



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:35 AM UTC

PDB ID : 5ZQ5 / pdb_00005zq5
Title : SidE-Ubi
Authors : Wang, Y.; Gao, A.; Gao, P.
Deposited on : 2018-04-17
Resolution : 2.49 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
Mogul : 2022.3.0, CSD as543be (2022)
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

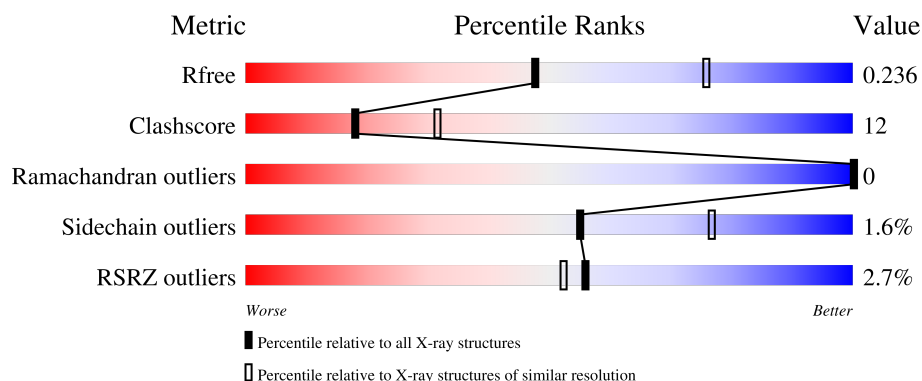
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	845	% 81%16%.
1	C	845	3% 74%21%..
2	B	79	77%19%.
2	D	79	13% 42%51%...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14624 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 Side.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	828	Total	C	N	O	S	Se	0	0	0
			6606	4164	1153	1267	6	16			
1	C	824	Total	C	N	O	S	Se	0	0	0
			6578	4149	1149	1258	6	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	MSE	-	initiating methionine	UNP Q6RCR1
A	1058	LEU	-	expression tag	UNP Q6RCR1
A	1059	GLU	-	expression tag	UNP Q6RCR1
A	1060	HIS	-	expression tag	UNP Q6RCR1
A	1061	HIS	-	expression tag	UNP Q6RCR1
A	1062	HIS	-	expression tag	UNP Q6RCR1
A	1063	HIS	-	expression tag	UNP Q6RCR1
A	1064	HIS	-	expression tag	UNP Q6RCR1
A	1065	HIS	-	expression tag	UNP Q6RCR1
C	221	MSE	-	initiating methionine	UNP Q6RCR1
C	1058	LEU	-	expression tag	UNP Q6RCR1
C	1059	GLU	-	expression tag	UNP Q6RCR1
C	1060	HIS	-	expression tag	UNP Q6RCR1
C	1061	HIS	-	expression tag	UNP Q6RCR1
C	1062	HIS	-	expression tag	UNP Q6RCR1
C	1063	HIS	-	expression tag	UNP Q6RCR1
C	1064	HIS	-	expression tag	UNP Q6RCR1
C	1065	HIS	-	expression tag	UNP Q6RCR1

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	0
			595	375	102	117	1			

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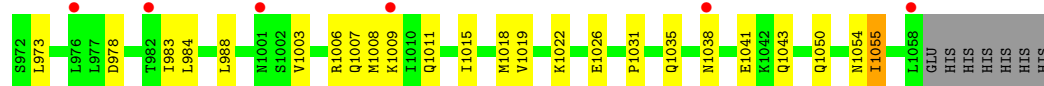
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	76	Total	C	N	O	S	0	0	0
			595	375	102	117	1			

There are 8 discrepancies between the modelled and reference sequences:

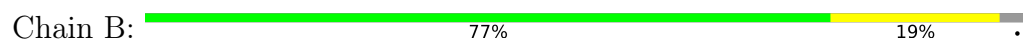
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P0CG48
B	-1	GLY	-	expression tag	UNP P0CG48
B	0	SER	-	expression tag	UNP P0CG48
B	42	ALA	ARG	engineered mutation	UNP P0CG48
D	-2	GLY	-	expression tag	UNP P0CG48
D	-1	GLY	-	expression tag	UNP P0CG48
D	0	SER	-	expression tag	UNP P0CG48
D	42	ALA	ARG	engineered mutation	UNP P0CG48

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	138	Total	O	0	0
			138	138		
3	B	3	Total	O	0	0
			3	3		
3	D	2	Total	O	0	0
			2	2		
3	C	107	Total	O	0	0
			107	107		



- Molecule 2: Ubiquitin



- Molecule 2: Ubiquitin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.67Å 129.08Å 191.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.69 – 2.49 48.69 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.69-2.49) 99.5 (48.69-2.49)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.190 , 0.233 0.199 , 0.236	Depositor DCC
