



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:40 PM UTC

PDB ID : 3W5K / pdb_00003w5k
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	:	4-5-2 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

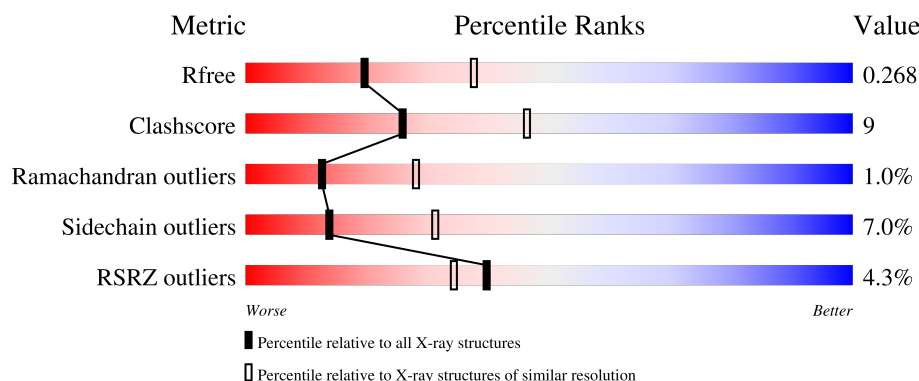
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

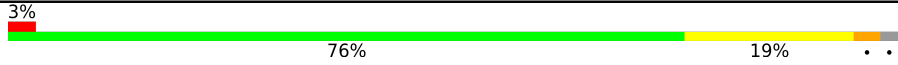
The reported resolution of this entry is 2.60 Å.

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	876	
2	B	264	

2 Entry composition

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 (CCD ID: ZN) (formula: Zn).

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

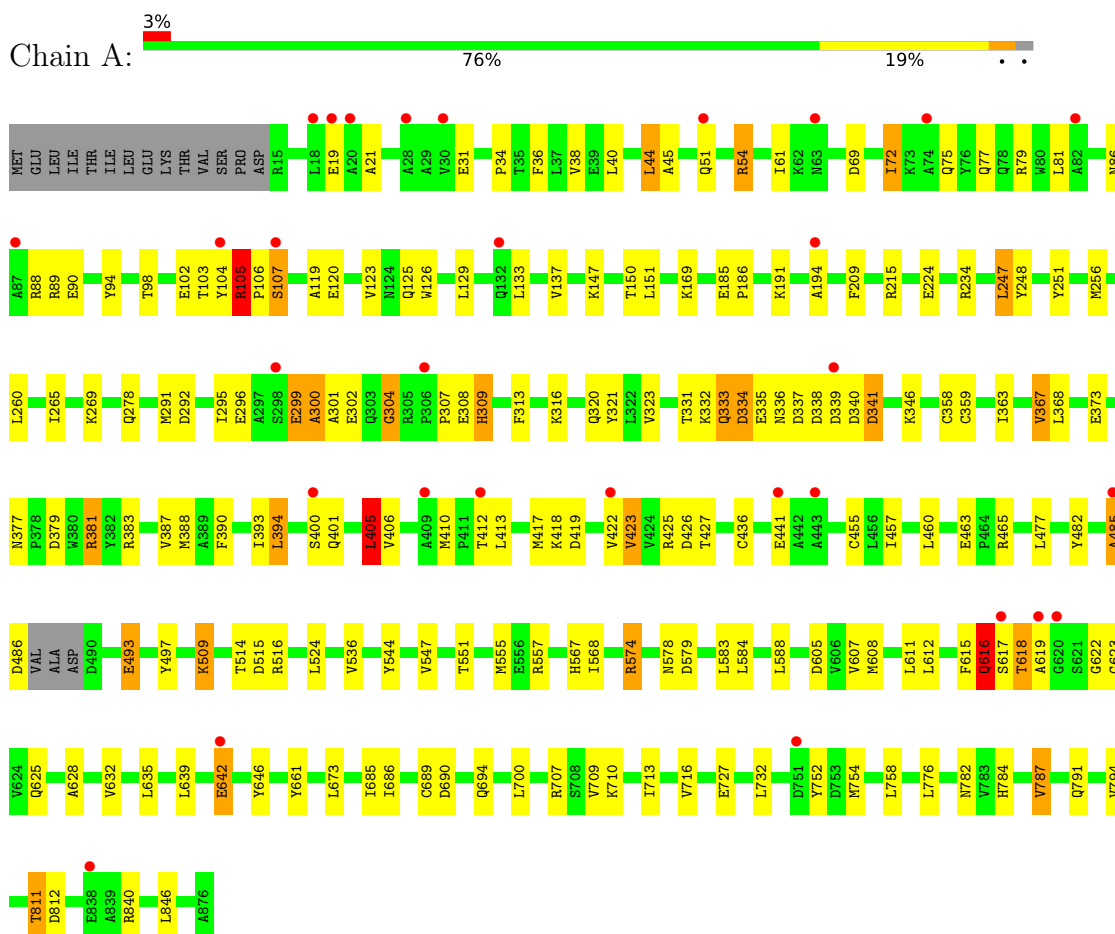
- Molecule 4 is water.

