Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 10:47 AM EST

PDB ID	:	3W5K
Title	:	Crystal structure of Snail1 and importin beta complex
Authors	:	Choi, S.; Yamashita, E.; Yasuhara, N.; Song, J.; Son, S.Y.; Won, Y.H.; Shin, Y.S.; Sekimoto, T.; Park, I.Y.; Yoneda, Y.; Lee, S.J.
Deposited on	:	2013-01-30
Resolution	:	2.60 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:

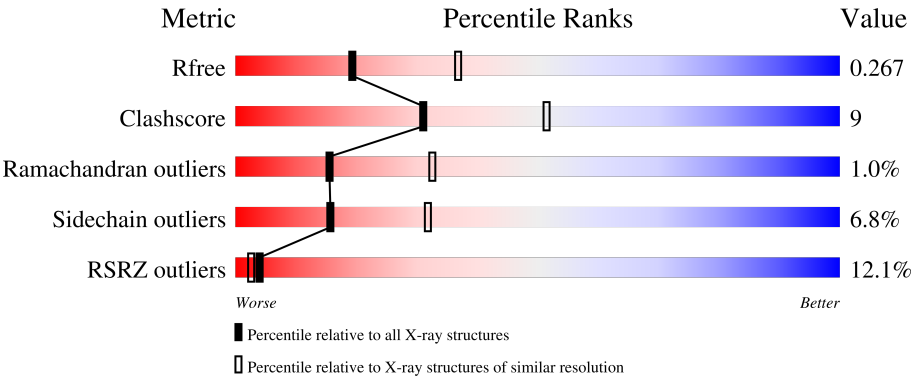
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	876	9% 76% 19%
2	B	264	14% 30% 10% 58%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7588 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 Importin subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	859	Total	C	N	O	S	0	0	0
			6676	4203	1123	1304	46			

- Molecule 2 is a protein called Zinc finger protein SNAI1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	110	Total	C	N	O	S	0	0	0
			848	523	168	144	13			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Zn	0	0
			4	4		

- Molecule 4 is water.

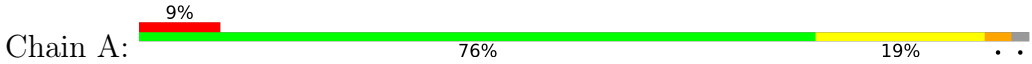
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O	0	0
			49	49		
4	B	11	Total	O	0	0
			11	11		

