



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2022 – 04:08 PM JST

PDB ID : 7XYU  
Title : Crystal structure of ZER1 bound to TFLH degran  
Authors : Dong, C.; Yan, X.; Li, Y.  
Deposited on : 2022-06-02  
Resolution : 2.70 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

<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>.

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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)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

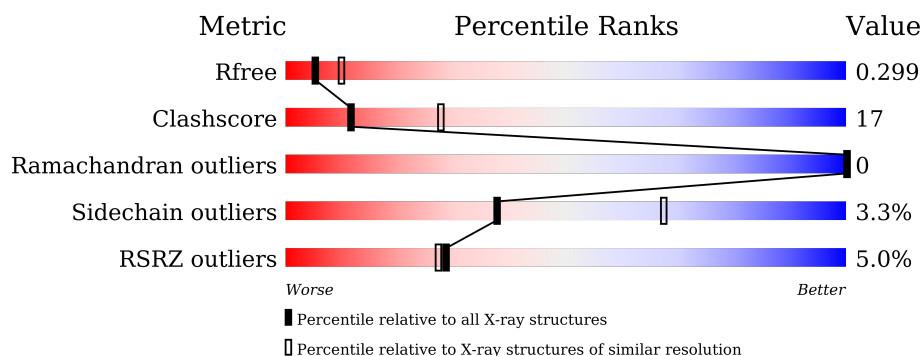
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	251	<div> <div>2%</div> <div>68% 28% . .</div> </div>
1	B	251	<div> <div>61% 32% . .</div> </div>
1	C	251	<div> <div>4%</div> <div>63% 29% . .</div> </div>
1	D	251	<div> <div>14%</div> <div>53% 37% . 7%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7850 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 Protein zer-1 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	243	Total	C	N	O	S	0	0	0
			1975	1265	332	359	19			
1	A	245	Total	C	N	O	S	0	0	0
			1992	1276	334	363	19			
1	C	241	Total	C	N	O	S	0	0	0
			1959	1257	329	355	18			
1	D	234	Total	C	N	O	S	0	0	0
			1901	1219	321	343	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	516	THR	-	expression tag	UNP Q7Z7L7
B	517	PHE	-	expression tag	UNP Q7Z7L7
B	518	LEU	-	expression tag	UNP Q7Z7L7
B	519	HIS	-	expression tag	UNP Q7Z7L7
A	516	THR	-	expression tag	UNP Q7Z7L7
A	517	PHE	-	expression tag	UNP Q7Z7L7
A	518	LEU	-	expression tag	UNP Q7Z7L7
A	519	HIS	-	expression tag	UNP Q7Z7L7
C	516	THR	-	expression tag	UNP Q7Z7L7
C	517	PHE	-	expression tag	UNP Q7Z7L7
C	518	LEU	-	expression tag	UNP Q7Z7L7
C	519	HIS	-	expression tag	UNP Q7Z7L7
D	516	THR	-	expression tag	UNP Q7Z7L7
D	517	PHE	-	expression tag	UNP Q7Z7L7
D	518	LEU	-	expression tag	UNP Q7Z7L7
D	519	HIS	-	expression tag	UNP Q7Z7L7

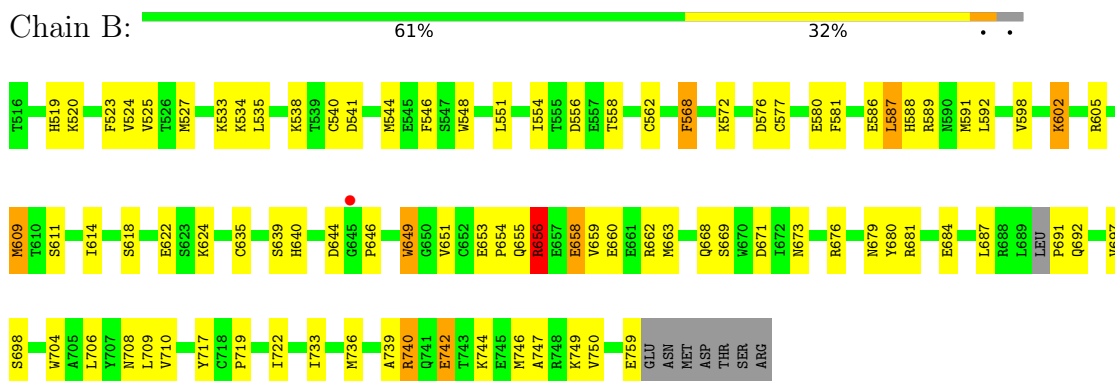
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total 5	O 5	0	0
2	A	11	Total 11	O 11	0	0
2	C	2	Total 2	O 2	0	0
2	D	5	Total 5	O 5	0	0

