



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2017 – 11:46 AM EST

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029077

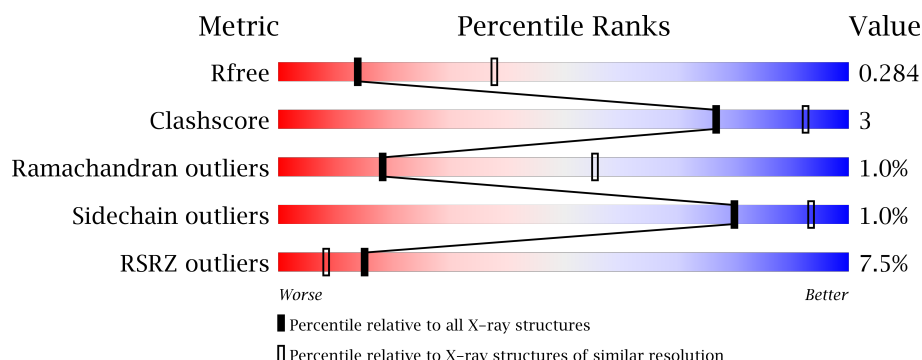
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>4%</div> <div>84%</div> <div>7%</div> <div>8%</div> </div>
1	B	927	<div> <div>5%</div> <div>84%</div> <div>7%</div> <div>8%</div> </div>
1	C	927	<div> <div>11%</div> <div>83%</div> <div>8%</div> <div>8%</div> </div>
1	D	927	<div> <div>7%</div> <div>84%</div> <div>7%</div> <div>8%</div> </div>

## 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

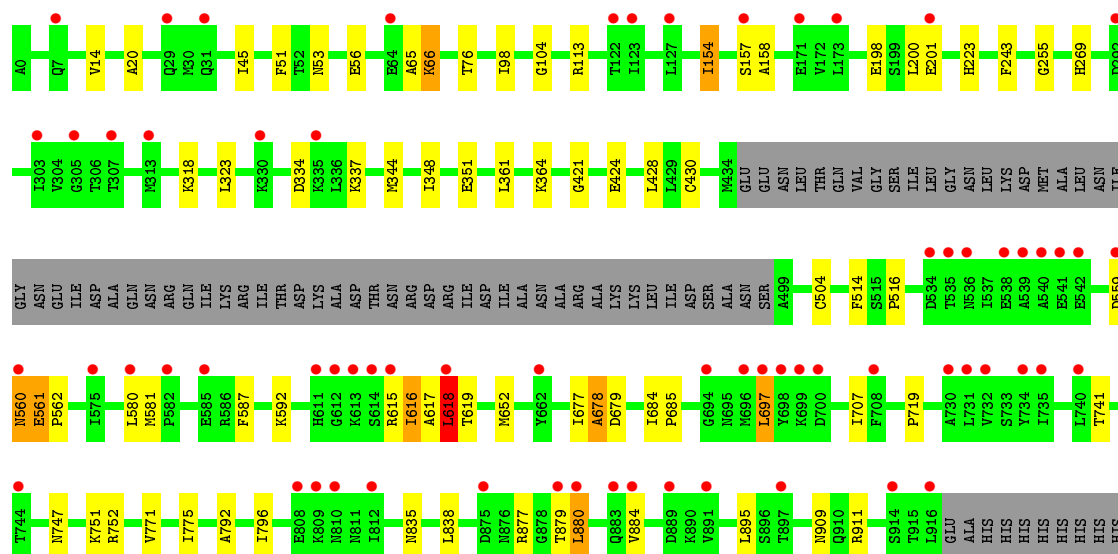
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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