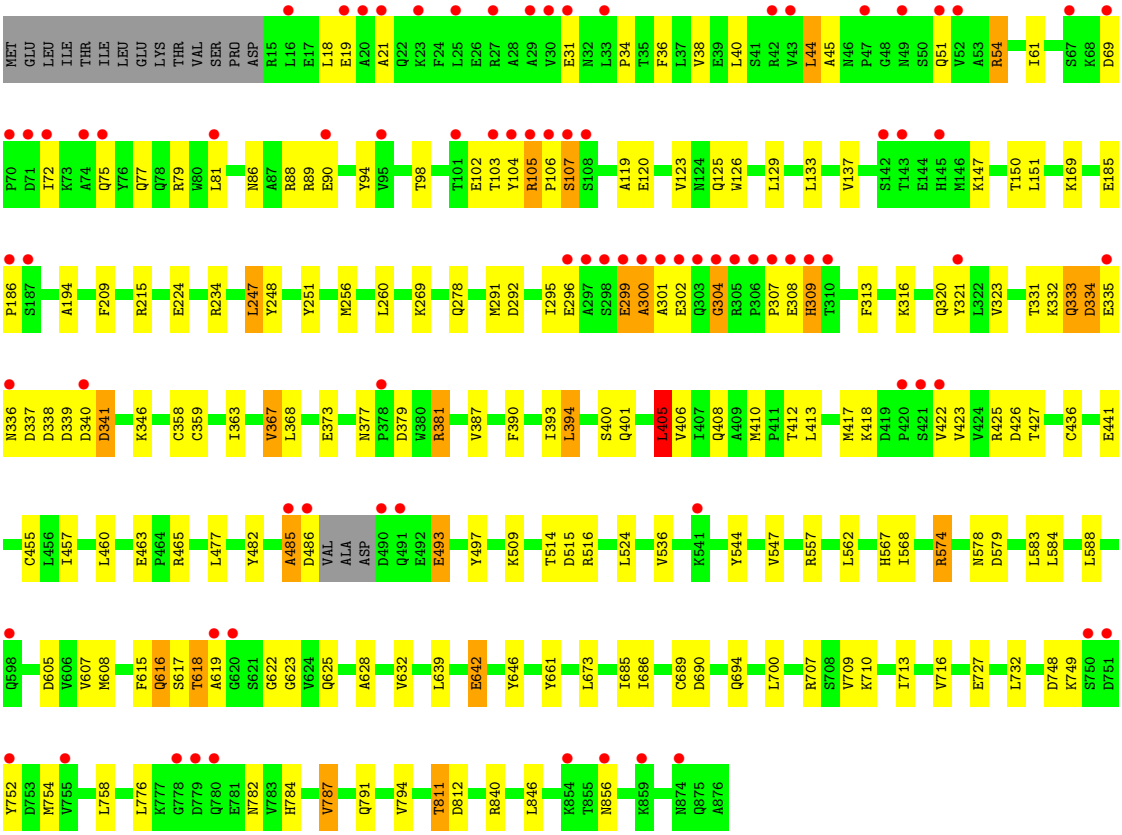
3 Residue-property plots (i)

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: Importin subunit beta-1

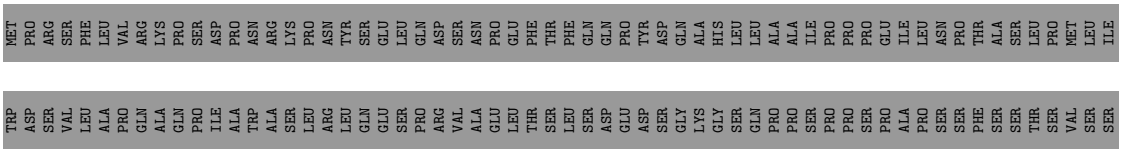
Chain A:

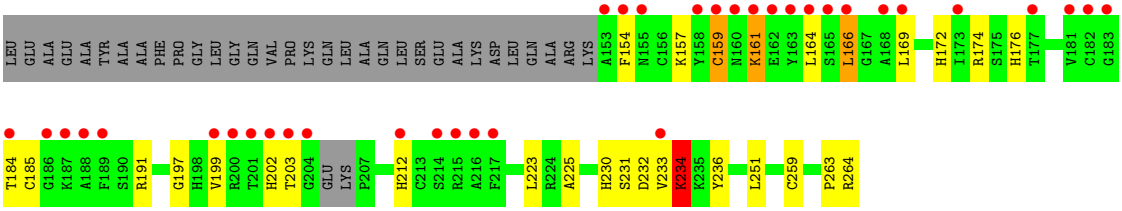




• Molecule 2: Zinc finger protein SNAI1

Chain B:




LEU GLU ALA GLU ALA TYR ALA ALA PHE PRO GLY LEU GLY GLN VAL PRO LYS GLN LEU ALA GLN LEU SER GLU ALA LYS ASP LEU GLN ALA ARG LYS
A153 F154 N155 C156 K157 Y158 C159 N160 K161 E162 Y163 L164 S165 L166 G167 A168 L169 H172 I173 R174 S175 H176 T177 V181 C182 G183
T184 C185 G186 K187 A188 F189 S190 R191 G197 H198 V199 R200 T201 H202 T203 G204 GLU LYS P207 H212 C213 S214 R215 A216 F217 L223 R224 A225 H230 S231 D232 V233 K234 K235 Y236 L251 C259 P263 R264