R_{free} test set	4061 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14624	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.44	7/6720 (0.1%)	0.50	6/9053 (0.1%)
1	C	0.53	6/6692 (0.1%)	0.55	11/9016 (0.1%)
2	B	0.47	1/601 (0.2%)	0.45	0/809
2	D	0.84	3/601 (0.5%)	0.92	2/809 (0.2%)
All	All	0.51	17/14614 (0.1%)	0.54	19/19687 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	37	PRO	C-O	-8.97	1.17	1.24
2	D	37	PRO	CA-C	-7.69	1.47	1.52
1	C	823	PRO	C-O	-6.94	1.15	1.24
1	C	826	ILE	C-O	-6.86	1.16	1.24
1	A	597	ASN	C-O	-6.59	1.15	1.23
1	A	596	PRO	C-O	-6.31	1.16	1.23
1	A	365	LEU	C-O	-6.07	1.16	1.24
1	A	369	VAL	C-O	-5.90	1.17	1.24
1	A	364	THR	C-O	-5.75	1.17	1.24
1	C	408	VAL	C-O	-5.69	1.17	1.23
1	A	599	ASP	C-O	-5.69	1.16	1.24
2	B	61	ILE	C-O	-5.63	1.18	1.24
1	C	824	ARG	C-O	-5.62	1.17	1.24
1	C	951	PHE	N-CA	-5.54	1.39	1.46
1	A	408	VAL	C-O	-5.48	1.17	1.23
1	C	825	THR	C-O	-5.35	1.16	1.23
2	D	37	PRO	N-CD	5.01	1.54	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	LEU	N-CA-C	9.20	121.39	111.36
1	C	509	GLN	N-CA-C	-8.21	99.46	110.55
1	C	473	VAL	N-CA-C	8.11	120.54	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	LEU	N-CA-C	7.61	122.73	108.65
1	C	826	ILE	N-CA-C	7.10	117.20	110.53
1	A	598	MSE	N-CA-CB	-7.09	99.70	110.12
1	A	364	THR	N-CA-C	6.95	118.94	111.36
1	C	476	GLN	N-CA-C	-6.54	104.16	111.28
1	C	410	VAL	N-CA-C	6.33	117.54	111.91
1	C	1055	ILE	CB-CA-C	-6.28	103.65	110.37
1	C	478	GLY	N-CA-C	6.26	120.24	112.73
1	C	392	ASP	N-CA-C	6.19	118.11	111.36
1	C	343	TYR	N-CA-C	-6.10	104.63	111.28
1	C	364	THR	N-CA-C	5.96	117.86	111.36
1	A	506	GLU	N-CA-C	5.47	117.75	110.53
1	C	477	ASP	N-CA-C	-5.42	103.32	110.43
2	D	36	ILE	N-CA-C	-5.26	101.73	107.73
1	A	410	VAL	N-CA-C	5.17	116.51	111.91
2	D	25	ASN	N-CA-CB	-5.08	102.37	109.94

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	6606	0	6542	108	0
1	C	6578	0	6522	192	0
2	B	595	0	621	9	0
2	D	595	0	621	49	0
3	A	138	0	0	5	0
3	B	3	0	0	0	0
3	C	107	0	0	4	0
3	D	2	0	0	1	0
All	All	14624	0	14306	349	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 12.

All (349) 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:C:474:ILE:HG21	1:C:510:ARG:NH2	1.35	1.39
1:C:474:ILE:CG2	1:C:510:ARG:HG3	1.66	1.25
1:C:482:ARG:HB2	1:C:496:LEU:HA	1.18	1.18
2:D:5:VAL:HG12	2:D:67:LEU:HB2	1.24	1.17
1:C:482:ARG:CB	1:C:496:LEU:HA	1.81	1.09
1:C:343:TYR:CE2	1:C:347:HIS:CD2	2.49	1.01
1:C:474:ILE:HG23	1:C:510:ARG:HG3	1.41	1.01
1:C:474:ILE:CG2	1:C:510:ARG:NH2	2.27	0.97
1:C:685:THR:O	1:C:689:THR:HG22	1.68	0.93
2:D:31:GLN:O	2:D:35:GLY:HA2	1.72	0.89
2:D:22:THR:H	2:D:25:ASN:ND2	1.70	0.89
1:C:474:ILE:HG21	1:C:510:ARG:HH21	1.25	0.89
1:C:343:TYR:CZ	1:C:347:HIS:NE2	2.40	0.89
1:C:474:ILE:HG21	1:C:510:ARG:HG3	1.54	0.89
1:C:477:ASP:OD1	1:C:478:GLY:N	2.06	0.88
1:A:279:THR:HG22	1:A:283:MSE:HE2	1.56	0.87