RCSB  
PDB

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.18 Å   204.97 Å   130.88 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.96 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.248   ,   0.293 0.243   ,   0.284	Depositor DCC
$R_{free}$ test set	4884 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical 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	0.32	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 [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	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:B:1:MET:CE	1:B:7:GLN:HE21	2.06	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: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: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: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: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: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:559:ASP:O	1:D:560:ASN:CB	2.56	0.52
1:D:255:GLY:CA	1:D:587:PHE:CE1	2.89	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: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: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:A:65:ALA:O	1:A:66:LYS:HB3	2.13	0.49
1:D:560:ASN:CG	1:D:561:GLU:N	2.66	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:A:53:ASN:HB3	1:A:56:GLU:HB2	1.96	0.48
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:A:113:ARG:HH11	1:A:113:ARG:CG	2.27	0.47
1:A:396:ASN:N	1:A:396:ASN:OD1	2.44	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:A:421:GLY:H	1:A:424:GLU:HG3	1.81	0.46
1:B:678:ALA:O	1:B:679:ASP:HB2	2.15	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: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: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:603:TYR:CE1	1:B:692:ASN:HB2	2.52	0.44
1:B:547:ASP:OD2	1:C:545:SER:HB2	2.17	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:C:344:MET:HA	1:C:348:ILE:HD12	1.99	0.44
1:C:98:ILE:O	1:C:104:GLY:HA3	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:882:GLY:C	1:B:884:VAL:H	2.22	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: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: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: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:353:ASN:HA	1:C:356:LYS:HD2	2.01	0.41
1:C:276:SER:OG	1:C:761:LYS:HD2	2.20	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
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: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:877:ARG:HG3	1:D:877:ARG:H	1.75	0.41
1:C:147:GLU:HG3	1:C:564:ASN:OD1	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: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

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	847/927 (91%)	812 (96%)	27 (3%)	8 (1%)	20	58
1	B	848/927 (92%)	812 (96%)	27 (3%)	9 (1%)	17	53
1	C	848/927 (92%)	812 (96%)	28 (3%)	8 (1%)	20	58
1	D	849/927 (92%)	804 (95%)	35 (4%)	10 (1%)	15	50
All	All	3392/3708 (92%)	3240 (96%)	117 (3%)	35 (1%)	18	55

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 ⓘ

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%)	85	95
1	B	768/831 (92%)	762 (99%)	6 (1%)	85	95
1	C	768/831 (92%)	759 (99%)	9 (1%)	75	92
1	D	768/831 (92%)	757 (99%)	11 (1%)	71	90
All	All	3071/3324 (92%)	3039 (99%)	32 (1%)	80	93

