Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 02:34 PM GMT

PDB ID	:	3ZUS
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

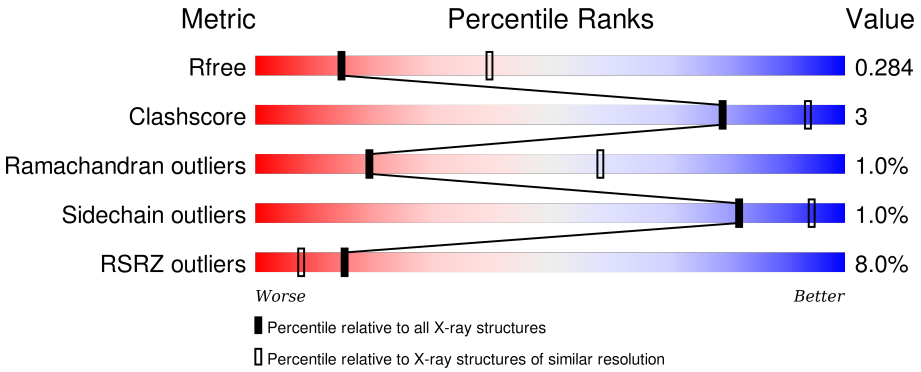
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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. 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 <=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	4% 84% 7% 8%
1	B	927	6% 84% 7% • 8%
1	C	927	11% 83% 8% 8%
1	D	927	8% 84% 7% • 8%

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, SYNAPTOSOMAL-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 72 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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	GLU	-	EXPRESSION TAG	UNP P10845
B	27	ALA	VAL	VARIANT	UNP P10845
B	466	ARG	PRO	SEE REMARK 999	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	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	916	LEU	-	EXPRESSION TAG	UNP P10845
D	917	GLU	-	EXPRESSION TAG	UNP P10845
D	918	ALA	-	EXPRESSION TAG	UNP P10845

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Chain	Residue	Modelled	Actual	Comment	Reference
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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

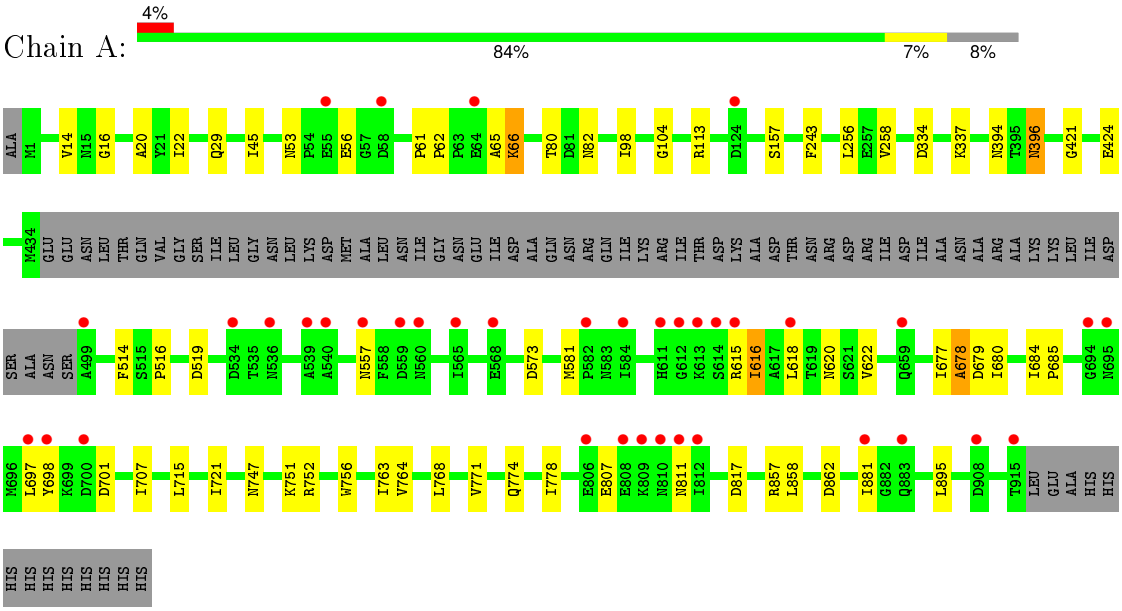
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O 27 27	0	0
3	B	21	Total O 21 21	0	0
3	C	9	Total O 9 9	0	0
3	D	13	Total O 13 13	0	0

3 Residue-property plots (i)

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.

