



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:01 PM UTC

PDB ID : 2A97 / pdb_00002a97
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 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

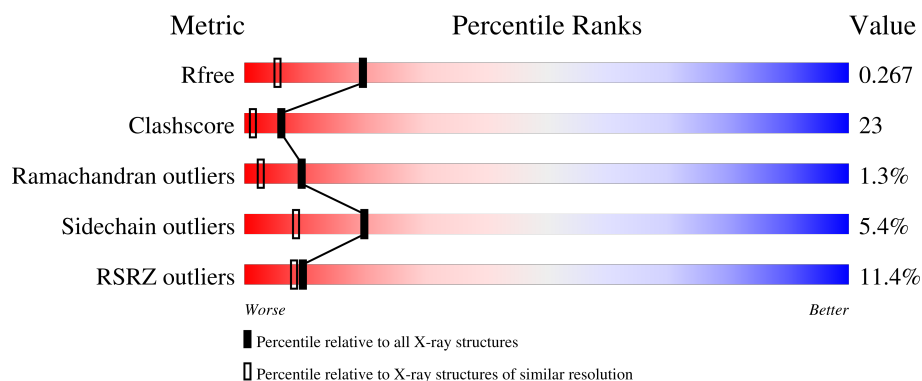
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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	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 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 (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 CADMIUM ION (CCD ID: CD) (formula: Cd).

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

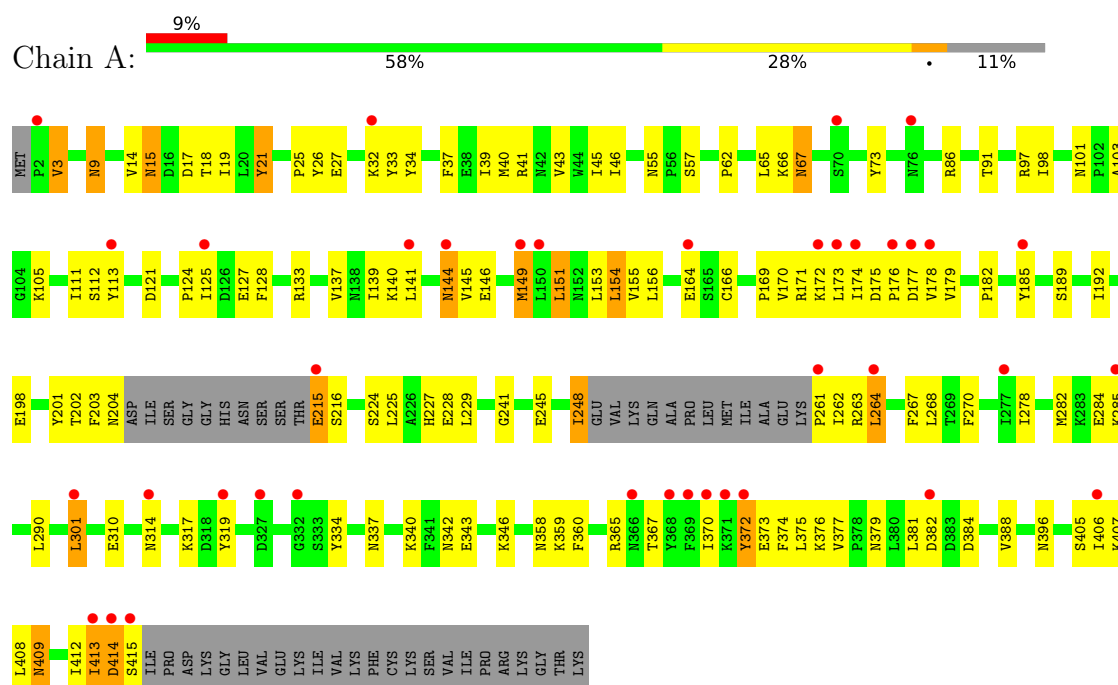
- Molecule 4 is water.

