



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 03:56 PM UTC

PDB ID : 3ZUS / pdb_00003zus
Title : Crystal structure of an engineered botulinum neurotoxin type A- SNARE23 derivative, LC-A-SNAP23-Hn-A
Authors : Masuyer, G.; Stancombe, P.; Chaddock, J.A.; Acharya, K.R.
Deposited on : 2011-07-19
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

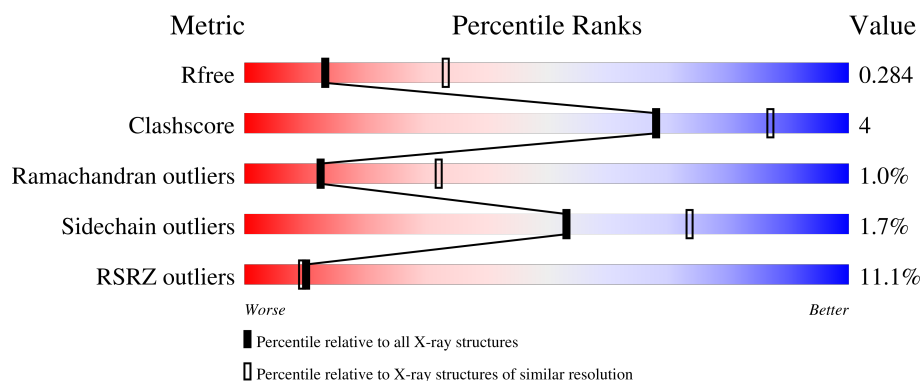
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	927	
1	B	927	
1	C	927	
1	D	927	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27661 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BOTULINUM NEUROTOXIN TYPE A, SYNAPTOSOMA L-ASSOCIATED PROTEIN 23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	851	Total	C	N	O	S	0	0	0
			6889	4427	1112	1329	21			
1	B	851	Total	C	N	O	S	0	1	0
			6898	4432	1113	1332	21			
1	C	852	Total	C	N	O	S	0	0	0
			6898	4432	1113	1332	21			
1	D	853	Total	C	N	O	S	0	0	0
			6902	4436	1114	1331	21			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP P10845
A	1	MET	-	expression tag	UNP P10845
A	2	GLU	-	expression tag	UNP P10845
A	27	ALA	VAL	variant	UNP P10845
A	466	ARG	PRO	SEE REMARK 999	UNP O00161
A	496	ALA	-	linker	UNP O00161
A	497	ASN	-	linker	UNP O00161
A	498	SER	-	linker	UNP O00161
A	499	ALA	-	linker	UNP O00161
A	500	LEU	-	linker	UNP O00161
A	501	ALA	-	linker	UNP O00161
A	502	LEU	-	linker	UNP O00161
A	503	GLN	-	linker	UNP O00161
A	916	LEU	-	expression tag	UNP P10845
A	917	GLU	-	expression tag	UNP P10845
A	918	ALA	-	expression tag	UNP P10845
A	919	HIS	-	expression tag	UNP P10845
A	920	HIS	-	expression tag	UNP P10845
A	921	HIS	-	expression tag	UNP P10845
A	922	HIS	-	expression tag	UNP P10845

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Chain	Residue	Modelled	Actual	Comment	Reference
A	923	HIS	-	expression tag	UNP P10845
A	924	HIS	-	expression tag	UNP P10845
A	925	HIS	-	expression tag	UNP P10845
A	926	HIS	-	expression tag	UNP P10845
A	927	HIS	-	expression tag	UNP P10845
A	928	HIS	-	expression tag	UNP P10845
B	0	ALA	-	expression tag	UNP P10845
B	1	MET	-	expression tag	UNP P10845
B	2	GLU	-	expression tag	UNP P10845
B	27	ALA	VAL	variant	UNP P10845
B	466	ARG	PRO	SEE REMARK 999	UNP O00161
B	496	ALA	-	linker	UNP O00161
B	497	ASN	-	linker	UNP O00161
B	498	SER	-	linker	UNP O00161
B	499	ALA	-	linker	UNP O00161
B	500	LEU	-	linker	UNP O00161
B	501	ALA	-	linker	UNP O00161
B	502	LEU	-	linker	UNP O00161
B	503	GLN	-	linker	UNP O00161
B	916	LEU	-	expression tag	UNP P10845
B	917	GLU	-	expression tag	UNP P10845
B	918	ALA	-	expression tag	UNP P10845
B	919	HIS	-	expression tag	UNP P10845
B	920	HIS	-	expression tag	UNP P10845
B	921	HIS	-	expression tag	UNP P10845
B	922	HIS	-	expression tag	UNP P10845
B	923	HIS	-	expression tag	UNP P10845
B	924	HIS	-	expression tag	UNP P10845
B	925	HIS	-	expression tag	UNP P10845
B	926	HIS	-	expression tag	UNP P10845
B	927	HIS	-	expression tag	UNP P10845
B	928	HIS	-	expression tag	UNP P10845
C	0	ALA	-	expression tag	UNP P10845
C	1	MET	-	expression tag	UNP P10845
C	2	GLU	-	expression tag	UNP P10845
C	27	ALA	VAL	variant	UNP P10845
C	466	ARG	PRO	SEE REMARK 999	UNP O00161
C	496	ALA	-	linker	UNP O00161
C	497	ASN	-	linker	UNP O00161
C	498	SER	-	linker	UNP O00161
C	499	ALA	-	linker	UNP O00161
C	500	LEU	-	linker	UNP O00161

