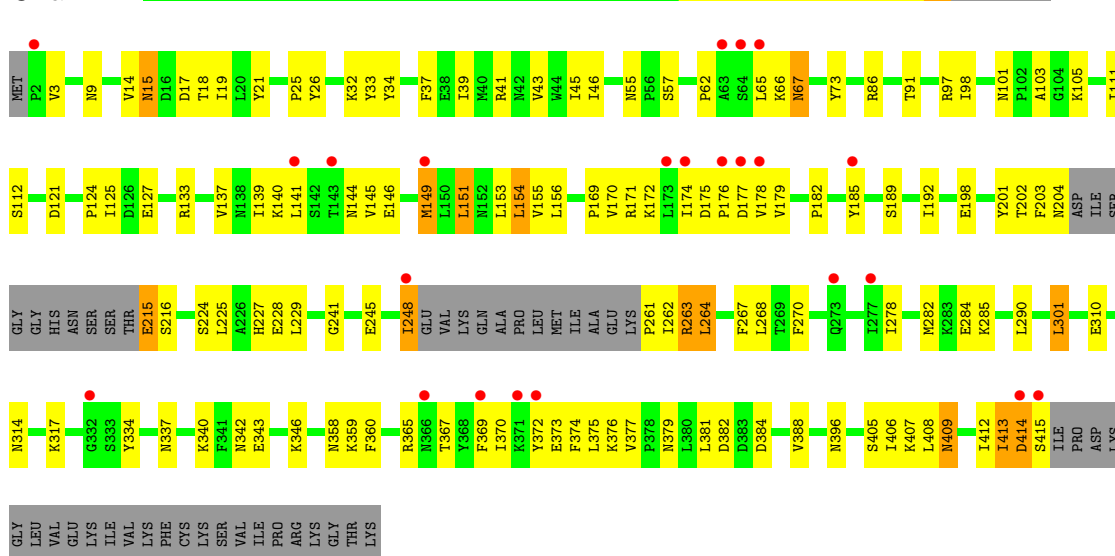
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	132	Total	O	0	0
			132	132		

### 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.

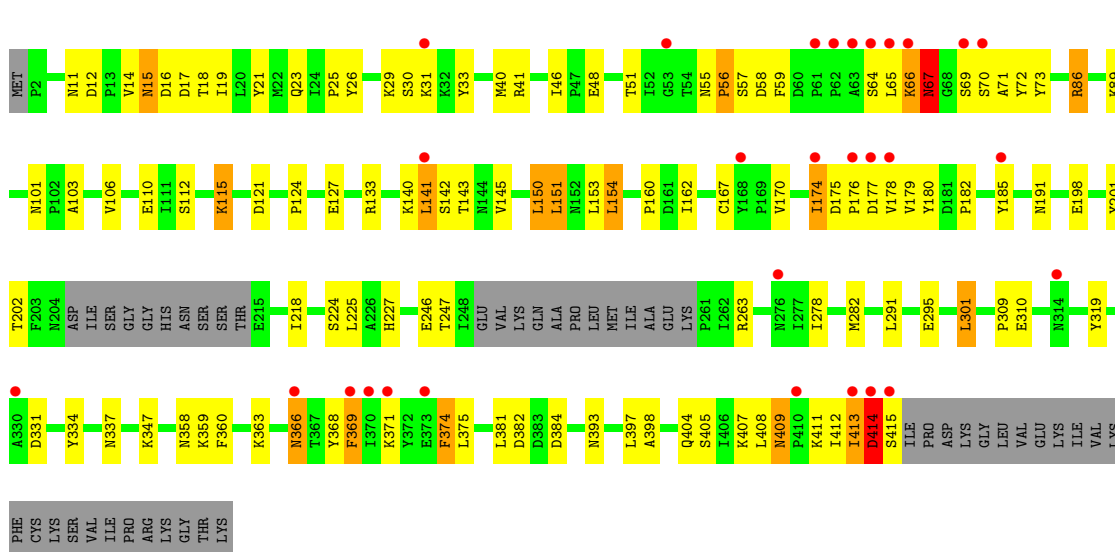
#### • Molecule 1: Botulinum neurotoxin type F

Chain A:



#### • Molecule 1: Botulinum neurotoxin type F

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.40Å 53.24Å 113.87Å 90.00° 119.17° 90.00°	Depositor
Resolution (Å)	26.05 – 1.80 26.05 – 1.80	Depositor EDS
% Data completeness (in resolution range)	76.6 (26.05-1.80) 76.8 (26.05-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.241 , 0.269 0.240 , 0.267	Depositor DCC
$R_{free}$ test set	1974 reflections (3.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 40.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 69805 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CD

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	0.34	0/3245	0.62	0/4407
1	B	0.36	0/3245	0.61	0/4407
All	All	0.35	0/6490	0.61	0/8814

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3168	0	3090	155	0
1	B	3168	0	3090	124	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	2	0	0	0	0
4	A	109	0	0	14	0
4	B	132	0	0	13	0
All	All	6586	0	6180	274	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (274) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:86:ARG:HH11	1:B:86:ARG:HB2	1.04	1.11
1:A:174:ILE:HG22	1:A:176:PRO:HD2	1.30	1.09
1:A:365:ARG:HD3	1:A:370:ILE:HD13	1.44	0.97
1:B:363:LYS:H	1:B:404:GLN:HE22	1.04	0.96
1:A:67:ASN:HD21	1:A:73:TYR:H	1.05	0.96
1:A:407:LYS:HG3	1:A:408:LEU:HD22	1.50	0.91
1:B:86:ARG:HB2	1:B:86:ARG:NH1	1.84	0.91
1:B:103:ALA:HB2	1:B:359:LYS:HD3	1.51	0.91
1:B:174:ILE:HG23	1:B:176:PRO:HD2	1.50	0.91
1:A:365:ARG:HD3	1:A:370:ILE:CD1	2.05	0.86
1:B:67:ASN:HD21	1:B:73:TYR:H	1.17	0.86
1:A:370:ILE:HD12	1:A:372:TYR:CD1	2.12	0.85
1:B:141:LEU:HD13	1:B:142:SER:H	1.41	0.84
1:B:178:VAL:HG22	1:B:179:VAL:H	1.43	0.83
1:A:375:LEU:HD21	1:A:415:SER:H	1.44	0.81
1:A:285:LYS:HE2	4:A:5580:HOH:O	1.79	0.81