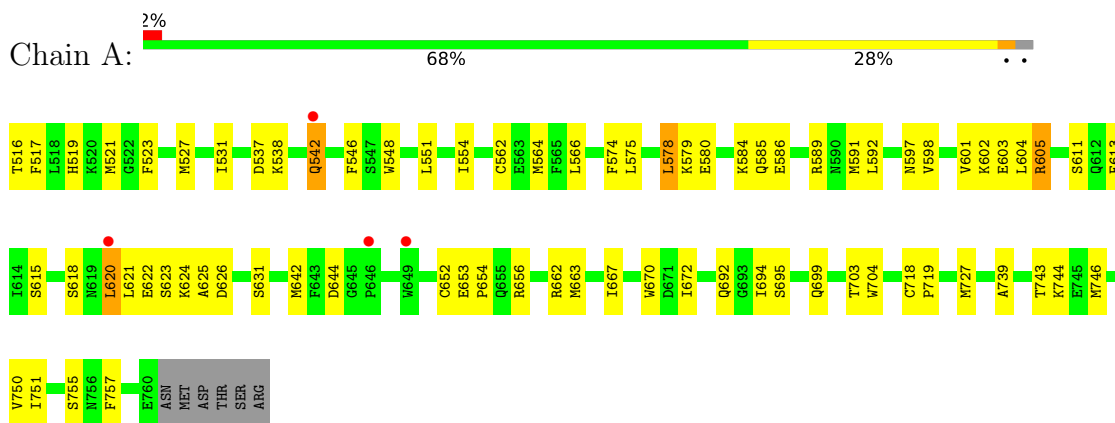
### 3 Residue-property plots

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

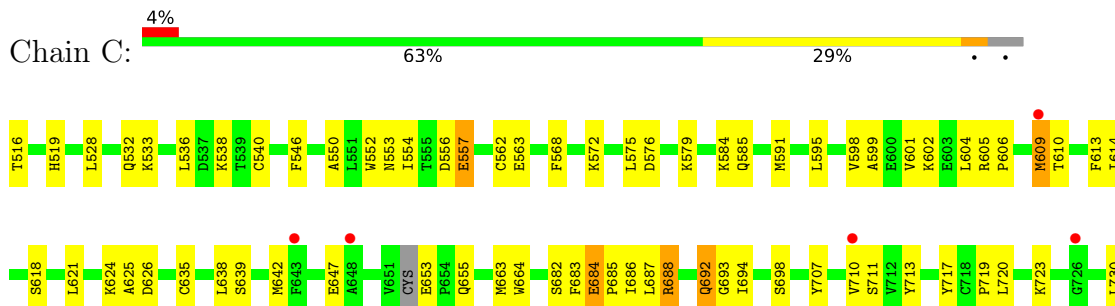
#### • Molecule 1: Protein zer-1 homolog

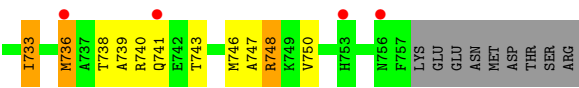


#### • Molecule 1: Protein zer-1 homolog

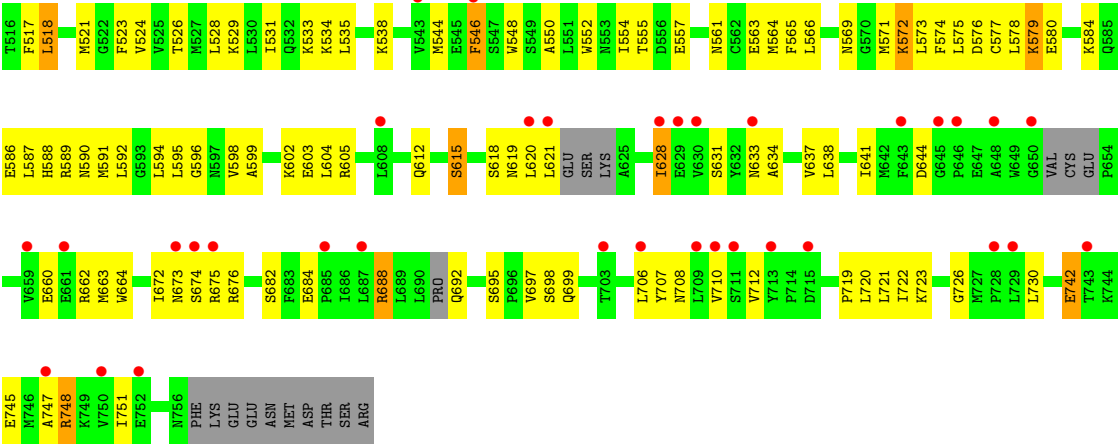


#### • Molecule 1: Protein zer-1 homolog





● Molecule 1: Protein zer-1 homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.78Å 67.78Å 418.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.90 – 2.70 48.05 – 2.39	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.90-2.70) 99.8 (48.05-2.39)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.248 , 0.304 0.248 , 0.299	Depositor DCC
$R_{free}$ test set	2010 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.096 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7850	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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