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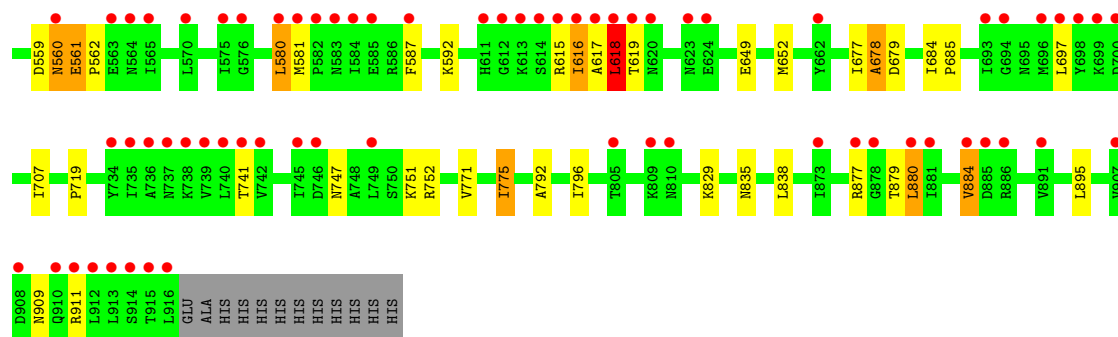
Chain	Residue	Modelled	Actual	Comment	Reference
C	501	ALA	-	linker	UNP O00161
C	502	LEU	-	linker	UNP O00161
C	503	GLN	-	linker	UNP O00161
C	916	LEU	-	expression tag	UNP P10845
C	917	GLU	-	expression tag	UNP P10845
C	918	ALA	-	expression tag	UNP P10845
C	919	HIS	-	expression tag	UNP P10845
C	920	HIS	-	expression tag	UNP P10845
C	921	HIS	-	expression tag	UNP P10845
C	922	HIS	-	expression tag	UNP P10845
C	923	HIS	-	expression tag	UNP P10845
C	924	HIS	-	expression tag	UNP P10845
C	925	HIS	-	expression tag	UNP P10845
C	926	HIS	-	expression tag	UNP P10845
C	927	HIS	-	expression tag	UNP P10845
C	928	HIS	-	expression tag	UNP P10845
D	0	ALA	-	expression tag	UNP P10845
D	1	MET	-	expression tag	UNP P10845
D	2	GLU	-	expression tag	UNP P10845
D	27	ALA	VAL	variant	UNP P10845
D	466	ARG	PRO	SEE REMARK 999	UNP O00161
D	496	ALA	-	linker	UNP O00161
D	497	ASN	-	linker	UNP O00161
D	498	SER	-	linker	UNP O00161
D	499	ALA	-	linker	UNP O00161
D	500	LEU	-	linker	UNP O00161
D	501	ALA	-	linker	UNP O00161
D	502	LEU	-	linker	UNP O00161
D	503	GLN	-	linker	UNP O00161
D	916	LEU	-	expression tag	UNP P10845
D	917	GLU	-	expression tag	UNP P10845
D	918	ALA	-	expression tag	UNP P10845
D	919	HIS	-	expression tag	UNP P10845
D	920	HIS	-	expression tag	UNP P10845
D	921	HIS	-	expression tag	UNP P10845
D	922	HIS	-	expression tag	UNP P10845
D	923	HIS	-	expression tag	UNP P10845
D	924	HIS	-	expression tag	UNP P10845
D	925	HIS	-	expression tag	UNP P10845
D	926	HIS	-	expression tag	UNP P10845
D	927	HIS	-	expression tag	UNP P10845
D	928	HIS	-	expression tag	UNP P10845

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total 27	O 27	0	0
3	B	21	Total 21	O 21	0	0
3	C	9	Total 9	O 9	0	0
3	D	13	Total 13	O 13	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.18Å 204.97Å 130.88Å 90.00° 91.91° 90.00°	Depositor
Resolution (Å)	130.81 – 2.95 130.81 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (130.81-2.95) 99.3 (130.81-2.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.248 , 0.293 0.243 , 0.284	Depositor DCC
R_{free} test set	4885 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	27661	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.90% 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 [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	0.40	0/7033	0.75	2/9526 (0.0%)
1	B	0.41	1/7042 (0.0%)	0.76	0/9538
1	C	0.40	0/7042	0.75	0/9538
1	D	0.41	0/7046	0.76	0/9544
All	All	0.41	1/28163 (0.0%)	0.75	2/38146 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	851	ILE	CA-CB	6.12	1.57	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	684	ILE	CA-C-N	5.29	124.80	119.19
1	A	684	ILE	C-N-CA	5.29	124.80	119.19

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	6889	0	6799	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6898	0	6804	61	0
1	C	6898	0	6805	49	0
1	D	6902	0	6817	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	0	0	0
3	B	21	0	0	0	0
3	C	9	0	0	0	0
3	D	13	0	0	0	0
All	All	27661	0	27225	199	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 4.

