Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 04:09 pm BST

PDB ID	:	5ZQ5
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 following versions of software and data (see references ⓘ) were used in the production of this report:

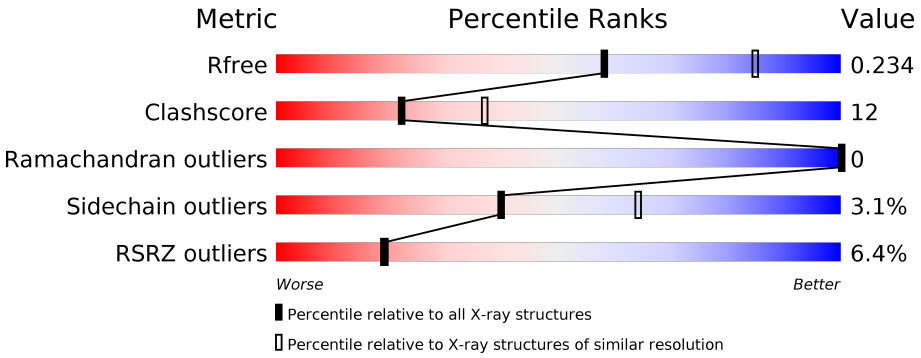
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (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 on 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 <=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% 17% .
1	C	845	5% 74% 22% ..
2	B	79	19% 78% 18% .
2	D	79	57% 44% 47% 5% .

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.

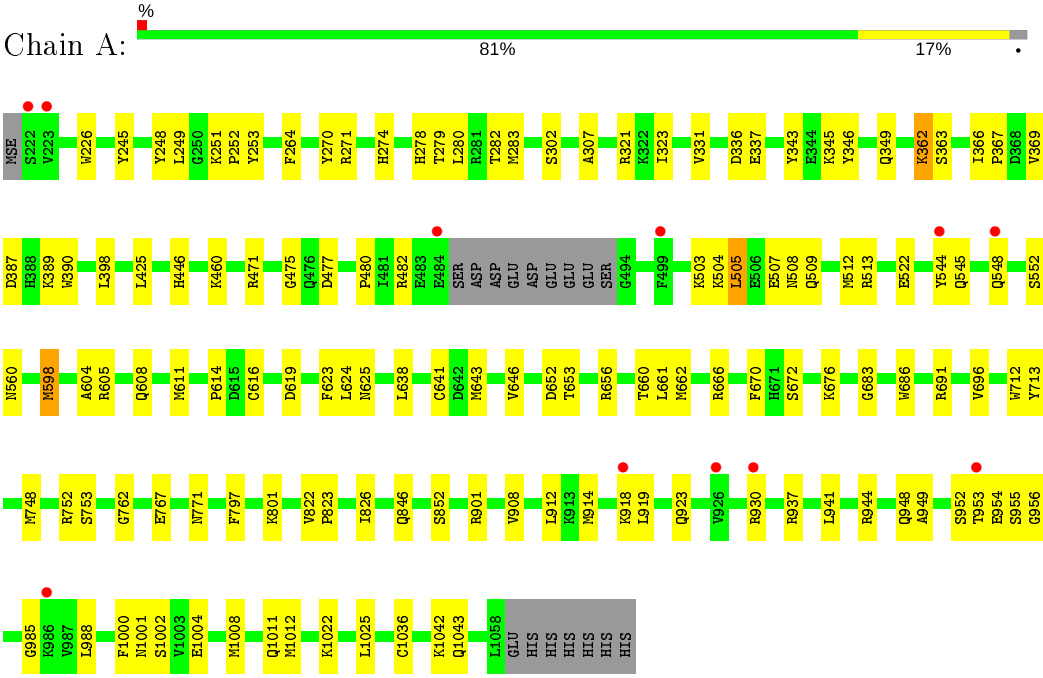
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	138	Total	O	0	0
			138	138		
3	B	3	Total	O	0	0
			3	3		
3	D	2	Total	O	0	0
			2	2		
3	C	107	Total	O	0	0
			107	107		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