1:A:653:THR:HG22	1:A:656:ARG:HH21	1.38	0.86
2:D:22:THR:O	2:D:25:ASN:HB2	1.74	0.85
2:D:22:THR:C	2:D:25:ASN:HB2	2.02	0.83
1:A:956:GLY:O	1:A:959:THR:HG22	1.79	0.82
1:C:311:THR:HG22	1:C:313:ALA:H	1.43	0.81
2:D:22:THR:HA	2:D:55:THR:HA	1.62	0.81
1:C:476:GLN:HG3	1:C:477:ASP:N	1.95	0.80
2:D:23:ILE:CG2	2:D:52:ASP:HA	2.13	0.79
1:C:475:GLY:HA2	1:C:509:GLN:HG2	1.65	0.79
1:A:641:CYS:HB2	1:A:643:MSE:HE3	1.67	0.77
1:C:474:ILE:HG22	1:C:510:ARG:O	1.84	0.77
2:D:31:GLN:O	2:D:35:GLY:CA	2.32	0.77
1:C:473:VAL:HG22	1:C:499:PHE:CE1	2.20	0.76
1:C:279:THR:HG22	1:C:283:MSE:HE2	1.66	0.76
1:C:343:TYR:CD2	1:C:347:HIS:CD2	2.73	0.76
1:C:474:ILE:HG23	1:C:510:ARG:CG	2.13	0.76
1:C:820:ILE:O	1:C:823:PRO:HD2	1.86	0.75
1:C:475:GLY:N	1:C:481:ILE:HD11	2.01	0.75
1:C:474:ILE:HD11	1:C:478:GLY:O	1.87	0.75
1:C:482:ARG:HB2	1:C:496:LEU:CA	2.10	0.75
1:A:949:ALA:O	1:A:958:LYS:HD2	1.88	0.73
1:C:984:LEU:HD22	1:C:1019:VAL:HG23	1.70	0.73
1:A:248:TYR:O	1:A:271:ARG:NH1	2.21	0.73
1:A:611:MSE:HE3	1:A:738:LEU:HD22	1.68	0.73
1:A:1008:MSE:HE2	1:A:1012:MSE:HE2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:VAL:HG22	2:B:13:ILE:HB	1.70	0.73
1:C:343:TYR:CZ	1:C:347:HIS:CD2	2.76	0.73
1:C:498:PHE:HD1	1:C:499:PHE:N	1.89	0.71
1:C:515:ASP:O	1:C:519:LYS:CG	2.39	0.71
2:D:22:THR:N	2:D:25:ASN:ND2	2.38	0.70
2:D:6:LYS:HG3	2:D:12:THR:HG22	1.73	0.70
1:C:474:ILE:CG2	1:C:510:ARG:HH21	1.93	0.70
2:D:56:LEU:HD12	2:D:61:ILE:HD13	1.73	0.70
2:D:37:PRO:HG2	2:D:40:GLN:HG3	1.73	0.70
1:A:643:MSE:HE2	1:A:646:VAL:HG21	1.74	0.69
2:D:22:THR:O	2:D:25:ASN:CB	2.40	0.69
1:A:362:LYS:HG2	1:A:366:ILE:HD12	1.73	0.69
1:C:482:ARG:HB3	1:C:496:LEU:HA	1.75	0.69
1:C:343:TYR:CD2	1:C:347:HIS:HD2	2.10	0.68
1:A:672:SER:HB2	1:A:712:TRP:HA	1.76	0.68
1:C:665:GLU:OE1	1:C:731:LYS:NZ	2.26	0.68
1:A:941:LEU:HD11	1:A:1008:MSE:HE1	1.74	0.67
1:A:949:ALA:O	1:A:958:LYS:CD	2.41	0.67
1:C:944:ARG:HG3	1:C:1008:MSE:HE3	1.75	0.67
1:A:941:LEU:HD21	1:A:1008:MSE:HE1	1.76	0.67
1:C:672:SER:HB2	1:C:712:TRP:HA	1.77	0.67
2:D:23:ILE:HG22	2:D:52:ASP:HA	1.76	0.67
1:C:362:LYS:O	1:C:366:ILE:HG22	1.95	0.66
1:A:545:GLN:HA	1:A:548:GLN:HE21	1.59	0.66
1:C:472:TYR:CE1	1:C:496:LEU:HD11	2.31	0.65
1:C:515:ASP:O	1:C:519:LYS:HG2	1.96	0.65
1:C:245:TYR:HA	1:C:249:LEU:HB2	1.79	0.64
1:C:577:LYS:NZ	3:C:1107:HOH:O	2.29	0.64
1:C:343:TYR:CE1	1:C:347:HIS:NE2	2.63	0.64
1:C:473:VAL:HG23	1:C:481:ILE:HB	1.79	0.64
1:C:473:VAL:O	1:C:481:ILE:HD13	1.97	0.64
2:D:5:VAL:HG12	2:D:67:LEU:CB	2.16	0.64
2:D:31:GLN:O	2:D:35:GLY:N	2.30	0.63
1:A:957:TYR:HB2	1:A:1000:PHE:CD1	2.34	0.63
1:C:971:GLN:HG3	1:C:983:ILE:HD11	1.81	0.63
1:C:479:ASN:HB3	1:C:480:PRO:HD2	1.81	0.62
1:A:505:LEU:HD23	1:A:509:GLN:OE1	2.00	0.62
1:C:474:ILE:HD12	1:C:479:ASN:O	1.99	0.62
2:D:13:ILE:HG23	2:D:33:LYS:HD3	1.81	0.61
1:C:659:ASP:OD1	1:C:686:TRP:NE1	2.28	0.61
1:C:481:ILE:HD12	1:C:481:ILE:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:HD23	1:A:283:MSE:HE3	1.82	0.61