All (199) 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:874:TYR:CD2	1:B:877:ARG:NH2	1.94	1.33
1:B:874:TYR:CE2	1:B:877:ARG:NH2	1.99	1.29
1:B:1:MET:HE3	1:B:7:GLN:HE21	1.12	1.10
1:B:880:LEU:O	1:B:881:ILE:HG22	1.55	1.07
1:D:255:GLY:HA3	1:D:587:PHE:CD1	1.91	1.05
1:B:1:MET:HE3	1:B:7:GLN:NE2	1.74	1.02
1:C:560:ASN:O	1:C:561:GLU:HG3	1.61	1.00
1:B:881:ILE:HG13	1:B:882:GLY:H	1.27	0.96
1:D:617:ALA:O	1:D:618:LEU:HB2	1.64	0.96
1:B:880:LEU:O	1:B:881:ILE:CG2	2.17	0.93
1:B:874:TYR:HD2	1:B:877:ARG:HH21	1.16	0.92
1:A:678:ALA:O	1:A:680:ILE:N	2.05	0.89
1:D:560:ASN:OD1	1:D:561:GLU:N	2.07	0.85
1:B:881:ILE:HG13	1:B:882:GLY:N	1.91	0.85
1:B:874:TYR:O	1:B:877:ARG:HG3	1.79	0.83
1:D:255:GLY:HA3	1:D:587:PHE:CE1	2.13	0.83
1:B:634:THR:HG22	1:B:789:GLN:OE1	1.82	0.79
1:A:243:PHE:HE2	1:A:516:PRO:HB3	1.47	0.78
1:D:877:ARG:HB3	1:D:884:VAL:HG21	1.66	0.77
1:D:617:ALA:CB	1:D:796:ILE:HG12	2.16	0.75
1:B:615:ARG:O	1:B:616:ILE:HB	1.86	0.75
1:A:678:ALA:C	1:A:680:ILE:H	1.94	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649[A]:GLU:H	1:B:649[A]:GLU:CD	1.95	0.74
1:C:634:THR:HG22	1:C:789:GLN:OE1	1.86	0.74
1:A:615:ARG:O	1:A:616:ILE:HB	1.87	0.73
1:B:880:LEU:C	1:B:881:ILE:HG22	2.15	0.71
1:D:559:ASP:O	1:D:560:ASN:HB3	1.90	0.70
1:B:103:LEU:HA	1:B:106:MET:HE3	1.72	0.69
1:A:677:ILE:O	1:A:678:ALA:HB3	1.93	0.69
1:A:103:LEU:HA	1:A:106:MET:HE3	1.76	0.68
1:D:617:ALA:O	1:D:618:LEU:CB	2.41	0.68
1:D:559:ASP:OD1	1:D:560:ASN:N	2.27	0.68
1:D:580:LEU:HD22	1:D:580:LEU:H	1.60	0.67
1:D:617:ALA:HB1	1:D:796:ILE:HG12	1.74	0.67
1:B:14:VAL:HG13	1:B:20:ALA:HA	1.77	0.66
1:D:14:VAL:HG13	1:D:20:ALA:HA	1.78	0.66
1:D:198:GLU:HG2	1:D:361:LEU:HD11	1.78	0.65
1:D:269:HIS:HE1	1:D:909:ASN:HB2	1.61	0.65
1:B:1:MET:CE	1:B:7:GLN:NE2	2.57	0.64
1:D:580:LEU:HD22	1:D:580:LEU:N	2.12	0.64
1:B:876:ASN:O	1:B:880:LEU:HG	1.98	0.64
1:B:881:ILE:HG23	1:B:882:GLY:N	2.12	0.64
1:A:243:PHE:CE2	1:A:516:PRO:HB3	2.31	0.62
1:C:556:PHE:HB3	1:C:558:PHE:CE2	2.34	0.62
1:B:201:GLU:HG3	1:B:361:LEU:HD11	1.81	0.62
1:A:14:VAL:HG13	1:A:20:ALA:HA	1.80	0.61
1:B:649[A]:GLU:CD	1:B:649[A]:GLU:N	2.58	0.61
1:B:874:TYR:HE2	1:B:877:ARG:HH22	1.46	0.60
1:C:559:ASP:O	1:C:560:ASN:HB2	2.01	0.60
1:C:560:ASN:C	1:C:561:GLU:HG3	2.27	0.60
1:D:560:ASN:CG	1:D:561:GLU:H	2.08	0.60
1:C:754:GLU:O	1:C:758:GLU:HG2	2.02	0.60
1:D:560:ASN:O	1:D:561:GLU:HB2	2.00	0.60
1:C:113:ARG:HH22	1:C:557:ASN:HB3	1.65	0.60
1:B:67:GLN:HE22	1:B:587:PHE:H	1.50	0.59
1:D:430:CYS:HG	1:D:504:CYS:HG	1.45	0.59
1:A:394:ASN:HB2	1:B:13:PRO:HB3	1.84	0.58
1:D:243:PHE:HE1	1:D:516:PRO:HB3	1.69	0.58
1:C:622:VAL:HG13	1:C:624:GLU:H	1.69	0.57
1:D:113:ARG:HA	1:D:562:PRO:HG3	1.86	0.57
1:A:344:MET:HE1	1:A:556:PHE:CE1	2.39	0.57
1:D:880:LEU:O	1:D:884:VAL:HG23	2.05	0.57
1:C:14:VAL:HG13	1:C:20:ALA:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:GLU:HG2	1:C:361:LEU:HD11	1.88	0.56
1:C:205:ASN:HD22	1:C:400:ASN:HA	1.71	0.56
1:D:580:LEU:H	1:D:580:LEU:CD2	2.19	0.56
1:A:677:ILE:O	1:A:678:ALA:CB	2.53	0.56
