



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:46 PM UTC

PDB ID : 7XYU / pdb_00007xyu
Title : Crystal structure of ZER1 bound to TFLH degron
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

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

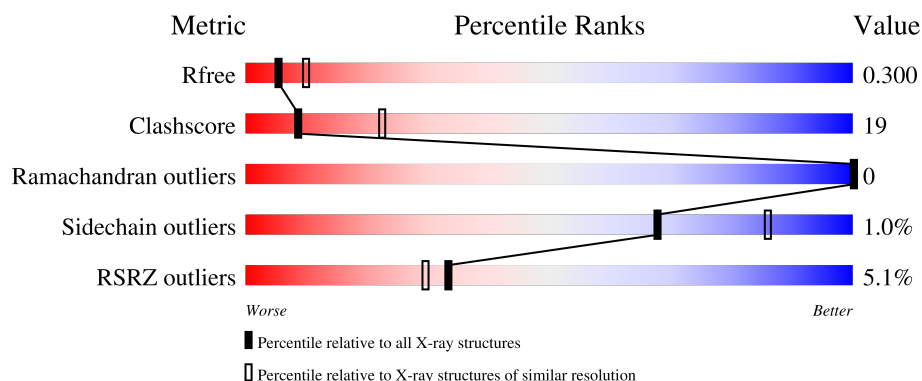
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 ≥ 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	2% 67% 30% ..
1	B	251	2% 61% 34% ..
1	C	251	5% 62% 31% ..
1	D	251	10% 51% 39% 7%

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

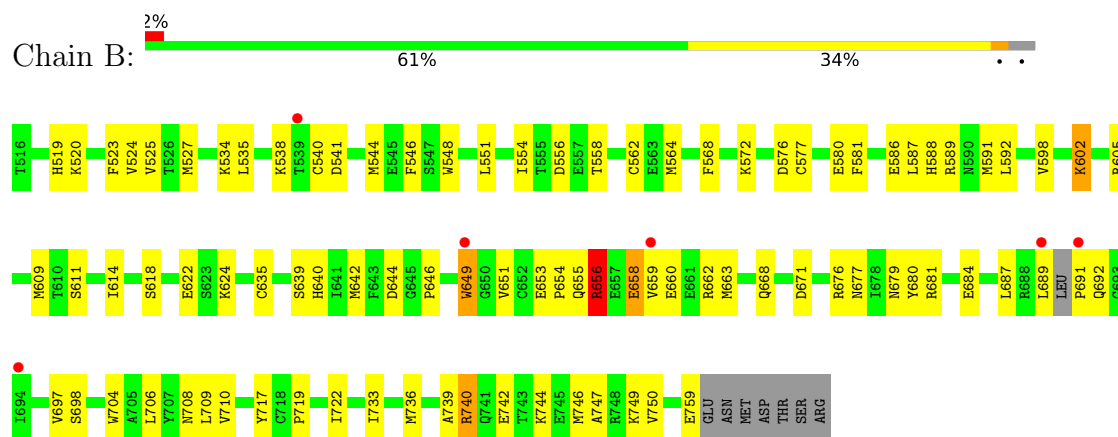
- Molecule 2 is water.