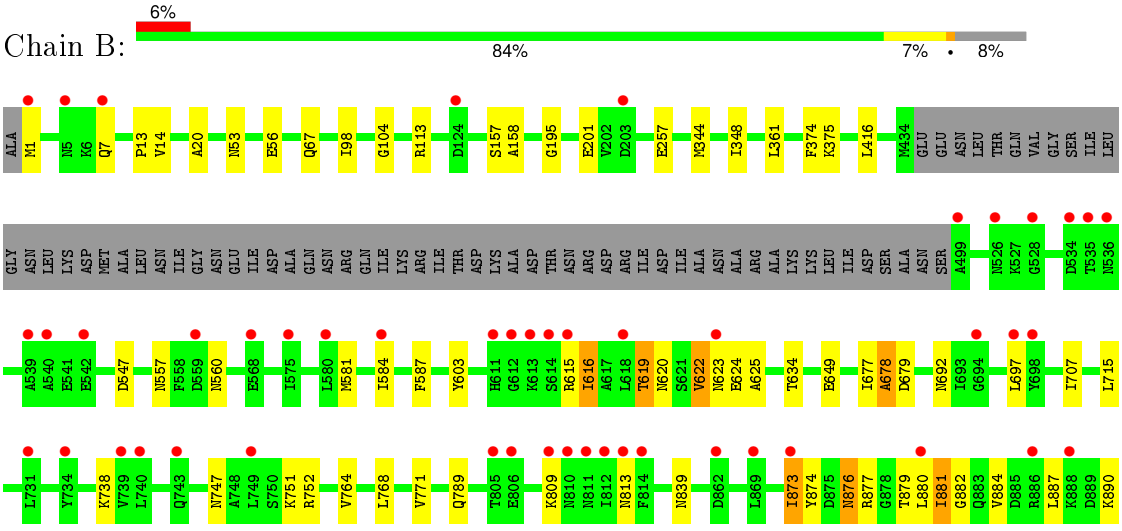
• Molecule 1: BOTULINUM NEUROTOXIN TYPE A, SYNAPTOSOMAL-ASSOCIATED PROTEIN 23

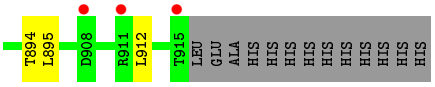
Chain A:



• Molecule 1: BOTULINUM NEUROTOXIN TYPE A, SYNAPTOSOMAL-ASSOCIATED PROTEIN 23

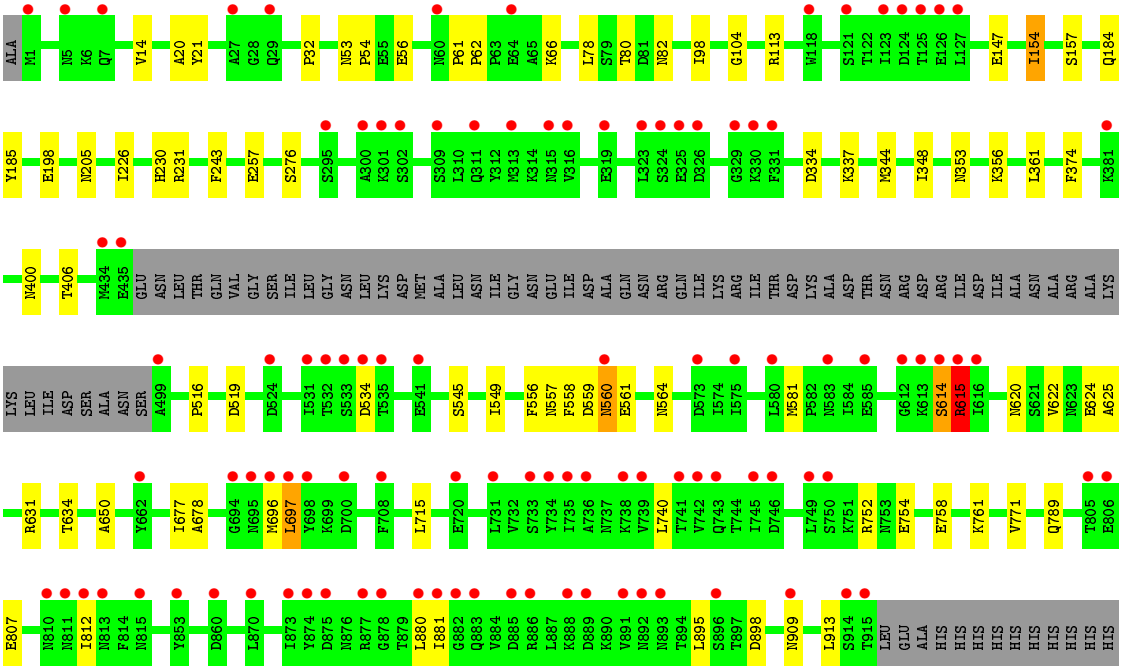
Chain B:





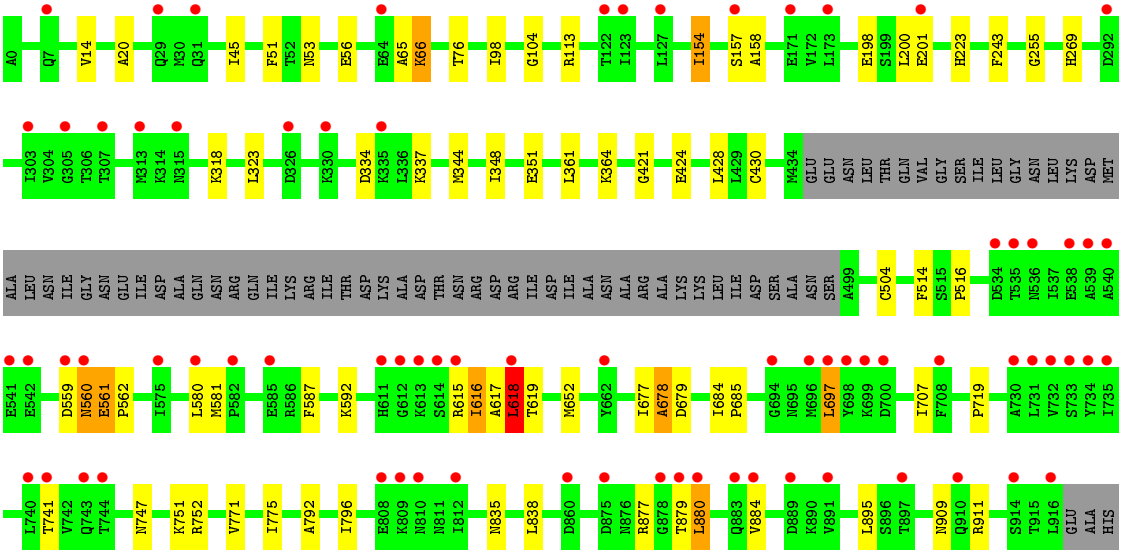
• Molecule 1: BOTULINUM NEUROTOXIN TYPE A, SYNAPTOSOMAL-ASSOCIATED PROTEIN 23

