Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:00 AM GMT

PDB ID	:	2Z5J
Title	:	Free Transportin 1
Authors	:	Imasaki, T.; Shimizu, T.; Hashimoto, H.; Hidaka, Y.; Yamada, M.; Sato, M.
Deposited on	:	2007-07-13
Resolution	:	3.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

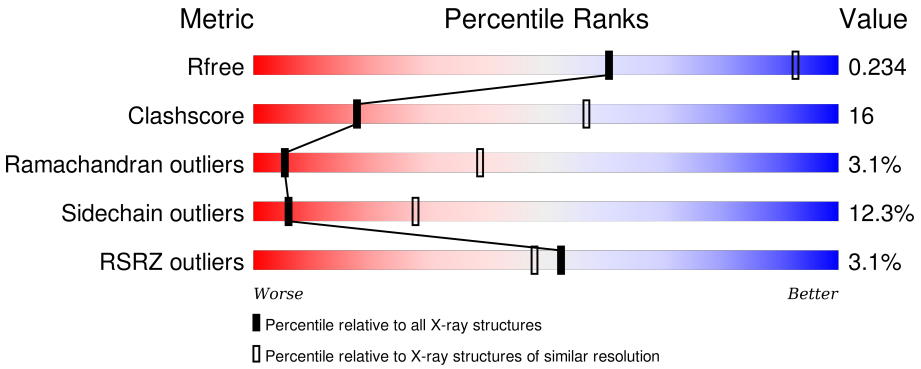
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.40 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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. 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	890	3%, 53%, 34%, 6%, 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6652 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 Transportin-1.

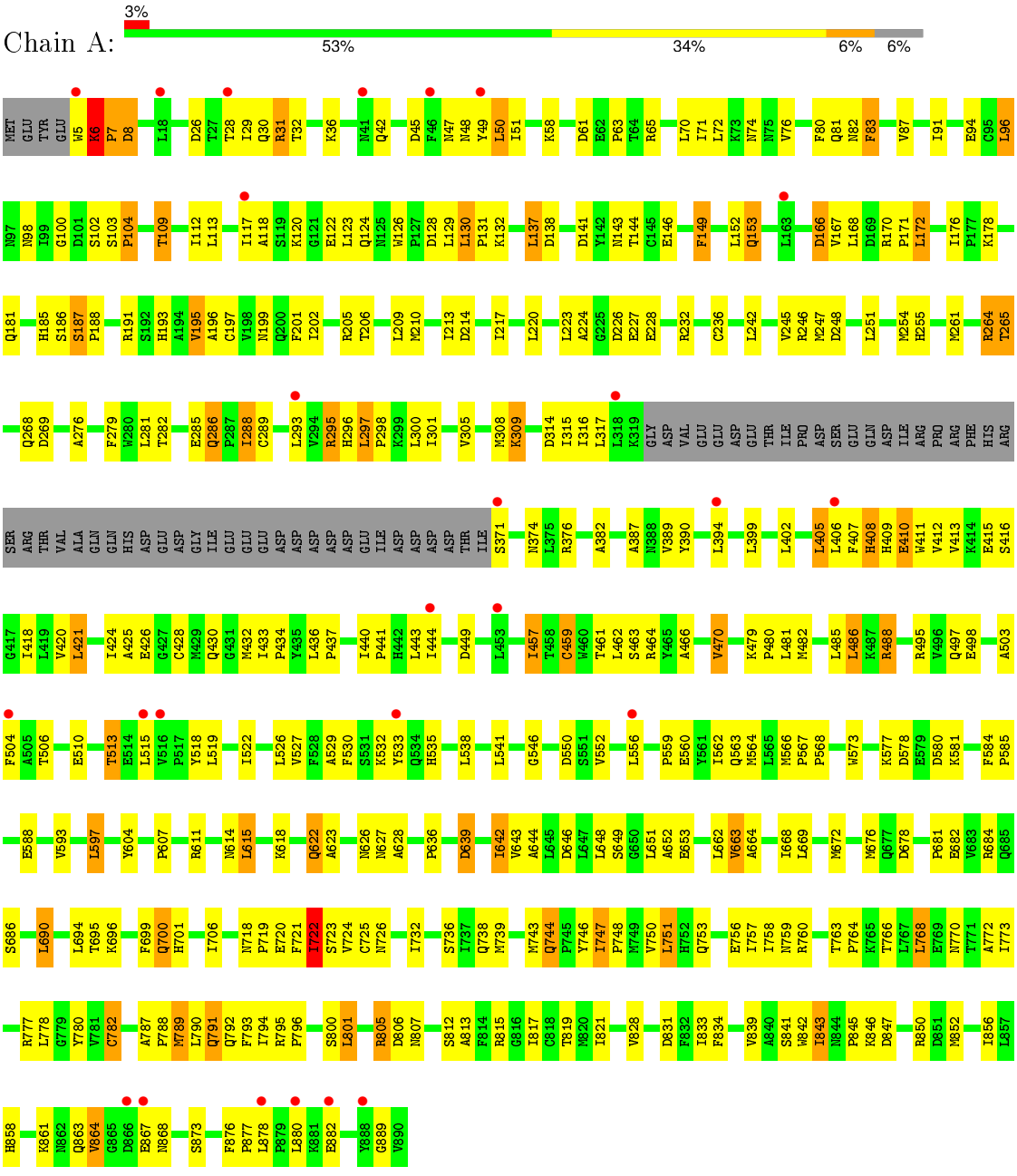
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	835	6652	4268	1109	1224	51	0	0	0

