



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:17 pm BST

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 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

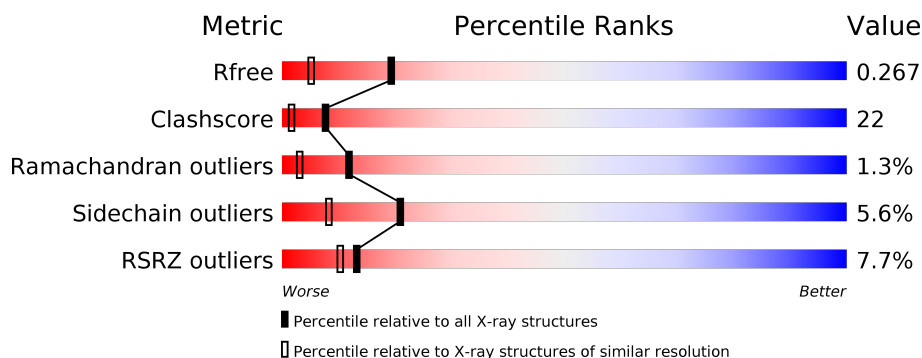
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 ≥ 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	439	<div> <div>6%</div> <div> <div></div> <div>59%</div> <div>27%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	439	<div> <div>8%</div> <div> <div></div> <div>62%</div> <div>23%</div> <div>•</div> <div>11%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6586 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 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		

These plots are drawn for all protein, RNA and DNA 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.

Chain A:

Chain B:

8% 62% 23% 11%

MET P2 N11 D12 V14 D16 D17 T18 I19 L20 M22 Q23 T24 P25 Y26 K29 S30 K31 K32 Y33 M40 R41 I46 P47 E48 T51 F52 G53 T54 N55 P56 S57 D58 F59 D60 P61 P62 A63 S64 L65 R66 R67 G68 S69 S70 A71 Y72 Y73 R86 Y90

M101 P102 A103 V106 E110 I111 S112 K115 D121 P124 E127 R133 K140 S141 S142 T143 M144 V145 H149 L150 L151 M152 L153 L154 P160 D161 I162 C167 Y168 P169 V170 I174 D175 I277 I278 L282 R263 M276 K411 I412 I413 D414 S415 ILE PRO ASP LYS GLY VAL GLU LYS Y319 D331 Y334 N337 K347 N358 K359 F360 K363 N366 T367 Y368 F369 I370 K371 Y372 E373 F374 L375 L381 D382 D383 D384 N393 L397 A398 Q404 S405 I406 K407 L408 N409 P410 K411 I412 I413 D414 S415 ILE PRO ASP LYS GLY VAL GLU LYS

VAL
LYS
PHE
CYS
LYS
SER
VAL
ILE
PRO
ARG
LYS
GLY
THR
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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) 76.7 (26.05-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (2.83%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6586	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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, 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 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	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

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 22.