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	228.21Å 77.53Å 72.02Å 90.00° 100.96° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 45.95 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.8 (40.00-2.60) 97.7 (45.95-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.94 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.215 , 0.264 0.216 , 0.267	Depositor DCC
R_{free} test set	2117 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	64.4	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 74.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7588	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.23	0/6785	0.44	2/9209 (0.0%)
2	B	0.53	2/869 (0.2%)	0.56	0/1166
All	All	0.28	2/7654 (0.0%)	0.46	2/10375 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	197	GLY	C-N	-8.98	1.13	1.34
2	B	225	ALA	C-N	5.01	1.45	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	LEU	CA-CB-CG	6.29	129.76	115.30
1	A	304	GLY	N-CA-C	-5.24	100.00	113.10

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	6676	0	6661	100	0
2	B	848	0	809	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
4	A	49	0	0	4	0
4	B	11	0	0	3	0
All	All	7588	0	7470	136	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 9.

All (136) 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)
2:B:233:VAL:HA	2:B:234:LYS:CB	1.43	1.44
2:B:233:VAL:HA	2:B:234:LYS:HB3	1.15	1.14
2:B:233:VAL:HA	2:B:234:LYS:HB2	1.30	1.14
2:B:233:VAL:CA	2:B:234:LYS:CB	2.30	1.08
2:B:233:VAL:CA	2:B:234:LYS:HB2	1.93	0.95
2:B:232:ASP:O	2:B:234:LYS:HB2	1.73	0.88
1:A:615:PHE:O	1:A:617:SER:N	2.13	0.81
1:A:368:LEU:HD11	1:A:405:LEU:HD11	1.66	0.77
2:B:259:CYS:SG	4:B:601:HOH:O	2.43	0.75
1:A:482:TYR:OH	1:A:493:GLU:OE2	2.03	0.75
2:B:159:CYS:SG	2:B:161:LYS:NZ	2.55	0.74
1:A:410:MET:HA	1:A:413:LEU:HD12	1.71	0.72
1:A:69:ASP:HB3	1:A:72:ILE:HG22	1.71	0.71
2:B:184:THR:HG22	2:B:184:THR:O	1.91	0.71
2:B:154:PHE:HB3	2:B:169:LEU:HD22	1.74	0.70
1:A:44:LEU:O	1:A:54:ARG:NH1	2.25	0.69
2:B:212:HIS:HD2	2:B:230:HIS:CD2	2.11	0.69
2:B:184:THR:HG21	2:B:202:HIS:CG	2.29	0.67
1:A:256:MET:HA	1:A:260:LEU:HB2	1.77	0.67
1:A:588:LEU:HD13	1:A:607:VAL:HG13	1.77	0.66
1:A:90:GLU:HG2	1:A:94:TYR:HE2	1.60	0.66
1:A:426:ASP:OD2	2:B:264:ARG:NH2	2.27	0.66
2:B:184:THR:CG2	2:B:202:HIS:CE1	2.78	0.66
1:A:316:LYS:NZ	1:A:358:CYS:SG	2.59	0.65
2:B:231:SER:OG	2:B:232:ASP:N	2.30	0.64
2:B:236:TYR:HB3	2:B:251:LEU:HD22	1.79	0.64
2:B:174:ARG:NH1	4:B:607:HOH:O	2.28	0.62