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 errors 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: Transportin-1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	107.47Å 107.47Å 194.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 3.40 49.36 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.36-3.40) 95.1 (49.36-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.303 0.229 , 0.234	Depositor DCC
R_{free} test set	791 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	97.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 120.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Outliers	0 of 15585 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6652	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.40	0/6795	0.56	0/9228

There are no bond length outliers.

There are no bond angle outliers.

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	6652	0	6718	213	0
All	All	6652	0	6718	213	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 16.

All (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LYS:HB3	1:A:7:PRO:HD2	1.22	1.09
1:A:130:LEU:H	1:A:130:LEU:HD12	1.40	0.85
1:A:518:TYR:O	1:A:522:ILE:HG12	1.78	0.83
1:A:611:ARG:O	1:A:615:LEU:HD12	1.86	0.75
1:A:6:LYS:HB3	1:A:7:PRO:CD	2.10	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:HB2	1:A:390:TYR:OH	1.87	0.75
1:A:470:VAL:HG21	1:A:510:GLU:HB3	1.69	0.74
1:A:664:ALA:HB2	1:A:701:HIS:CE1	2.23	0.73
1:A:584:PHE:HB2	1:A:585:PRO:HD3	1.69	0.73
1:A:48:ASN:HD21	1:A:87:VAL:HG22	1.55	0.72
1:A:6:LYS:CB	1:A:7:PRO:HD2	2.08	0.71
1:A:817:ILE:O	1:A:821:ILE:HG13	1.90	0.71
1:A:562:ILE:HG12	1:A:597:LEU:HD21	1.72	0.71
1:A:546:GLY:O	1:A:550:ASP:HB2	1.91	0.71
1:A:255:HIS:CE1	1:A:295:ARG:HE	2.10	0.68
1:A:286:GLN:HB2	1:A:288:ILE:HD12	1.76	0.68
1:A:739:MET:HB2	1:A:743:MET:HG2	1.75	0.67
1:A:573:TRP:CZ2	1:A:611:ARG:HG2	2.30	0.67
1:A:387:ALA:HA	1:A:394:LEU:HD22	1.78	0.66
1:A:768:LEU:HD23	1:A:800:SER:HB2	1.77	0.66
1:A:433:ILE:HA	1:A:436:LEU:HD12	1.79	0.65
1:A:772:ALA:HB3	1:A:801:LEU:HD13	1.78	0.65