Chain C:



• Molecule 1: BOTULINUM NEUROTOXIN TYPE A, SYNAPTOSOMAL-ASSOCIATED PROTEIN 23

Chain D:



HIS
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4 Data and refinement statistics (i)

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 46.31 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (130.81-2.95) 99.4 (46.31-2.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.26%)	DCC
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 , 37.5	EDS
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 97778 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.32	0/7033	0.45	0/9526
1	B	0.33	0/7042	0.46	0/9538
1	C	0.32	0/7042	0.45	0/9538
1	D	0.33	0/7046	0.45	0/9544
All	All	0.33	0/28163	0.45	0/38146

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	6889	0	6799	36	0
1	B	6898	0	6804	59	0
1	C	6898	0	6805	45	0
1	D	6902	0	6817	51	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	189	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 3.

All (189) 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: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: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: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:D:559:ASP:O	1:D:560:ASN:HB3	1.90	0.70
1:A:678:ALA:C	1:A:680:ILE:H	1.94	0.70
1:B:649[A]:GLU:CD	1:B:649[A]:GLU:H	1.95	0.70
1:A:677:ILE:O	1:A:678:ALA:HB3	1.93	0.69
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:B:1:MET:CE	1:B:7:GLN:HE21	2.06	0.68
1:B:1:MET:CE	1:B:7:GLN:NE2	2.57	0.67
1:D:580:LEU:HD22	1:D:580:LEU:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:880:LEU:C	1:B:881:ILE:HG22	2.15	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:B:1:MET:HE3	1:B:7:GLN:NE2	2.11	0.65
1:D:269:HIS:HE1	1:D:909:ASN:HB2	1.61	0.65
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: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:B:1:MET:HE3	1:B:7:GLN:HE21	1.66	0.60
1:D:560:ASN:O	1:D:561:GLU:HB2	2.00	0.60
1:C:754:GLU:O	1:C:758:GLU:HG2	2.02	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: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:D:430:CYS:HG	1:D:504:CYS:HG	1.46	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: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
1:B:649[A]:GLU:N	1:B:649[A]:GLU:CD	2.58	0.56
1:C:205:ASN:HD22	1:C:400:ASN:HA	1.71	0.56
1:C:198:GLU:HG2	1:C:361:LEU:HD11	1.88	0.56
1:D:580:LEU:CD2	1:D:580:LEU:H	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:560:ASN:C	1:C:561:GLU:HG3	2.27	0.55
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:B:344:MET:HA	1:B:348:ILE:HD12	1.89	0.54
1:A:752:ARG:HD3	1:A:895:LEU:CD2	2.38	0.54
1:B:1:MET:HE2	1:B:7:GLN:NE2	2.23	0.54
1:D:65:ALA:O	1:D:66:LYS:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:MET:HE2	1:B:7:GLN:HE21	1.75	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:C:560:ASN:O	1:C:561:GLU:CG	2.46	0.51