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

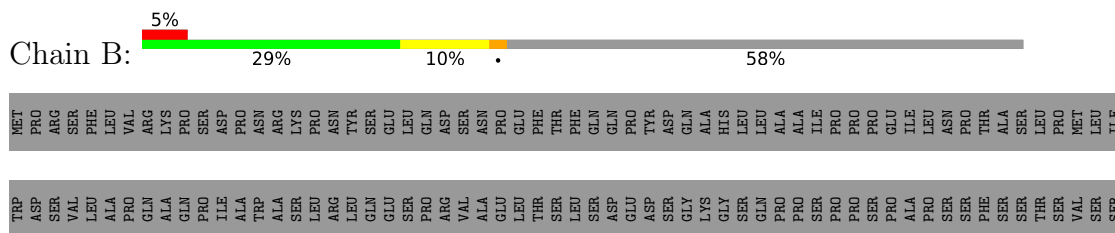
3 Residue-property plots

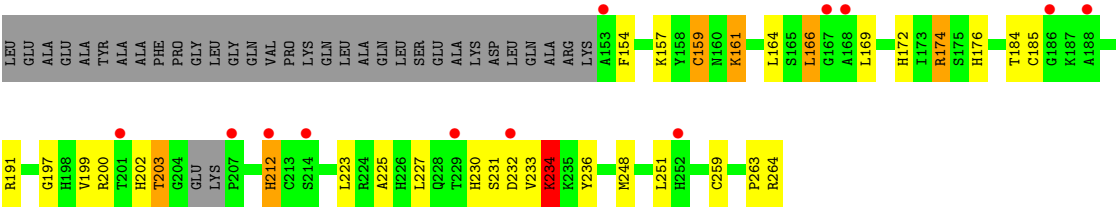
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 2: Zinc finger protein SNAI1





4 Data and refinement statistics

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 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (40.00-2.60) 97.8 (40.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.94 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.215 , 0.264 0.218 , 0.268	Depositor DCC
R_{free} test set	2117 reflections (4.98%)	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)	0.36 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

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](#)

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	0.34	0/6785	0.80	4/9209 (0.0%)
2	B	0.76	2/869 (0.2%)	0.89	3/1166 (0.3%)
All	All	0.41	2/7654 (0.0%)	0.81	7/10375 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	197	GLY	C-N	-15.10	1.13	1.33
2	B	225	ALA	C-N	8.88	1.45	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	GLY	N-CA-C	-6.75	100.00	111.27
1	A	105	ARG	CA-C-N	-6.74	112.86	119.87
1	A	105	ARG	C-N-CA	-6.74	112.86	119.87
2	B	212	HIS	N-CA-C	6.14	117.97	111.28
2	B	200	ARG	N-CA-C	-5.92	104.90	111.71
2	B	203	THR	N-CA-C	-5.65	106.36	113.20
1	A	616	GLN	N-CA-C	5.40	122.29	110.80

There are no chirality outliers.

There are no planarity outliers.

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	6676	0	6661	105	0
2	B	848	0	809	43	0
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	142	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 (142) 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:388:MET:HE1	2:B:264:ARG:HD3	1.66	0.78
1:A:368:LEU:HD11	1:A:405:LEU:HD11	1.66	0.77
2:B:159:CYS:SG	2:B:161:LYS:NZ	2.55	0.76
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
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
2:B:227:LEU:HD11	2:B:248:MET:HE3	1.77	0.65
1:A:316:LYS:NZ	1:A:358:CYS:SG	2.59	0.65
2:B:232:ASP:C	2:B:234:LYS:HB2	2.22	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:137:VAL:HA	1:A:147:LYS:HG2	1.84	0.59
1:A:605:ASP:OD1	1:A:646:TYR:OH	2.16	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:299:GLU:O	1:A:301:ALA:N	2.38	0.56
1:A:608:MET:HE1	1:A:632:VAL:HG22	1.85	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:608:MET:HE2	1:A:611:LEU:HD12	1.90	0.53
1:A:339:ASP:OD1	1:A:346:LYS:NZ	2.36	0.52
1:A:608:MET:HE3	1:A:635:LEU:HD23	1.91	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:400:SER:OG	1:A:401:GLN:N	2.43	0.49
1:A:19:GLU:C	1:A:21:ALA:H	2.18	0.49
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
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:103:THR:O	1:A:103:THR:OG1	2.24	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
2:B:263:PRO:HA	2:B:264:ARG:C	2.40	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:383:ARG:HH21	1:A:419:ASP:CG	2.26	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
1:A:551:THR:HG22	1:A:555:MET:HE2	2.03	0.40
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