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

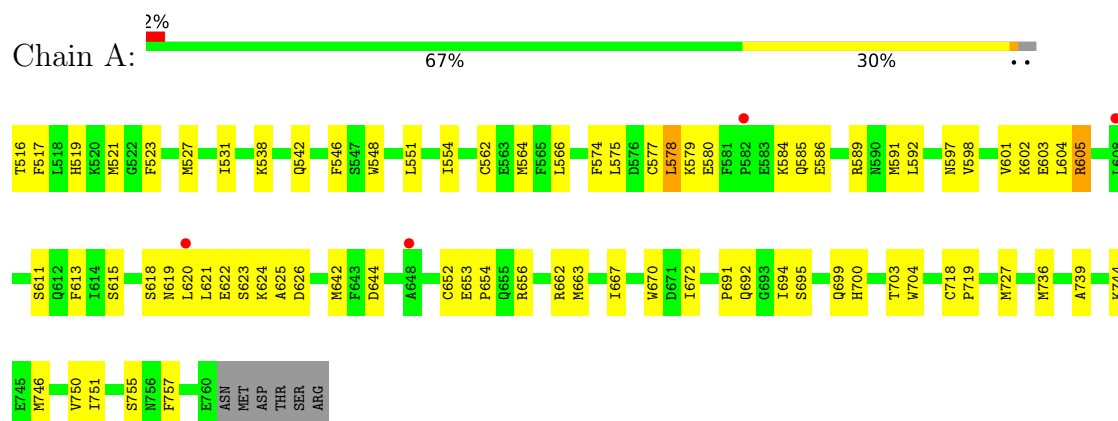
3 Residue-property plots

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.