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 [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 carbohydrates 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	851/927 (91%)	0.22	33 (3%) 40 25	20, 44, 72, 85	0
1	B	851/927 (91%)	0.28	50 (5%) 23 14	23, 47, 93, 118	0
1	C	852/927 (91%)	0.61	106 (12%) 4 2	25, 59, 117, 140	0
1	D	853/927 (92%)	0.40	67 (7%) 13 7	23, 52, 97, 118	0
All	All	3407/3708 (91%)	0.38	256 (7%) 15 8	20, 50, 100, 140	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	736	ALA	8.2
1	C	885	ASP	8.0
1	C	499	ALA	6.8
1	A	614	SER	6.8
1	B	811	ASN	6.4
1	D	612	GLY	6.3
1	C	915	THR	5.9
1	C	742	VAL	5.5
1	C	535	THR	5.4
1	C	739	VAL	5.3
1	D	697	LEU	5.2
1	D	914	SER	5.2
1	C	738	LYS	5.2
1	A	811	ASN	5.1
1	C	881	ILE	5.0
1	C	877	ARG	4.9
1	A	915	THR	4.8
1	D	534	ASP	4.7
1	B	614	SER	4.7
1	B	612	GLY	4.6
1	C	541	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	536	ASN	4.6
1	C	697	LEU	4.5
1	C	615	ARG	4.5
1	B	539	ALA	4.4
1	C	735	ILE	4.4
1	B	740	LEU	4.4
1	D	698	TYR	4.3
1	C	914	SER	4.3
1	C	745	ILE	4.3
1	D	740	LEU	4.3
1	C	882	GLY	4.2
1	C	534	ASP	4.1
1	C	810	ASN	4.1
1	B	535	THR	4.0
1	D	538	GLU	4.0
1	B	694	GLY	4.0
1	D	809	LYS	4.0
1	B	534	ASP	4.0
1	C	524	ASP	4.0
1	D	541	GLU	4.0
1	A	700	ASP	4.0
1	C	734	TYR	4.0
1	D	614	SER	3.9
1	C	886	ARG	3.9
1	D	536	ASN	3.9
1	D	696	MET	3.8
1	D	611	HIS	3.8
1	C	29	GLN	3.8
1	C	323	LEU	3.7
1	C	614	SER	3.7
1	C	326	ASP	3.7
1	A	613	LYS	3.7
1	C	330	LYS	3.7
1	D	810	ASN	3.7
1	D	539	ALA	3.7
1	C	731	LEU	3.7
1	D	699	LYS	3.6
1	D	582	PRO	3.6
1	C	746	ASP	3.6
1	D	535	THR	3.6
1	A	539	ALA	3.6
1	D	575	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	612	GLY	3.6
1	C	694	GLY	3.6
1	D	560	ASN	3.6
1	D	916	LEU	3.5
1	C	700	ASP	3.5
1	C	889	ASP	3.5
1	C	125	THR	3.5
1	C	805	THR	3.5
1	A	694	GLY	3.5
1	D	732	VAL	3.5
1	D	542	GLU	3.4
1	C	878	GLY	3.4
1	C	612	GLY	3.4
1	C	733	SER	3.4
1	C	880	LEU	3.4
1	A	698	TYR	3.4
1	C	698	TYR	3.4
1	D	700	ASP	3.3
1	B	915	THR	3.3
1	C	870	LEU	3.3
1	A	810	ASN	3.2
1	B	536	ASN	3.2
1	B	615	ARG	3.2
1	B	540	ALA	3.2
1	C	891	VAL	3.2
1	D	730	ALA	3.2
1	B	869	LEU	3.2
1	C	575	ILE	3.1
1	D	808	GLU	3.1
1	C	811	ASN	3.1
1	A	540	ALA	3.1
1	A	534	ASP	3.1
1	D	884	VAL	3.1
1	C	533	SER	3.0
1	C	1	MET	3.0
1	C	893	ASN	3.0
1	D	29	GLN	3.0
1	B	697	LEU	3.0
1	C	325	GLU	3.0
1	A	582	PRO	3.0
1	D	559	ASP	3.0
1	B	880	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	809	LYS	3.0
1	D	171	GLU	3.0
1	C	127	LEU	2.9
1	D	585	GLU	2.9
1	D	122	THR	2.9
1	D	123	ILE	2.9
1	D	313	MET	2.9
1	C	883	GLN	2.9
1	D	883	GLN	2.9
1	B	1	MET	2.9
1	C	319	GLU	2.9
1	B	542	GLU	2.9