1:A:202:THR:O	1:A:372:TYR:HB3	1.82	0.79
1:A:373:GLU:HG2	1:A:374:PHE:H	1.46	0.79
1:B:363:LYS:H	1:B:404:GLN:NE2	1.84	0.76
1:A:365:ARG:HD2	1:A:367:THR:O	1.84	0.76
1:B:301:LEU:HD12	1:B:334:TYR:CE1	2.21	0.75
1:A:412:ILE:HG13	4:A:5571:HOH:O	1.87	0.74
1:A:174:ILE:HG22	1:A:176:PRO:CD	2.16	0.73
1:B:366:ASN:HD22	1:B:366:ASN:N	1.87	0.73
1:B:202:THR:HG22	1:B:218:ILE:HG22	1.70	0.72
1:A:41:ARG:HG3	1:A:112:SER:OG	1.89	0.72
1:B:174:ILE:HG23	1:B:176:PRO:CD	2.19	0.72
1:B:409:ASN:HD21	1:B:411:LYS:HB2	1.54	0.72
1:B:67:ASN:ND2	1:B:73:TYR:H	1.88	0.71
1:B:309:PRO:HG2	1:B:310:GLU:OE2	1.91	0.71
1:B:41:ARG:HG2	4:B:5585:HOH:O	1.88	0.71
1:A:216:SER:HB3	1:A:406:ILE:HD12	1.73	0.71
1:B:178:VAL:HG22	1:B:179:VAL:N	2.05	0.70
1:B:368:TYR:HB3	4:B:5599:HOH:O	1.91	0.70
1:A:15:ASN:ND2	1:A:17:ASP:H	1.90	0.70
1:A:111:ILE:HD11	1:A:229:LEU:HB3	1.74	0.69
1:A:375:LEU:CD2	1:A:415:SER:H	2.05	0.69
1:A:370:ILE:HD12	1:A:372:TYR:HD1	1.57	0.69
1:B:150:LEU:O	1:B:150:LEU:HD12	1.93	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:270:PHE:HZ	1:A:365:ARG:HG3	1.57	0.68
1:B:363:LYS:N	1:B:404:GLN:HE22	1.86	0.68
1:A:15:ASN:HD22	1:A:17:ASP:H	1.40	0.68
1:B:141:LEU:HD13	1:B:142:SER:N	2.08	0.67
1:B:15:ASN:HD22	1:B:17:ASP:H	1.41	0.67
1:B:86:ARG:HH11	1:B:86:ARG:CB	1.95	0.67
1:B:15:ASN:ND2	1:B:17:ASP:H	1.92	0.67
1:B:15:ASN:HD21	1:B:18:THR:H	1.43	0.66
1:A:174:ILE:HD12	1:A:178:VAL:HG13	1.77	0.66
1:A:171:ARG:HB2	1:A:171:ARG:HH11	1.60	0.65
1:A:124:PRO:HB2	1:A:127:GLU:HG2	1.79	0.65
1:A:204:ASN:ND2	1:A:372:TYR:HE2	1.96	0.64
1:B:70:SER:O	1:B:71:ALA:HB3	1.98	0.64
1:B:153:LEU:HD23	1:B:154:LEU:N	2.13	0.63
1:B:278:ILE:N	1:B:278:ILE:HD12	2.12	0.63
1:A:171:ARG:HB2	1:A:171:ARG:NH1	2.13	0.63
1:A:43:VAL:HG13	1:A:153:LEU:HD22	1.79	0.63
1:A:365:ARG:CD	1:A:370:ILE:HD13	2.22	0.63
1:B:371:LYS:HE2	1:B:371:LYS:HA	1.81	0.63
1:A:384:ASP:HB2	1:B:381:LEU:HD13	1.81	0.63
1:A:301:LEU:HD21	1:A:317:LYS:HG2	1.82	0.62
1:A:406:ILE:HA	1:A:414:ASP:OD1	1.98	0.62
1:B:15:ASN:HD21	1:B:19:ILE:H	1.47	0.62
1:A:176:PRO:HG2	1:A:178:VAL:HG12	1.81	0.61
1:B:393:ASN:HD21	1:B:404:GLN:HE21	1.49	0.61