1:A:774:GLN:O	1:A:778:ILE:HD12	2.10	0.51
1:B:53:ASN:HB3	1:B:56:GLU:HB2	1.92	0.50
1:C:147:GLU:CD	1:C:564:ASN:HD21	2.15	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:D:560:ASN:CG	1:D:561:GLU:N	2.66	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:B:623:ASN:C	1:B:625:ALA:H	2.16	0.49
1:D:752:ARG:HD3	1:D:895:LEU:CD2	2.41	0.48
1:C:21:TYR:HB3	1:C:32:PRO:HB2	1.95	0.48
1:A:53:ASN:HB3	1:A:56:GLU:HB2	1.96	0.48
1:B:620:ASN:ND2	1:B:622:VAL:HG12	2.29	0.48
1:A:396:ASN:N	1:A:396:ASN:OD1	2.44	0.47
1:A:113:ARG:HH11	1:A:113:ARG:CG	2.27	0.47
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:B:678:ALA:O	1:B:679:ASP:HB2	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:LYS:HB2	1:B:416:LEU:HD11	1.97	0.46
1:D:792:ALA:O	1:D:796:ILE:HG13	2.16	0.46
1:D:45:ILE:HB	1:D:154:ILE:HG23	1.98	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:D:775:ILE:HG23	1:D:838:LEU:HB3	1.98	0.45
1:B:715:LEU:HD21	1:B:771:VAL:HG13	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:D:678:ALA:O	1:D:679:ASP:HB2	2.17	0.44
1:B:890:LYS:O	1:B:894:THR:HG22	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
1:D:580:LEU:N	1:D:580:LEU:CD2	2.78	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:C:98:ILE:O	1:C:104:GLY:HA3	2.18	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:D:201:GLU:OE2	1:D:361:LEU:HD13	2.19	0.43
1:A:16:GLY:HA2	1:A:20:ALA:HB2	1.99	0.43
1:D:747:ASN:O	1:D:751:LYS:HB2	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: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:D:835:ASN:HB3	1:D:911:ARG:HH21	1.83	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:882:GLY:C	1:B:884:VAL:H	2.22	0.42
1:A:61:PRO:HA	1:A:62:PRO:HD3	1.83	0.42
1:A:22:ILE:HD11	1:A:45:ILE:HD11	2.01	0.42
1:D:157:SER:O	1:D:158:ALA:C	2.57	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:C:752:ARG:HD3	1:C:895:LEU:CD2	2.50	0.42
1:C:556:PHE:HB3	1:C:558:PHE:CZ	2.55	0.42
1:A:756:TRP:CE3	1:A:858:LEU:HD13	2.55	0.42
1:B:157:SER:O	1:B:158:ALA:C	2.58	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: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: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:A:684:ILE:HA	1:A:685:PRO:HD3	1.81	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:B:201:GLU:HG3	1:B:361:LEU:CD1	2.49	0.41
1:A:764:VAL:O	1:A:768:LEU:HB2	2.20	0.41
1:B:839:ASN:OD1	1:B:912:LEU:HD23	2.20	0.41
1:D:877:ARG:HG3	1:D:877:ARG:H	1.75	0.41
1:C:620:ASN:ND2	1:C:622:VAL:HG12	2.36	0.41
1:C:147:GLU:HG3	1:C:564:ASN:OD1	2.21	0.41
1:C:650:ALA:HB1	1:C:812:ILE:HD11	2.02	0.41
1:A:807:GLU:O	1:A:811:ASN:HB3	2.21	0.41
1:D:719:PRO:HG3	1:D:771:VAL:CG2	2.50	0.41
1:B:195:GLY:HA3	1:B:374:PHE:HE1	1.85	0.41
1:C:61:PRO:HA	1:C:62:PRO:HD3	1.89	0.40
1:B:113:ARG:NH2	1:B:557:ASN:O	2.53	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