1:B:874:TYR:CE2	1:B:877:ARG:CZ	2.85	0.56
1:C:243:PHE:HE2	1:C:516:PRO:HB3	1.70	0.55
1:D:835:ASN:HB3	1:D:911:ARG:NH2	2.22	0.55
1:C:344:MET:HE2	1:C:552:TYR:HD2	1.72	0.55
1:A:752:ARG:HD3	1:A:895:LEU:CD2	2.38	0.54
1:B:344:MET:HA	1:B:348:ILE:HD12	1.89	0.54
1:C:147:GLU:CD	1:C:564:ASN:HD21	2.15	0.54
1:D:560:ASN:CG	1:D:561:GLU:N	2.66	0.54
1:B:623:ASN:C	1:B:625:ALA:H	2.16	0.54
1:D:65:ALA:O	1:D:66:LYS:HB3	2.08	0.53
1:A:678:ALA:C	1:A:680:ILE:N	2.60	0.53
1:B:620:ASN:HD21	1:B:622:VAL:HG12	1.74	0.53
1:C:614:SER:O	1:C:615:ARG:HB3	2.09	0.53
1:A:98:ILE:O	1:A:104:GLY:HA3	2.10	0.52
1:B:881:ILE:CG1	1:B:882:GLY:H	1.99	0.52
1:B:881:ILE:HG23	1:B:882:GLY:H	1.74	0.52
1:D:255:GLY:CA	1:D:587:PHE:CE1	2.89	0.52
1:D:559:ASP:O	1:D:560:ASN:CB	2.56	0.52
1:B:98:ILE:O	1:B:104:GLY:HA3	2.09	0.52
1:B:873:ILE:HD11	1:B:887:LEU:HB3	1.91	0.51
1:B:874:TYR:CD2	1:B:877:ARG:CZ	2.88	0.51
1:A:715:LEU:HD21	1:A:771:VAL:HG13	1.92	0.51
1:A:80:THR:HG22	1:A:82:ASN:H	1.75	0.51
1:A:774:GLN:O	1:A:778:ILE:HD12	2.10	0.51
1:C:560:ASN:O	1:C:561:GLU:CG	2.46	0.51
1:B:53:ASN:HB3	1:B:56:GLU:HB2	1.92	0.50
1:D:421:GLY:H	1:D:424:GLU:HG3	1.74	0.50
1:A:721:ILE:HD11	1:A:763:ILE:HG12	1.93	0.50
1:C:909:ASN:O	1:C:913:LEU:HG	2.12	0.50
1:A:677:ILE:HG12	1:A:707:ILE:HA	1.94	0.49
1:B:677:ILE:HG12	1:B:707:ILE:HA	1.93	0.49
1:C:696:MET:HE3	1:C:701:ASP:HB3	1.94	0.49
1:C:103:LEU:HA	1:C:106:MET:HE3	1.93	0.49
1:A:65:ALA:O	1:A:66:LYS:HB3	2.13	0.49
1:D:53:ASN:HB3	1:D:56:GLU:HB2	1.94	0.49
1:D:752:ARG:HD3	1:D:895:LEU:CD2	2.41	0.48
1:A:53:ASN:HB3	1:A:56:GLU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:TYR:HB3	1:C:32:PRO:HB2	1.95	0.48
1:B:620:ASN:ND2	1:B:622:VAL:HG12	2.29	0.48
1:B:880:LEU:C	1:B:881:ILE:CG2	2.81	0.47
1:A:113:ARG:HH11	1:A:113:ARG:CG	2.27	0.47
1:A:396:ASN:OD1	1:A:396:ASN:N	2.44	0.47
1:B:882:GLY:C	1:B:884:VAL:H	2.22	0.47
1:D:157:SER:O	1:D:158:ALA:C	2.57	0.47
1:B:157:SER:O	1:B:158:ALA:C	2.58	0.46
1:A:334:ASP:HB3	1:A:337:LYS:HB2	1.97	0.46
1:C:80:THR:HG22	1:C:82:ASN:H	1.81	0.46
1:C:715:LEU:HD21	1:C:771:VAL:HG13	1.98	0.46
1:A:421:GLY:H	1:A:424:GLU:HG3	1.81	0.46
1:C:374:PHE:CE1	1:C:406:THR:HG21	2.51	0.46
1:A:698:TYR:HB2	1:A:701:ASP:HB2	1.98	0.46
1:C:334:ASP:HB3	1:C:337:LYS:HB2	1.97	0.46
1:C:614:SER:O	1:C:615:ARG:CB	2.64	0.46
1:B:375:LYS:HB2	1:B:416:LEU:HD11	1.97	0.46
1:C:696:MET:HE2	1:C:705:ALA:HB2	1.97	0.46
1:D:45:ILE:HB	1:D:154:ILE:HG23	1.98	0.46
1:D:792:ALA:O	1:D:796:ILE:HG13	2.16	0.46
1:B:678:ALA:O	1:B:679:ASP:HB2	2.15	0.46
1:C:348:ILE:HG23	1:C:549:ILE:HG12	1.97	0.46
1:D:344:MET:HA	1:D:348:ILE:HB	1.97	0.45
1:A:113:ARG:NH2	1:A:557:ASN:O	2.45	0.45
1:D:677:ILE:HG12	1:D:707:ILE:HA	1.97	0.45
1:A:752:ARG:HD2	1:A:862:ASP:OD1	2.17	0.45
1:B:747:ASN:O	1:B:751:LYS:HB2	2.16	0.45
1:B:715:LEU:HD21	1:B:771:VAL:HG13	1.98	0.45
1:D:775:ILE:HG23	1:D:838:LEU:HB3	1.98	0.45
1:D:269:HIS:CE1	1:D:909:ASN:HB2	2.47	0.45
1:A:256:LEU:HG	1:A:258:VAL:HG23	1.99	0.45
1:A:620:ASN:ND2	1:A:622:VAL:HG12	2.32	0.45
1:A:747:ASN:O	1:A:751:LYS:HB2	2.17	0.45