1:B:65:LEU:HD13	1:B:67:ASN:N	2.16	0.61
1:A:15:ASN:HD21	1:A:18:THR:H	1.49	0.60
1:B:15:ASN:C	1:B:15:ASN:HD22	2.04	0.60
1:A:370:ILE:HD12	1:A:372:TYR:CE1	2.35	0.60
1:A:39:ILE:HD11	1:A:45:ILE:HB	1.83	0.60
1:A:86:ARG:NH2	1:A:379:ASN:HD21	1.99	0.60
1:B:412:ILE:O	1:B:413:ILE:HB	2.01	0.60
1:B:67:ASN:HD21	1:B:73:TYR:N	1.95	0.60
1:B:366:ASN:ND2	1:B:366:ASN:N	2.49	0.59
1:A:140:LYS:HG2	4:A:5589:HOH:O	2.01	0.59
1:B:66:LYS:HB3	1:B:66:LYS:NZ	2.17	0.59
1:A:178:VAL:HG22	1:A:179:VAL:N	2.18	0.59
1:A:203:PHE:HA	1:A:372:TYR:CD2	2.37	0.59
1:A:407:LYS:HG2	4:A:5616:HOH:O	2.02	0.59
1:A:178:VAL:HG22	1:A:179:VAL:H	1.68	0.59
1:B:246:GLU:HG2	1:B:282:MET:SD	2.42	0.59
1:A:141:LEU:CD1	1:A:145:VAL:HB	2.32	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:103:ALA:HB2	1:A:359:LYS:HD3	1.84	0.59
1:B:141:LEU:HB2	1:B:145:VAL:HB	1.83	0.58
1:A:373:GLU:CG	1:A:374:PHE:H	2.17	0.58
1:A:409:ASN:HD22	1:A:409:ASN:C	2.06	0.58
1:A:406:ILE:HG23	1:A:414:ASP:CG	2.24	0.58
1:A:15:ASN:C	1:A:15:ASN:HD22	2.07	0.58
1:A:55:ASN:HD21	1:A:57:SER:HB3	1.67	0.57
1:A:270:PHE:CZ	1:A:365:ARG:HG3	2.39	0.57
1:A:67:ASN:HD21	1:A:73:TYR:N	1.89	0.57
1:A:406:ILE:HG23	1:A:414:ASP:OD1	2.04	0.57
1:B:413:ILE:HG22	1:B:414:ASP:N	2.20	0.57
1:A:241:GLY:O	1:A:245:GLU:HG3	2.05	0.57
1:A:413:ILE:HG23	1:A:413:ILE:O	2.05	0.57
1:A:370:ILE:HB	1:A:372:TYR:CE1	2.40	0.56
1:A:174:ILE:CG2	1:A:176:PRO:HD2	2.19	0.56
1:A:62:PRO:HG2	1:A:65:LEU:HB3	1.87	0.56
1:A:373:GLU:HG2	1:A:374:PHE:N	2.18	0.56
1:A:154:LEU:HD23	1:A:155:VAL:N	2.20	0.56
1:B:167:CYS:SG	1:B:191:ASN:OD1	2.58	0.56
1:B:86:ARG:HD3	4:B:5625:HOH:O	2.06	0.56
1:A:261:PRO:C	1:A:262:ILE:HD12	2.27	0.55
1:B:15:ASN:HD21	1:B:18:THR:N	2.04	0.55
1:A:125:ILE:N	1:A:125:ILE:HD12	2.22	0.55
1:A:101:ASN:HB3	1:A:360:PHE:CZ	2.42	0.55
1:A:175:ASP:N	1:A:176:PRO:HD2	2.22	0.55
1:A:182:PRO:HG2	1:A:189:SER:HB3	1.88	0.55
1:B:150:LEU:C	1:B:150:LEU:HD12	2.27	0.54
1:A:141:LEU:HD12	1:A:145:VAL:HB	1.89	0.54
1:A:98:ILE:CD1	1:A:225:LEU:HD12	2.37	0.54
1:B:174:ILE:CG2	1:B:176:PRO:HG2	2.37	0.54
1:A:133:ARG:HG2	1:A:170:VAL:HG11	1.90	0.54