### 5.1 Standard geometry

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	0.39	1/2038 (0.0%)	0.69	6/2753 (0.2%)
1	B	0.51	2/2020 (0.1%)	0.73	7/2726 (0.3%)
1	C	0.41	0/2004	0.71	7/2707 (0.3%)
1	D	0.53	2/1942 (0.1%)	1.02	13/2619 (0.5%)
All	All	0.46	5/8004 (0.1%)	0.80	33/10805 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	748	ARG	CB-CG	-7.95	1.31	1.52
1	B	602	LYS	CD-CE	7.72	1.70	1.51
1	A	605	ARG	CG-CD	5.97	1.66	1.51
1	D	748	ARG	CZ-NH2	-5.54	1.25	1.33
1	B	742	GLU	CB-CG	5.24	1.62	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	748	ARG	NE-CZ-NH2	-14.55	113.02	120.30
1	D	748	ARG	NE-CZ-NH1	14.43	127.52	120.30
1	D	748	ARG	CG-CD-NE	-11.87	86.86	111.80
1	D	572	LYS	CD-CE-NZ	-11.29	85.73	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	609	MET	CB-CG-SD	10.09	142.67	112.40
1	D	742	GLU	CA-CB-CG	9.54	134.38	113.40
1	A	578	LEU	CA-CB-CG	9.18	136.42	115.30
1	D	603	GLU	CB-CA-C	-8.81	92.77	110.40
1	B	749	LYS	CD-CE-NZ	-8.64	91.82	111.70
1	D	675	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	D	675	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	A	620	LEU	CB-CG-CD1	7.38	123.54	111.00
1	A	605	ARG	CG-CD-NE	6.67	125.80	111.80
1	D	684	GLU	CA-CB-CG	6.64	128.02	113.40
1	D	603	GLU	CA-CB-CG	6.31	127.28	113.40
1	B	649	TRP	CA-CB-CG	6.22	125.53	113.70
1	A	605	ARG	CB-CG-CD	6.22	127.77	111.60
1	B	658	GLU	CA-CB-CG	6.20	127.04	113.40
1	D	546	PHE	CB-CA-C	-6.02	98.37	110.40
1	C	748	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	C	736	MET	CA-CB-CG	5.77	123.11	113.30
1	C	684	GLU	N-CA-CB	-5.73	100.29	110.60
1	C	557	GLU	CA-CB-CG	5.71	125.97	113.40
1	B	740	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	684	GLU	N-CA-CB	-5.63	100.46	110.60
1	B	740	ARG	CA-CB-CG	5.63	125.79	113.40
1	A	605	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	579	LYS	CA-CB-CG	5.44	125.36	113.40
1	C	733	ILE	CB-CA-C	5.30	122.20	111.60
1	C	733	ILE	CG1-CB-CG2	5.29	123.04	111.40
1	B	740	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	656	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	674	SER	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	656	ARG	Sidechain
1	C	748	ARG	Sidechain
1	D	628	ILE	Peptide
1	D	748	ARG	Sidechain

## 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	1992	0	1983	64	3
1	B	1975	0	1966	80	1
1	C	1959	0	1952	66	2
1	D	1901	0	1896	78	0
2	A	11	0	0	1	0
2	B	5	0	0	2	0
2	C	2	0	0	0	0
2	D	5	0	0	2	0
All	All	7850	0	7797	273	3

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 17.