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	855/876 (98%)	817 (96%)	30 (4%)	8 (1%)	14	30
2	B	106/264 (40%)	99 (93%)	5 (5%)	2 (2%)	6	13
All	All	961/1140 (84%)	916 (95%)	35 (4%)	10 (1%)	12	28

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

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%)	684 (93%)	51 (7%)	14	32
2	B	91/228 (40%)	84 (92%)	7 (8%)	12	27
All	All	826/979 (84%)	768 (93%)	58 (7%)	14	31

All (58) 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	72	ILE
1	A	75	GLN
1	A	79	ARG
1	A	191	LYS
1	A	224	GLU
1	A	234	ARG
1	A	247	LEU
1	A	265	ILE
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	412	THR
1	A	422	VAL
1	A	423	VAL
1	A	477	LEU
1	A	493	GLU
1	A	497	TYR
1	A	509	LYS
1	A	514	THR
1	A	524	LEU
1	A	574	ARG
1	A	583	LEU
1	A	584	LEU
1	A	612	LEU
1	A	618	THR
1	A	642	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	661	TYR
1	A	673	LEU
1	A	709	VAL
1	A	752	TYR
1	A	758	LEU
1	A	782	ASN
1	A	787	VAL
1	A	811	THR
1	A	846	LEU
2	B	157	LYS
2	B	159	CYS
2	B	161	LYS
2	B	166	LEU
2	B	174	ARG
2	B	223	LEU
2	B	234	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	51	GLN
1	A	200	ASN
1	A	445	ASN
1	A	576	GLN
1	A	589	GLN
1	A	616	GLN
1	A	744	GLN
1	A	856	ASN
2	B	212	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 [i](#)

There are no oligosaccharides 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 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	859/876 (98%)	0.27	30 (3%) 47 41	39, 69, 121, 170	0
2	B	110/264 (41%)	0.77	12 (10%) 10 8	47, 99, 138, 156	0
All	All	969/1140 (85%)	0.33	42 (4%) 40 34	39, 71, 128, 170	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	ALA	4.0
2	B	167	GLY	3.5
1	A	20	ALA	3.4
1	A	19	GLU	3.4
2	B	232	ASP	3.3
2	B	207	PRO	3.3
1	A	751	ASP	3.2
1	A	298	SER	3.0
1	A	642	GLU	2.9
1	A	107	SER	2.9
1	A	104	TYR	2.8
2	B	188	ALA	2.8
1	A	18	LEU	2.8
1	A	400	SER	2.7
1	A	306	PRO	2.6
1	A	339	ASP	2.5
1	A	619	ALA	2.5
1	A	620	GLY	2.5
1	A	63	ASN	2.5
1	A	132	GLN	2.4
1	A	485	ALA	2.4
2	B	212	HIS	2.4
1	A	422	VAL	2.4
2	B	168	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	186	GLY	2.4
1	A	30	VAL	2.3
1	A	838	GLU	2.3
2	B	252	HIS	2.3
1	A	441	GLU	2.3
1	A	28	ALA	2.2
2	B	214	SER	2.2
1	A	74	ALA	2.2
1	A	443	ALA	2.2
2	B	201	THR	2.2
1	A	82	ALA	2.2
1	A	87	ALA	2.2
2	B	229	THR	2.2
1	A	194	ALA	2.1
2	B	153	ALA	2.1
1	A	51	GLN	2.1
1	A	412	THR	2.1
1	A	617	SER	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](#)

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, 95th 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($\text{\AA}^2$)	Q<0.9
3	ZN	B	502	1/1	0.93	0.09	174,174,174,174	0
3	ZN	B	503	1/1	0.95	0.07	107,107,107,107	0
3	ZN	B	501	1/1	0.97	0.06	147,147,147,147	0
3	ZN	B	504	1/1	1.00	0.02	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.