1:A:375:LEU:HD21	1:A:415:SER:N	2.21	0.54
1:B:103:ALA:CB	1:B:359:LYS:HD3	2.31	0.54
1:A:140:LYS:HE2	1:A:146:GLU:HG2	1.89	0.53
1:B:393:ASN:HB3	1:B:398:ALA:HA	1.90	0.53
1:A:202:THR:O	1:A:372:TYR:CB	2.55	0.53
1:A:268:LEU:HD21	1:A:278:ILE:HD13	1.91	0.53
1:A:15:ASN:HD21	1:A:19:ILE:H	1.57	0.53
1:B:178:VAL:CG2	1:B:179:VAL:H	2.18	0.53
1:B:25:PRO:O	1:B:26:TYR:HB2	2.08	0.52
1:A:414:ASP:HA	4:A:5556:HOH:O	2.08	0.52
1:A:225:LEU:C	1:A:225:LEU:HD13	2.28	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:55:ASN:ND2	1:A:57:SER:HB3	2.25	0.52
1:A:301:LEU:HD22	1:A:334:TYR:CE1	2.44	0.52
1:A:263:ARG:HH11	1:A:263:ARG:HG2	1.74	0.51
1:A:154:LEU:HD23	1:A:154:LEU:C	2.31	0.51
1:A:202:THR:CG2	1:A:406:ILE:HD11	2.40	0.51
1:A:154:LEU:HD22	1:A:156:LEU:HG	1.91	0.51
1:A:15:ASN:HD21	1:A:18:THR:N	2.08	0.51
1:A:262:ILE:N	1:A:262:ILE:HD12	2.26	0.51
1:B:16:ASP:OD1	1:B:141:LEU:HD22	2.10	0.51
1:B:177:ASP:HB3	4:B:5609:HOH:O	2.09	0.51
1:B:374:PHE:N	4:B:5535:HOH:O	2.44	0.51
1:A:139:ILE:HD13	1:A:149:MET:HG3	1.93	0.51
1:A:176:PRO:O	1:A:177:ASP:HB2	2.11	0.51
1:B:375:LEU:HD21	1:B:415:SER:HA	1.93	0.51
1:B:110:GLU:OE2	1:B:347:LYS:HD2	2.11	0.51
1:A:376:LYS:HD3	1:A:377:VAL:N	2.26	0.51
1:A:111:ILE:CD1	1:A:229:LEU:HB3	2.39	0.50
1:B:67:ASN:ND2	1:B:72:TYR:HA	2.26	0.50
1:B:160:PRO:HG2	4:B:5594:HOH:O	2.11	0.50
1:B:405:SER:O	1:B:408:LEU:O	2.28	0.50
1:A:248:ILE:HG23	1:A:267:PHE:HE1	1.76	0.50
1:A:263:ARG:CG	1:A:263:ARG:HH11	2.24	0.50
1:B:151:LEU:N	1:B:151:LEU:HD13	2.26	0.50
1:B:247:THR:HG22	1:B:263:ARG:HA	1.92	0.50
1:B:15:ASN:ND2	1:B:19:ILE:H	2.09	0.50
1:A:62:PRO:HG2	1:A:65:LEU:CB	2.42	0.50
1:A:86:ARG:HH21	1:A:379:ASN:HD21	1.60	0.50
1:A:65:LEU:HD13	1:A:67:ASN:N	2.26	0.49
1:B:66:LYS:HB3	1:B:66:LYS:HZ3	1.76	0.49
1:A:202:THR:CG2	1:A:375:LEU:HD12	2.42	0.49
1:B:174:ILE:HG23	1:B:176:PRO:CG	2.42	0.49
1:B:141:LEU:HD12	1:B:143:THR:H	1.77	0.49
1:B:101:ASN:ND2	1:B:103:ALA:H	2.10	0.49
1:A:204:ASN:HA	1:A:215:GLU:O	2.12	0.49
1:A:384:ASP:HA	1:B:89:LYS:HD3	1.94	0.49
1:A:337:ASN:HB3	1:A:340:LYS:HG3	1.94	0.49