All (273) 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:A:602:LYS:HB2	1:A:605:ARG:NH1	1.52	1.23
1:B:588:HIS:O	1:B:592:LEU:HD23	1.57	1.04
1:B:605:ARG:NH1	1:B:640:HIS:O	2.02	0.93
1:A:516:THR:HG23	1:C:552:TRP:HE1	1.36	0.89
1:A:602:LYS:CB	1:A:605:ARG:NH1	2.37	0.86
1:B:602:LYS:HA	1:B:605:ARG:HG3	1.61	0.82
1:A:574:PHE:O	1:A:578:LEU:HB2	1.81	0.81
1:A:602:LYS:HB2	1:A:605:ARG:HH12	1.45	0.79
1:B:740:ARG:HG3	1:B:742:GLU:OE1	1.84	0.78
1:C:736:MET:CE	1:C:738:THR:HB	2.13	0.78
1:D:526:THR:O	1:D:529:LYS:HB2	1.84	0.78
1:C:736:MET:HE3	1:C:738:THR:HB	1.65	0.77
1:C:585:GLN:OE1	1:C:625:ALA:HA	1.84	0.77
1:D:672:ILE:C	1:D:673:ASN:HD22	1.89	0.77
1:A:605:ARG:HH21	1:A:644:ASP:CG	1.87	0.76
1:B:588:HIS:O	1:B:592:LEU:CD2	2.31	0.76
1:D:695:SER:OG	1:D:698:SER:OG	2.03	0.75
1:C:692:GLN:HG2	1:C:694:ILE:H	1.53	0.73
1:A:602:LYS:HB2	1:A:605:ARG:CZ	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:710:VAL:HG21	1:C:750:VAL:HG13	1.71	0.73
1:C:591:MET:O	1:C:595:LEU:HD22	1.90	0.72
1:A:620:LEU:HB3	1:A:623:SER:HB2	1.70	0.71
1:D:521:MET:HG2	1:D:564:MET:SD	2.30	0.70
1:B:736:MET:HG3	1:B:739:ALA:HB2	1.73	0.70
1:D:533:LYS:HE3	1:D:534:LYS:HG3	1.73	0.69
1:D:742:GLU:O	1:D:745:GLU:HB3	1.91	0.69
1:B:602:LYS:NZ	1:B:644:ASP:HB2	2.08	0.69
1:C:585:GLN:OE1	1:C:626:ASP:N	2.24	0.69
1:B:709:LEU:HB3	1:B:717:TYR:CD2	2.26	0.69
1:D:644:ASP:OD2	2:D:801:HOH:O	2.10	0.68
1:C:609:MET:HA	1:C:614:ILE:HD11	1.74	0.68
1:B:519:HIS:CD2	1:B:554:ILE:HG12	2.29	0.68
1:C:605:ARG:HH22	1:C:688:ARG:HH22	1.39	0.68
1:A:602:LYS:HA	1:A:605:ARG:HB2	1.75	0.68
1:C:599:ALA:O	1:C:605:ARG:NH1	2.29	0.66
1:C:746:MET:O	1:C:750:VAL:HG23	1.96	0.66
1:D:595:LEU:HA	1:D:598:VAL:HG12	1.78	0.65
1:D:692:GLN:HE21	1:D:699:GLN:HG3	1.61	0.65
1:D:576:ASP:HA	1:D:579:LYS:HE3	1.79	0.64
1:C:532:GLN:O	1:C:536:LEU:HD22	1.97	0.64
1:C:707:TYR:O	1:C:711:SER:OG	2.13	0.64
1:B:646:PRO:HB3	1:B:656:ARG:NH1	2.14	0.63
1:C:740:ARG:O	1:C:743:THR:OG1	2.16	0.63
1:D:557:GLU:OE2	2:D:802:HOH:O	2.15	0.62
1:A:605:ARG:NH2	1:A:644:ASP:OD2	2.33	0.62
1:A:605:ARG:NH2	1:A:644:ASP:OD1	2.32	0.62
1:C:591:MET:O	1:C:595:LEU:CD2	2.47	0.62
1:C:618:SER:HA	1:C:621:LEU:HD23	1.80	0.61
1:D:563:GLU:HG2	1:D:604:LEU:HD21	1.83	0.61
1:B:520:LYS:HB3	1:B:523:PHE:CE2	2.35	0.61
1:B:658:GLU:O	1:B:662:ARG:HG3	2.01	0.61
1:D:730:LEU:HB2	1:D:751:ILE:HD11	1.83	0.60
1:B:739:ALA:HB3	1:B:744:LYS:HE2	1.82	0.60
1:B:635:CYS:O	1:B:639:SER:OG	2.19	0.60
1:C:572:LYS:NZ	1:C:576:ASP:OD2	2.22	0.60
1:D:596:GLY:HA2	1:D:637:VAL:HG12	1.84	0.60
1:C:639:SER:HB3	1:C:698:SER:HA	1.83	0.59
1:B:649:TRP:HB3	1:B:656:ARG:NH2	2.17	0.59
1:B:668:GLN:NE2	2:B:801:HOH:O	2.17	0.59
1:B:602:LYS:NZ	1:B:644:ASP:CB	2.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:PHE:HZ	1:C:550:ALA:HB1	1.68	0.59
1:D:672:ILE:O	1:D:708:ASN:ND2	2.34	0.58
1:D:673:ASN:HA	1:D:712:VAL:HG21	1.85	0.58
1:B:520:LYS:H	1:B:523:PHE:HD2	1.50	0.58
1:D:588:HIS:O	1:D:592:LEU:HD23	2.03	0.58
1:D:586:GLU:HB3	1:D:589:ARG:NH1	2.19	0.57
1:A:597:ASN:HD21	1:C:516:THR:N	2.02	0.57
1:B:659:VAL:O	1:B:663:MET:HG3	2.05	0.57
1:B:609:MET:HE1	1:B:651:VAL:H	1.69	0.57
1:B:649:TRP:HB3	1:B:656:ARG:HH21	1.70	0.56
1:B:660:GLU:HA	1:B:663:MET:HE3	1.86	0.56
1:A:521:MET:HG3	1:A:564:MET:SD	2.45	0.56
1:A:699:GLN:O	1:A:703:THR:HG23	2.05	0.56
1:B:706:LEU:O	1:B:710:VAL:HG22	2.05	0.56
1:B:602:LYS:HZ2	1:B:644:ASP:CB	2.19	0.56
1:C:736:MET:HG2	1:C:739:ALA:N	2.21	0.56
1:B:609:MET:SD	1:B:649:TRP:HA	2.46	0.56
1:A:642:MET:HG2	1:A:656:ARG:CZ	2.36	0.56
1:B:646:PRO:CA	1:B:656:ARG:NH1	2.69	0.56
1:C:736:MET:HG2	1:C:739:ALA:H	1.70	0.55
1:B:538:LYS:NZ	1:B:580:GLU:OE1	2.27	0.55
1:D:550:ALA:O	1:D:554:ILE:HG13	2.06	0.55
1:B:646:PRO:HA	1:B:656:ARG:NH1	2.22	0.55
1:A:603:GLU:OE1	1:A:603:GLU:N	2.27	0.55
1:C:736:MET:HE2	1:C:738:THR:HB	1.88	0.54
1:D:726:GLY:O	1:D:730:LEU:HG	2.06	0.54
1:C:692:GLN:HG2	1:C:693:GLY:N	2.22	0.54
1:D:747:ALA:O	1:D:751:ILE:HG13	2.07	0.54
1:C:635:CYS:O	1:C:639:SER:OG	2.23	0.54
1:B:681:ARG:HG3	1:D:517:PHE:CE2	2.43	0.53
1:C:683:PHE:HB3	1:C:687:LEU:HD13	1.89	0.53
1:B:679:ASN:ND2	1:D:518:LEU:HD12	2.23	0.53