2:D:23:ILE:HG21	2:D:51:GLU:C	2.26	0.61
1:C:935:LEU:HD23	1:C:973:LEU:HD12	1.83	0.60
2:D:59:TYR:HB2	2:D:61:ILE:CD1	2.31	0.60
1:C:319:GLU:O	1:C:323:ILE:HG12	2.01	0.60
1:A:956:GLY:O	1:A:959:THR:N	2.34	0.60
1:C:474:ILE:CG2	1:C:510:ARG:CG	2.59	0.60
1:C:472:TYR:CD1	1:C:496:LEU:HD11	2.37	0.60
1:C:475:GLY:CA	1:C:481:ILE:HD11	2.33	0.59
1:A:251:LYS:O	1:A:271:ARG:NH1	2.36	0.59
1:A:605:ARG:NH1	1:C:978:ASP:OD2	2.35	0.59
1:A:343:TYR:OH	1:A:385:ASP:OD2	2.20	0.59
1:C:598:MSE:HG3	1:C:908:VAL:HG21	1.83	0.59
1:A:762:GLY:HA3	1:A:823:PRO:HB3	1.85	0.58
1:C:515:ASP:O	1:C:519:LYS:HG3	2.03	0.58
2:B:22:THR:HG23	2:B:25:ASN:H	1.68	0.58
1:A:953:THR:OG1	1:A:954:GLU:N	2.34	0.58
1:C:476:GLN:HG3	1:C:477:ASP:H	1.67	0.58
1:A:767:GLU:O	1:A:771:ASN:ND2	2.36	0.57
2:D:59:TYR:HB2	2:D:61:ILE:HD12	1.85	0.57
1:A:1008:MSE:HE3	1:A:1011:GLN:HB2	1.86	0.57
1:C:656:ARG:HG3	1:C:696:VAL:HG12	1.85	0.57
2:D:49:GLN:NE2	1:C:709:ASN:O	2.35	0.57
1:A:653:THR:HG22	1:A:656:ARG:NH2	2.16	0.57
1:A:274:HIS:HB3	1:A:331:VAL:HG11	1.85	0.56
1:A:302:SER:HA	3:A:1107:HOH:O	2.04	0.56
1:C:390:TRP:CE3	1:C:390:TRP:HA	2.40	0.56
1:C:538:LEU:HD23	1:C:539:PRO:HD2	1.88	0.56
1:A:948:GLN:NE2	1:A:1004:GLU:HB2	2.20	0.56
1:C:944:ARG:HD3	1:C:947:ARG:NH1	2.20	0.56
2:D:73:LEU:HB2	1:C:849:THR:CG2	2.36	0.56
1:C:472:TYR:CZ	1:C:496:LEU:HD11	2.41	0.56
1:C:237:VAL:HG23	1:C:321:ARG:HG3	1.88	0.56
1:C:744:ASN:HB3	1:C:748:MSE:HE2	1.89	0.56
1:C:474:ILE:HG21	1:C:510:ARG:HH22	1.60	0.55
1:A:1008:MSE:HE3	1:A:1008:MSE:HA	1.88	0.55
1:C:323:ILE:HD12	1:C:395:ALA:HA	1.87	0.55
1:C:510:ARG:NH2	1:C:510:ARG:HG3	2.22	0.55
1:C:510:ARG:HG3	1:C:510:ARG:HH21	1.71	0.55
1:C:807:GLN:HB2	3:C:1194:HOH:O	2.07	0.55
2:D:22:THR:HG23	2:D:25:ASN:ND2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:TYR:O	1:C:520:LEU:HG	2.07	0.55
2:D:23:ILE:HG21	2:D:51:GLU:O	2.06	0.55
1:C:842:LEU:HB3	1:C:860:ILE:HD12	1.89	0.54
1:A:598:MSE:HG2	1:A:908:VAL:HG21	1.90	0.54
1:C:470:GLY:HA3	1:C:498:PHE:CE1	2.42	0.54
1:A:941:LEU:HD21	1:A:1008:MSE:CE	2.37	0.54
1:C:1009:LYS:HB3	1:C:1009:LYS:HZ2	1.73	0.54
1:C:474:ILE:HG21	1:C:510:ARG:CZ	2.26	0.53
1:C:971:GLN:CG	1:C:983:ILE:HD11	2.37	0.53
1:C:338:GLU:OE2	1:C:340:SER:OG	2.26	0.53
1:A:245:TYR:HA	1:A:249:LEU:HB2	1.89	0.53
1:A:323:ILE:HD13	1:A:398:LEU:HD12	1.89	0.53
1:A:477:ASP:OD1	1:A:477:ASP:N	2.42	0.53
1:C:474:ILE:HD11	1:C:478:GLY:C	2.34	0.52
1:A:386:LYS:HE2	1:A:387:ASP:OD2	2.08	0.52
1:A:826:ILE:HD11	2:B:8:LEU:HG	1.91	0.52
1:C:481:ILE:N	1:C:481:ILE:CD1	2.72	0.52
1:C:954:GLU:OE2	1:C:956:GLY:N	2.43	0.52
1:A:345:LYS:O	1:A:349:GLN:HG3	2.10	0.52
1:C:822:VAL:HB	1:C:823:PRO:HD3	1.91	0.52
1:A:480:PRO:HB3	1:A:512:MSE:HE3	1.92	0.52
2:D:8:LEU:HG	1:C:826:ILE:HD11	1.91	0.52
1:A:475:GLY:HA2	1:A:509:GLN:HG2	1.92	0.52
1:C:1006:ARG:HA	1:C:1009:LYS:HZ2	1.75	0.52
2:D:23:ILE:HG21	2:D:52:ASP:HA	1.90	0.51