1:C:696:MET:O	1:C:697:LEU:HB2	2.17	0.44
1:B:881:ILE:CG1	1:B:882:GLY:N	2.61	0.44
1:B:890:LYS:O	1:B:894:THR:HG22	2.17	0.44
1:D:678:ALA:O	1:D:679:ASP:HB2	2.17	0.44
1:B:547:ASP:OD2	1:C:545:SER:HB2	2.17	0.44
1:B:603:TYR:CE1	1:B:692:ASN:HB2	2.52	0.44
1:B:619:THR:HG23	1:B:634:THR:CG2	2.47	0.44
1:C:625:ALA:HA	1:C:631:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ILE:O	1:C:104:GLY:HA3	2.18	0.44
1:C:344:MET:HA	1:C:348:ILE:HD12	1.99	0.44
1:D:200:LEU:HD23	1:D:364:LYS:HG3	1.99	0.44
1:D:580:LEU:N	1:D:580:LEU:CD2	2.78	0.44
1:D:334:ASP:HB3	1:D:337:LYS:HB2	1.99	0.44
1:C:113:ARG:NH2	1:C:557:ASN:O	2.51	0.43
1:A:16:GLY:HA2	1:A:20:ALA:HB2	1.99	0.43
1:D:201:GLU:OE2	1:D:361:LEU:HD13	2.19	0.43
1:C:226:ILE:HG22	1:C:230:HIS:CE1	2.52	0.43
1:D:428:LEU:HD23	1:D:592:LYS:HG3	2.01	0.43
1:D:747:ASN:O	1:D:751:LYS:HB2	2.19	0.43
1:C:154:ILE:HD11	1:C:185:TYR:HB3	1.99	0.43
1:C:559:ASP:O	1:C:560:ASN:CB	2.64	0.43
1:C:807:GLU:O	1:C:812:ILE:HG12	2.19	0.43
1:D:318:LYS:HA	1:D:323:LEU:HD12	2.01	0.43
1:D:835:ASN:HB3	1:D:911:ARG:HH21	1.83	0.43
1:B:615:ARG:O	1:B:616:ILE:CB	2.62	0.43
1:C:184:GLN:OE1	1:C:231:ARG:HD3	2.18	0.43
1:A:22:ILE:HD11	1:A:45:ILE:HD11	2.01	0.42
1:A:61:PRO:HA	1:A:62:PRO:HD3	1.83	0.42
1:D:98:ILE:O	1:D:104:GLY:HA3	2.19	0.42
1:B:752:ARG:HD3	1:B:895:LEU:CD2	2.48	0.42
1:B:764:VAL:O	1:B:768:LEU:HB2	2.20	0.42
1:B:812:ILE:O	1:B:813:ASN:C	2.62	0.42
1:C:752:ARG:HD3	1:C:895:LEU:CD2	2.50	0.42
1:A:756:TRP:CE3	1:A:858:LEU:HD13	2.55	0.42
1:C:556:PHE:HB3	1:C:558:PHE:CZ	2.55	0.42
1:D:684:ILE:HA	1:D:685:PRO:HD3	1.89	0.42
1:A:29:GLN:HG3	1:A:573:ASP:OD2	2.20	0.41
1:B:678:ALA:C	1:B:680:ILE:H	2.28	0.41
1:B:738:LYS:HA	1:B:879:THR:CG2	2.50	0.41
1:B:738:LYS:HA	1:B:879:THR:HG22	2.02	0.41
1:A:684:ILE:HA	1:A:685:PRO:HD3	1.81	0.41
1:C:276:SER:OG	1:C:761:LYS:HD2	2.20	0.41
1:C:353:ASN:HA	1:C:356:LYS:HD2	2.01	0.41
1:C:53:ASN:HB3	1:C:56:GLU:HB2	2.01	0.41
1:C:677:ILE:O	1:C:678:ALA:HB3	2.20	0.41
1:D:223:HIS:ND1	1:D:351:GLU:OE1	2.49	0.41
1:C:53:ASN:HA	1:C:54:PRO:HD3	1.96	0.41
1:A:764:VAL:O	1:A:768:LEU:HB2	2.20	0.41
1:B:201:GLU:HG3	1:B:361:LEU:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:839:ASN:OD1	1:B:912:LEU:HD23	2.20	0.41
1:A:807:GLU:O	1:A:811:ASN:HB3	2.21	0.41
1:C:147:GLU:HG3	1:C:564:ASN:OD1	2.21	0.41
1:C:620:ASN:ND2	1:C:622:VAL:HG12	2.36	0.41
1:C:650:ALA:HB1	1:C:812:ILE:HD11	2.02	0.41
1:D:719:PRO:HG3	1:D:771:VAL:CG2	2.50	0.41
1:D:877:ARG:H	1:D:877:ARG:HG3	1.75	0.41
1:B:195:GLY:HA3	1:B:374:PHE:HE1	1.85	0.41
1:B:113:ARG:NH2	1:B:557:ASN:O	2.53	0.40
1:C:61:PRO:HA	1:C:62:PRO:HD3	1.89	0.40
1:D:65:ALA:O	1:D:66:LYS:CB	2.69	0.40
1:B:881:ILE:CG2	1:B:882:GLY:H	2.31	0.40
1:B:882:GLY:C	1:B:884:VAL:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	847/927 (91%)	812 (96%)	27 (3%)	8 (1%)	14	34
1	B	848/927 (92%)	812 (96%)	27 (3%)	9 (1%)	11	29
1	C	848/927 (92%)	812 (96%)	28 (3%)	8 (1%)	14	34
1	D	849/927 (92%)	804 (95%)	35 (4%)	10 (1%)	10	28
All	All	3392/3708 (92%)	3240 (96%)	117 (3%)	35 (1%)	12	32

