



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:57 AM UTC

PDB ID : 2Z5J / pdb_00002z5j
Title : Free Transportin 1
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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

<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

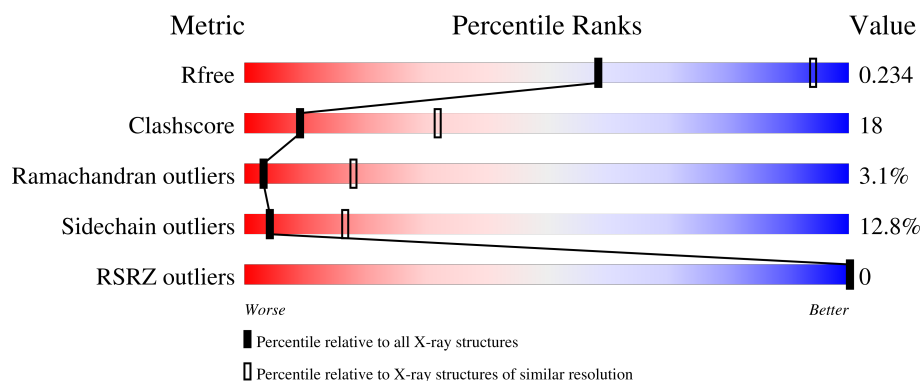
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	890	

2 Entry composition

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

- Molecule 1: Transportin-1



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	792 reflections (5.08%)	wwPDB-VP
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 , 121.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

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 ⓘ

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	0.50	2/6795 (0.0%)	0.93	13/9228 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	ILE	CA-CB	5.21	1.56	1.54
1	A	564	MET	CG-SD	5.02	1.93	1.80

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	SER	CA-C-N	8.44	130.39	119.84
1	A	103	SER	C-N-CA	8.44	130.39	119.84
1	A	841	SER	N-CA-C	-7.48	106.09	114.62
1	A	43	TYR	CA-C-N	7.05	128.65	119.84
1	A	43	TYR	C-N-CA	7.05	128.65	119.84
1	A	187	SER	CA-C-N	6.34	126.09	119.05
1	A	187	SER	C-N-CA	6.34	126.09	119.05
1	A	6	LYS	CA-C-N	5.69	126.95	119.84
1	A	6	LYS	C-N-CA	5.69	126.95	119.84
1	A	718	ASN	CA-C-N	5.20	125.28	119.87
1	A	718	ASN	C-N-CA	5.20	125.28	119.87
1	A	228	GLU	CA-C-N	5.10	124.71	119.56
1	A	228	GLU	C-N-CA	5.10	124.71	119.56

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	243	0
All	All	6652	0	6718	243	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 18.