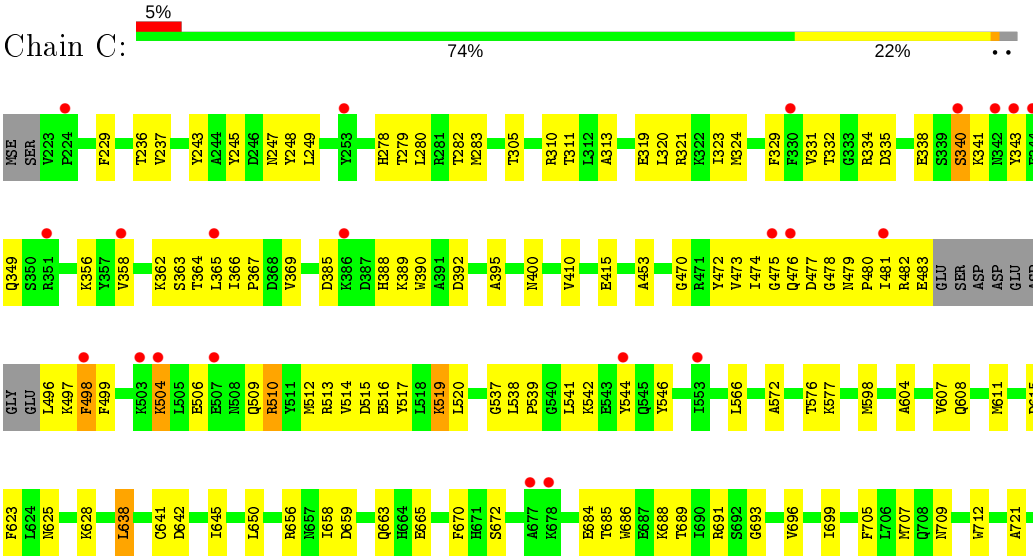
- Molecule 1: SidE

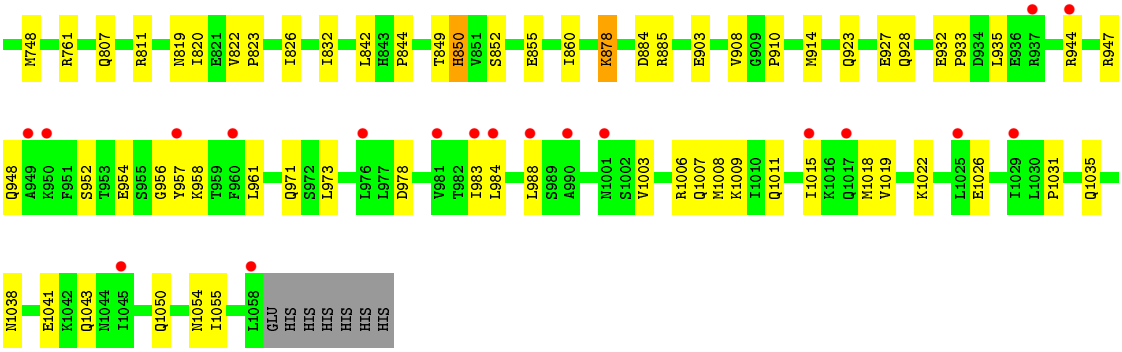
Chain A:



- Molecule 1: SidE

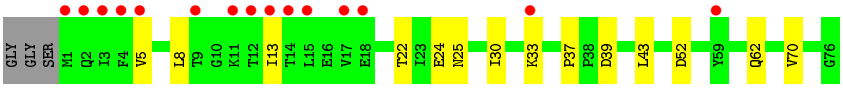
Chain C:





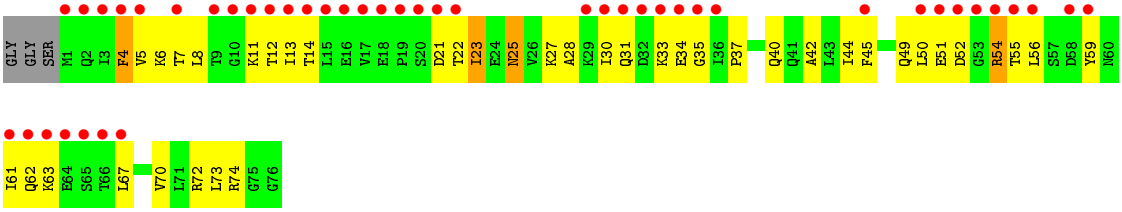
- Molecule 2: Ubiquitin

Chain B:



- Molecule 2: Ubiquitin

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.28 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.190 , 0.233 0.194 , 0.234	Depositor DCC
R_{free} test set	4061 reflections (5.02%)	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)	0.34 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.41	0/6720	0.50	1/9053 (0.0%)
1	C	0.46	0/6692	0.52	0/9016
2	B	0.38	0/601	0.52	0/809
2	D	0.53	0/601	0.70	0/809
All	All	0.44	0/14614	0.52	1/19687 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	598	MSE	N-CA-CB	-6.05	99.70	110.60