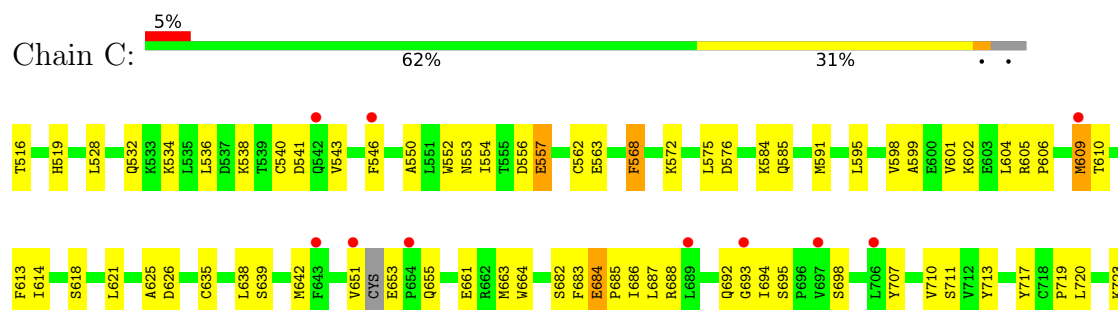
• Molecule 1: Protein zer-1 homolog

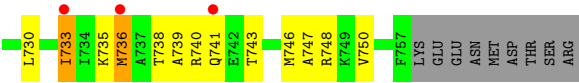


• Molecule 1: Protein zer-1 homolog

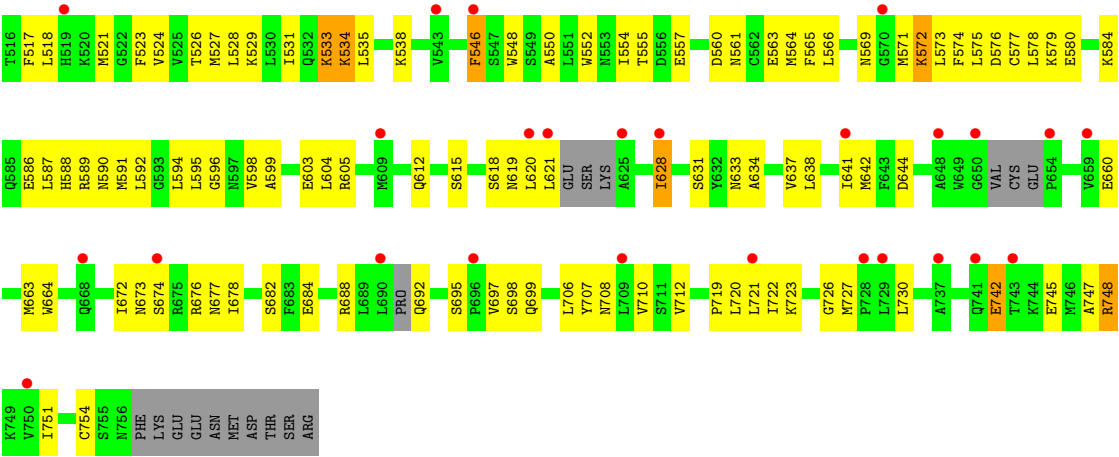


• Molecule 1: Protein zer-1 homolog





● Molecule 1: Protein zer-1 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	67.78Å 67.78Å 418.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.90 – 2.70 44.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.90-2.70) 100.0 (44.90-2.70)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.248 , 0.304 0.249 , 0.300	Depositor DCC
R_{free} test set	2010 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.096 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7850	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.45	1/2038 (0.0%)	0.75	6/2753 (0.2%)
1	B	0.46	1/2020 (0.0%)	0.75	5/2726 (0.2%)
1	C	0.46	1/2004 (0.0%)	0.85	9/2707 (0.3%)
1	D	0.51	2/1942 (0.1%)	1.07	21/2619 (0.8%)
All	All	0.47	5/8004 (0.1%)	0.86	41/10805 (0.4%)

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	A	691	PRO	CA-CB	-12.40	1.45	1.53
1	D	748	ARG	CB-CG	-7.12	1.31	1.52
1	C	733	ILE	CG1-CD1	-6.49	1.26	1.51
1	B	602	LYS	CD-CE	6.04	1.70	1.52
1	D	748	ARG	CZ-NH2	-5.85	1.25	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	748	ARG	CG-CD-NE	-11.43	86.86	112.00
1	D	742	GLU	CA-CB-CG	10.14	134.38	114.10
1	C	609	MET	CB-CG-SD	9.99	142.67	112.70
1	D	603	GLU	CB-CA-C	-9.65	92.77	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	674	SER	CA-C-N	9.40	134.21	120.87
1	D	674	SER	C-N-CA	9.40	134.21	120.87
1	D	572	LYS	CD-CE-NZ	-8.18	85.73	111.90
1	C	543	VAL	N-CA-C	-7.66	101.55	112.35