1:D:673:ASN:HA	1:D:712:VAL:CG2	2.39	0.52
1:C:638:LEU:O	1:C:642:MET:HB2	2.10	0.52
1:D:633:ASN:O	1:D:637:VAL:HG13	2.10	0.52
1:D:719:PRO:O	1:D:723:LYS:HB2	2.09	0.52
1:D:566:LEU:HD12	1:D:604:LEU:HD22	1.91	0.52
1:D:673:ASN:HD22	1:D:673:ASN:N	2.06	0.52
1:C:618:SER:O	1:C:621:LEU:HB2	2.09	0.52
1:D:615:SER:O	1:D:619:ASN:HB2	2.10	0.52
1:C:556:ASP:O	1:C:557:GLU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:PRO:HD3	1:A:757:PHE:CE2	2.44	0.52
1:D:555:THR:HG21	1:D:594:LEU:CD1	2.40	0.52
1:A:602:LYS:CB	1:A:605:ARG:CZ	2.85	0.52
1:B:709:LEU:HD22	1:B:717:TYR:CE2	2.45	0.51
1:D:660:GLU:HG3	1:D:697:VAL:HG21	1.92	0.51
1:D:628:ILE:HD11	1:D:676:ARG:CZ	2.40	0.51
1:D:706:LEU:HD22	1:D:721:LEU:HD22	1.93	0.51
1:A:605:ARG:NH2	1:A:644:ASP:CG	2.62	0.51
1:C:741:GLN:O	1:C:741:GLN:HG2	2.10	0.51
1:D:535:LEU:HD22	1:D:573:LEU:HD22	1.92	0.51
1:A:574:PHE:HA	1:A:591:MET:HE2	1.93	0.50
1:B:659:VAL:HG12	1:B:662:ARG:HD3	1.93	0.50
1:A:755:SER:HB3	1:D:564:MET:HE1	1.94	0.50
1:C:682:SER:HA	1:C:720:LEU:HD21	1.93	0.50
1:B:704:TRP:CD1	1:B:746:MET:HE1	2.47	0.50
1:C:707:TYR:HA	1:C:750:VAL:HG22	1.93	0.50
1:A:566:LEU:HD12	1:A:604:LEU:HD22	1.94	0.50
1:D:552:TRP:CE3	1:D:590:ASN:HA	2.48	0.49
1:D:682:SER:HA	1:D:720:LEU:HD21	1.94	0.49
1:B:676:ARG:NH1	1:B:708:ASN:OD1	2.45	0.49
1:A:546:PHE:CZ	1:C:550:ALA:HB1	2.47	0.49
1:B:646:PRO:CB	1:B:656:ARG:NH1	2.75	0.49
1:B:523:PHE:HB3	1:D:546:PHE:HE1	1.78	0.48
1:B:525:VAL:HG13	1:B:568:PHE:CE2	2.48	0.48
1:D:605:ARG:HH12	1:D:688:ARG:HH22	1.59	0.48
1:A:642:MET:HA	1:A:656:ARG:HH22	1.77	0.48
1:A:562:CYS:HB3	1:A:598:VAL:HG22	1.95	0.48
1:C:733:ILE:N	1:C:733:ILE:HD12	2.28	0.48
1:D:722:ILE:HG13	1:D:723:LYS:N	2.28	0.48
1:C:733:ILE:HG13	1:C:736:MET:SD	2.54	0.48
1:A:694:ILE:HD12	1:A:694:ILE:H	1.78	0.48
1:C:635:CYS:SG	1:C:663:MET:HG2	2.53	0.48
1:C:733:ILE:O	1:C:736:MET:HB3	2.14	0.48
1:D:524:VAL:O	1:D:528:LEU:HD12	2.14	0.48
1:D:634:ALA:O	1:D:637:VAL:HG22	2.13	0.48
1:B:653:GLU:OE2	1:B:655:GLN:HG2	2.12	0.48
1:B:679:ASN:HD22	1:D:518:LEU:HD12	1.78	0.48
1:B:747:ALA:O	1:B:750:VAL:HG12	2.14	0.48
1:B:548:TRP:CE3	1:B:591:MET:HG2	2.48	0.48
1:B:602:LYS:HZ1	1:B:644:ASP:HB2	1.79	0.48
1:A:739:ALA:HB3	1:A:744:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:706:LEU:O	1:D:710:VAL:HG22	2.14	0.48
1:C:683:PHE:O	1:C:686:ILE:HG12	2.14	0.47
1:A:746:MET:O	1:A:750:VAL:HG23	2.14	0.47
1:B:639:SER:HB3	1:B:698:SER:HA	1.96	0.47
1:D:612:GLN:HA	1:D:615:SER:HB3	1.95	0.47
1:B:524:VAL:HG23	1:B:551:LEU:HD22	1.97	0.47
1:B:562:CYS:HB3	1:B:598:VAL:HG22	1.97	0.47
1:B:587:LEU:HD23	1:B:588:HIS:HD2	1.78	0.47
1:A:670:TRP:HB2	1:A:704:TRP:CZ2	2.50	0.47
1:A:672:ILE:HD11	1:A:704:TRP:HE1	1.79	0.47
1:A:692:GLN:NE2	1:A:695:SER:O	2.48	0.47
1:D:620:LEU:O	1:D:631:SER:HB3	2.15	0.47
1:A:718:CYS:N	1:A:719:PRO:HD2	2.30	0.46
1:D:538:LYS:HD2	1:D:580:GLU:CD	2.36	0.46
1:A:538:LYS:HE3	1:A:580:GLU:OE1	2.16	0.46
1:C:562:CYS:HB3	1:C:598:VAL:HG22	1.97	0.46
1:D:569:ASN:HB2	1:D:572:LYS:HD2	1.97	0.46
1:B:680:TYR:HB2	1:B:717:TYR:CE1	2.51	0.46
1:A:642:MET:HA	1:A:656:ARG:NH2	2.31	0.46
1:C:563:GLU:HG2	1:C:604:LEU:HD21	1.97	0.46
1:B:614:ILE:HG21	1:B:649:TRP:CZ2	2.51	0.45
1:B:660:GLU:HG3	1:B:697:VAL:HG11	1.97	0.45
1:D:548:TRP:CE3	1:D:591:MET:HG2	2.51	0.45
1:B:544:MET:HE2	1:B:587:LEU:HD11	1.97	0.45
1:B:534:LYS:HE3	1:B:541:ASP:OD2	2.16	0.45
1:C:664:TRP:CH2	1:C:740:ARG:HG3	2.52	0.45
1:D:533:LYS:HE2	1:D:533:LYS:HB3	1.46	0.45
1:A:519:HIS:CE1	1:A:554:ILE:HG13	2.50	0.45
1:A:575:LEU:O	1:A:578:LEU:HB3	2.17	0.45
1:C:605:ARG:HH22	1:C:688:ARG:NH2	2.08	0.45
1:C:713:TYR:HB2	1:C:717:TYR:HD2	1.81	0.45
1:C:733:ILE:HA	1:C:736:MET:HB2	1.98	0.45
1:A:653:GLU:HA	1:A:654:PRO:C	2.37	0.45
1:A:727:MET:HE1	1:A:751:ILE:HA	1.99	0.45
1:D:524:VAL:HG21	1:D:561:ASN:HB3	1.98	0.45
1:D:535:LEU:HD13	1:D:577:CYS:SG	2.57	0.45
1:D:719:PRO:HA	1:D:722:ILE:HG12	1.98	0.45
1:A:585:GLN:OE1	1:A:625:ALA:HA	2.17	0.45
1:B:646:PRO:CA	1:B:656:ARG:HH12	2.29	0.45
1:B:646:PRO:CB	1:B:656:ARG:HH12	2.29	0.45
1:B:680:TYR:HB2	1:B:717:TYR:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:LYS:HB3	1:B:605:ARG:NH2	2.33	0.44