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	106	0
1	C	6578	0	6522	181	0
2	B	595	0	621	9	0
2	D	595	0	621	47	0
3	A	138	0	0	6	0
3	B	3	0	0	0	0
3	C	107	0	0	4	0
3	D	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14624	0	14306	334	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 (334) 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
1:C:474:ILE:HG21	1:C:510:ARG:HH21	1.25	0.89
2:D:22:THR:H	2:D:25:ASN:ND2	1.70	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
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
2:D:22:THR:C	2:D:25:ASN:HB2	2.02	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1008:MSE:HE2	1:A:1012:MSE:HE2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:481:ILE:HD12	2.16	0.61
1:A:280:LEU:HD23	1:A:283:MSE:HE3	1.82	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:A:389:LYS:NZ	3:A:1110:HOH:O	2.35	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:1009:LYS:HZ2	1:C:1009:LYS:HB3	1.70	0.56
1:C:390:TRP:HA	1:C:390:TRP:CE3	2.40	0.56
1:C:538:LEU:HD23	1:C:539:PRO:HD2	1.88	0.56
2:D:23:ILE:HG21	2:D:51:GLU:C	2.26	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
1:C:472:TYR:CZ	1:C:496:LEU:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:LEU:HB2	1:C:849:THR:CG2	2.36	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:HA	1:A:1008:MSE:HE3	1.88	0.55
1:C:323:ILE:HD12	1:C:395:ALA:HA	1.87	0.55
1:C:510:ARG:HG3	1:C:510:ARG:HH21	1.71	0.55
1:C:510:ARG:NH2	1:C:510:ARG:HG3	2.22	0.55
1:C:807:GLN:HB2	3:C:1194:HOH:O	2.07	0.55
1:C:517:TYR:O	1:C:520:LEU:HG	2.07	0.55
2:D:22:THR:HG23	2:D:25:ASN:ND2	2.22	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: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: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:CD1	1:C:481:ILE:N	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
2:D:23:ILE:HG21	2:D:52:ASP:HA	1.90	0.51
1:C:1006:ARG:HA	1:C:1009:LYS:NZ	2.25	0.51
1:C:470:GLY:HA3	1:C:498:PHE:HE1	1.75	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:948:GLN:HE21	1:A:1004:GLU:HB2	1.76	0.51
1:A:279:THR:O	1:A:283:MSE:HG3	2.10	0.51
1:A:949:ALA:O	1:A:958:LYS:HD3	2.10	0.51
1:C:237:VAL:HG11	1:C:324:MSE:HE3	1.91	0.51
2:D:21:ASP:HB3	2:D:25:ASN:OD1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:691:ARG:NH1	1:C:693:GLY:O	2.32	0.50
1:C:638:LEU:HG	1:C:721:ALA:HA	1.94	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
1:C:475:GLY:N	1:C:481:ILE:CD1	2.73	0.50
2:D:56:LEU:HD11	2:D:61:ILE:HG21	1.93	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: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
1:C:933:PRO:HG2	1:C:935:LEU:HD11	1.93	0.48
2:D:45:PHE:HB2	2:D:67:LEU:HD22	1.94	0.48
1:A:559:GLU:HB3	3:A:1112:HOH:O	2.12	0.48
1:C:1038:ASN:HA	1:C:1041:GLU:HG2	1.95	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
2:D:72:ARG:NH2	1:C:855:GLU:OE1	2.47	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:954:GLU:HG3	1:A:1002:SER:HB3	1.96	0.48
1:A:937:ARG:HH21	1:A:1011:GLN:NE2	2.12	0.48
1:A:611:MSE:HE1	1:A:738:LEU:HD13	1.95	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:C:474:ILE:HD11	1:C:478:GLY:C	2.34	0.48
1:A:643:MSE:CE	1:A:646:VAL:HG21	2.43	0.47
1:C:278:HIS:O	1:C:282:THR:HG23	2.15	0.47
2:D:5:VAL:HA	2:D:67:LEU:O	2.14	0.47
1:A:822:VAL:HB	1:A:823:PRO:HD3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:THR:O	1:C:283:MSE:HG3	2.14	0.47
1:A:1042:LYS:HB3	1:A:1042:LYS:HE3	1.65	0.47
1:A:1043:GLN:N	1:A:1043:GLN:OE1	2.47	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
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:C:1043:GLN:OE1	1:C:1043:GLN:N	2.48	0.47