All (274) 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: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
1:A:270:PHE:HZ	1:A:365:ARG:HG3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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:373:GLU:HG2	1:A:374:PHE:N	2.18	0.56
1:A:62:PRO:HG2	1:A:65:LEU:HB3	1.87	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:A:125:ILE:N	1:A:125:ILE:HD12	2.22	0.55
1:B:15:ASN:HD21	1:B:18:THR:N	2.04	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:HD12	1:B:150:LEU:C	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:C	1:A:225:LEU:HD13	2.28	0.52
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:154:LEU:HD22	1:A:156:LEU:HG	1.91	0.51
1:A:202:THR:CG2	1:A:406:ILE:HD11	2.40	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:A:376:LYS:HD3	1:A:377:VAL:N	2.26	0.51
1:B:110:GLU:OE2	1:B:347:LYS:HD2	2.11	0.51
1:B:375:LEU:HD21	1:B:415:SER:HA	1.93	0.51
1:A:111:ILE:CD1	1:A:229:LEU:HB3	2.39	0.50
1:B:160:PRO:HG2	4:B:5594:HOH:O	2.11	0.50
1:B:67:ASN:ND2	1:B:72:TYR:HA	2.26	0.50
1:A:248:ILE:HG23	1:A:267:PHE:HE1	1.76	0.50
1:B:405:SER:O	1:B:408:LEU:O	2.28	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:86:ARG:HH21	1:A:379:ASN:HD21	1.60	0.50
1:A:62:PRO:HG2	1:A:65:LEU:CB	2.42	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:141:LEU:HD12	1:B:143:THR:H	1.77	0.49
1:B:174:ILE:HG23	1:B:176:PRO:CG	2.42	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:337:ASN:HB3	1:A:340:LYS:HG3	1.94	0.49
1:A:384:ASP:HA	1:B:89:LYS:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:227:HIS:HE1	4:A:5585:HOH:O	1.97	0.48
1:B:201:TYR:HA	4:B:5535:HOH:O	2.13	0.48
1:B:278:ILE:N	1:B:278:ILE:CD1	2.76	0.48
1:B:70:SER:O	1:B:71:ALA:CB	2.60	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:227:HIS:CE1	4:A:5585:HOH:O	2.67	0.47
1:A:248:ILE:HG23	1:A:267:PHE:CE1	2.49	0.47
1:A:45:ILE:HD12	1:A:91:THR:HG21	1.97	0.47
1:A:32:LYS:HE3	1:A:34:TYR:CE1	2.50	0.47
1:A:379:ASN:HB3	1:A:382:ASP:OD2	2.15	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:125:ILE:HD12	1:A:125:ILE:H	1.78	0.47
1:A:14:VAL:HG21	1:A:21:TYR:CE1	2.50	0.47
1:A:264:LEU:HD11	1:A:282:MET:CG	2.44	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:A:97:ARG:HA	1:A:388:VAL:HG13	1.98	0.46
1:B:65:LEU:HD22	1:B:66:LYS:H	1.80	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:146:GLU:N	4:A:5589:HOH:O	2.49	0.45
1:A:153:LEU:HD23	1:A:153:LEU:C	2.36	0.45
1:B:40:MET:HE3	1:B:112:SER:HB3	1.97	0.45
1:B:40:MET:CE	1:B:112:SER:HB3	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:382:ASP:OD1	1:B:384:ASP:HB3	2.17	0.44
1:B:409:ASN:ND2	1:B:411:LYS:HB2	2.26	0.44
1:A:137:VAL:HG13	1:A:151:LEU:HD11	1.98	0.44
1:B:178:VAL:CG2	1:B:179:VAL:N	2.76	0.44
1:A:412:ILE:C	1:A:414:ASP:N	2.71	0.44
1:A:141:LEU:HG	1:A:145:VAL:HB	1.99	0.44
1:B:176:PRO:CD	4:B:5518:HOH:O	2.65	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:151:LEU:HD13	1:A:151:LEU:N	2.34	0.43
1:A:133:ARG:HG2	1:A:170:VAL:CG1	2.47	0.43
1:B:65:LEU:HD13	1:B:66:LYS:N	2.34	0.43
1:B:198:GLU:HB2	4:B:5544:HOH:O	2.19	0.43
1:B:224:SER:O	1:B:227:HIS:HB3	2.19	0.43
1:B:337:ASN:OD1	1:B:337:ASN:C	2.56	0.43
1:A:314:ASN:ND2	4:A:5602:HOH:O	2.52	0.43
1:A:379:ASN:ND2	1:A:382:ASP:OD2	2.52	0.43
1:B:371:LYS:HE2	1:B:371:LYS:CA	2.48	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:A:358:ASN:ND2	4:A:5553:HOH:O	2.50	0.42
1:B:150:LEU:CD1	1:B:150:LEU:C	2.88	0.42
1:A:268:LEU:CD2	1:A:278:ILE:HD13	2.48	0.42
1:A:412:ILE:O	1:A:414:ASP:N	2.53	0.42
1:B:86:ARG:NH1	1:B:86:ARG:CB	2.69	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:A:264:LEU:HD21	1:A:278:ILE:HG12	2.01	0.42
1:B:409:ASN:C	1:B:409:ASN:HD22	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:202:THR:HG22	1:A:406:ILE:HD11	2.01	0.41
1:B:41:ARG:NH1	4:B:5585:HOH:O	2.54	0.41
1:B:66:LYS:HG3	1:B:66:LYS:O	2.21	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: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:B:414:ASP:HB3	1:B:415:SER:H	1.55	0.41
1:B:66:LYS:O	1:B:67:ASN:C	2.59	0.41
1:A:227:HIS:HD2	1:A:228:GLU:OE2	2.04	0.40
1:A:405:SER:OG	1:A:408:LEU:HD23	2.21	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:A:101:ASN:N	1:A:105:LYS:HZ2	2.19	0.40
1:B:141:LEU:HB3	1:B:145:VAL:H	1.87	0.40
1:B:162:ILE:O	1:B:162:ILE:HG22	2.20	0.40
1:B:310:GLU:N	1:B:310:GLU:CD	2.74	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%)	29	15
1	B	386/439 (88%)	358 (93%)	20 (5%)	8 (2%)	7	1
All	All	772/878 (88%)	731 (95%)	31 (4%)	10 (1%)	12	3