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	616	ILE
1	B	616	ILE

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Mol	Chain	Res	Type
1	C	615	ARG
1	D	618	LEU
1	D	619	THR
1	A	679	ASP
1	B	813	ASN
1	A	514	PHE
1	C	581	MET
1	C	614	SER
1	A	157	SER
1	A	581	MET
1	B	581	MET
1	B	624	GLU
1	B	678	ALA
1	B	881	ILE
1	C	257	GLU
1	D	560	ASN
1	D	581	MET
1	D	697	LEU
1	A	66	LYS
1	B	257	GLU
1	B	560	ASN
1	C	157	SER
1	C	560	ASN
1	D	66	LYS
1	D	616	ILE
1	D	678	ALA
1	A	678	ALA
1	A	881	ILE
1	B	809	LYS
1	C	66	LYS
1	D	514	PHE
1	C	881	ILE
1	D	561	GLU

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	767/831 (92%)	756 (99%)	11 (1%)	59	77
1	B	768/831 (92%)	757 (99%)	11 (1%)	59	77
1	C	768/831 (92%)	756 (98%)	12 (2%)	55	75
1	D	768/831 (92%)	750 (98%)	18 (2%)	44	67
All	All	3071/3324 (92%)	3019 (98%)	52 (2%)	53	73

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ARG
1	A	154	ILE
1	A	396	ASN
1	A	565	ILE
1	A	618	LEU
1	A	641	VAL
1	A	697	LEU
1	A	725	VAL
1	A	775	ILE
1	A	778	ILE
1	A	857	ARG
1	B	154	ILE
1	B	257	GLU
1	B	565	ILE
1	B	584	ILE
1	B	618	LEU
1	B	619	THR
1	B	622	VAL
1	B	649[A]	GLU
1	B	649[B]	GLU
1	B	775	ILE
1	B	873	ILE
1	C	78	LEU
1	C	154	ILE
1	C	244	LYS
1	C	565	ILE
1	C	615	ARG
1	C	619	THR
1	C	641	VAL
1	C	697	LEU
1	C	740	LEU
1	C	775	ILE
1	C	880	LEU

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Mol	Chain	Res	Type
1	C	910	GLN
1	D	51	PHE
1	D	76	THR
1	D	154	ILE
1	D	293	ILE
1	D	500	LEU
1	D	537	ILE
1	D	580	LEU
1	D	615	ARG
1	D	616	ILE
1	D	618	LEU
1	D	649	GLU
1	D	652	MET
1	D	741	THR
1	D	775	ILE
1	D	829	LYS
1	D	879	THR
1	D	880	LEU
1	D	884	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	29	GLN
1	A	82	ASN
1	A	170	HIS
1	A	569	ASN
1	A	620	ASN
1	A	623	ASN
1	A	737	ASN
1	A	883	GLN
1	A	909	ASN
1	B	7	GLN
1	B	26	ASN
1	B	29	GLN
1	B	31	GLN
1	B	40	ASN
1	B	67	GLN
1	B	133	ASN
1	B	174	ASN
1	B	396	ASN

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Mol	Chain	Res	Type
1	B	557	ASN
1	B	560	ASN
1	B	620	ASN
1	B	659	GLN
1	B	743	GLN
1	B	848	ASN
1	C	29	GLN
1	C	40	ASN
1	C	67	GLN
1	C	205	ASN
1	C	227	HIS
1	C	377	ASN
1	C	391	ASN
1	C	557	ASN
1	C	623	ASN
1	C	848	ASN
1	C	883	GLN
1	D	9	ASN
1	D	29	GLN
1	D	82	ASN
1	D	139	GLN
1	D	240	ASN
1	D	269	HIS
1	D	391	ASN
1	D	396	ASN
1	D	410	ASN
1	D	737	ASN
1	D	743	GLN
1	D	811	ASN
1	D	848	ASN
1	D	892	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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	851/927 (91%)	0.51	57 (6%) 24 20	20, 44, 72, 85	0
1	B	851/927 (91%)	0.62	85 (9%) 12 11	23, 47, 93, 118	1 (0%)
1	C	852/927 (91%)	0.91	139 (16%) 4 4	25, 59, 117, 140	0
1	D	853/927 (92%)	0.73	96 (11%) 10 9	23, 52, 97, 118	0
All	All	3407/3708 (91%)	0.69	377 (11%) 10 9	20, 50, 100, 140	1 (0%)