1:C:923:GLN:O	1:C:927:GLU:HG3	2.15	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: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:280:LEU:HD23	1:A:283:MSE:CE	2.46	0.46
1:A:274:HIS:ND1	1:A:337:GLU:OE2	2.32	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:1031:PRO:O	1:C:1035:GLN:HG3	2.16	0.46
1:C:305:THR:O	3:C:1101:HOH:O	2.21	0.46
1:C:691:ARG:CZ	1:C:699:ILE:HG12	2.46	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:A:624:LEU:HA	1:A:624:LEU:HD23	1.72	0.45
1:A:507:GLU:O	1:A:508:ASN:HB2	2.17	0.45
1:C:910:PRO:O	1:C:914:MSE:HG3	2.16	0.45
2:D:34:GLU:OE2	2:D:34:GLU:HA	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: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
1:A:503:LYS:O	1:A:503:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:VAL:CG2	1:C:481:ILE:HB	2.46	0.45
1:C:320:LEU:O	1:C:324:MSE:HG3	2.16	0.44
2:D:61:ILE:O	2:D:62:GLN:HG3	2.17	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:247:ASN:C	1:C:248:TYR:CD1	2.90	0.44
1:A:366:ILE:CG2	1:A:367:PRO:HA	2.47	0.44
1:C:480:PRO:HB3	1:C:512:MSE:CE	2.48	0.44
2:D:59:TYR:HB2	2:D:61:ILE:HD11	2.00	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:820:ILE:C	1:C:823:PRO:HD2	2.38	0.43
1:C:935:LEU:HD12	1:C:935:LEU:H	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: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
2:B:33:LYS:C	2:B:33:LYS:HD3	2.39	0.42
1:C:954:GLU:OE2	1:C:957:TYR:N	2.30	0.42
1:C:474:ILE:HG12	1:C:510:ARG:NH2	2.33	0.42
2:D:52:ASP:O	2:D:54:ARG:NH2	2.52	0.42
1:C:903:GLU:HA	1:C:903:GLU:OE1	2.19	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:912:LEU:HD13	1:C:932:GLU:HB3	2.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:C:504:LYS:H	1.72	0.42
1:C:541:LEU:HA	1:C:541:LEU:HD23	1.92	0.42
1:A:253:TYR:CZ	1:A:271:ARG:HG2	2.54	0.42
1:C:1018:MSE:HB3	1:C:1018:MSE:HE2	1.89	0.42
1:C:331:VAL:HG22	1:C:334:ARG:HD2	2.02	0.42
1:C:641:CYS:O	1:C:811:ARG:NH1	2.47	0.42
2:D:7:THR:HG22	2:D:11:LYS:O	2.19	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:74:ARG:HG2	1:C:705:PHE:HB2	2.02	0.41
2:D:8:LEU:HD22	1:C:819:ASN:HD21	1.85	0.41
1:A:385:ASP:CG	1:A:390:TRP:HE1	2.23	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
1:C:473:VAL:CG2	1:C:499:PHE:CZ	3.04	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:A:367:PRO:HA	1:A:370:PHE:O	2.21	0.41
1:C:480:PRO:HB3	1:C:512:MSE:HE3	2.02	0.41
3:D:102:HOH:O	1:C:849:THR:HG22	2.19	0.41
1:A:264:PHE:HB2	1:A:556:ALA:HB2	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: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:A:988:LEU:HA	1:A:988:LEU:HD23	1.89	0.41
1:C:849:THR:C	1:C:850:HIS:HD1	2.22	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
2:D:27:LYS:O	2:D:28:ALA:C	2.57	0.41
1:A:959:THR:CG2	1:A:960:PHE:N	2.84	0.41
2:B:30:ILE:HD12	2:B:43:LEU:HD11	2.03	0.41
1:A:336:ASP:OD1	1:A:346:TYR:OH	2.24	0.41
1:A:614:PRO:HG2	1:A:660:THR:HG22	2.02	0.41
1:A:985:GLY:O	1:A:988:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:PRO:HB2	2:B:39:ASP:OD1	2.21	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: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: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:473:VAL:C	1:C:481:ILE:HD13	2.41	0.40
1:C:280:LEU:HA	1:C:283:MSE:HE3	2.03	0.40
1:C:707:MSE:HE2	1:C:707:MSE:HB3	2.01	0.40
1:C:650:LEU:O	1:C:745:LYS:HE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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
All	All	1792/1848 (97%)	1754 (98%)	38 (2%)	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	719/719 (100%)	697 (97%)	22 (3%)	40	64
1	C	716/719 (100%)	694 (97%)	22 (3%)	40	64
2	B	67/68 (98%)	66 (98%)	1 (2%)	65	83
2	D	67/68 (98%)	63 (94%)	4 (6%)	19	34
All	All	1569/1574 (100%)	1520 (97%)	49 (3%)	40	64