1:B:310:GLU:CD	1:B:310:GLU:H	2.16	0.48
1:A:33:TYR:CE1	1:A:140:LYS:HG3	2.48	0.48
1:B:29:LYS:O	1:B:31:LYS:HD2	2.14	0.48
1:A:171:ARG:CB	1:A:171:ARG:HH11	2.26	0.48
1:A:375:LEU:HD13	1:A:414:ASP:HB3	1.95	0.48
1:B:180:TYR:CE2	1:B:182:PRO:HG3	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:215:GLU:HG2	4:A:5579:HOH:O	2.12	0.48
1:A:407:LYS:CG	1:A:408:LEU:HD22	2.33	0.48
1:A:381:LEU:HD13	1:B:384:ASP:HB2	1.96	0.48
1:B:201:TYR:HA	4:B:5535:HOH:O	2.13	0.48
1:A:227:HIS:HE1	4:A:5585:HOH:O	1.97	0.48
1:B:70:SER:O	1:B:71:ALA:CB	2.60	0.48
1:B:278:ILE:N	1:B:278:ILE:CD1	2.76	0.48
1:A:9:ASN:ND2	1:B:397:LEU:HG	2.29	0.47
1:B:133:ARG:HG2	1:B:170:VAL:HG11	1.96	0.47
1:A:45:ILE:HD12	1:A:91:THR:HG21	1.97	0.47
1:A:248:ILE:HG23	1:A:267:PHE:CE1	2.49	0.47
1:A:227:HIS:CE1	4:A:5585:HOH:O	2.67	0.47
1:A:414:ASP:OD2	1:A:414:ASP:N	2.45	0.47
1:B:101:ASN:HD22	1:B:103:ALA:H	1.61	0.47
1:A:379:ASN:HB3	1:A:382:ASP:OD2	2.15	0.47
1:A:125:ILE:HD12	1:A:125:ILE:H	1.78	0.47
1:A:32:LYS:HE3	1:A:34:TYR:CE1	2.50	0.47
1:A:264:LEU:HD11	1:A:282:MET:CG	2.44	0.47
1:A:14:VAL:HG21	1:A:21:TYR:CE1	2.50	0.47
1:B:106:VAL:O	1:B:110:GLU:HG2	2.15	0.47
1:B:150:LEU:HD13	4:B:5521:HOH:O	2.13	0.47
1:A:33:TYR:CE2	1:A:140:LYS:HE3	2.50	0.46
1:A:409:ASN:ND2	1:A:409:ASN:C	2.69	0.46
1:A:198:GLU:OE1	1:A:198:GLU:HA	2.16	0.46
1:B:65:LEU:HD22	1:B:66:LYS:H	1.80	0.46
1:A:97:ARG:HA	1:A:388:VAL:HG13	1.98	0.46
1:A:264:LEU:HD11	1:A:282:MET:HG3	1.98	0.46
1:A:65:LEU:CD1	1:A:67:ASN:HA	2.45	0.46
1:A:98:ILE:HD11	1:A:225:LEU:HD12	1.97	0.46
1:B:413:ILE:CG2	1:B:414:ASP:N	2.79	0.46
1:B:175:ASP:C	1:B:177:ASP:H	2.20	0.46
1:A:153:LEU:HD23	1:A:153:LEU:C	2.36	0.45
1:A:146:GLU:N	4:A:5589:HOH:O	2.49	0.45
1:B:40:MET:CE	1:B:112:SER:HB3	2.45	0.45
1:B:40:MET:HE3	1:B:112:SER:HB3	1.97	0.45
1:B:412:ILE:O	1:B:413:ILE:CB	2.64	0.45
1:B:51:THR:HG22	1:B:59:PHE:CZ	2.50	0.45
1:B:51:THR:HG22	1:B:59:PHE:CE2	2.51	0.45
1:A:285:LYS:HE3	1:A:285:LYS:HB3	1.74	0.45
1:B:115:LYS:HD3	1:B:319:TYR:CZ	2.52	0.45
1:A:224:SER:O	1:A:227:HIS:HB3	2.17	0.45
1:B:291:LEU:O	1:B:295:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:396:ASN:HB3	1:B:12:ASP:OD1	2.17	0.45