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%)	21	8
1	B	354/395 (90%)	334 (94%)	20 (6%)	21	8
All	All	708/790 (90%)	668 (94%)	40 (6%)	21	8

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 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 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.

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	392/439 (89%)	0.46	27 (6%) 16 13	16, 28, 41, 52	0
1	B	392/439 (89%)	0.49	33 (8%) 11 8	13, 26, 43, 51	0
All	All	784/878 (89%)	0.47	60 (7%) 13 10	13, 27, 42, 52	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	369	PHE	13.0
1	A	414	ASP	12.1
1	A	415	SER	9.4
1	A	2	PRO	8.2
1	B	414	ASP	7.9
1	A	372	TYR	7.4
1	B	415	SER	6.4
1	B	65	LEU	6.3
1	B	177	ASP	6.3
1	B	63	ALA	5.4
1	A	177	ASP	4.9
1	B	64	SER	4.9
1	B	185	TYR	4.5
1	B	178	VAL	4.4
1	A	277	ILE	4.2
1	B	70	SER	4.2
1	B	371	LYS	4.1
1	B	69	SER	4.0
1	B	413	ILE	3.7
1	A	369	PHE	3.6
1	A	64	SER	3.6
1	A	65	LEU	3.5
1	B	62	PRO	3.5
1	A	185	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	366	ASN	3.4
1	B	410	PRO	3.3
1	A	176	PRO	3.2
1	B	66	LYS	3.2
1	B	373	GLU	3.1
1	B	176	PRO	3.1
1	A	178	VAL	3.0
1	B	141	LEU	3.0
1	A	143	THR	3.0
1	A	273	GLN	2.9
1	B	366	ASN	2.8
1	A	141	LEU	2.8
1	B	31	LYS	2.8
1	A	63	ALA	2.7
1	A	371	LYS	2.7
1	B	53	GLY	2.7
1	B	276	ASN	2.7
1	A	149	MET	2.6
1	A	174	ILE	2.6
1	B	174	ILE	2.6
1	B	61	PRO	2.6
1	A	248	ILE	2.5
1	A	173	LEU	2.4
1	B	309	PRO	2.3
1	A	314	ASN	2.3
1	B	215	GLU	2.2
1	A	373	GLU	2.2
1	A	43	VAL	2.2
1	B	149	MET	2.2
1	B	41	ARG	2.2
1	B	168	TYR	2.2
1	B	222	ALA	2.1
1	B	314	ASN	2.1
1	A	113	TYR	2.1
1	A	332	GLY	2.1
1	B	370	ILE	2.1

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 [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. 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(\AA^2)	Q<0.9
3	CD	A	5504	1/1	0.98	0.02	45,45,45,45	0
3	CD	A	5506	1/1	0.98	0.08	39,39,39,39	0
3	CD	B	5505	1/1	0.98	0.11	53,53,53,53	0
2	ZN	B	2437	1/1	0.99	0.14	17,17,17,17	0
3	CD	A	5507	1/1	0.99	0.05	29,29,29,29	0
2	ZN	A	1437	1/1	0.99	0.16	18,18,18,18	0
3	CD	B	5503	1/1	0.99	0.04	46,46,46,46	0
3	CD	A	5500	1/1	1.00	0.06	21,21,21,21	0
3	CD	A	5502	1/1	1.00	0.02	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.