1:C:470:GLY:HA3	1:C:498:PHE:HE1	1.75	0.51
1:C:1006:ARG:HA	1:C:1009:LYS:NZ	2.25	0.51
1:C:513:ARG:NE	1:C:516:GLU:OE2	2.44	0.51
1:C:390:TRP:CE3	1:C:400:ASN:HB2	2.45	0.51
1:A:279:THR:O	1:A:283:MSE:HG3	2.10	0.51
1:A:948:GLN:HE21	1:A:1004:GLU:HB2	1.76	0.51
1:A:949:ALA:O	1:A:958:LYS:HD3	2.10	0.51
2:D:21:ASP:HB3	2:D:25:ASN:OD1	2.10	0.51
1:C:237:VAL:HG11	1:C:324:MSE:HE3	1.91	0.51
1:C:984:LEU:O	1:C:988:LEU:HD23	2.10	0.51
1:C:745:LYS:HA	1:C:748:MSE:HE3	1.93	0.51
1:C:638:LEU:HG	1:C:721:ALA:HA	1.94	0.50
1:C:691:ARG:NH1	1:C:693:GLY:O	2.32	0.50
1:C:685:THR:HG22	1:C:689:THR:HG21	1.93	0.50
1:A:504:LYS:O	1:A:505:LEU:HD12	2.11	0.50
2:D:56:LEU:HD11	2:D:61:ILE:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:GLY:N	1:C:481:ILE:CD1	2.73	0.50
1:C:684:GLU:O	1:C:688:LYS:HG2	2.11	0.50
1:C:329:PHE:HA	1:C:332:THR:HG23	1.94	0.50
1:C:1015:ILE:HA	1:C:1018:MSE:HE2	1.94	0.49
1:C:410:VAL:HG12	1:C:453:ALA:HB2	1.93	0.49
1:C:878:LYS:NZ	1:C:884:ASP:OD1	2.45	0.49
1:C:952:SER:HB3	1:C:958:LYS:HG3	1.95	0.49
1:C:247:ASN:C	1:C:248:TYR:CD1	2.90	0.49
1:A:919:LEU:O	1:A:923:GLN:HG3	2.12	0.49
1:A:446:HIS:HE1	3:A:1234:HOH:O	1.96	0.49
1:C:345:LYS:O	1:C:349:GLN:HG3	2.13	0.49
1:A:937:ARG:HH21	1:A:1011:GLN:HE22	1.61	0.48
1:C:685:THR:CG2	1:C:689:THR:HG21	2.43	0.48
1:C:844:PRO:HB3	1:C:860:ILE:HD11	1.95	0.48
2:D:45:PHE:HB2	2:D:67:LEU:HD22	1.94	0.48
1:C:933:PRO:HG2	1:C:935:LEU:HD11	1.93	0.48
1:A:559:GLU:HB3	3:A:1112:HOH:O	2.12	0.48
1:C:685:THR:C	1:C:689:THR:HG22	2.38	0.48
1:C:358:VAL:HA	1:C:365:LEU:CD2	2.43	0.48
1:C:685:THR:HG22	1:C:689:THR:CG2	2.43	0.48
1:C:1038:ASN:HA	1:C:1041:GLU:HG2	1.95	0.48
2:D:72:ARG:NH2	1:C:855:GLU:OE1	2.47	0.48
1:C:820:ILE:C	1:C:823:PRO:HD2	2.38	0.48
2:D:42:ALA:HB3	2:D:70:VAL:HG23	1.96	0.48
1:C:625:ASN:HB2	1:C:914:MSE:HB3	1.96	0.48
1:A:611:MSE:HE1	1:A:738:LEU:HD13	1.95	0.48
1:A:937:ARG:HH21	1:A:1011:GLN:NE2	2.12	0.48
1:A:954:GLU:HG3	1:A:1002:SER:HB3	1.96	0.48
2:B:24:GLU:HG3	2:B:52:ASP:HB3	1.95	0.48
2:D:49:GLN:OE1	2:D:72:ARG:NH1	2.47	0.48
1:A:643:MSE:CE	1:A:646:VAL:HG21	2.43	0.47
2:D:5:VAL:HA	2:D:67:LEU:O	2.14	0.47
1:C:278:HIS:O	1:C:282:THR:HG23	2.15	0.47
1:A:822:VAL:HB	1:A:823:PRO:HD3	1.96	0.47
2:B:33:LYS:HD3	2:B:33:LYS:C	2.39	0.47
1:A:611:MSE:CE	1:A:738:LEU:HD13	2.44	0.47
1:A:954:GLU:OE2	1:A:1002:SER:N	2.39	0.47
1:C:279:THR:O	1:C:283:MSE:HG3	2.14	0.47
1:A:652:ASP:HB3	1:A:696:VAL:HG11	1.96	0.47
1:A:955:SER:HA	1:A:956:GLY:HA2	1.66	0.47
1:A:1042:LYS:HE3	1:A:1042:LYS:HB3	1.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:GLN:OE1	1:A:1043:GLN:N	2.47	0.47
2:D:22:THR:HG23	2:D:25:ASN:HD22	1.78	0.47
1:A:226:TRP:HB3	3:A:1167:HOH:O	2.14	0.47
1:C:621:HIS:CG	1:C:628:LYS:HD2	2.49	0.47
1:A:604:ALA:O	1:A:608:GLN:HG3	2.14	0.47
1:C:516:GLU:O	1:C:520:LEU:CD2	2.62	0.47
1:C:923:GLN:O	1:C:927:GLU:HG3	2.15	0.47
1:C:1043:GLN:OE1	1:C:1043:GLN:N	2.48	0.47
1:C:482:ARG:HA	1:C:497:LYS:H	1.79	0.47