1	D	546	PHE	CB-CA-C	-7.48	98.37	110.79
1	C	695	SER	O-C-N	-7.32	116.88	121.27
1	A	605	ARG	CB-CG-CD	7.16	127.77	111.30
1	D	684	GLU	CA-CB-CG	6.96	128.02	114.10
1	D	748	ARG	NE-CZ-NH2	-6.86	113.02	119.20
1	D	603	GLU	CA-CB-CG	6.59	127.28	114.10
1	C	684	GLU	N-CA-CB	-6.54	100.29	110.43
1	B	658	GLU	CA-CB-CG	6.47	127.04	114.10
1	B	649	TRP	CA-CB-CG	6.28	125.53	113.60
1	B	749	LYS	CD-CE-NZ	-6.28	91.82	111.90
1	A	605	ARG	CG-CD-NE	6.27	125.80	112.00
1	D	748	ARG	NE-CZ-NH1	6.01	127.52	121.50
1	C	557	GLU	CA-CB-CG	5.93	125.97	114.10
1	B	740	ARG	CA-CB-CG	5.84	125.79	114.10
1	D	534	LYS	CA-CB-CG	-5.79	102.52	114.10
1	A	578	LEU	CA-CB-CG	5.75	136.42	116.30
1	D	684	GLU	N-CA-CB	-5.68	100.46	110.34
1	A	579	LYS	CA-CB-CG	5.63	125.36	114.10
1	D	742	GLU	N-CA-CB	5.57	118.88	110.30
1	B	656	ARG	CB-CG-CD	-5.51	98.62	111.30
1	D	533	LYS	CA-C-N	-5.50	113.09	122.56
1	D	533	LYS	C-N-CA	-5.50	113.09	122.56
1	D	603	GLU	N-CA-CB	5.48	118.66	110.22
1	A	619	ASN	CA-C-N	-5.46	114.42	122.83
1	A	619	ASN	C-N-CA	-5.46	114.42	122.83
1	C	568	PHE	N-CA-C	-5.38	107.26	112.97
1	D	572	LYS	CB-CG-CD	-5.22	99.28	111.30
1	D	533	LYS	CB-CA-C	-5.19	102.97	110.96
1	C	736	MET	CB-CA-C	-5.18	101.21	109.75
1	D	572	LYS	CG-CD-CE	5.17	123.20	111.30
1	D	534	LYS	CB-CG-CD	5.13	123.09	111.30
1	C	735	LYS	CA-C-N	5.02	129.65	122.72
1	C	735	LYS	C-N-CA	5.02	129.65	122.72

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 [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	1992	0	1983	67	3
1	B	1975	0	1966	88	1
1	C	1959	0	1952	67	2
1	D	1901	0	1896	89	0
2	A	11	0	0	0	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	294	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 19.