1:A:334:ASP:N	1:A:334:ASP:OD1	2.32	0.62
2:B:233:VAL:CA	2:B:234:LYS:HB3	2.09	0.62
1:A:333:GLN:O	1:A:381:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:THR:HG21	2:B:202:HIS:CE1	2.36	0.61
2:B:212:HIS:HD2	2:B:230:HIS:HD2	1.48	0.61
1:A:616:GLN:H	1:A:625:GLN:HE21	1.49	0.60
2:B:212:HIS:CD2	2:B:230:HIS:CD2	2.90	0.60
2:B:232:ASP:C	2:B:234:LYS:HB2	2.22	0.60
1:A:137:VAL:HA	1:A:147:LYS:HG2	1.84	0.59
2:B:184:THR:HG21	2:B:202:HIS:CD2	2.38	0.59
1:A:436:CYS:O	4:A:901:HOH:O	2.16	0.59
1:A:427:THR:OG1	2:B:264:ARG:NH1	2.36	0.58
1:A:707:ARG:NH1	1:A:754:MET:SD	2.77	0.58
1:A:784:HIS:O	1:A:787:VAL:HG23	2.04	0.57
2:B:203:THR:HG22	2:B:203:THR:O	2.04	0.57
1:A:301:ALA:HB1	1:A:307:PRO:HD3	1.85	0.57
2:B:184:THR:HG22	2:B:202:HIS:CE1	2.39	0.57
1:A:209:PHE:O	1:A:215:ARG:NE	2.35	0.57
1:A:441:GLU:HG3	2:B:166:LEU:HD23	1.87	0.57
1:A:103:THR:O	1:A:103:THR:OG1	2.24	0.56
1:A:299:GLU:O	1:A:301:ALA:N	2.38	0.56
1:A:686:ILE:HD13	1:A:727:GLU:HG3	1.89	0.55
1:A:86:ASN:OD1	1:A:89:ARG:NH2	2.39	0.55
1:A:574:ARG:NH1	1:A:578:ASN:OD1	2.39	0.55
2:B:184:THR:O	2:B:184:THR:CG2	2.55	0.55
1:A:536:VAL:HG13	1:A:547:VAL:HG13	1.88	0.55
1:A:120:GLU:HB3	1:A:125:GLN:HB3	1.89	0.55
1:A:579:ASP:OD1	2:B:191:ARG:NH2	2.32	0.55
2:B:164:LEU:HB2	4:B:606:HOH:O	2.07	0.54
1:A:460:LEU:O	1:A:516:ARG:NH1	2.41	0.54
1:A:313:PHE:HD2	1:A:316:LYS:HG3	1.73	0.54
1:A:400:SER:OG	1:A:401:GLN:N	2.43	0.52
1:A:44:LEU:HD22	1:A:98:THR:HG21	1.90	0.51
1:A:337:ASP:OD1	1:A:338:ASP:N	2.44	0.51
1:A:608:MET:HE1	1:A:632:VAL:HG22	1.92	0.51
1:A:605:ASP:OD1	1:A:646:TYR:OH	2.16	0.51
1:A:700:LEU:HD22	1:A:710:LYS:HG3	1.93	0.51
1:A:123:VAL:HG23	1:A:125:GLN:HB2	1.93	0.51
2:B:184:THR:HG21	2:B:202:HIS:ND1	2.26	0.50
1:A:390:PHE:HZ	1:A:406:VAL:HA	1.77	0.50
1:A:413:LEU:O	1:A:417:MET:HG2	2.12	0.50
1:A:248:TYR:HB3	1:A:251:TYR:HD2	1.76	0.50
1:A:151:LEU:HD13	1:A:194:ALA:HB2	1.95	0.48
1:A:331:THR:HG23	1:A:381:ARG:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD12	1:A:61:ILE:HD12	1.95	0.48
1:A:90:GLU:HG2	1:A:94:TYR:CE2	2.45	0.48
1:A:169:LYS:NZ	4:A:919:HOH:O	2.47	0.48
2:B:184:THR:CG2	2:B:202:HIS:NE2	2.77	0.48
1:A:425:ARG:NH1	1:A:463:GLU:OE2	2.46	0.48
1:A:622:GLY:HA3	1:A:623:GLY:HA2	1.62	0.48
1:A:102:GLU:OE1	1:A:107:SER:HB2	2.14	0.47
1:A:441:GLU:HG3	2:B:166:LEU:CD2	2.44	0.47
1:A:690:ASP:O	1:A:694:GLN:HG2	2.14	0.47
1:A:301:ALA:O	1:A:302:GLU:HG2	2.14	0.47
1:A:639:LEU:HB3	1:A:642:GLU:OE1	2.15	0.47
1:A:493:GLU:HG2	1:A:544:TYR:OH	2.13	0.47
1:A:45:ALA:HB2	1:A:94:TYR:HB3	1.97	0.47