1:C:605:ARG:NH2	1:C:688:ARG:HH22	2.11	0.44
1:C:684:GLU:N	1:C:685:PRO:HD2	2.33	0.44
1:A:603:GLU:H	1:A:603:GLU:CD	2.16	0.44
1:D:664:TRP:CZ2	1:D:697:VAL:HG22	2.52	0.44
1:C:606:PRO:HA	1:C:609:MET:HG3	1.98	0.44
1:B:586:GLU:HG2	1:B:589:ARG:NH2	2.32	0.44
1:B:622:GLU:OE1	1:B:662:ARG:NH2	2.46	0.44
1:C:528:LEU:HD13	1:C:568:PHE:HB3	2.00	0.44
1:D:638:LEU:HA	1:D:641:ILE:HG12	2.00	0.44
1:B:687:LEU:O	1:B:691:PRO:HG3	2.18	0.44
1:A:523:PHE:O	1:A:527:MET:HG3	2.17	0.44
1:A:586:GLU:OE1	1:A:589:ARG:NH2	2.49	0.44
1:A:602:LYS:CA	1:A:605:ARG:NH1	2.80	0.44
1:A:618:SER:HA	1:A:621:LEU:HD12	1.99	0.44
1:C:519:HIS:CE1	1:C:554:ILE:HD13	2.53	0.44
1:D:521:MET:SD	1:D:564:MET:HG3	2.57	0.44
1:D:572:LYS:HA	1:D:575:LEU:HD12	2.00	0.44
1:D:599:ALA:O	1:D:605:ARG:NH1	2.44	0.44
1:D:742:GLU:C	1:D:745:GLU:HB3	2.38	0.44
1:A:755:SER:CB	1:D:564:MET:HE1	2.47	0.44
1:D:531:ILE:O	1:D:535:LEU:N	2.50	0.44
1:A:624:LYS:HA	1:A:624:LYS:HD3	1.74	0.44
1:D:571:MET:O	1:D:575:LEU:HG	2.17	0.44
1:B:602:LYS:HZ2	1:B:644:ASP:HB2	1.77	0.43
1:A:551:LEU:HA	1:A:554:ILE:HG22	2.00	0.43
1:A:592:LEU:HA	1:A:592:LEU:HD13	1.83	0.43
1:B:572:LYS:HE3	1:B:572:LYS:HB3	1.90	0.43
1:A:642:MET:HE3	1:A:642:MET:HB2	1.39	0.43
1:D:719:PRO:O	1:D:722:ILE:HG13	2.18	0.43
1:A:611:SER:O	1:A:615:SER:HB2	2.19	0.43
1:C:621:LEU:HD21	1:C:638:LEU:HD12	1.99	0.43
1:C:719:PRO:O	1:C:723:LYS:HB2	2.19	0.43
1:B:540:CYS:HB2	1:B:581:PHE:CD1	2.54	0.43
1:B:646:PRO:O	1:B:656:ARG:NH2	2.51	0.43
1:A:601:VAL:O	1:A:605:ARG:HG3	2.19	0.43
1:D:605:ARG:HH22	1:D:688:ARG:HH22	1.66	0.43
1:B:618:SER:OG	1:B:659:VAL:HG11	2.19	0.43
1:A:743:THR:OG1	2:A:801:HOH:O	2.22	0.43
1:B:535:LEU:HD11	1:B:576:ASP:HB3	2.00	0.42
1:B:556:ASP:O	1:B:558:THR:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:LYS:HE2	1:B:624:LYS:HB2	1.92	0.42
1:B:671:ASP:OD2	2:B:802:HOH:O	2.21	0.42
1:A:602:LYS:HA	1:A:605:ARG:CB	2.46	0.42
1:A:602:LYS:N	1:A:605:ARG:HH11	2.16	0.42
1:C:610:THR:O	1:C:614:ILE:HD12	2.19	0.42
1:C:713:TYR:HB2	1:C:717:TYR:CD2	2.53	0.42
1:C:733:ILE:N	1:C:733:ILE:CD1	2.81	0.42
1:C:736:MET:HG2	1:C:739:ALA:CB	2.49	0.42
1:B:548:TRP:CD2	1:B:591:MET:HG2	2.54	0.42
1:D:578:LEU:HD23	1:D:578:LEU:HA	1.83	0.42
1:D:584:LYS:HA	1:D:584:LYS:HE2	2.01	0.42
1:B:523:PHE:HB3	1:D:546:PHE:CE1	2.54	0.42
1:B:733:ILE:HD13	1:B:736:MET:SD	2.60	0.42
1:D:618:SER:O	1:D:621:LEU:HB2	2.19	0.42
1:A:622:GLU:CD	1:A:662:ARG:HH21	2.23	0.42
1:B:742:GLU:OE1	1:B:742:GLU:N	2.49	0.42
1:A:516:THR:N	1:C:556:ASP:OD1	2.53	0.42
1:A:575:LEU:HD11	1:A:613:PHE:HE1	1.84	0.42
1:C:730:LEU:HB3	1:C:747:ALA:HB1	2.02	0.42
1:B:520:LYS:HB3	1:B:520:LYS:HE3	1.83	0.42
1:B:719:PRO:O	1:B:722:ILE:HG13	2.19	0.42
1:A:517:PHE:HB2	1:C:553:ASN:OD1	2.20	0.42
1:C:638:LEU:HB3	1:C:663:MET:HE1	2.01	0.42
1:D:571:MET:O	1:D:574:PHE:HB3	2.19	0.42
1:A:584:LYS:HD3	1:A:584:LYS:HA	1.91	0.41
1:B:653:GLU:HA	1:B:654:PRO:C	2.41	0.41
1:C:736:MET:HG2	1:C:739:ALA:HB2	2.01	0.41
1:C:584:LYS:HD2	1:C:584:LYS:HA	1.72	0.41
1:C:602:LYS:HG2	1:C:605:ARG:NH2	2.35	0.41
1:D:555:THR:HG21	1:D:594:LEU:HD12	2.00	0.41
1:D:565:PHE:CE1	1:D:594:LEU:HD21	2.54	0.41
1:D:577:CYS:HB2	1:D:591:MET:HE3	2.03	0.41
1:B:546:PHE:HD1	1:D:523:PHE:CD1	2.39	0.41
1:C:692:GLN:HG2	1:C:694:ILE:N	2.28	0.41
1:D:587:LEU:O	1:D:591:MET:HG3	2.20	0.41
1:A:663:MET:O	1:A:667:ILE:HG13	2.20	0.41
1:A:531:ILE:HD13	1:A:548:TRP:CE2	2.55	0.41
1:D:605:ARG:HH12	1:D:688:ARG:NH2	2.18	0.41
1:B:527:MET:HB2	1:B:551:LEU:HD21	2.03	0.41
1:B:709:LEU:HD22	1:B:717:TYR:HE2	1.85	0.41
1:C:575:LEU:HD11	1:C:613:PHE:HE1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:LEU:HD12	1:B:577:CYS:SG	2.61	0.40
1:B:523:PHE:CD1	1:D:546:PHE:HD1	2.40	0.40
1:B:611:SER:HB3	1:B:653:GLU:O	2.21	0.40
1:A:602:LYS:HA	1:A:605:ARG:CG	2.52	0.40
1:C:601:VAL:HG11	1:C:604:LEU:HD12	2.03	0.40
1:D:663:MET:HG3	1:D:697:VAL:HG11	2.03	0.40
1:D:672:ILE:HD11	1:D:707:TYR:CD2	2.56	0.40
1:A:652:CYS:O	1:A:653:GLU:HG2	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ILE:CD1	1:C:653:GLU:OE1[1_655]	1.55	0.65
1:A:694:ILE:CG1	1:C:653:GLU:OE1[1_655]	1.91	0.29
1:B:759:GLU:OE2	1:A:542:GLN:OE1[1_665]	2.13	0.07