1:B:124:PRO:HB2	1:B:127:GLU:HG2	1.98	0.45
1:B:409:ASN:ND2	1:B:411:LYS:HB2	2.26	0.44
1:B:382:ASP:OD1	1:B:384:ASP:HB3	2.17	0.44
1:B:178:VAL:CG2	1:B:179:VAL:N	2.76	0.44
1:A:137:VAL:HG13	1:A:151:LEU:HD11	1.98	0.44
1:A:412:ILE:C	1:A:414:ASP:N	2.71	0.44
1:B:176:PRO:CD	4:B:5518:HOH:O	2.65	0.44
1:A:141:LEU:HG	1:A:145:VAL:HB	1.99	0.44
1:A:65:LEU:HD22	1:A:66:LYS:N	2.33	0.44
1:A:154:LEU:HD13	1:A:192:ILE:HD12	2.00	0.44
1:A:154:LEU:CD2	1:A:154:LEU:C	2.86	0.44
1:B:55:ASN:ND2	1:B:57:SER:OG	2.48	0.43
1:A:133:ARG:HG2	1:A:170:VAL:CG1	2.47	0.43
1:A:151:LEU:HD13	1:A:151:LEU:N	2.34	0.43
1:B:65:LEU:HD13	1:B:66:LYS:N	2.34	0.43
1:B:224:SER:O	1:B:227:HIS:HB3	2.19	0.43
1:B:198:GLU:HB2	4:B:5544:HOH:O	2.19	0.43
1:B:337:ASN:OD1	1:B:337:ASN:C	2.56	0.43
1:B:371:LYS:HE2	1:B:371:LYS:CA	2.48	0.43
1:A:379:ASN:ND2	1:A:382:ASP:OD2	2.52	0.43
1:A:314:ASN:ND2	4:A:5602:HOH:O	2.52	0.43
1:A:65:LEU:HD22	1:A:66:LYS:H	1.84	0.43
1:B:101:ASN:HB3	1:B:360:PHE:CZ	2.54	0.43
1:B:150:LEU:C	1:B:150:LEU:CD1	2.88	0.42
1:A:358:ASN:ND2	4:A:5553:HOH:O	2.50	0.42
1:B:86:ARG:NH1	1:B:86:ARG:CB	2.69	0.42
1:A:412:ILE:O	1:A:414:ASP:N	2.53	0.42
1:A:268:LEU:CD2	1:A:278:ILE:HD13	2.48	0.42
1:B:14:VAL:HG21	1:B:21:TYR:CE1	2.54	0.42
1:A:264:LEU:HD22	1:A:268:LEU:CD1	2.50	0.42
1:B:21:TYR:HB2	1:B:140:LYS:HB2	2.01	0.42
1:B:409:ASN:C	1:B:409:ASN:HD22	2.22	0.42
1:A:264:LEU:HD21	1:A:278:ILE:HG12	2.01	0.42
1:B:55:ASN:OD1	1:B:58:ASP:OD2	2.37	0.42
1:A:171:ARG:NH1	1:A:179:VAL:HG11	2.34	0.42
1:A:201:TYR:HA	1:A:373:GLU:O	2.19	0.41
1:B:358:ASN:ND2	4:B:5597:HOH:O	2.53	0.41
1:A:202:THR:HG22	1:A:406:ILE:HD11	2.01	0.41
1:A:141:LEU:CG	1:A:145:VAL:HB	2.50	0.41
1:A:25:PRO:O	1:A:26:TYR:HB2	2.21	0.41
1:B:66:LYS:HG3	1:B:66:LYS:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:41:ARG:NH1	4:B:5585:HOH:O	2.54	0.41
1:A:125:ILE:CD1	1:A:125:ILE:H	2.34	0.41
1:B:198:GLU:HA	1:B:198:GLU:OE1	2.21	0.41
1:A:172:LYS:HE2	4:A:5614:HOH:O	2.20	0.41
1:B:16:ASP:OD1	1:B:141:LEU:HD13	2.21	0.41
1:B:30:SER:O	1:B:31:LYS:HB2	2.21	0.41