1:A:425:ALA:HB3	1:A:464:ARG:HH11	1.62	0.65
1:A:113:LEU:O	1:A:117:ILE:HG12	1.98	0.64
1:A:440:ILE:O	1:A:444:ILE:HG12	1.97	0.64
1:A:102:SER:HA	1:A:143:ASN:HD22	1.63	0.64
1:A:130:LEU:HB2	1:A:131:PRO:HD3	1.80	0.63
1:A:26:ASP:HB3	1:A:29:ILE:HB	1.81	0.63
1:A:141:ASP:HB3	1:A:144:THR:OG1	1.99	0.62
1:A:644:ALA:O	1:A:648:LEU:HB2	2.00	0.62
1:A:245:VAL:HG12	1:A:246:ARG:HG2	1.81	0.61
1:A:51:ILE:HD13	1:A:91:ILE:HA	1.83	0.61
1:A:831:ASP:O	1:A:834:PHE:HB2	1.99	0.61
1:A:852:MET:O	1:A:856:ILE:HG12	2.01	0.61
1:A:747:ILE:N	1:A:748:PRO:HD2	2.15	0.61
1:A:217:ILE:HD12	1:A:242:LEU:HD21	1.81	0.61
1:A:529:ALA:HB3	1:A:541:LEU:HD21	1.81	0.61
1:A:623:ALA:HB2	1:A:636:PRO:HG3	1.83	0.61
1:A:205:ARG:HE	1:A:245:VAL:HG13	1.65	0.60
1:A:261:MET:O	1:A:265:THR:HB	2.01	0.59
1:A:481:LEU:O	1:A:485:LEU:HB2	2.02	0.59
1:A:535:HIS:O	1:A:538:LEU:HB3	2.02	0.59
1:A:81:GLN:CD	1:A:81:GLN:H	2.05	0.59
1:A:410:GLU:HG3	1:A:413:VAL:HB	1.84	0.59
1:A:584:PHE:HB2	1:A:585:PRO:CD	2.33	0.59
1:A:185:HIS:O	1:A:191:ARG:HD3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ILE:HB	1:A:441:PRO:HD3	1.85	0.58
1:A:309:LYS:HA	1:A:416:SER:OG	2.03	0.58
1:A:415:GLU:HG2	1:A:457:ILE:HG13	1.84	0.57
1:A:763:THR:HB	1:A:768:LEU:CD1	2.34	0.57
1:A:117:ILE:HB	1:A:126:TRP:HZ3	1.70	0.57
1:A:806:ASP:OD2	1:A:843:ILE:HG12	2.05	0.57
1:A:639:ASP:O	1:A:643:VAL:HG23	2.05	0.56
1:A:626:ASN:C	1:A:628:ALA:H	2.09	0.56
1:A:232:ARG:HD2	1:A:264:ARG:HD2	1.87	0.56
1:A:374:ASN:ND2	1:A:376:ARG:HB3	2.20	0.56
1:A:255:HIS:CE1	1:A:295:ARG:NE	2.74	0.56
1:A:410:GLU:HB2	1:A:413:VAL:H	1.71	0.56
1:A:585:PRO:HA	1:A:588:GLU:OE1	2.07	0.54
1:A:736:SER:HA	1:A:743:MET:HG3	1.88	0.54
1:A:639:ASP:HA	1:A:642:ILE:HD12	1.89	0.54
1:A:877:PRO:HD2	1:A:880:LEU:HD23	1.88	0.54
1:A:301:ILE:O	1:A:305:VAL:HG23	2.08	0.54
1:A:255:HIS:HE1	1:A:295:ARG:HE	1.53	0.54
1:A:622:GLN:HB3	1:A:636:PRO:HB3	1.89	0.54
1:A:482:MET:O	1:A:486:LEU:HB2	2.08	0.54
1:A:118:ALA:O	1:A:122:GLU:O	2.26	0.54
1:A:389:VAL:HB	1:A:390:TYR:HD1	1.73	0.53
1:A:410:GLU:C	1:A:412:VAL:H	2.12	0.53
1:A:753:GLN:O	1:A:757:ILE:HG12	2.08	0.53
1:A:399:LEU:HA	1:A:402:LEU:HD12	1.91	0.53