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

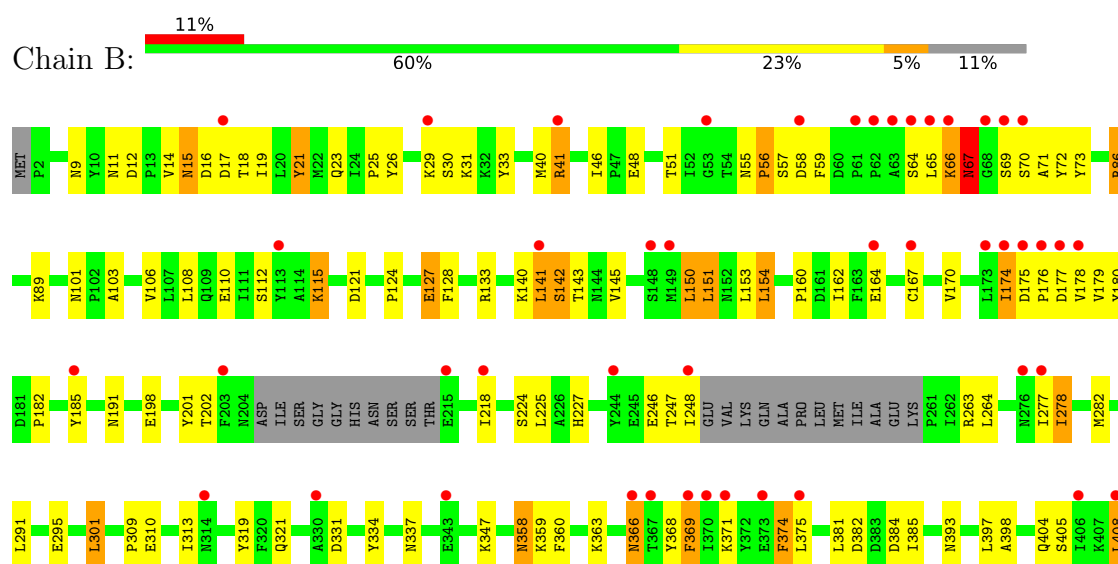
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Botulinum neurotoxin type F



• Molecule 1: Botulinum neurotoxin type F



M409	F410	K411	I412	I413	D414	S415	ILE	PRO	ASP	LYS	GLY	LEU	VAL	GLU	LYS	ILE	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)	0.39 , 46.0	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	0.38	0/3245	0.91	7/4407 (0.2%)
1	B	0.40	0/3245	0.89	11/4407 (0.2%)
All	All	0.39	0/6490	0.90	18/8814 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ASN	N-CA-C	-6.79	98.85	109.72
1	B	9	ASN	N-CA-C	-6.74	98.42	109.40
1	A	372	TYR	N-CA-C	6.55	116.71	108.45
1	A	128	PHE	N-CA-C	-6.11	99.24	108.96
1	B	277	ILE	N-CA-C	-6.08	104.11	113.16
1	B	408	LEU	N-CA-C	-5.99	101.66	110.52
1	B	164	GLU	N-CA-C	5.93	118.91	109.24
1	B	313	ILE	N-CA-C	5.84	116.49	110.36
1	B	127	GLU	N-CA-C	5.78	117.57	108.96
1	A	164	GLU	N-CA-C	5.68	118.79	109.76
1	B	128	PHE	N-CA-C	-5.66	99.50	108.73
1	A	21	TYR	N-CA-C	-5.47	100.39	109.46
1	B	142	SER	N-CA-C	-5.39	105.96	112.54
1	A	144	ASN	N-CA-C	5.38	119.12	111.92
1	B	21	TYR	N-CA-C	-5.36	100.56	109.46
1	B	321	GLN	N-CA-C	-5.14	105.57	111.07
1	A	166	CYS	N-CA-C	5.12	115.30	108.38
1	B	385	ILE	N-CA-C	5.09	116.39	112.12

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	160	0
1	B	3168	0	3090	128	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	15	0
4	B	132	0	0	14	0
All	All	6586	0	6180	283	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 23.