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%)	21	61
1	B	848/927 (92%)	812 (96%)	27 (3%)	9 (1%)	17	56
1	C	848/927 (92%)	812 (96%)	28 (3%)	8 (1%)	21	61
1	D	849/927 (92%)	804 (95%)	35 (4%)	10 (1%)	16	53
All	All	3392/3708 (92%)	3240 (96%)	117 (3%)	35 (1%)	19	58

All (35) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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 (i)

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%)	761 (99%)	6 (1%)	86 95
1	B	768/831 (92%)	762 (99%)	6 (1%)	86 95
1	C	768/831 (92%)	759 (99%)	9 (1%)	78 93
1	D	768/831 (92%)	757 (99%)	11 (1%)	74 92
All	All	3071/3324 (92%)	3039 (99%)	32 (1%)	82 94

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	396	ASN
1	A	519	ASP
1	A	618	LEU
1	A	697	LEU
1	A	817	ASP
1	A	857	ARG
1	B	584	ILE
1	B	619	THR

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Mol	Chain	Res	Type
1	B	622	VAL
1	B	697	LEU
1	B	873	ILE
1	B	876	ASN
1	C	78	LEU
1	C	154	ILE
1	C	519	ASP
1	C	534	ASP
1	C	615	ARG
1	C	697	LEU
1	C	740	LEU
1	C	880	LEU
1	C	898	ASP
1	D	51	PHE
1	D	76	THR
1	D	154	ILE
1	D	615	ARG
1	D	616	ILE
1	D	618	LEU
1	D	652	MET
1	D	697	LEU
1	D	741	THR
1	D	879	THR
1	D	880	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	40	ASN
1	A	86	ASN
1	A	620	ASN
1	A	623	ASN
1	A	772	ASN
1	B	7	GLN
1	B	29	GLN
1	B	67	GLN
1	B	86	ASN
1	B	133	ASN
1	B	396	ASN
1	B	560	ASN
1	B	620	ASN

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Mol	Chain	Res	Type
1	B	743	GLN
1	C	29	GLN
1	C	40	ASN
1	C	205	ASN
1	C	503	GLN
1	C	772	ASN
1	C	839	ASN
1	C	848	ASN
1	C	876	ASN
1	D	29	GLN
1	D	86	ASN
1	D	240	ASN
1	D	269	HIS
1	D	396	ASN
1	D	743	GLN
1	D	772	ASN
1	D	848	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 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

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^{th} 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%)	0.24	38 (4%) 37 21	20, 44, 72, 85	0
1	B	851/927 (91%)	0.29	52 (6%) 25 13	23, 47, 93, 118	0
1	C	852/927 (91%)	0.63	106 (12%) 5 2	25, 59, 117, 140	0
1	D	853/927 (92%)	0.42	75 (8%) 12 6	23, 52, 97, 118	0
All	All	3407/3708 (91%)	0.39	271 (7%) 15 8	20, 50, 100, 140	0