1:A:566:MET:HG3	1:A:604:TYR:CE1	2.43	0.53
1:A:440:ILE:HB	1:A:441:PRO:CD	2.39	0.53
1:A:415:GLU:HA	1:A:418:ILE:HD12	1.90	0.53
1:A:593:VAL:O	1:A:597:LEU:HB2	2.09	0.53
1:A:314:ASP:C	1:A:316:ILE:H	2.11	0.52
1:A:206:THR:O	1:A:210:MET:HG2	2.08	0.52
1:A:58:LYS:HE2	1:A:65:ARG:HH22	1.74	0.52
1:A:410:GLU:CG	1:A:413:VAL:HB	2.39	0.52
1:A:482:MET:HG3	1:A:504:PHE:HE1	1.73	0.52
1:A:5:TRP:O	1:A:6:LYS:HB2	2.09	0.52
1:A:719:PRO:HB2	1:A:760:ARG:HH22	1.75	0.52
1:A:443:LEU:HB3	1:A:462:LEU:HD21	1.92	0.52
1:A:130:LEU:CD1	1:A:130:LEU:H	2.17	0.51
1:A:858:HIS:CE1	1:A:889:GLY:HA3	2.46	0.51
1:A:519:LEU:HD21	1:A:552:VAL:HG11	1.93	0.51
1:A:434:PRO:O	1:A:437:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:LYS:HA	1:A:738:GLN:HE21	1.75	0.50
1:A:746:TYR:C	1:A:748:PRO:HD2	2.32	0.50
1:A:276:ALA:O	1:A:279:PHE:HB3	2.11	0.50
1:A:864:VAL:HG22	1:A:868:ASN:CB	2.41	0.50
1:A:560:GLU:O	1:A:563:GLN:HB2	2.11	0.50
1:A:732:ILE:O	1:A:736:SER:HB2	2.12	0.50
1:A:750:VAL:HG23	1:A:751:LEU:N	2.28	0.49
1:A:466:ALA:O	1:A:470:VAL:HG22	2.11	0.49
1:A:96:LEU:HD12	1:A:132:LYS:HG2	1.95	0.49
1:A:718:ASN:HD21	1:A:720:GLU:HB2	1.78	0.49
1:A:8:ASP:HB3	1:A:49:TYR:OH	2.11	0.49
1:A:529:ALA:CB	1:A:541:LEU:HD21	2.42	0.49
1:A:780:TYR:CE1	1:A:815:ARG:HG2	2.48	0.48
1:A:199:ASN:HA	1:A:202:ILE:HD12	1.95	0.48
1:A:559:PRO:O	1:A:563:GLN:HG2	2.12	0.48
1:A:117:ILE:HB	1:A:126:TRP:CZ3	2.48	0.48
1:A:526:LEU:O	1:A:529:ALA:HB3	2.14	0.48
1:A:747:ILE:HG23	1:A:778:LEU:HD22	1.95	0.48
1:A:479:LYS:HB3	1:A:480:PRO:HD3	1.95	0.48
1:A:297:LEU:N	1:A:298:PRO:CD	2.76	0.48
1:A:739:MET:CB	1:A:743:MET:HG2	2.44	0.48
1:A:420:VAL:O	1:A:424:ILE:HG13	2.14	0.48
1:A:648:LEU:HD12	1:A:648:LEU:HA	1.77	0.47
1:A:488:ARG:NE	1:A:488:ARG:HA	2.28	0.47
1:A:374:ASN:HD21	1:A:376:ARG:HB3	1.80	0.47
1:A:649:SER:HA	1:A:652:ALA:HB3	1.97	0.47
1:A:806:ASP:HB3	1:A:842:TRP:CZ3	2.50	0.47
1:A:47:ASN:O	1:A:50:LEU:HB2	2.15	0.47
1:A:873:SER:HA	1:A:876:PHE:CE2	2.50	0.47
1:A:100:GLY:HA3	1:A:144:THR:HA	1.96	0.46
1:A:226:ASP:O	1:A:228:GLU:N	2.48	0.46
1:A:149:PHE:CD2	1:A:193:HIS:HB3	2.51	0.46