## 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	243/251 (97%)	231 (95%)	12 (5%)	0	100	100
1	B	239/251 (95%)	230 (96%)	9 (4%)	0	100	100
1	C	237/251 (94%)	231 (98%)	6 (2%)	0	100	100
1	D	226/251 (90%)	216 (96%)	10 (4%)	0	100	100
All	All	945/1004 (94%)	908 (96%)	37 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	222/228 (97%)	218 (98%)	4 (2%)	59	83
1	B	220/228 (96%)	212 (96%)	8 (4%)	35	64
1	C	218/228 (96%)	208 (95%)	10 (5%)	27	54
1	D	211/228 (92%)	204 (97%)	7 (3%)	38	67
All	All	871/912 (96%)	842 (97%)	29 (3%)	38	67

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	533	LYS
1	B	568	PHE
1	B	587	LEU
1	B	609	MET
1	B	669	SER
1	B	673	ASN
1	B	684	GLU
1	B	692	GLN
1	A	537	ASP
1	A	542	GLN
1	A	626	ASP
1	A	631	SER
1	C	533	LYS
1	C	538	LYS
1	C	540	CYS
1	C	546	PHE
1	C	579	LYS
1	C	624	LYS
1	C	647	GLU
1	C	655	GLN
1	C	688	ARG
1	C	692	GLN
1	D	518	LEU
1	D	544	MET