1:C:572:ALA:O	1:C:576:THR:HG23	2.14	0.46
1:A:307:ALA:O	3:A:1101:HOH:O	2.20	0.46
1:C:761:ARG:HD2	3:C:1118:HOH:O	2.15	0.46
1:A:274:HIS:ND1	1:A:337:GLU:OE2	2.32	0.46
1:A:280:LEU:HD23	1:A:283:MSE:CE	2.46	0.46
1:A:385:ASP:CG	1:A:390:TRP:HE1	2.23	0.46
1:C:243:TYR:OH	1:C:356:LYS:HG2	2.15	0.46
1:C:616:CYS:HB2	1:C:623:PHE:O	2.16	0.46
1:C:305:THR:O	3:C:1101:HOH:O	2.21	0.46
1:C:473:VAL:C	1:C:481:ILE:HD13	2.41	0.46
1:C:691:ARG:CZ	1:C:699:ILE:HG12	2.46	0.46
1:C:1031:PRO:O	1:C:1035:GLN:HG3	2.16	0.46
1:A:245:TYR:CE1	1:A:560:ASN:HA	2.51	0.46
1:C:537:GLY:HA2	1:C:546:TYR:CZ	2.51	0.46
1:A:662:MSE:HG3	1:A:686:TRP:CD1	2.51	0.46
1:A:954:GLU:OE2	1:A:1001:ASN:N	2.49	0.46
1:C:849:THR:C	1:C:850:HIS:HD1	2.22	0.46
1:A:624:LEU:HD23	1:A:624:LEU:HA	1.72	0.45
1:A:507:GLU:O	1:A:508:ASN:HB2	2.17	0.45
2:D:27:LYS:O	2:D:28:ALA:C	2.57	0.45
2:D:34:GLU:OE2	2:D:34:GLU:HA	2.16	0.45
1:C:910:PRO:O	1:C:914:MSE:HG3	2.16	0.45
1:A:545:GLN:HA	1:A:548:GLN:NE2	2.27	0.45
1:C:335:ASP:OD2	1:C:349:GLN:NE2	2.49	0.45
1:C:607:VAL:O	1:C:611:MSE:HG2	2.17	0.45
1:C:984:LEU:HD13	1:C:1022:LYS:HG2	1.98	0.45
1:A:1025:LEU:HD23	1:A:1025:LEU:HA	1.75	0.45
2:D:4:PHE:HD1	2:D:14:THR:HG1	1.60	0.45
2:D:45:PHE:HB3	2:D:50:LEU:HD21	1.98	0.45
1:A:336:ASP:OD1	1:A:346:TYR:OH	2.24	0.45
1:A:822:VAL:HA	1:A:826:ILE:HD13	1.99	0.45
1:C:1050:GLN:HG2	1:C:1054:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:594:ARG:HE	1:C:864:GLU:CD	2.24	0.45
1:A:503:LYS:O	1:A:503:LYS:HG2	2.16	0.45
1:C:473:VAL:CG2	1:C:481:ILE:HB	2.46	0.45
2:D:61:ILE:O	2:D:62:GLN:HG3	2.17	0.44
1:C:320:LEU:O	1:C:324:MSE:HG3	2.16	0.44
1:C:335:ASP:CG	1:C:349:GLN:HE22	2.25	0.44
1:C:1003:VAL:O	1:C:1007:GLN:HG3	2.18	0.44
1:A:280:LEU:HA	1:A:283:MSE:HE3	2.00	0.44
1:C:408:VAL:C	1:C:409:ARG:HG2	2.42	0.44
1:A:366:ILE:CG2	1:A:367:PRO:HA	2.47	0.44
2:D:59:TYR:HB2	2:D:61:ILE:HD11	2.00	0.44
1:C:480:PRO:HB3	1:C:512:MSE:CE	2.48	0.44
1:A:611:MSE:HE1	1:A:661:LEU:HD22	2.00	0.44
1:C:516:GLU:O	1:C:520:LEU:HD23	2.18	0.43
1:C:642:ASP:HB3	1:C:645:ILE:HD12	2.00	0.43
1:A:252:PRO:HG3	1:A:270:TYR:CE1	2.54	0.43
1:C:472:TYR:CD1	1:C:496:LEU:CD1	3.01	0.43
1:C:935:LEU:H	1:C:935:LEU:HD12	1.83	0.43
1:A:503:LYS:HG2	1:A:505:LEU:HD13	2.00	0.43
1:C:415:GLU:HB2	1:C:514:VAL:HG21	2.01	0.43
1:C:236:THR:HG21	1:C:369:VAL:HG21	2.01	0.43
1:C:498:PHE:CD1	1:C:499:PHE:N	2.79	0.43
1:A:744:ASN:O	1:A:748:MSE:HG3	2.19	0.43
1:C:410:VAL:HA	1:C:453:ALA:HB2	2.01	0.43
1:C:496:LEU:HD12	1:C:496:LEU:C	2.43	0.43
1:C:510:ARG:NH1	1:C:516:GLU:OE2	2.51	0.43
1:C:229:PHE:HZ	1:C:324:MSE:HE2	1.84	0.43
1:C:472:TYR:CE2	1:C:496:LEU:HD11	2.54	0.43
1:C:744:ASN:O	1:C:748:MSE:HG3	2.18	0.43
1:A:482:ARG:NH2	1:A:522:GLU:OE2	2.50	0.43
1:A:753:SER:OG	1:A:846:GLN:HB2	2.19	0.43
2:D:44:ILE:HD13	2:D:49:GLN:HA	2.01	0.43
1:C:954:GLU:OE2	1:C:957:TYR:N	2.30	0.42
2:D:52:ASP:O	2:D:54:ARG:NH2	2.52	0.42
1:C:474:ILE:HG12	1:C:510:ARG:NH2	2.33	0.42