1	B	613	LYS	2.9
1	A	618	LEU	2.9
1	C	434	MET	2.9
1	B	886	ARG	2.9
1	D	694	GLY	2.8
1	C	580	LEU	2.8
1	B	739	VAL	2.8
1	B	805	THR	2.8
1	C	573	ASP	2.8
1	C	331	PHE	2.8
1	C	316	VAL	2.8
1	C	613	LYS	2.7
1	C	696	MET	2.7
1	A	812	ILE	2.7
1	D	31	GLN	2.7
1	B	813	ASN	2.7
1	C	892	ASN	2.7
1	D	157	SER	2.7
1	C	874	TYR	2.7
1	C	741	THR	2.7
1	B	580	LEU	2.7
1	C	695	ASN	2.7
1	C	301	LYS	2.7
1	A	557	ASN	2.7
1	C	27	ALA	2.7
1	D	335	LYS	2.7
1	C	749	LEU	2.7
1	C	309	SER	2.6
1	A	611	HIS	2.6
1	C	60	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	697	LEU	2.6
1	C	860	ASP	2.6
1	B	812	ILE	2.6
1	B	810	ASN	2.6
1	D	891	VAL	2.6
1	B	743	GLN	2.5
1	B	873	ILE	2.5
1	B	568	GLU	2.5
1	C	806	GLU	2.5
1	D	731	LEU	2.5
1	D	615	ARG	2.5
1	C	873	ILE	2.5
1	D	735	ILE	2.5
1	A	584	ILE	2.5
1	C	909	ASN	2.5
1	C	300	ALA	2.5
1	D	880	LEU	2.5
1	A	499	ALA	2.5
1	D	7	GLN	2.5
1	B	575	ILE	2.5
1	B	559	ASP	2.5
1	B	698	TYR	2.5
1	C	329	GLY	2.5
1	D	540	ALA	2.5
1	B	731	LEU	2.5
1	C	616	ILE	2.4
1	B	911	ARG	2.4
1	B	203	ASP	2.4
1	D	307	THR	2.4
1	C	123	ILE	2.4
1	C	896	SER	2.4
1	D	201	GLU	2.4
1	A	615	ARG	2.4
1	B	734	TYR	2.4
1	A	559	ASP	2.4
1	C	302	SER	2.4
1	B	618	LEU	2.4
1	C	815	ASN	2.4
1	A	560	ASN	2.4
1	C	118	TRP	2.4
1	B	814	PHE	2.3
1	B	809	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	662	TYR	2.3
1	D	875	ASP	2.3
1	D	580	LEU	2.3
1	C	435	GLU	2.3
1	C	5	ASN	2.3
1	B	499	ALA	2.3
1	C	531	ILE	2.3
1	C	295	SER	2.3
1	D	305	GLY	2.3
1	C	743	GLN	2.3
1	A	64	GLU	2.3
1	C	381	LYS	2.3
1	C	888	LYS	2.3
1	D	303	ILE	2.3
1	B	806	GLU	2.3
1	C	121	SER	2.2
1	B	124	ASP	2.2
1	D	613	LYS	2.2
1	D	734	TYR	2.2
1	D	897	THR	2.2
1	C	585	GLU	2.2
1	B	5	ASN	2.2
1	C	324	SER	2.2
1	C	875	ASP	2.2
1	A	55	GLU	2.2
1	C	126	GLU	2.2
1	C	315	ASN	2.2
1	D	127	LEU	2.2
1	D	708	PHE	2.2
1	B	749	LEU	2.2
1	D	292	ASP	2.2
1	A	565	ILE	2.2
1	D	618	LEU	2.2
1	D	889	ASP	2.2
1	C	708	PHE	2.2
1	C	750	SER	2.2
1	B	584	ILE	2.2
1	C	532	THR	2.2
1	B	888	LYS	2.2
1	D	173	LEU	2.1
1	C	720	GLU	2.1
1	B	528	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	812	ILE	2.1
1	C	853	TYR	2.1
1	C	583	ASN	2.1
1	B	611	HIS	2.1
1	A	806	GLU	2.1
1	D	662	TYR	2.1
1	B	7	GLN	2.1
1	C	7	GLN	2.1
1	C	813	ASN	2.1
1	C	64	GLU	2.1
1	B	623	ASN	2.1
1	C	313	MET	2.1
1	C	311	GLN	2.0
1	A	908	ASP	2.0
1	B	908	ASP	2.0
1	A	881	ILE	2.0
1	D	879	THR	2.0
1	A	659	GLN	2.0
1	A	58	ASP	2.0
1	D	330	LYS	2.0
1	C	124	ASP	2.0
1	D	64	GLU	2.0
1	D	812	ILE	2.0
1	D	744	THR	2.0
1	C	560	ASN	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<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	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.