1:A:338:ASP:O	1:A:341:ASP:HB2	2.14	0.47
1:A:133:LEU:HD22	1:A:150:THR:HG23	1.96	0.46
1:A:335:GLU:HG3	1:A:423:VAL:HG13	1.97	0.46
1:A:269:LYS:NZ	1:A:321:TYR:OH	2.48	0.46
1:A:19:GLU:C	1:A:21:ALA:H	2.18	0.46
1:A:34:PRO:O	1:A:38:VAL:HG23	2.15	0.46
1:A:69:ASP:HB3	1:A:72:ILE:CG2	2.44	0.46
1:A:417:MET:HG3	1:A:455:CYS:SG	2.57	0.45
1:A:339:ASP:OD1	1:A:346:LYS:NZ	2.36	0.45
1:A:105:ARG:HB3	1:A:106:PRO:HD2	1.99	0.44
1:A:457:ILE:HG23	1:A:509:LYS:HG3	1.98	0.44
1:A:394:LEU:HD13	1:A:394:LEU:HA	1.81	0.44
1:A:515:ASP:OD2	1:A:557:ARG:NH1	2.50	0.44
1:A:323:VAL:HG13	1:A:367:VAL:HG23	1.99	0.44
1:A:618:THR:HA	1:A:619:ALA:HA	1.57	0.44
1:A:732:LEU:HD11	1:A:776:LEU:HD11	2.00	0.43
1:A:811:THR:OG1	1:A:812:ASP:N	2.50	0.43
1:A:36:PHE:CZ	1:A:40:LEU:HD11	2.54	0.43
1:A:51:GLN:HG3	1:A:104:TYR:CD1	2.54	0.43
1:A:567:HIS:CD2	1:A:568:ILE:HG23	2.53	0.43
2:B:236:TYR:CD2	2:B:236:TYR:N	2.86	0.43
2:B:203:THR:O	2:B:203:THR:CG2	2.67	0.43
1:A:307:PRO:HA	1:A:308:GLU:CB	2.49	0.43
1:A:291:MET:O	1:A:295:ILE:HG13	2.19	0.42
1:A:339:ASP:HA	1:A:341:ASP:N	2.34	0.42
1:A:185:GLU:HA	1:A:186:PRO:HD2	1.89	0.42
1:A:300:ALA:O	1:A:304:GLY:N	2.52	0.42
1:A:81:LEU:HA	1:A:88:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:ARG:H	2:B:264:ARG:HG2	1.46	0.42
1:A:316:LYS:HE3	1:A:359:CYS:HA	2.01	0.42
1:A:77:GLN:HG2	1:A:119:ALA:HB2	2.01	0.42
1:A:713:ILE:O	1:A:716:VAL:HG12	2.19	0.42
2:B:161:LYS:HE2	2:B:172:HIS:CE1	2.55	0.42
2:B:263:PRO:HA	2:B:264:ARG:C	2.40	0.42
1:A:574:ARG:HD2	1:A:619:ALA:HB1	2.02	0.42
1:A:840:ARG:NH1	4:A:905:HOH:O	2.35	0.42
1:A:418:LYS:HD3	1:A:418:LYS:HA	1.75	0.41
1:A:296:GLU:OE1	1:A:309:HIS:HB2	2.20	0.41
1:A:685:ILE:HG23	1:A:689:CYS:SG	2.60	0.41
1:A:485:ALA:HA	1:A:486:ASP:HA	1.69	0.41
1:A:247:LEU:HD12	1:A:247:LEU:HA	1.92	0.41
1:A:126:TRP:CH2	1:A:129:LEU:HD13	2.56	0.41
1:A:465:ARG:NH1	4:A:923:HOH:O	2.53	0.41
1:A:544:TYR:HA	1:A:547:VAL:HB	2.02	0.41
2:B:199:VAL:HG13	2:B:202:HIS:HD2	1.85	0.40
1:A:377:ASN:OD1	1:A:379:ASP:N	2.47	0.40
1:A:628:ALA:O	1:A:632:VAL:HG23	2.21	0.40
1:A:791:GLN:HA	1:A:794:VAL:HG23	2.03	0.40
2:B:159:CYS:SG	2:B:176:HIS:HE1	2.42	0.40
1:A:406:VAL:O	1:A:410:MET:N	2.55	0.40
1:A:390:PHE:O	1:A:393:ILE:HG12	2.22	0.40
2:B:234:LYS:O	2:B:236:TYR:CE2	2.74	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	855/876 (98%)	817 (96%)	30 (4%)	8 (1%)	17 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	106/264 (40%)	99 (93%)	5 (5%)	2 (2%)	8 15
All	All	961/1140 (84%)	916 (95%)	35 (4%)	10 (1%)	15 32