1:C:310:ARG:HH22	1:C:319:GLU:CD	2.27	0.42
1:A:912:LEU:HD13	1:C:932:GLU:HB3	2.00	0.42
1:C:472:TYR:CG	1:C:496:LEU:HD11	2.53	0.42
1:C:483:GLU:HG2	1:C:497:LYS:HB2	2.01	0.42
1:A:625:ASN:HB2	1:A:914:MSE:HG2	2.02	0.42
1:C:280:LEU:HD22	1:C:566:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:ILE:HG23	1:C:474:ILE:O	2.19	0.42
1:C:878:LYS:HZ2	1:C:878:LYS:HG2	1.75	0.42
1:C:957:TYR:CZ	1:C:961:LEU:HD11	2.54	0.42
1:A:1008:MSE:HE2	1:A:1012:MSE:CE	2.44	0.42
1:C:504:LYS:H	1:C:504:LYS:HG2	1.72	0.42
1:C:541:LEU:HD23	1:C:541:LEU:HA	1.92	0.42
1:A:253:TYR:CZ	1:A:271:ARG:HG2	2.54	0.42
1:C:331:VAL:HG22	1:C:334:ARG:HD2	2.02	0.42
1:C:477:ASP:CG	1:C:478:GLY:N	2.76	0.42
1:C:641:CYS:O	1:C:811:ARG:NH1	2.47	0.42
1:C:1018:MSE:HE2	1:C:1018:MSE:HB3	1.89	0.42
2:D:7:THR:HG22	2:D:11:LYS:O	2.19	0.42
2:D:19:PRO:C	2:D:21:ASP:H	2.27	0.42
1:A:666:ARG:HA	1:A:683:GLY:HA3	2.02	0.42
1:A:941:LEU:HD12	1:A:941:LEU:HA	1.83	0.42
1:C:604:ALA:O	1:C:608:GLN:HG3	2.20	0.41
1:C:832:ILE:HD12	1:C:885:ARG:HD2	2.02	0.41
2:B:39:ASP:OD1	2:B:39:ASP:N	2.51	0.41
2:D:8:LEU:HD22	1:C:819:ASN:HD21	1.85	0.41
2:D:74:ARG:HG2	1:C:705:PHE:HB2	2.02	0.41
1:A:318:GLU:CD	1:A:318:GLU:H	2.28	0.41
1:A:762:GLY:CA	1:A:823:PRO:HB3	2.49	0.41
1:A:919:LEU:HD12	1:A:919:LEU:H	1.84	0.41
2:D:5:VAL:HG21	2:D:30:ILE:HD13	2.01	0.41
2:D:62:GLN:HB3	2:D:63:LYS:H	1.72	0.41
1:C:473:VAL:CG2	1:C:499:PHE:CZ	3.04	0.41
1:A:367:PRO:HA	1:A:370:PHE:O	2.21	0.41
3:D:102:HOH:O	1:C:849:THR:HG22	2.19	0.41
1:C:474:ILE:HG22	1:C:510:ARG:C	2.44	0.41
1:C:480:PRO:HB3	1:C:512:MSE:HE3	2.02	0.41
2:D:31:GLN:C	2:D:35:GLY:H	2.28	0.41
1:A:264:PHE:HB2	1:A:556:ALA:HB2	2.01	0.41
1:A:273:HIS:CD2	1:A:273:HIS:C	2.98	0.41
1:C:366:ILE:HA	1:C:367:PRO:HA	1.76	0.41
1:C:611:MSE:HE1	1:C:658:ILE:HA	2.01	0.41
1:C:1007:GLN:O	1:C:1011:GLN:HG2	2.21	0.41
1:C:1022:LYS:NZ	1:C:1026:GLU:OE1	2.54	0.41
1:A:988:LEU:HD23	1:A:988:LEU:HA	1.89	0.41
1:A:278:HIS:O	1:A:282:THR:HG23	2.21	0.41
1:A:712:TRP:CZ3	1:A:713:TYR:HB2	2.56	0.41
1:C:366:ILE:HG13	1:C:367:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:PRO:HG2	1:A:660:THR:HG22	2.02	0.41
1:A:959:THR:CG2	1:A:960:PHE:N	2.84	0.41
1:A:985:GLY:O	1:A:988:LEU:HB2	2.21	0.41
2:B:30:ILE:HD12	2:B:43:LEU:HD11	2.03	0.41
2:B:37:PRO:HB2	2:B:39:ASP:OD1	2.21	0.41
1:C:474:ILE:CD1	1:C:479:ASN:C	2.94	0.41
1:C:903:GLU:OE1	1:C:903:GLU:HA	2.19	0.41
1:C:385:ASP:OD1	1:C:388:HIS:HA	2.21	0.41
1:A:321:ARG:HE	1:A:369:VAL:HG22	1.86	0.40
1:C:659:ASP:O	1:C:663:GLN:HG3	2.20	0.40
1:A:1004:GLU:H	1:A:1004:GLU:CD	2.30	0.40
1:A:1008:MSE:CE	1:A:1011:GLN:HB2	2.50	0.40
2:B:8:LEU:HD12	2:B:70:VAL:HG12	2.03	0.40
1:C:343:TYR:CD2	1:C:343:TYR:C	2.99	0.40
1:A:460:LYS:HB3	1:A:513:ARG:HD2	2.03	0.40
1:A:616:CYS:HB2	1:A:623:PHE:O	2.21	0.40
1:A:797:PHE:CZ	1:A:801:LYS:HD2	2.57	0.40
1:C:310:ARG:NH2	1:C:319:GLU:OE1	2.55	0.40
1:C:280:LEU:HA	1:C:283:MSE:HE3	2.03	0.40