All (283) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:41:ARG:HG2	4:B:5585:HOH:O	1.88	0.71
1:B:309:PRO:HG2	1:B:310:GLU:OE2	1.91	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:HD12	1:B:150:LEU:O	1.93	0.69
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:15:ASN:HD22	1:B:17:ASP:H	1.41	0.67
1:B:141:LEU:HD13	1:B:142:SER:N	2.08	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:HH11	1:A:171:ARG:HB2	1.60	0.65
1:B:15:ASN:HD22	1:B:15:ASN:C	2.04	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:15:ASN:HD22	1:A:15:ASN:C	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:406:ILE:HG23	1:A:414:ASP:CG	2.24	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:A:409:ASN:HD22	1:A:409:ASN:C	2.06	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: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:A:261:PRO:C	1:A:262:ILE:HD12	2.27	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:N	1:B:366:ASN:ND2	2.49	0.59
1:A:140:LYS:HG2	4:A:5589:HOH:O	2.01	0.59
1:B:66:LYS:NZ	1:B:66:LYS:HB3	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:150:LEU:HD12	1:B:150:LEU:C	2.27	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
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: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:225:LEU:HD13	1:A:225:LEU:C	2.28	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:62:PRO:HG2	1:A:65:LEU:HB3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:C	1:A:154:LEU:HD23	2.31	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:125:ILE:HD12	1:A:125:ILE:N	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:A:98:ILE:CD1	1:A:225:LEU:HD12	2.37	0.54
1:A:141:LEU:HD12	1:A:145:VAL:HB	1.89	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:310:GLU:CD	1:B:310:GLU:H	2.16	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: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:HG2	1:A:263:ARG:HH11	1.74	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:HD12	1:A:262:ILE:N	2.26	0.51
1:A:409:ASN:C	1:A:409:ASN:ND2	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:248:ILE:HG23	1:A:267:PHE:HE1	1.76	0.50
1:B:175:ASP:C	1:B:177:ASP:H	2.20	0.50
1:B:405:SER:O	1:B:408:LEU:O	2.28	0.50
1:A:153:LEU:HD23	1:A:153:LEU:C	2.36	0.50
1:A:263:ARG:HH11	1:A:263:ARG:CG	2.24	0.50
1:B:151:LEU:HD13	1:B:151:LEU:N	2.26	0.50
1:B:247:THR:HG22	1:B:263:ARG:HA	1.92	0.50
1:A:3:VAL:HG21	1:A:40:MET:HE3	1.93	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: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:A:154:LEU:C	1:A:154:LEU:CD2	2.86	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:HH11	1:A:171:ARG:CB	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
1:A:215:GLU:HG2	4:A:5579:HOH:O	2.12	0.48
1:A:381:LEU:HD13	1:B:384:ASP:HB2	1.96	0.48
1:A:407:LYS:CG	1:A:408:LEU:HD22	2.33	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:337:ASN:C	1:B:337:ASN:OD1	2.56	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: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:412:ILE:C	1:A:414:ASP:N	2.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:HE3	1:A:34:TYR:CE1	2.50	0.47
1:A:125:ILE:HD12	1:A:125:ILE:H	1.78	0.47
1:A:379:ASN:HB3	1:A:382:ASP:OD2	2.15	0.47
1:A:414:ASP:N	1:A:414:ASP:OD2	2.45	0.47
1:B:101:ASN:HD22	1:B:103:ALA:H	1.61	0.47
1:B:150:LEU:C	1:B:150:LEU:CD1	2.88	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: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:409:ASN:C	1:B:409:ASN:HD22	2.22	0.46
1:A:146:GLU:N	4:A:5589:HOH:O	2.49	0.45
1:A:198:GLU:OE1	1:A:198:GLU:HA	2.16	0.45
1:B:40:MET:CE	1:B:112:SER:HB3	2.45	0.45
1:B:51:THR:HG22	1:B:59:PHE:CZ	2.50	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:CE2	2.51	0.45
1:B:66:LYS:O	1:B:67:ASN:C	2.59	0.45
1:A:113:TYR:O	1:A:319:TYR:OH	2.32	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
1:B:310:GLU:CD	1:B:310:GLU:N	2.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ILE:C	4:B:5560:HOH:O	2.60	0.43
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:246:GLU:C	1:B:264:LEU:HD23	2.44	0.43
1:A:412:ILE:C	1:A:414:ASP:H	2.27	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:A:144:ASN:C	4:A:5589:HOH:O	2.62	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:B:409:ASN:C	1:B:409:ASN:ND2	2.75	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: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:40:MET:HE1	1:B:108:LEU:O	2.19	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: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:25:PRO:O	1:A:26:TYR:HB2	2.21	0.41
1:A:141:LEU:CG	1:A:145:VAL:HB	2.50	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:O	1:B:66:LYS:HG3	2.21	0.41
1:A:25:PRO:C	1:A:27:GLU:H	2.29	0.41
1:A:125:ILE:H	1:A:125:ILE:CD1	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:B:66:LYS:HB3	1:B:66:LYS:HZ2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:23:GLN:HG3	1:B:33:TYR:CE1	2.56	0.41
1:B:31:LYS:HD2	1:B:31:LYS:N	2.36	0.41
1:B:414:ASP:HB3	1:B:415:SER:H	1.55	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:101:ASN:N	1:A:105:LYS:HZ2	2.19	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: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:151:LEU:C	1:B:151:LEU:HD22	2.47	0.40
1:B:369:PHE:CD1	1:B:369:PHE:N	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%)	24	14
1	B	386/439 (88%)	358 (93%)	20 (5%)	8 (2%)	5	1
All	All	772/878 (88%)	731 (95%)	31 (4%)	10 (1%)	9	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%)	336 (95%)	18 (5%)	21	9
1	B	354/395 (90%)	334 (94%)	20 (6%)	19	8
All	All	708/790 (90%)	670 (95%)	38 (5%)	20	8

All (38) 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	149	MET
1	A	151	LEU
1	A	154	LEU
1	A	173	LEU
1	A	185	TYR
1	A	215	GLU
1	A	248	ILE
1	A	264	LEU
1	A	284	GLU
1	A	290	LEU