All (243) 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:HD12	1:A:130:LEU:H	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
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:199:ASN:HB3	1:A:241:MET:HE1	1.76	0.65
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:81:GLN:CD	1:A:81:GLN:H	2.05	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:672:MET:HE1	1:A:691:LEU:HA	1.81	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:817:ILE:HA	1:A:820:MET:HE3	1.82	0.60
1:A:247:MET:HE3	1:A:288:ILE:HD11	1.84	0.59
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:626:ASN:C	1:A:628:ALA:H	2.09	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
1:A:410:GLU:C	1:A:412:VAL:H	2.12	0.58
1:A:309:LYS:HA	1:A:416:SER:OG	2.03	0.58
1:A:440:ILE:HB	1:A:441:PRO:HD3	1.85	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:314:ASP:C	1:A:316:ILE:H	2.11	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: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:746:TYR:C	1:A:748:PRO:HD2	2.32	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:58:LYS:HE2	1:A:65:ARG:HH22	1.74	0.52
1:A:206:THR:O	1:A:210:MET:HG2	2.08	0.52
1:A:482:MET:HE1	1:A:518:TYR:CD1	2.44	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:H	1:A:130:LEU:CD1	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
1:A:696:LYS:HA	1:A:738:GLN:HE21	1.75	0.50
1:A:710:MET:HE2	1:A:746:TYR:HB3	1.93	0.50
1:A:276:ALA:O	1:A:279:PHE:HB3	2.11	0.50
1:A:560:GLU:O	1:A:563:GLN:HB2	2.11	0.50
1:A:839:VAL:C	1:A:841:SER:H	2.20	0.50
1:A:864:VAL:HG22	1:A:868:ASN:CB	2.41	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:199:ASN:HA	1:A:202:ILE:HD12	1.95	0.48
1:A:780:TYR:CE1	1:A:815:ARG:HG2	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:420:VAL:O	1:A:424:ILE:HG13	2.14	0.48
1:A:739:MET:CB	1:A:743:MET:HG2	2.44	0.48
1:A:530:PHE:C	1:A:532:LYS:H	2.22	0.47
1:A:488:ARG:NE	1:A:488:ARG:HA	2.28	0.47
1:A:648:LEU:HD12	1:A:648:LEU:HA	1.77	0.47
1:A:374:ASN:HD21	1:A:376:ARG:HB3	1.80	0.47
1:A:815:ARG:HG3	1:A:852:MET:HE1	1.96	0.47
1:A:649:SER:HA	1:A:652:ALA:HB3	1.97	0.47
1:A:726:ASN:OD1	1:A:726:ASN:C	2.57	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:149:PHE:CD2	1:A:193:HIS:HB3	2.51	0.46
1:A:226:ASP:O	1:A:228:GLU:N	2.48	0.46
1:A:130:LEU:HB2	1:A:131:PRO:CD	2.45	0.46
1:A:411:TRP:CD1	1:A:411:TRP:H	2.31	0.46
1:A:646:ASP:OD1	1:A:686:SER:HB2	2.16	0.46
1:A:82:ASN:O	1:A:83:PHE:C	2.59	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:676:MET:O	1:A:684:ARG:HD2	2.15	0.46
1:A:864:VAL:HG22	1:A:868:ASN:HB2	1.98	0.46
1:A:195:VAL:O	1:A:196:ALA:C	2.60	0.45
1:A:756:GLU:OE2	1:A:756:GLU:HA	2.17	0.45
1:A:795:ARG:HG2	1:A:831:ASP:OD1	2.17	0.45
1:A:626:ASN:C	1:A:628:ALA:N	2.74	0.45
1:A:223:LEU:O	1:A:224:ALA:C	2.60	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:HE21	1:A:700:GLN:HB3	1.63	0.45
1:A:428:CYS:O	1:A:432:MET:HG2	2.17	0.44
1:A:583:LEU:O	1:A:584:PHE:C	2.60	0.44
1:A:791:GLN:HG2	1:A:792:GLN:HG3	1.99	0.44
1:A:109:THR:O	1:A:112:ILE:HB	2.16	0.44
1:A:166:ASP:CG	1:A:170:ARG:HH21	2.25	0.44
1:A:408:HIS:O	1:A:410:GLU:N	2.50	0.44
1:A:61:ASP:OD2	1:A:63:PRO:HD2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:153:GLN:HA	1:A:197:CYS:SG	2.58	0.44
1:A:676:MET:HE3	1:A:688:PHE:HE2	1.83	0.44
1:A:751:LEU:HD11	1:A:789:MET:SD	2.58	0.44
1:A:421:LEU:HB3	1:A:461:THR:HG21	1.99	0.44
1:A:669:LEU:HA	1:A:672:MET:HB2	1.99	0.44
1:A:722:ILE:HD12	1:A:723:SER:H	1.82	0.44
1:A:787:ALA:N	1:A:788:PRO:CD	2.80	0.44
1:A:187:SER:HA	1:A:188:PRO:HD3	1.78	0.43
1:A:26:ASP:O	1:A:30:GLN:HG2	2.18	0.43
1:A:556:LEU:O	1:A:556:LEU:HG	2.17	0.43
1:A:562:ILE:CG1	1:A:597:LEU:HD21	2.47	0.43
1:A:787:ALA:C	1:A:789:MET:H	2.26	0.43
1:A:744:GLN:HG2	1:A:782:CYS:SG	2.58	0.43
1:A:846:LYS:O	1:A:847:ASP:C	2.62	0.43
1:A:6:LYS:CB	1:A:7:PRO:CD	2.85	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:601:PHE:C	1:A:603:PRO:HD2	2.44	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:94:GLU:O	1:A:98:ASN:HB2	2.19	0.42
1:A:777:ARG:HE	1:A:812:SER:HB3	1.84	0.42
1:A:141:ASP:HB3	1:A:144:THR:HG1	1.84	0.42
1:A:311:SER:C	1:A:313:ILE:H	2.27	0.42
1:A:676:MET:HE3	1:A:688:PHE:CE2	2.53	0.42
1:A:72:LEU:HD21	1:A:91:ILE:HD12	2.01	0.42
1:A:695:THR:O	1:A:699:PHE:HB2	2.20	0.42
1:A:864:VAL:HG22	1:A:868:ASN:HB3	2.00	0.42
1:A:126:TRP:CG	1:A:129:LEU:HB2	2.55	0.42
1:A:706:ILE:HD13	1:A:706:ILE:HA	1.94	0.42
1:A:721:PHE:HB3	1:A:724:VAL:HB	2.01	0.42
1:A:722:ILE:CD1	1:A:723:SER:H	2.33	0.42
1:A:791:GLN:HG2	1:A:792:GLN:N	2.34	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:791:GLN:HE21	1:A:792:GLN:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:PHE:C	1:A:862:ASN:H	2.28	0.42
1:A:166:ASP:OD2	1:A:166:ASP:N	2.49	0.41
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: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:137:LEU:HD11	1:A:152:LEU:HD12	2.02	0.41
1:A:584:PHE:CD2	1:A:643:VAL:HG21	2.55	0.41
1:A:651:LEU:C	1:A:653:GLU:N	2.77	0.41
1:A:773:ILE:HG13	1:A:801:LEU:HD11	2.01	0.41
1:A:201:PHE:HB3	1:A:206:THR:HG21	2.01	0.41
1:A:584:PHE:O	1:A:585:PRO:C	2.63	0.41
1:A:44:PRO:C	1:A:46:PHE:H	2.27	0.41
1:A:71:ILE:O	1:A:74:ASN:HB2	2.20	0.41
1:A:457:ILE:O	1:A:458:THR:C	2.63	0.41
1:A:795:ARG:N	1:A:796:PRO:HD2	2.35	0.41
1:A:389:VAL:HB	1:A:390:TYR:CD1	2.52	0.41
1:A:405:LEU:C	1:A:407:PHE:H	2.28	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:439:LEU:O	1:A:440:ILE:C	2.63	0.41
1:A:459:CYS:SG	1:A:503:ALA:HB2	2.61	0.41
1:A:690:LEU:CD2	1:A:694:LEU:HG	2.51	0.41
1:A:797:TRP:O	1:A:798:CYS:C	2.64	0.41
1:A:176:ILE:HG21	1:A:209:LEU:HA	2.03	0.41
1:A:668:ILE:HG23	1:A:669:LEU:N	2.35	0.41
1:A:678:ASP:O	1:A:684:ARG:HD3	2.21	0.41
1:A:773:ILE:HG23	1:A:813:ALA:HB2	2.03	0.41
1:A:794:ILE:HG12	1:A:828:VAL:HG12	2.03	0.41
1:A:220:LEU:O	1:A:223:LEU:HB3	2.19	0.41
1:A:406:LEU:C	1:A:414:LYS:HG3	2.45	0.40
1:A:763:THR:O	1:A:764:PRO:C	2.63	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:839:VAL:O	1:A:841:SER:N	2.46	0.40
1:A:408:HIS:C	1:A:410:GLU:H	2.29	0.40
1:A:651:LEU:C	1:A:653:GLU:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:ILE:HG12	1:A:796:PRO:HB2	2.04	0.40
1:A:170:ARG:N	1:A:171:PRO:HD3	2.36	0.40
1:A:213:ILE:HD13	1:A:246:ARG:HG3	2.04	0.40
1:A:651:LEU:O	1:A:653:GLU:N	2.54	0.40
1:A:805:ARG:O	1:A:807:ASN:N	2.48	0.40
1:A:845:PRO:HB2	1:A:850:ARG:HB2	2.03	0.40
1:A:663:VAL:HG22	1:A:668:ILE:HG21	2.04	0.40
1:A:884:LEU:C	1:A:886:ALA:H	2.29	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	831/890 (93%)	666 (80%)	139 (17%)	26 (3%)	3 18