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	616	GLN
2	B	234	LYS
1	A	336	ASN
1	A	405	LEU
2	B	185	CYS
1	A	105	ARG
1	A	107	SER
1	A	300	ALA
1	A	485	ALA
1	A	309	HIS

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	735/751 (98%)	685 (93%)	50 (7%)	16 32
2	B	91/228 (40%)	85 (93%)	6 (7%)	16 33
All	All	826/979 (84%)	770 (93%)	56 (7%)	16 32

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	44	LEU
1	A	54	ARG
1	A	75	GLN
1	A	79	ARG
1	A	224	GLU

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Mol	Chain	Res	Type
1	A	234	ARG
1	A	247	LEU
1	A	278	GLN
1	A	292	ASP
1	A	299	GLU
1	A	320	GLN
1	A	332	LYS
1	A	333	GLN
1	A	334	ASP
1	A	340	ASP
1	A	341	ASP
1	A	363	ILE
1	A	367	VAL
1	A	373	GLU
1	A	381	ARG
1	A	387	VAL
1	A	394	LEU
1	A	405	LEU
1	A	408	GLN
1	A	412	THR
1	A	422	VAL
1	A	477	LEU
1	A	493	GLU
1	A	497	TYR
1	A	514	THR
1	A	524	LEU
1	A	562	LEU
1	A	574	ARG
1	A	583	LEU
1	A	584	LEU
1	A	618	THR
1	A	642	GLU
1	A	661	TYR
1	A	673	LEU
1	A	709	VAL
1	A	748	ASP
1	A	749	LYS
1	A	752	TYR
1	A	758	LEU
1	A	782	ASN
1	A	787	VAL
1	A	811	THR

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Mol	Chain	Res	Type
1	A	846	LEU
1	A	856	ASN
2	B	157	LYS
2	B	159	CYS
2	B	161	LYS
2	B	166	LEU
2	B	223	LEU
2	B	234	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	366	HIS
1	A	576	GLN
2	B	212	HIS

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)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	197:GLY	C	198:HIS	N	1.13