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Mol	Chain	Res	Type
1	A	301	LEU
1	A	310	GLU
1	A	343	GLU
1	A	409	ASN
1	B	15	ASN
1	B	41	ARG
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	278	ILE
1	B	301	LEU
1	B	358	ASN
1	B	366	ASN
1	B	369	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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	184	ASN
1	A	204	ASN
1	A	227	HIS
1	A	314	ASN
1	A	329	ASN
1	A	358	ASN
1	A	366	ASN
1	A	379	ASN
1	A	393	ASN
1	A	401	ASN

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Mol	Chain	Res	Type
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	204	ASN
1	B	321	GLN
1	B	329	ASN
1	B	339	ASN
1	B	358	ASN
1	B	366	ASN
1	B	401	ASN
1	B	404	GLN
1	B	409	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 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	392/439 (89%)	0.78	39 (9%) 13 11	16, 28, 41, 52	0
1	B	392/439 (89%)	0.75	50 (12%) 7 6	13, 26, 43, 51	0
All	All	784/878 (89%)	0.77	89 (11%) 10 8	13, 27, 42, 52	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	ASP	10.6
1	B	369	PHE	8.8
1	A	372	TYR	8.5
1	A	415	SER	6.2
1	B	414	ASP	6.2
1	A	185	TYR	5.2
1	A	2	PRO	5.1
1	B	366	ASN	5.1
1	B	185	TYR	5.1
1	B	177	ASP	4.9
1	B	413	ILE	4.6
1	A	366	ASN	4.4
1	B	141	LEU	4.3
1	A	174	ILE	4.3
1	A	149	MET	4.1
1	A	370	ILE	3.7
1	A	177	ASP	3.7
1	B	408	LEU	3.6
1	A	215	GLU	3.5
1	B	178	VAL	3.5
1	A	141	LEU	3.5
1	B	415	SER	3.5
1	A	413	ILE	3.5
1	B	149	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	65	LEU	3.4
1	B	314	ASN	3.4
1	B	53	GLY	3.3
1	A	369	PHE	3.3
1	A	314	ASN	3.3
1	B	174	ILE	3.2
1	A	172	LYS	3.2
1	B	63	ALA	3.2
1	B	64	SER	3.1
1	A	382	ASP	3.1
1	B	176	PRO	3.1
1	B	68	GLY	3.1
1	B	330	ALA	3.1
1	A	178	VAL	2.9
1	B	248	ILE	2.9
1	A	368	TYR	2.8
1	B	218	ILE	2.8
1	A	176	PRO	2.8
1	B	370	ILE	2.8
1	A	150	LEU	2.7
1	B	406	ILE	2.7
1	B	167	CYS	2.6
1	B	371	LYS	2.6
1	B	277	ILE	2.6
1	B	41	ARG	2.6
1	A	319	TYR	2.6
1	B	70	SER	2.6
1	B	373	GLU	2.5
1	B	375	LEU	2.5
1	B	62	PRO	2.5
1	B	244	TYR	2.5
1	B	276	ASN	2.4
1	A	32	LYS	2.4
1	B	215	GLU	2.3
1	B	29	LYS	2.3
1	B	69	SER	2.3
1	A	70	SER	2.3
1	A	327	ASP	2.3
1	B	173	LEU	2.3
1	B	343	GLU	2.2
1	B	58	ASP	2.2
1	A	144	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	203	PHE	2.2
1	A	277	ILE	2.2
1	A	332	GLY	2.2
1	B	113	TYR	2.2
1	A	76	ASN	2.2
1	A	173	LEU	2.2
1	A	285	LYS	2.2
1	A	164	GLU	2.1
1	A	261	PRO	2.1
1	A	113	TYR	2.1
1	A	125	ILE	2.1
1	B	367	THR	2.1
1	A	371	LYS	2.1
1	B	66	LYS	2.1
1	A	264	LEU	2.1
1	B	61	PRO	2.1
1	B	410	PRO	2.1
1	A	301	LEU	2.1
1	B	175	ASP	2.1
1	A	406	ILE	2.0
1	B	17	ASP	2.0
1	B	164	GLU	2.0
1	B	148	SER	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CD	A	5506	1/1	0.95	0.06	39,39,39,39	0
3	CD	A	5504	1/1	0.98	0.08	45,45,45,45	0
2	ZN	B	2437	1/1	0.98	0.08	17,17,17,17	0
3	CD	A	5507	1/1	0.98	0.03	29,29,29,29	0
3	CD	B	5503	1/1	0.98	0.05	46,46,46,46	0
3	CD	B	5505	1/1	0.98	0.06	53,53,53,53	0
3	CD	A	5502	1/1	0.99	0.06	32,32,32,32	0
2	ZN	A	1437	1/1	0.99	0.11	18,18,18,18	0
3	CD	A	5500	1/1	1.00	0.02	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.