1:A:130:LEU:HB2	1:A:131:PRO:CD	2.45	0.46
1:A:646:ASP:OD1	1:A:686:SER:HB2	2.16	0.46
1:A:80:PHE:HA	1:A:83:PHE:CD2	2.50	0.46
1:A:201:PHE:HB3	1:A:206:THR:CG2	2.46	0.46
1:A:405:LEU:O	1:A:407:PHE:N	2.48	0.46
1:A:864:VAL:HG22	1:A:868:ASN:HB2	1.98	0.46
1:A:676:MET:O	1:A:684:ARG:HD2	2.15	0.46
1:A:839:VAL:C	1:A:841:SER:H	2.20	0.45
1:A:795:ARG:HG2	1:A:831:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:GLU:OE2	1:A:756:GLU:HA	2.17	0.45
1:A:662:LEU:HD12	1:A:662:LEU:H	1.82	0.45
1:A:251:LEU:HA	1:A:254:MET:HB2	1.99	0.45
1:A:700:GLN:HB3	1:A:700:GLN:HE21	1.63	0.45
1:A:428:CYS:O	1:A:432:MET:HG2	2.17	0.44
1:A:791:GLN:HG2	1:A:792:GLN:HG3	1.99	0.44
1:A:408:HIS:O	1:A:410:GLU:N	2.50	0.44
1:A:109:THR:O	1:A:112:ILE:HB	2.16	0.44
1:A:61:ASP:OD2	1:A:63:PRO:HD2	2.16	0.44
1:A:777:ARG:HE	1:A:812:SER:CB	2.30	0.44
1:A:213:ILE:HG23	1:A:214:ASP:H	1.81	0.44
1:A:864:VAL:O	1:A:868:ASN:HB2	2.17	0.44
1:A:751:LEU:HD11	1:A:789:MET:SD	2.58	0.44
1:A:153:GLN:HA	1:A:197:CYS:SG	2.58	0.44
1:A:669:LEU:HA	1:A:672:MET:HB2	1.99	0.44
1:A:421:LEU:HB3	1:A:461:THR:HG21	1.99	0.44
1:A:787:ALA:N	1:A:788:PRO:CD	2.80	0.44
1:A:722:ILE:HD12	1:A:723:SER:H	1.82	0.44
1:A:556:LEU:HG	1:A:556:LEU:O	2.17	0.43
1:A:187:SER:HA	1:A:188:PRO:HD3	1.78	0.43
1:A:562:ILE:CG1	1:A:597:LEU:HD21	2.47	0.43
1:A:26:ASP:O	1:A:30:GLN:HG2	2.18	0.43
1:A:744:GLN:HG2	1:A:782:CYS:SG	2.58	0.43
1:A:6:LYS:CB	1:A:7:PRO:CD	2.85	0.43
1:A:530:PHE:C	1:A:532:LYS:H	2.22	0.43
1:A:213:ILE:HG23	1:A:214:ASP:N	2.34	0.43
1:A:281:LEU:HD23	1:A:382:ALA:HA	2.00	0.43
1:A:28:THR:O	1:A:31:ARG:HG3	2.18	0.43
1:A:747:ILE:H	1:A:747:ILE:HG12	1.61	0.43
1:A:668:ILE:HG23	1:A:669:LEU:HG	2.01	0.42
1:A:76:VAL:HG11	1:A:117:ILE:HD13	2.01	0.42
1:A:777:ARG:HE	1:A:812:SER:HB3	1.84	0.42
1:A:94:GLU:O	1:A:98:ASN:HB2	2.19	0.42
1:A:141:ASP:HB3	1:A:144:THR:HG1	1.84	0.42
1:A:726:ASN:C	1:A:726:ASN:OD1	2.57	0.42
1:A:72:LEU:HD21	1:A:91:ILE:HD12	2.01	0.42
1:A:864:VAL:HG22	1:A:868:ASN:HB3	2.00	0.42
1:A:695:THR:O	1:A:699:PHE:HB2	2.20	0.42
1:A:126:TRP:CG	1:A:129:LEU:HB2	2.55	0.42
1:A:706:ILE:HA	1:A:706:ILE:HD13	1.94	0.42