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	885	ASP	8.2
1	C	736	ALA	8.2
1	A	614	SER	6.9
1	C	499	ALA	6.8
1	B	811	ASN	6.6
1	D	612	GLY	6.4
1	C	915	THR	6.1
1	C	535	THR	5.6
1	C	742	VAL	5.5
1	C	739	VAL	5.4
1	D	914	SER	5.3
1	D	697	LEU	5.3
1	A	811	ASN	5.3
1	C	738	LYS	5.3
1	C	881	ILE	5.1
1	A	915	THR	4.9
1	D	534	ASP	4.9
1	B	614	SER	4.8
1	C	877	ARG	4.7
1	A	536	ASN	4.7
1	C	541	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	612	GLY	4.7
1	C	697	LEU	4.6
1	C	735	ILE	4.4
1	B	740	LEU	4.4
1	D	698	TYR	4.4
1	C	914	SER	4.4
1	C	745	ILE	4.4
1	B	539	ALA	4.4
1	C	615	ARG	4.3
1	D	740	LEU	4.3
1	C	882	GLY	4.2
1	C	534	ASP	4.2
1	C	810	ASN	4.2
1	B	535	THR	4.2
1	D	538	GLU	4.1
1	B	534	ASP	4.1
1	C	524	ASP	4.1
1	A	700	ASP	4.1
1	D	809	LYS	4.1
1	D	541	GLU	4.1
1	B	694	GLY	4.1
1	C	734	TYR	4.1
1	D	614	SER	4.0
1	D	536	ASN	4.0
1	D	696	MET	3.9
1	C	29	GLN	3.9
1	D	611	HIS	3.9
1	C	326	ASP	3.8
1	C	614	SER	3.8
1	D	810	ASN	3.8
1	C	323	LEU	3.8
1	A	613	LYS	3.8
1	C	330	LYS	3.8
1	D	582	PRO	3.8
1	C	731	LEU	3.7
1	C	746	ASP	3.7
1	C	886	ARG	3.7
1	D	535	THR	3.7
1	D	699	LYS	3.7
1	D	560	ASN	3.7
1	D	539	ALA	3.7
1	C	700	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	889	ASP	3.6
1	D	575	ILE	3.6
1	C	125	THR	3.6
1	A	612	GLY	3.6
1	C	805	THR	3.6
1	C	694	GLY	3.6
1	D	916	LEU	3.6
1	A	539	ALA	3.6
1	D	542	GLU	3.5
1	A	694	GLY	3.5
1	C	733	SER	3.5
1	D	732	VAL	3.5
1	C	878	GLY	3.5
1	C	612	GLY	3.5
1	A	698	TYR	3.5
1	D	700	ASP	3.4
1	C	698	TYR	3.4
1	C	880	LEU	3.4
1	B	915	THR	3.4
1	A	810	ASN	3.4
1	B	536	ASN	3.4
1	C	870	LEU	3.4
1	C	811	ASN	3.2
1	B	869	LEU	3.2
1	D	808	GLU	3.2
1	C	891	VAL	3.2
1	A	534	ASP	3.2
1	C	575	ILE	3.2
1	B	540	ALA	3.1
1	D	730	ALA	3.1
1	C	533	SER	3.1
1	C	893	ASN	3.1
1	C	1	MET	3.1
1	B	615	ARG	3.1
1	D	29	GLN	3.1
1	A	540	ALA	3.1
1	D	884	VAL	3.1
1	A	582	PRO	3.1
1	C	325	GLU	3.1
1	D	559	ASP	3.1
1	B	697	LEU	3.0
1	D	171	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	809	LYS	3.0
1	D	585	GLU	3.0
1	D	122	THR	3.0
1	D	313	MET	3.0
1	C	883	GLN	3.0
1	D	883	GLN	3.0
1	B	880	LEU	3.0
1	C	127	LEU	3.0
1	B	1	MET	3.0
1	C	319	GLU	3.0
1	B	542	GLU	3.0
1	D	123	ILE	3.0
1	C	434	MET	3.0
1	B	613	LYS	3.0
1	A	618	LEU	2.9
1	D	694	GLY	2.9
1	C	573	ASP	2.9
1	B	805	THR	2.9
1	C	580	LEU	2.8
1	D	31	GLN	2.8
1	B	813	ASN	2.8
1	C	613	LYS	2.8
1	C	892	ASN	2.8
1	C	331	PHE	2.8
1	C	696	MET	2.8
1	B	739	VAL	2.8
1	C	695	ASN	2.8
1	C	741	THR	2.8
1	C	316	VAL	2.8
1	D	157	SER	2.8
1	A	557	ASN	2.8
1	C	874	TYR	2.8
1	A	812	ILE	2.8
1	B	886	ARG	2.7
1	C	301	LYS	2.7
1	B	580	LEU	2.7
1	D	335	LYS	2.7