1:C:650:LEU:O	1:C:745:LYS:HE2	2.21	0.40
1:C:707:MSE:HE2	1:C:707:MSE:HB3	2.01	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	824/845 (98%)	804 (98%)	20 (2%)	0	100	100
1	C	820/845 (97%)	806 (98%)	14 (2%)	0	100	100
2	B	74/79 (94%)	73 (99%)	1 (1%)	0	100	100
2	D	74/79 (94%)	71 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1792/1848 (97%)	1754 (98%)	38 (2%)	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	719/719 (100%)	712 (99%)	7 (1%)	68	84
1	C	716/719 (100%)	701 (98%)	15 (2%)	47	71
2	B	67/68 (98%)	66 (98%)	1 (2%)	57	78
2	D	67/68 (98%)	65 (97%)	2 (3%)	36	61
All	All	1569/1574 (100%)	1544 (98%)	25 (2%)	55	77

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	SER
1	A	425	LEU
1	A	471	ARG
1	A	505	LEU
1	A	638	LEU
1	A	952	SER
1	A	958	LYS
2	B	62	GLN
2	D	23	ILE
2	D	25	ASN
1	C	340	SER
1	C	341	LYS
1	C	363	SER
1	C	364	THR
1	C	365	LEU
1	C	389	LYS
1	C	392	ASP

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Mol	Chain	Res	Type
1	C	474	ILE
1	C	481	ILE
1	C	504	LYS
1	C	506	GLU
1	C	510	ARG
1	C	519	LYS
1	C	638	LEU
1	C	1055	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	HIS
1	A	342	ASN
1	A	347	HIS
1	A	361	ASN
1	A	545	GLN
1	A	548	GLN
1	A	551	ASN
1	A	609	GLN
1	A	775	ASN
1	A	787	HIS
1	A	915	GLN
1	A	923	GLN
1	A	1011	GLN
2	B	60	ASN
2	D	25	ASN
1	C	361	ASN
1	C	388	HIS
1	C	568	GLN
1	C	595	GLN
1	C	608	GLN
1	C	657	ASN
1	C	718	ASN
1	C	843	HIS
1	C	923	GLN
1	C	928	GLN
1	C	974	ASN
1	C	1035	GLN
1	C	1054	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 oligosaccharides 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, 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	812/845 (96%)	-0.14	12 (1%) 72 69	26, 48, 93, 122	0
1	C	808/845 (95%)	0.13	26 (3%) 50 47	28, 63, 105, 141	0
2	B	76/79 (96%)	0.33	0 100 100	46, 71, 93, 103	0
2	D	76/79 (96%)	1.14	10 (13%) 7 5	62, 121, 171, 178	0
All	All	1772/1848 (95%)	0.06	48 (2%) 56 52	26, 58, 109, 178	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	475	GLY	3.7
1	C	224	PRO	3.6
1	C	223	VAL	3.4
1	C	1058	LEU	3.4
1	C	366	ILE	3.1
1	C	950	LYS	3.0
1	C	365	LEU	3.0
2	D	36	ILE	2.9
1	C	481	ILE	2.8
1	A	505	LEU	2.8
1	C	951	PHE	2.8
2	D	63	LYS	2.8
1	C	624	LEU	2.8
2	D	66	THR	2.7
1	A	484	GLU	2.7
1	A	620	ASP	2.6
1	C	343	TYR	2.6
2	D	20	SER	2.6
2	D	59	TYR	2.6
1	C	340	SER	2.5
1	A	956	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	15	LEU	2.4
1	A	494	GLY	2.4
1	C	474	ILE	2.4
2	D	13	ILE	2.4
1	C	505	LEU	2.4
2	D	4	PHE	2.4
1	A	981	VAL	2.3
2	D	54	ARG	2.3
1	A	504	LYS	2.3
1	C	953	THR	2.3
1	C	976	LEU	2.3
1	C	1001	ASN	2.2
1	C	659	ASP	2.2
1	A	951	PHE	2.2
1	C	342	ASN	2.2
1	C	478	GLY	2.2
1	A	260	THR	2.1
1	C	1009	LYS	2.1
1	A	499	PHE	2.1
1	C	390	TRP	2.1
1	A	982	THR	2.1
1	C	499	PHE	2.1
2	D	17	VAL	2.1
1	C	458	GLU	2.0
1	A	222	SER	2.0
1	C	1038	ASN	2.0
1	C	982	THR	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.