1:A:722:ILE:CD1	1:A:723:SER:H	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:PHE:HB3	1:A:724:VAL:HB	2.01	0.42
1:A:791:GLN:HG2	1:A:792:GLN:N	2.34	0.42
1:A:791:GLN:HE21	1:A:792:GLN:HG3	1.84	0.42
1:A:32:THR:O	1:A:36:LYS:HG2	2.18	0.42
1:A:567:PRO:HB2	1:A:568:PRO:HD3	2.02	0.42
1:A:470:VAL:CG2	1:A:510:GLU:HB3	2.44	0.41
1:A:649:SER:HB3	1:A:690:LEU:HA	2.02	0.41
1:A:166:ASP:N	1:A:166:ASP:OD2	2.49	0.41
1:A:790:LEU:HA	1:A:793:PHE:CE2	2.55	0.41
1:A:7:PRO:HB2	1:A:8:ASP:H	1.73	0.41
1:A:584:PHE:CD2	1:A:643:VAL:HG21	2.55	0.41
1:A:773:ILE:HG13	1:A:801:LEU:HD11	2.01	0.41
1:A:137:LEU:HD11	1:A:152:LEU:HD12	2.02	0.41
1:A:201:PHE:HB3	1:A:206:THR:HG21	2.01	0.41
1:A:795:ARG:N	1:A:796:PRO:HD2	2.35	0.41
1:A:82:ASN:O	1:A:83:PHE:C	2.59	0.41
1:A:71:ILE:O	1:A:74:ASN:HB2	2.20	0.41
1:A:389:VAL:HB	1:A:390:TYR:CD1	2.52	0.41
1:A:497:GLN:HB3	1:A:533:TYR:HE1	1.86	0.41
1:A:529:ALA:HB1	1:A:533:TYR:CD2	2.56	0.41
1:A:81:GLN:HE22	1:A:120:LYS:NZ	2.18	0.41
1:A:103:SER:HA	1:A:104:PRO:HD2	1.74	0.41
1:A:527:VAL:HG21	1:A:564:MET:HB2	2.02	0.41
1:A:213:ILE:O	1:A:217:ILE:HG12	2.21	0.41
1:A:690:LEU:CD2	1:A:694:LEU:HG	2.51	0.41
1:A:459:CYS:SG	1:A:503:ALA:HB2	2.61	0.41
1:A:773:ILE:HG23	1:A:813:ALA:HB2	2.03	0.41
1:A:678:ASP:O	1:A:684:ARG:HD3	2.21	0.41
1:A:668:ILE:HG23	1:A:669:LEU:N	2.35	0.41
1:A:794:ILE:HG12	1:A:828:VAL:HG12	2.03	0.41
1:A:176:ILE:HG21	1:A:209:LEU:HA	2.03	0.41
1:A:220:LEU:O	1:A:223:LEU:HB3	2.19	0.41
1:A:195:VAL:O	1:A:196:ALA:C	2.60	0.40
1:A:839:VAL:O	1:A:841:SER:N	2.46	0.40
1:A:172:LEU:HD13	1:A:176:ILE:HG12	2.02	0.40
1:A:282:THR:O	1:A:285:GLU:HB2	2.20	0.40
1:A:758:ILE:HG12	1:A:796:PRO:HB2	2.04	0.40
1:A:213:ILE:HD13	1:A:246:ARG:HG3	2.04	0.40
1:A:845:PRO:HB2	1:A:850:ARG:HB2	2.03	0.40
1:A:805:ARG:O	1:A:807:ASN:N	2.48	0.40
1:A:170:ARG:N	1:A:171:PRO:HD3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:LEU:O	1:A:653:GLU:N	2.54	0.40
1:A:663:VAL:HG22	1:A:668:ILE:HG21	2.04	0.40
1:A:223:LEU:O	1:A:224:ALA:C	2.60	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	831/890 (93%)	666 (80%)	139 (17%)	26 (3%)	5 39