1	C	309	SER	2.7
1	C	749	LEU	2.7
1	C	60	ASN	2.7
1	C	860	ASP	2.7
1	A	611	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	810	ASN	2.7
1	B	743	GLN	2.6
1	C	27	ALA	2.6
1	A	697	LEU	2.6
1	B	568	GLU	2.6
1	C	806	GLU	2.6
1	C	909	ASN	2.6
1	B	812	ILE	2.6
1	B	873	ILE	2.6
1	D	7	GLN	2.6
1	D	891	VAL	2.6
1	D	731	LEU	2.6
1	B	559	ASP	2.6
1	C	873	ILE	2.6
1	D	735	ILE	2.6
1	A	584	ILE	2.5
1	D	880	LEU	2.5
1	B	698	TYR	2.5
1	B	203	ASP	2.5
1	B	575	ILE	2.5
1	D	307	THR	2.5
1	C	329	GLY	2.5
1	B	731	LEU	2.5
1	C	300	ALA	2.5
1	A	559	ASP	2.5
1	A	499	ALA	2.5
1	C	616	ILE	2.5
1	D	201	GLU	2.5
1	C	896	SER	2.5
1	C	815	ASN	2.5
1	C	302	SER	2.4
1	A	560	ASN	2.4
1	B	734	TYR	2.4
1	C	118	TRP	2.4
1	D	615	ARG	2.4
1	C	123	ILE	2.4
1	D	540	ALA	2.4
1	D	875	ASP	2.4
1	B	618	LEU	2.4
1	C	5	ASN	2.4
1	B	809	LYS	2.4
1	C	662	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	814	PHE	2.4
1	C	435	GLU	2.4
1	D	580	LEU	2.4
1	C	743	GLN	2.4
1	C	295	SER	2.4
1	A	64	GLU	2.3
1	B	124	ASP	2.3
1	B	911	ARG	2.3
1	C	381	LYS	2.3
1	C	888	LYS	2.3
1	B	806	GLU	2.3
1	C	531	ILE	2.3
1	C	121	SER	2.3
1	D	305	GLY	2.3
1	C	875	ASP	2.3
1	D	613	LYS	2.3
1	B	5	ASN	2.3
1	A	615	ARG	2.3
1	D	303	ILE	2.3
1	D	897	THR	2.3
1	C	585	GLU	2.3
1	C	315	ASN	2.3
1	D	734	TYR	2.3
1	A	55	GLU	2.3
1	D	292	ASP	2.3
1	B	499	ALA	2.3
1	C	324	SER	2.3
1	C	126	GLU	2.3
1	D	889	ASP	2.3
1	D	708	PHE	2.2
1	C	750	SER	2.2
1	C	532	THR	2.2
1	D	127	LEU	2.2
1	B	749	LEU	2.2
1	C	720	GLU	2.2
1	B	888	LYS	2.2
1	C	708	PHE	2.2
1	A	565	ILE	2.2
1	D	618	LEU	2.2
1	C	583	ASN	2.2
1	B	584	ILE	2.2
1	B	7	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	7	GLN	2.2
1	C	813	ASN	2.2
1	D	173	LEU	2.2
1	A	806	GLU	2.2
1	B	623	ASN	2.2
1	C	853	TYR	2.2
1	B	528	GLY	2.2
1	C	64	GLU	2.2
1	D	662	TYR	2.2
1	C	812	ILE	2.1
1	B	611	HIS	2.1
1	A	908	ASP	2.1
1	B	908	ASP	2.1
1	C	311	GLN	2.1
1	C	313	MET	2.1
1	A	58	ASP	2.1
1	A	659	GLN	2.1
1	D	879	THR	2.1
1	C	124	ASP	2.1
1	C	560	ASN	2.1
1	D	64	GLU	2.1
1	D	330	LYS	2.1
1	A	124	ASP	2.1
1	D	744	THR	2.1
1	D	743	GLN	2.1
1	A	881	ILE	2.1
1	D	741	THR	2.1
1	D	326	ASP	2.0
1	B	526	ASN	2.0
1	A	808	GLU	2.0
1	D	812	ILE	2.0
1	A	695	ASN	2.0
1	D	315	ASN	2.0
1	D	878	GLY	2.0
1	A	568	GLU	2.0
1	B	862	ASP	2.0
1	D	860	ASP	2.0
1	A	883	GLN	2.0
1	D	910	GLN	2.0
1	D	733	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	D	1917	1/1	0.95	0.16	-	83,83,83,83	0
2	ZN	C	1916	1/1	0.97	0.14	-	45,45,45,45	0
2	ZN	A	1916	1/1	0.99	0.13	-	38,38,38,38	0
2	ZN	B	1916	1/1	0.94	0.17	-	74,74,74,74	0

6.5 Other polymers (i)

There are no such residues in this entry.