All (294) 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:C:736:MET:HE3	1:C:738:THR:HB	1.49	0.95
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:605:ARG:HH21	1:A:644:ASP:CG	1.87	0.81
1:D:672:ILE:C	1:D:673:ASN:HD22	1.89	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:585:GLN:OE1	1:C:625:ALA:HA	1.84	0.77
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
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:C:642:MET:HE3	1:C:663:MET:HE1	1.73	0.70
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:A:642:MET:HE1	1:A:663:MET:SD	2.37	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:A:574:PHE:HA	1:A:591:MET:HE2	1.80	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:727:MET:HE1	1:A:751:ILE:HA	1.84	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
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:527:MET:HE3	1:D:546:PHE:CD2	2.39	0.57
1:B:659:VAL:O	1:B:663:MET:HG3	2.05	0.57
1:B:649:TRP:HB3	1:B:656:ARG:HH21	1.70	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:D:574:PHE:HD2	1:D:591:MET:HE2	1.71	0.55
1:A:605:ARG:NH2	1:A:644:ASP:CG	2.62	0.55
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:B:642:MET:HE1	1:B:656:ARG:HG2	1.87	0.55
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:D:527:MET:HE2	1:D:527:MET:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:MET:HE1	1:B:651:VAL:H	1.71	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
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:A:577:CYS:HB2	1:A:591:MET:HE1	1.92	0.51
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:B:544:MET:HE2	1:B:587:LEU:HD11	1.93	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:D:538:LYS:HD2	1:D:580:GLU:CD	2.36	0.50
1:D:569:ASN:CG	1:D:572:LYS:HZ2	2.19	0.50
1:B:659:VAL:HG12	1:B:662:ARG:HD3	1.93	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:A:653:GLU:HA	1:A:654:PRO:C	2.37	0.49
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:660:GLU:HA	1:B:663:MET:HE3	1.93	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:A:603:GLU:H	1:A:603:GLU:CD	2.16	0.49
1:B:646:PRO:CB	1:B:656:ARG:NH1	2.75	0.49
1:D:521:MET:HE2	1:D:560:ASP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:742:GLU:C	1:D:745:GLU:HB3	2.38	0.48
1:A:642:MET:HA	1:A:656:ARG:HH22	1.77	0.48
1:B:564:MET:HE3	1:B:564:MET:HB2	1.71	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:A:755:SER:HB3	1:D:564:MET:HE1	1.95	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
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:D:642:MET:HE1	1:D:697:VAL:HB	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:622:GLU:CD	1:A:662:ARG:HH21	2.23	0.47
1:A:718:CYS:N	1:A:719:PRO:HD2	2.30	0.46
1:A:538:LYS:HE3	1:A:580:GLU:OE1	2.16	0.46
1:B:653:GLU:HA	1:B:654:PRO:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:MET:HE3	1:A:736:MET:HA	1.96	0.46
1:B:642:MET:HE3	1:B:663:MET:HE1	1.98	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: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:D:727:MET:HE1	1:D:754:CYS:SG	2.57	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
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:700:HIS:CE1	1:A:746:MET:HE2	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:531:ILE:O	1:D:535:LEU:N	2.50	0.44
1:D:663:MET:HE2	1:D:663:MET:HB3	1.80	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:C:642:MET:CE	1:C:663:MET:HE1	2.45	0.43
1:B:572:LYS:HE3	1:B:572:LYS:HB3	1.90	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:B:677:ASN:C	1:D:518:LEU:HD13	2.44	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
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:B:609:MET:HB3	1:B:609:MET:HE3	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:571:MET:O	1:D:574:PHE:HB3	2.19	0.42
1:B:609:MET:HE1	1:B:651:VAL:HG23	2.02	0.41
1:A:584:LYS:HD3	1:A:584:LYS:HA	1.91	0.41
1:D:672:ILE:C	1:D:708:ASN:HD22	2.23	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: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:577:CYS:HB2	1:D:591:MET:HE1	2.03	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:B:689:LEU:C	1:B:691:PRO:HD2	2.45	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:D:677:ASN:C	1:D:678:ILE:HG12	2.46	0.41
1:B:527:MET:HB2	1:B:551:LEU:HD21	2.03	0.41
1:C:534:LYS:HE2	1:C:541:ASP:CG	2.46	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
1:B:535:LEU:HD12	1:B:577:CYS:SG	2.61	0.40
1:A:755:SER:CB	1:D:564:MET:HE1	2.50	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
1:A:736:MET:O	1:A:744:LYS:NZ	2.49	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 [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	222/228 (97%)	221 (100%)	1 (0%)	81	92
1	B	220/228 (96%)	218 (99%)	2 (1%)	70	87
1	C	218/228 (96%)	212 (97%)	6 (3%)	38	68
1	D	211/228 (92%)	211 (100%)	0	100	100
All	All	871/912 (96%)	862 (99%)	9 (1%)	68	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	684	GLU
1	B	692	GLN
1	A	626	ASP
1	C	538	LYS
1	C	540	CYS
1	C	546	PHE
1	C	651	VAL
1	C	655	GLN
1	C	661	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	519	HIS
1	B	585	GLN
1	B	668	GLN
1	B	679	ASN
1	A	532	GLN
1	A	612	GLN
1	D	532	GLN
1	D	569	ASN
1	D	590	ASN
1	D	612	GLN
1	D	619	ASN
1	D	673	ASN
1	D	692	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	245/251 (97%)	0.27	4 (1%) 70 68	46, 71, 102, 122	0
1	B	243/251 (96%)	0.40	6 (2%) 58 55	50, 74, 104, 120	0
1	C	241/251 (96%)	0.46	13 (5%) 31 27	45, 80, 112, 134	0
1	D	234/251 (93%)	0.99	26 (11%) 10 8	55, 111, 140, 153	0
All	All	963/1004 (95%)	0.53	49 (5%) 33 29	45, 80, 127, 153	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	628	ILE	4.6
1	B	691	PRO	3.7
1	A	620	LEU	3.4
1	D	543	VAL	3.0
1	A	648	ALA	2.9
1	D	690	LEU	2.8
1	B	659	VAL	2.8
1	C	651	VAL	2.8
1	C	741	GLN	2.7
1	A	582	PRO	2.6
1	D	654	PRO	2.6
1	D	641	ILE	2.6
1	C	733	ILE	2.6
1	C	654	PRO	2.6
1	D	709	LEU	2.5
1	B	649	TRP	2.5
1	D	721	LEU	2.5
1	D	609	MET	2.5
1	D	729	LEU	2.5
1	D	625	ALA	2.4
1	D	728	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	546	PHE	2.4
1	D	620	LEU	2.4
1	D	650	GLY	2.4
1	C	643	PHE	2.4
1	C	736	MET	2.3
1	B	539	THR	2.3
1	C	542	GLN	2.3
1	D	741	GLN	2.3
1	D	570	GLY	2.2
1	D	696	PRO	2.2
1	C	706	LEU	2.2
1	C	609	MET	2.2
1	B	694	ILE	2.2
1	D	743	THR	2.1
1	C	689	LEU	2.1
1	D	519	HIS	2.1
1	D	621	LEU	2.1
1	D	659	VAL	2.1
1	D	750	VAL	2.1
1	A	608	LEU	2.1
1	D	737	ALA	2.0
1	D	546	PHE	2.0
1	D	648	ALA	2.0
1	D	674	SER	2.0
1	B	689	LEU	2.0
1	D	668	GLN	2.0
1	C	693	GLY	2.0
1	C	697	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.