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	227	GLU
1	A	289	CYS
1	A	722	ILE
1	A	847	ASP
1	A	8	ASP
1	A	409	HIS
1	A	513	THR
1	A	186	SER
1	A	248	ASP
1	A	295	ARG
1	A	405	LEU
1	A	406	LEU
1	A	627	ASN
1	A	764	PRO
1	A	6	LYS
1	A	83	PHE
1	A	104	PRO

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Mol	Chain	Res	Type
1	A	607	PRO
1	A	642	ILE
1	A	770	ASN
1	A	846	LYS
1	A	315	ILE
1	A	470	VAL
1	A	681	PRO
1	A	744	GLN

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	750/802 (94%)	658 (88%)	92 (12%)	6 28

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	31	ARG
1	A	42	GLN
1	A	45	ASP
1	A	50	LEU
1	A	70	LEU
1	A	96	LEU
1	A	109	THR
1	A	123	LEU
1	A	124	GLN
1	A	128	ASP
1	A	130	LEU
1	A	137	LEU
1	A	138	ASP
1	A	146	GLU
1	A	149	PHE
1	A	153	GLN
1	A	166	ASP

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Mol	Chain	Res	Type
1	A	167	VAL
1	A	168	LEU
1	A	172	LEU
1	A	178	LYS
1	A	181	GLN
1	A	187	SER
1	A	195	VAL
1	A	236	CYS
1	A	247	MET
1	A	264	ARG
1	A	265	THR
1	A	268	GLN
1	A	269	ASP
1	A	286	GLN
1	A	288	ILE
1	A	296	HIS
1	A	297	LEU
1	A	300	LEU
1	A	308	MET
1	A	309	LYS
1	A	317	LEU
1	A	371	SER
1	A	408	HIS
1	A	410	GLU
1	A	411	TRP
1	A	421	LEU
1	A	426	GLU
1	A	430	GLN
1	A	449	ASP
1	A	457	ILE
1	A	459	CYS
1	A	463	SER
1	A	486	LEU
1	A	488	ARG
1	A	495	ARG
1	A	498	GLU
1	A	506	THR
1	A	513	THR
1	A	515	LEU
1	A	577	LYS
1	A	578	ASP
1	A	580	ASP

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Mol	Chain	Res	Type
1	A	581	LYS
1	A	597	LEU
1	A	614	ASN
1	A	615	LEU
1	A	618	LYS
1	A	622	GLN
1	A	639	ASP
1	A	663	VAL
1	A	682	GLU
1	A	690	LEU
1	A	700	GLN
1	A	722	ILE
1	A	725	CYS
1	A	747	ILE
1	A	751	LEU
1	A	759	ASN
1	A	766	THR
1	A	768	LEU
1	A	782	CYS
1	A	789	MET
1	A	791	GLN
1	A	801	LEU
1	A	805	ARG
1	A	819	THR
1	A	833	ILE
1	A	843	ILE
1	A	861	LYS
1	A	863	GLN
1	A	864	VAL
1	A	867	GLU
1	A	878	LEU
1	A	882	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	42	GLN
1	A	47	ASN
1	A	48	ASN
1	A	79	HIS
1	A	81	GLN

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Mol	Chain	Res	Type
1	A	85	ASN
1	A	98	ASN
1	A	124	GLN
1	A	125	ASN
1	A	143	ASN
1	A	173	ASN
1	A	212	HIS
1	A	255	HIS
1	A	442	HIS
1	A	534	GLN
1	A	574	ASN
1	A	700	GLN
1	A	701	HIS
1	A	718	ASN
1	A	738	GLN
1	A	784	GLN
1	A	791	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no 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	835/890 (93%)	0.21	26 (3%) 52 48	112, 126, 136, 147	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	SER	4.6
1	A	888	TYR	3.8
1	A	394	LEU	3.7
1	A	318	LEU	3.6
1	A	880	LEU	3.5
1	A	293	LEU	3.2
1	A	504	PHE	3.2
1	A	406	LEU	3.1
1	A	516	VAL	3.1
1	A	28	THR	3.0
1	A	867	GLU	3.0
1	A	453	LEU	3.0
1	A	866	ASP	3.0
1	A	878	LEU	2.8
1	A	18	LEU	2.5
1	A	5	TRP	2.5
1	A	41	ASN	2.5
1	A	46	PHE	2.5
1	A	117	ILE	2.4
1	A	533	TYR	2.3
1	A	49	TYR	2.2
1	A	556	LEU	2.2
1	A	515	LEU	2.1
1	A	882	GLU	2.1
1	A	163	LEU	2.1
1	A	444	ILE	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.