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

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Mol	Chain	Res	Type
1	A	627	ASN
1	A	764	PRO
1	A	6	LYS
1	A	83	PHE
1	A	104	PRO
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%)	654 (87%)	96 (13%)	4 17

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	99	ILE
1	A	109	THR
1	A	117	ILE
1	A	123	LEU
1	A	124	GLN
1	A	128	ASP
1	A	130	LEU

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Mol	Chain	Res	Type
1	A	137	LEU
1	A	146	GLU
1	A	149	PHE
1	A	153	GLN
1	A	166	ASP
1	A	167	VAL
1	A	168	LEU
1	A	172	LEU
1	A	174	ILE
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	251	LEU
1	A	264	ARG
1	A	265	THR
1	A	268	GLN
1	A	269	ASP
1	A	281	LEU
1	A	286	GLN
1	A	288	ILE
1	A	296	HIS
1	A	297	LEU
1	A	300	LEU
1	A	309	LYS
1	A	313	ILE
1	A	317	LEU
1	A	371	SER
1	A	408	HIS
1	A	410	GLU
1	A	421	LEU
1	A	424	ILE
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

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Mol	Chain	Res	Type
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
1	A	590	LEU
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	641	MET
1	A	643	VAL
1	A	663	VAL
1	A	680	MET
1	A	682	GLU
1	A	690	LEU
1	A	700	GLN
1	A	722	ILE
1	A	747	ILE
1	A	751	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	13	GLN
1	A	41	ASN
1	A	42	GLN
1	A	48	ASN
1	A	79	HIS
1	A	81	GLN
1	A	85	ASN
1	A	124	GLN
1	A	125	ASN
1	A	143	ASN
1	A	173	ASN
1	A	181	GLN
1	A	212	HIS
1	A	255	HIS
1	A	266	GLN
1	A	286	GLN
1	A	442	HIS
1	A	445	GLN
1	A	534	GLN
1	A	554	HIS
1	A	574	ASN
1	A	610	GLN
1	A	626	ASN
1	A	700	GLN
1	A	701	HIS
1	A	718	ASN
1	A	738	GLN
1	A	759	ASN
1	A	784	GLN
1	A	791	GLN
1	A	803	ASN
1	A	858	HIS
1	A	875	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	835/890 (93%)	-0.39	0 100 100	112, 126, 136, 147	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.