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	LYS
1	A	363	SER
1	A	386	LYS
1	A	425	LEU
1	A	471	ARG
1	A	505	LEU
1	A	544	TYR
1	A	552	SER
1	A	619	ASP
1	A	638	LEU
1	A	670	PHE
1	A	676	LYS
1	A	691	ARG
1	A	752	ARG
1	A	852	SER
1	A	901	ARG
1	A	918	LYS
1	A	930	ARG
1	A	944	ARG
1	A	952	SER
1	A	1022	LYS
1	A	1036	CYS
2	B	62	GLN
2	D	4	PHE

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Mol	Chain	Res	Type
2	D	23	ILE
2	D	25	ASN
2	D	54	ARG
1	C	340	SER
1	C	341	LYS
1	C	363	SER
1	C	364	THR
1	C	389	LYS
1	C	392	ASP
1	C	498	PHE
1	C	504	LYS
1	C	506	GLU
1	C	510	ARG
1	C	519	LYS
1	C	542	LYS
1	C	544	TYR
1	C	615	ASP
1	C	638	LEU
1	C	670	PHE
1	C	850	HIS
1	C	852	SER
1	C	878	LYS
1	C	928	GLN
1	C	948	GLN
1	C	1055	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	HIS
1	A	548	GLN
1	A	609	GLN
1	A	1011	GLN
2	D	25	ASN
1	C	388	HIS
1	C	657	ASN
1	C	843	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	812/845 (96%)	0.15	12 (1%)	73	75	26, 48, 93, 122	0
1	C	808/845 (95%)	0.44	41 (5%)	28	29	28, 63, 105, 141	0
2	B	76/79 (96%)	1.22	15 (19%)	1	0	46, 71, 93, 103	0
2	D	76/79 (96%)	2.79	45 (59%)	0	0	62, 121, 171, 178	0
All	All	1772/1848 (95%)	0.44	113 (6%)	19	19	26, 58, 109, 178	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	59	TYR	8.8
2	D	36	ILE	8.0
2	D	53	GLY	7.8
2	D	20	SER	7.8
1	C	475	GLY	6.5
2	D	32	ASP	6.1
2	D	66	THR	5.5
2	D	15	LEU	5.2
2	D	30	ILE	5.0
2	D	19	PRO	4.9
2	D	55	THR	4.9
2	B	4	PHE	4.7
1	A	222	SER	4.7
2	D	22	THR	4.6
2	D	3	ILE	4.6
2	D	1	MET	4.5
2	D	4	PHE	4.5
2	B	33	LYS	4.5
2	D	63	LYS	4.5
2	D	11	LYS	4.4
2	D	13	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	1058	LEU	4.3
2	D	54	ARG	4.3
2	D	21	ASP	4.2
1	C	1001	ASN	4.2
2	B	15	LEU	4.1
2	D	61	ILE	4.1
2	D	14	THR	4.1
2	D	9	THR	4.0
2	D	12	THR	4.0
2	D	33	LYS	4.0
1	C	481	ILE	4.0
1	C	988	LEU	3.9
2	B	9	THR	3.9
2	D	16	GLU	3.9
2	D	64	GLU	3.8
1	A	223	VAL	3.8
1	C	553	ILE	3.8
2	B	3	ILE	3.7
2	D	10	GLY	3.7
2	B	2	GLN	3.6
2	D	17	VAL	3.5
1	A	930	ARG	3.5
1	C	340	SER	3.4
1	C	343	TYR	3.4
1	C	949	ALA	3.4
1	A	926	VAL	3.4
2	B	13	ILE	3.3
2	D	34	GLU	3.3
1	C	957	TYR	3.3
2	D	65	SER	3.2
2	D	29	LYS	3.2
1	C	476	GLN	3.2
2	D	67	LEU	3.2
2	B	17	VAL	3.2
1	C	1015	ILE	3.1
2	D	58	ASP	2.9
2	D	51	GLU	2.9
1	C	1029	ILE	2.9
2	B	14	THR	2.9
2	D	50	LEU	2.9
2	B	59	TYR	2.9
2	B	1	MET	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	5	VAL	2.9
2	D	2	GLN	2.9
1	A	484	GLU	2.8
1	A	960	PHE	2.8
2	D	56	LEU	2.8
1	C	983	ILE	2.8
2	B	11	LYS	2.8
1	C	984	LEU	2.7
1	C	503	LYS	2.7
1	C	224	PRO	2.7
1	A	953	THR	2.7
1	C	1045	ILE	2.7
1	C	386	LYS	2.7
2	D	52	ASP	2.7
1	A	544	TYR	2.6
1	C	544	TYR	2.6
1	C	976	LEU	2.6
1	C	990	ALA	2.6
1	C	981	VAL	2.6
1	C	351	ARG	2.6
2	D	35	GLY	2.6
2	D	45	PHE	2.5
1	A	499	PHE	2.5
1	C	504	LYS	2.5
1	A	548	GLN	2.5
1	C	344	GLU	2.5
1	C	1017	GLN	2.4
2	D	62	GLN	2.4
2	B	18	GLU	2.4
1	C	677	ALA	2.4
1	C	498	PHE	2.4
1	C	950	LYS	2.4
1	C	358	VAL	2.4
2	D	18	GLU	2.4
1	C	944	ARG	2.4
1	C	1025	LEU	2.3
1	C	342	ASN	2.3
2	B	5	VAL	2.3
1	C	960	PHE	2.3
2	B	12	THR	2.2
1	A	986	LYS	2.2
1	C	678	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	7	THR	2.2
1	C	365	LEU	2.2
1	C	507	GLU	2.1
1	C	937	ARG	2.1
2	D	31	GLN	2.0
1	C	330	PHE	2.0
1	A	918	LYS	2.0
1	C	253	TYR	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.