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	859/876 (98%)	0.54	81 (9%) 8 5	39, 69, 121, 170	0
2	B	110/264 (41%)	1.49	36 (32%) 0 0	47, 99, 138, 156	0
All	All	969/1140 (85%)	0.65	117 (12%) 4 2	39, 71, 128, 170	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	ARG	7.5
2	B	181	VAL	7.1
2	B	188	ALA	6.8
2	B	204	GLY	6.5
1	A	300	ALA	6.5
1	A	307	PRO	6.0
1	A	304	GLY	5.8
1	A	303	GLN	5.8
1	A	301	ALA	5.7
1	A	306	PRO	5.6
2	B	187	LYS	5.5
1	A	106	PRO	5.4
1	A	105	ARG	5.4
2	B	160	ASN	5.4
1	A	302	GLU	5.2
1	A	16	LEU	4.8
2	B	212	HIS	4.8
2	B	161	LYS	4.8
1	A	19	GLU	4.7
2	B	214	SER	4.7
1	A	299	GLU	4.7
2	B	216	ALA	4.7
1	A	51	GLN	4.5
2	B	164	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	158	TYR	4.5
1	A	43	VAL	4.4
2	B	201	THR	4.4
1	A	75	GLN	4.4
2	B	163	TYR	4.3
1	A	145	HIS	4.1
2	B	166	LEU	4.0
1	A	750	SER	4.0
1	A	620	GLY	4.0
2	B	155	ASN	4.0
1	A	340	ASP	4.0
1	A	752	TYR	3.9
1	A	297	ALA	3.9
1	A	336	ASN	3.8
2	B	203	THR	3.8
1	A	47	PRO	3.8
1	A	72	ILE	3.7
2	B	186	GLY	3.6
1	A	104	TYR	3.6
1	A	486	ASP	3.6
1	A	296	GLU	3.6
1	A	74	ALA	3.5
2	B	200	ARG	3.5
1	A	780	GLN	3.3
1	A	69	ASP	3.3
1	A	490	ASP	3.3
1	A	755	VAL	3.3
1	A	308	GLU	3.3
1	A	856	ASN	3.2
2	B	177	THR	3.2
1	A	485	ALA	3.2
1	A	71	ASP	3.1
1	A	42	ARG	3.1
1	A	298	SER	3.1
2	B	165	SER	3.1
1	A	27	ARG	3.1
1	A	422	VAL	3.0
1	A	21	ALA	3.0
1	A	101	THR	3.0
1	A	31	GLU	2.9
2	B	168	ALA	2.9
2	B	173	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	215	ARG	2.9
2	B	169	LEU	2.9
1	A	25	LEU	2.9
1	A	49	ASN	2.9
1	A	29	ALA	2.8
2	B	153	ALA	2.8
2	B	162	GLU	2.8
1	A	779	ASP	2.8
1	A	335	GLU	2.7
1	A	30	VAL	2.7
1	A	541	LYS	2.7
1	A	420	PRO	2.7
1	A	859	LYS	2.7
2	B	217	PHE	2.7
2	B	154	PHE	2.6
1	A	598	GLN	2.6
1	A	67	SER	2.5
1	A	309	HIS	2.5
2	B	184	THR	2.4
2	B	189	PHE	2.4
1	A	20	ALA	2.4
1	A	854	LYS	2.4
2	B	182	CYS	2.4
1	A	107	SER	2.3
1	A	70	PRO	2.3
1	A	90	GLU	2.3
2	B	202	HIS	2.3
1	A	619	ALA	2.3
2	B	183	GLY	2.3
1	A	95	VAL	2.3
1	A	186	PRO	2.3
2	B	159	CYS	2.3
1	A	491	GLN	2.2
2	B	233	VAL	2.2
1	A	108	SER	2.2
1	A	187	SER	2.2
1	A	103	THR	2.2
1	A	23	LYS	2.2
1	A	874	ASN	2.2
1	A	378	PRO	2.2
1	A	778	GLY	2.2
1	A	321	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	52	VAL	2.2
1	A	142	SER	2.2
1	A	81	LEU	2.1
1	A	421	SER	2.1
1	A	143	THR	2.1
1	A	33	LEU	2.1
1	A	310	THR	2.1
1	A	751	ASP	2.1
2	B	199	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	B	502	1/1	0.86	0.06	174,174,174,174	0
3	ZN	B	503	1/1	0.92	0.07	107,107,107,107	0
3	ZN	B	501	1/1	0.95	0.04	147,147,147,147	0
3	ZN	B	504	1/1	0.99	0.13	57,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.