1:A:342:ASN:O	1:A:346:LYS:HG3	2.21	0.41
1:B:11:ASN:ND2	4:B:5526:HOH:O	2.54	0.41
1:B:66:LYS:O	1:B:67:ASN:C	2.59	0.41
1:B:414:ASP:HB3	1:B:415:SER:H	1.55	0.41
1:A:101:ASN:O	1:A:105:LYS:HG3	2.20	0.41
1:B:31:LYS:N	1:B:31:LYS:HD2	2.36	0.41
1:B:23:GLN:HG3	1:B:33:TYR:CE1	2.56	0.41
1:A:405:SER:OG	1:A:408:LEU:HD23	2.21	0.40
1:A:227:HIS:HD2	1:A:228:GLU:OE2	2.04	0.40
1:A:169:PRO:HB3	4:A:5527:HOH:O	2.21	0.40
1:A:46:ILE:HB	1:A:156:LEU:HD23	2.03	0.40
1:A:198:GLU:HG2	4:A:5519:HOH:O	2.22	0.40
1:B:46:ILE:HG22	1:B:48:GLU:HG2	2.03	0.40
1:B:141:LEU:HB3	1:B:145:VAL:H	1.87	0.40
1:B:310:GLU:N	1:B:310:GLU:CD	2.74	0.40
1:A:101:ASN:N	1:A:105:LYS:HZ2	2.19	0.40
1:B:162:ILE:O	1:B:162:ILE:HG22	2.20	0.40
1:A:37:PHE:CD2	1:A:37:PHE:N	2.90	0.40
1:B:369:PHE:N	1:B:369:PHE:CD1	2.90	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	386/439 (88%)	373 (97%)	11 (3%)	2 (0%)	38	19
1	B	386/439 (88%)	358 (93%)	20 (5%)	8 (2%)	11	1
All	All	772/878 (88%)	731 (95%)	31 (4%)	10 (1%)	18	4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	ASN
1	B	69	SER
1	B	374	PHE
1	B	413	ILE
1	B	414	ASP
1	B	331	ASP
1	B	64	SER
1	A	414	ASP
1	B	56	PRO
1	A	413	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	354/395 (90%)	334 (94%)	20 (6%)	30	11
1	B	354/395 (90%)	334 (94%)	20 (6%)	30	11
All	All	708/790 (90%)	668 (94%)	40 (6%)	30	11

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	15	ASN
1	A	67	ASN
1	A	121	ASP
1	A	144	ASN
1	A	149	MET
1	A	151	LEU
1	A	154	LEU
1	A	185	TYR
1	A	215	GLU
1	A	248	ILE
1	A	263	ARG
1	A	264	LEU
1	A	284	GLU

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Mol	Chain	Res	Type
1	A	290	LEU
1	A	301	LEU
1	A	310	GLU
1	A	343	GLU
1	A	369	PHE
1	A	409	ASN
1	B	15	ASN
1	B	56	PRO
1	B	66	LYS
1	B	67	ASN
1	B	86	ARG
1	B	115	LYS
1	B	121	ASP
1	B	141	LEU
1	B	150	LEU
1	B	151	LEU
1	B	154	LEU
1	B	174	ILE
1	B	185	TYR
1	B	225	LEU
1	B	301	LEU
1	B	366	ASN
1	B	369	PHE
1	B	407	LYS
1	B	409	ASN
1	B	414	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	67	ASN
1	A	99	ASN
1	A	144	ASN
1	A	204	ASN
1	A	227	HIS
1	A	314	ASN