All (377) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	697	LEU	6.7
1	B	811	ASN	6.1
1	D	612	GLY	6.0
1	C	881	ILE	5.9
1	C	742	VAL	5.8
1	A	618	LEU	5.8
1	A	811	ASN	5.4
1	C	736	ALA	5.1
1	C	735	ILE	5.0
1	C	616	ILE	5.0
1	D	884	VAL	4.9
1	B	736	ALA	4.9
1	D	611	HIS	4.8
1	C	745	ILE	4.8
1	C	739	VAL	4.7
1	C	499	ALA	4.7
1	C	877	ARG	4.6
1	C	880	LEU	4.6
1	C	873	ILE	4.6
1	A	614	SER	4.6
1	D	699	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	741	THR	4.5
1	D	618	LEU	4.5
1	D	878	GLY	4.5
1	C	697	LEU	4.5
1	B	612	GLY	4.5
1	C	891	VAL	4.4
1	A	806	GLU	4.4
1	B	697	LEU	4.4
1	B	618	LEU	4.3
1	C	884	VAL	4.3
1	A	697	LEU	4.3
1	C	524	ASP	4.3
1	A	694	GLY	4.3
1	D	916	LEU	4.2
1	C	887	LEU	4.2
1	D	157	SER	4.2
1	A	539	ALA	4.2
1	B	617	ALA	4.1
1	B	806	GLU	4.1
1	C	874	TYR	4.1
1	C	882	GLY	4.1
1	C	915	THR	4.1
1	C	734	TYR	4.0
1	D	914	SER	4.0
1	D	696	MET	4.0
1	D	537	ILE	4.0
1	D	7	GLN	4.0
1	B	539	ALA	3.9
1	C	746	ASP	3.9
1	C	580	LEU	3.9
1	D	880	LEU	3.9
1	C	540	ALA	3.9
1	A	698	TYR	3.9
1	D	698	TYR	3.9
1	C	885	ASP	3.9
1	D	201	GLU	3.9
1	A	536	ASN	3.9
1	B	537	ILE	3.8
1	C	565	ILE	3.8
1	D	616	ILE	3.8
1	A	810	ASN	3.8
1	C	749	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	614	SER	3.7
1	C	738	LYS	3.7
1	B	740	LEU	3.7
1	C	750	SER	3.7
1	D	533	SER	3.7
1	C	615	ARG	3.7
1	A	735	ILE	3.7
1	C	570	LEU	3.6
1	B	614	SER	3.6
1	D	617	ALA	3.6
1	C	533	SER	3.6
1	D	881	ILE	3.6
1	C	698	TYR	3.6
1	C	888	LYS	3.5
1	C	541	GLU	3.5
1	D	0	ALA	3.5
1	D	539	ALA	3.5
1	B	616	ILE	3.5
1	C	539	ALA	3.5
1	B	814	PHE	3.5
1	C	612	GLY	3.5
1	B	750	SER	3.5
1	D	560	ASN	3.5
1	D	582	PRO	3.5
1	C	326	ASP	3.5
1	B	880	LEU	3.4
1	C	912	LEU	3.4
1	C	535	THR	3.4
1	D	570	LEU	3.4
1	C	806	GLU	3.4
1	C	893	ASN	3.4
1	B	570	LEU	3.3
1	A	616	ILE	3.3
1	B	735	ILE	3.3
1	A	612	GLY	3.3
1	A	51	PHE	3.3
1	C	51	PHE	3.3
1	D	662	TYR	3.3
1	B	881	ILE	3.3
1	C	737	ASN	3.2
1	C	562	PRO	3.2
1	B	576	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	531	ILE	3.2
1	C	889	ASP	3.2
1	B	623	ASN	3.2
1	B	739	VAL	3.2
1	C	744	THR	3.2
1	C	914	SER	3.2
1	A	540	ALA	3.2
1	B	542	GLU	3.2
1	B	812	ILE	3.2
1	B	580	LEU	3.1
1	C	740	LEU	3.1
1	D	615	ARG	3.1
1	C	662	TYR	3.1
1	B	624	GLU	3.1
1	B	809	LYS	3.1
1	C	733	SER	3.1
1	C	731	LEU	3.1
1	C	897	THR	3.1
1	D	580	LEU	3.1
1	C	748	ALA	3.1
1	B	566	SER	3.1
1	D	885	ASP	3.1
1	C	876	ASN	3.0
1	C	909	ASN	3.0
1	D	587	PHE	3.0
1	A	557	ASN	3.0
1	D	541	GLU	3.0
1	B	611	HIS	3.0
1	B	203	ASP	3.0
1	D	257	GLU	3.0
1	B	694	GLY	3.0
1	C	886	ARG	2.9
1	C	500	LEU	2.9
1	B	569	ASN	2.9
1	C	619	THR	2.9
1	B	565	ILE	2.9
1	D	694	GLY	2.9
1	B	810	ASN	2.9
1	C	913	LEU	2.9
1	C	614	SER	2.9
1	C	617	ALA	2.9
1	D	619	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	554	LEU	2.9
1	A	617	ALA	2.9
1	B	559	ASP	2.9
1	C	27	ALA	2.9
1	D	575	ILE	2.9
1	D	581	MET	2.8
1	B	813	ASN	2.8
1	D	620	ASN	2.8
1	D	542	GLU	2.8
1	A	611	HIS	2.8
1	D	623	ASN	2.8
1	B	908	ASP	2.8
1	D	693	ILE	2.8
1	A	915	THR	2.8
1	C	564	ASN	2.8
1	C	743	GLN	2.8
1	C	911	ARG	2.8
1	A	534	ASP	2.8
1	A	700	ASP	2.8
1	B	776	ASP	2.8
1	C	805	THR	2.8
1	D	700	ASP	2.8
1	C	870	LEU	2.7
1	B	536	ASN	2.7
1	D	583	ASN	2.7
1	C	566	SER	2.7
1	C	878	GLY	2.7
1	B	257	GLU	2.7
1	D	749	LEU	2.7
1	C	666	ASP	2.7
1	C	908	ASP	2.7
1	B	610	GLU	2.7
1	D	809	LYS	2.7
1	C	611	HIS	2.7
1	C	723	ILE	2.7
1	C	895	LEU	2.7
1	C	814	PHE	2.7
1	A	623	ASN	2.7
1	D	735	ILE	2.6
1	C	28	GLY	2.6
1	A	805	THR	2.6
1	B	894	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	541	GLU	2.6
1	B	584	ILE	2.6
1	D	565	ILE	2.6
1	C	732	VAL	2.6
1	C	810	ASN	2.6