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Mol	Chain	Res	Type
1	D	579	LYS
1	D	602	LYS
1	D	615	SER
1	D	662	ARG
1	D	688	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	519	HIS
1	A	612	GLN
1	D	532	GLN
1	D	569	ASN
1	D	673	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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, 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	245/251 (97%)	0.04	4 (1%) 72 74	46, 71, 102, 122	0
1	B	243/251 (96%)	0.14	1 (0%) 92 93	50, 74, 104, 120	0
1	C	241/251 (96%)	0.20	9 (3%) 41 41	45, 80, 112, 134	0
1	D	234/251 (93%)	0.88	34 (14%) 2 1	55, 111, 140, 153	0
All	All	963/1004 (95%)	0.31	48 (4%) 28 27	45, 80, 127, 153	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	628	ILE	7.7
1	D	675	ARG	5.3
1	D	710	VAL	5.0
1	D	674	SER	4.8
1	D	728	PRO	4.7
1	D	646	PRO	4.6
1	C	741	GLN	4.4
1	D	659	VAL	4.3
1	C	648	ALA	3.8
1	D	543	VAL	3.7
1	C	736	MET	3.7
1	D	650	GLY	3.5
1	D	703	THR	3.4
1	C	726	GLY	3.3
1	D	645	GLY	3.3
1	D	709	LEU	3.3
1	C	609	MET	3.3
1	D	687	LEU	3.1
1	D	743	THR	3.1
1	C	643	PHE	3.1
1	D	711	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	685	PRO	3.0
1	D	608	LEU	2.9
1	C	753	HIS	2.8
1	D	715	ASP	2.8
1	D	629	GLU	2.7
1	D	648	ALA	2.6
1	A	620	LEU	2.6
1	D	750	VAL	2.6
1	D	706	LEU	2.6
1	A	649	TRP	2.6
1	D	643	PHE	2.6
1	D	673	ASN	2.5
1	D	630	VAL	2.4
1	D	752	GLU	2.3
1	B	645	GLY	2.3
1	D	633	ASN	2.3
1	D	713	TYR	2.3
1	D	729	LEU	2.3
1	C	756	ASN	2.2
1	D	747	ALA	2.2
1	D	546	PHE	2.2
1	A	646	PRO	2.2
1	D	621	LEU	2.2
1	A	542	GLN	2.1
1	C	710	VAL	2.1
1	D	661	GLU	2.1
1	D	620	LEU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.