1	A	329	ASN
1	A	358	ASN
1	A	409	ASN
1	B	11	ASN
1	B	15	ASN

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Mol	Chain	Res	Type
1	B	55	ASN
1	B	67	ASN
1	B	99	ASN
1	B	101	ASN
1	B	122	HIS
1	B	329	ASN
1	B	339	ASN
1	B	358	ASN
1	B	366	ASN
1	B	404	GLN
1	B	409	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 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.

## 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, 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	392/439 (89%)	0.39	23 (5%)	22 16	16, 28, 41, 52	0
1	B	392/439 (89%)	0.42	29 (7%)	14 10	13, 26, 43, 51	0
All	All	784/878 (89%)	0.41	52 (6%)	18 13	13, 27, 42, 52	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	369	PHE	11.2
1	A	414	ASP	11.0
1	A	415	SER	7.9
1	B	414	ASP	7.5
1	A	2	PRO	6.5
1	A	372	TYR	6.5
1	B	65	LEU	6.0
1	B	415	SER	5.9
1	B	177	ASP	5.8
1	A	177	ASP	4.4
1	B	64	SER	4.3
1	A	277	ILE	4.0
1	B	63	ALA	4.0
1	B	185	TYR	4.0
1	B	70	SER	3.9
1	B	62	PRO	3.9
1	A	369	PHE	3.6
1	A	64	SER	3.5
1	B	371	LYS	3.4
1	B	413	ILE	3.3
1	B	178	VAL	3.2
1	A	176	PRO	3.1
1	B	66	LYS	3.1
1	B	69	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	366	ASN	3.1
1	A	185	TYR	3.1
1	A	65	LEU	3.0
1	A	371	LYS	2.9
1	B	176	PRO	2.8
1	B	410	PRO	2.8
1	B	141	LEU	2.8
1	A	178	VAL	2.7
1	A	63	ALA	2.7
1	B	61	PRO	2.5
1	A	248	ILE	2.5
1	B	276	ASN	2.5
1	B	373	GLU	2.5
1	B	53	GLY	2.5
1	B	366	ASN	2.5
1	A	141	LEU	2.4
1	A	273	GLN	2.4
1	B	31	LYS	2.3
1	B	370	ILE	2.3
1	B	314	ASN	2.2
1	A	143	THR	2.2
1	B	174	ILE	2.2
1	A	174	ILE	2.1
1	A	332	GLY	2.1
1	B	168	TYR	2.1
1	B	330	ALA	2.1
1	A	149	MET	2.0
1	A	173	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	A	1437	1/1	0.15	0.78	18,18,18,18	0
2	ZN	B	2437	1/1	0.12	0.34	17,17,17,17	0
3	CD	B	5505	1/1	0.10	-1.19	53,53,53,53	0
3	CD	B	5503	1/1	0.04	-1.35	46,46,46,46	0
3	CD	A	5506	1/1	0.07	-2.41	39,39,39,39	0
3	CD	A	5504	1/1	0.02	-2.55	45,45,45,45	0
3	CD	A	5500	1/1	0.06	-2.57	21,21,21,21	0
3	CD	A	5507	1/1	0.04	-2.93	29,29,29,29	0
3	CD	A	5502	1/1	0.02	-2.98	32,32,32,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.