1	B	567	ILE	2.6
1	A	559	ASP	2.6
1	B	534	ASP	2.6
1	B	533	SER	2.6
1	C	204	THR	2.6
1	C	584	ILE	2.6
1	A	678	ALA	2.6
1	D	534	ASP	2.6
1	D	540	ALA	2.6
1	A	740	LEU	2.6
1	C	618	LEU	2.6
1	D	912	LEU	2.6
1	D	891	VAL	2.6
1	C	883	GLN	2.6
1	D	810	ASN	2.6
1	C	875	ASP	2.6
1	C	335	LYS	2.5
1	B	882	GLY	2.5
1	B	696	MET	2.5
1	D	535	THR	2.5
1	C	304	VAL	2.5
1	B	558	PHE	2.5
1	A	396	ASN	2.5
1	B	886	ARG	2.5
1	A	533	SER	2.5
1	C	434	MET	2.5
1	D	913	LEU	2.5
1	D	745	ILE	2.5
1	C	530	GLU	2.5
1	B	805	THR	2.5
1	D	915	THR	2.5
1	B	615	ARG	2.5
1	C	569	ASN	2.5
1	D	613	LYS	2.5
1	A	867	ASP	2.5
1	C	309	SER	2.5
1	D	123	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	532	THR	2.5
1	D	27	ALA	2.5
1	D	741	THR	2.5
1	C	890	LYS	2.5
1	D	119	GLY	2.4
1	D	907	VAL	2.4
1	D	910	GLN	2.4
1	C	534	ASP	2.4
1	B	738	LYS	2.4
1	B	758	GLU	2.4
1	C	558	PHE	2.4
1	B	540	ALA	2.4
1	B	913	LEU	2.4
1	C	695	ASN	2.4
1	D	576	GLY	2.4
1	A	809	LYS	2.4
1	A	64	GLU	2.4
1	A	568	GLU	2.4
1	D	171	GLU	2.4
1	C	894	THR	2.4
1	A	739	VAL	2.4
1	A	908	ASP	2.4
1	B	568	GLU	2.4
1	A	295	SER	2.4
1	C	910	GLN	2.4
1	A	734	TYR	2.4
1	C	553	TYR	2.4
1	C	138	ILE	2.4
1	C	124	ASP	2.3
1	D	199	SER	2.3
1	A	532	THR	2.3
1	B	535	THR	2.3
1	B	741	THR	2.3
1	B	891	VAL	2.3
1	B	911	ARG	2.3
1	D	739	VAL	2.3
1	D	536	ASN	2.3
1	D	736	ALA	2.3
1	A	659	GLN	2.3
1	D	411	MET	2.3
1	C	572	SER	2.3
1	C	726	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	537	ILE	2.3
1	B	574	ILE	2.3
1	C	575	ILE	2.3
1	C	623	ASN	2.3
1	A	541	GLU	2.3
1	C	293	ILE	2.3
1	D	742	VAL	2.3
1	D	564	ASN	2.3
1	A	580	LEU	2.3
1	C	322	LEU	2.3
1	C	547	ASP	2.3
1	A	812	ILE	2.3
1	A	535	THR	2.3
1	C	555	THR	2.3
1	D	532	THR	2.3
1	D	877	ARG	2.3
1	A	499	ALA	2.2
1	C	869	LEU	2.2
1	B	700	ASP	2.2
1	A	565	ILE	2.2
1	D	873	ILE	2.2
1	A	615	ARG	2.2
1	B	915	THR	2.2
1	D	333	VAL	2.2
1	A	578	LEU	2.2
1	B	563	GLU	2.2
1	B	743	GLN	2.2
1	C	123	ILE	2.2
1	D	432	ASP	2.2
1	D	911	ARG	2.2
1	C	582	PRO	2.2
1	C	725	VAL	2.2
1	B	572	SER	2.2
1	B	698	TYR	2.2
1	B	499	ALA	2.2
1	D	563	GLU	2.2
1	A	543	ASN	2.2
1	C	693	ILE	2.2
1	C	700	ASP	2.2
1	D	585	GLU	2.2
1	B	303	ILE	2.2
1	D	584	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	203	ASP	2.2
1	B	326	ASP	2.2
1	D	307	THR	2.2
1	A	699	LYS	2.2
1	B	613	LYS	2.2
1	C	301	LYS	2.2
1	B	733	SER	2.2
1	C	147	GLU	2.2
1	B	531	ILE	2.1
1	A	596	ASP	2.1
1	D	746	ASP	2.1
1	D	908	ASP	2.1
1	B	555	THR	2.1
1	C	125	THR	2.1
1	D	805	THR	2.1
1	C	117	PHE	2.1
1	C	201	GLU	2.1
1	D	886	ARG	2.1
1	D	737	ASN	2.1
1	C	14	VAL	2.1
1	C	696	MET	2.1
1	A	555	THR	2.1
1	D	327	THR	2.1
1	C	59	LEU	2.1
1	C	525	LEU	2.1
1	C	552	TYR	2.1
1	C	678	ALA	2.1
1	C	853	TYR	2.1
1	D	734	TYR	2.1
1	D	624	GLU	2.1
1	B	699	LYS	2.1
1	C	526	ASN	2.1
1	D	738	LYS	2.1
1	B	912	LEU	2.1
1	C	548	LEU	2.1
1	D	203	ASP	2.1
1	D	740	LEU	2.1
1	B	807	GLU	2.1
1	C	180	TYR	2.1
1	D	295	SER	2.1
1	B	7	GLN	2.1
1	C	659	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	582	PRO	2.1
1	B	564	ASN	2.1
1	C	5	ASN	2.1
1	C	546	LEU	2.1
1	A	814	PHE	2.1
1	B	596	ASP	2.1
1	B	544	ILE	2.1
1	D	538	GLU	2.1
1	B	571	SER	2.0
1	A	732	VAL	2.0
1	A	695	ASN	2.0
1	D	322	LEU	2.0
1	B	57	GLY	2.0
1	C	419	PHE	2.0
1	C	899	ILE	2.0
1	C	64	GLU	2.0
1	B	1	MET	2.0
1	A	911	ARG	2.0
1	C	730	ALA	2.0
1	C	573	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	D	1917	1/1	0.94	0.09	83,83,83,83	0
2	ZN	B	1916	1/1	0.98	0.07	74,74,74,74	0
2	ZN	C	1916	1/1	0.99	0.02	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	1916	1/1	0.99	0.02	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.