



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 05:46 PM GMT

PDB ID : 2H4M
Title : Karyopherin Beta2/Transportin-M9NLS
Authors : Chook, Y.M.; Cansizoglu, A.E.
Deposited on : 2006-05-24
Resolution : 3.05 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

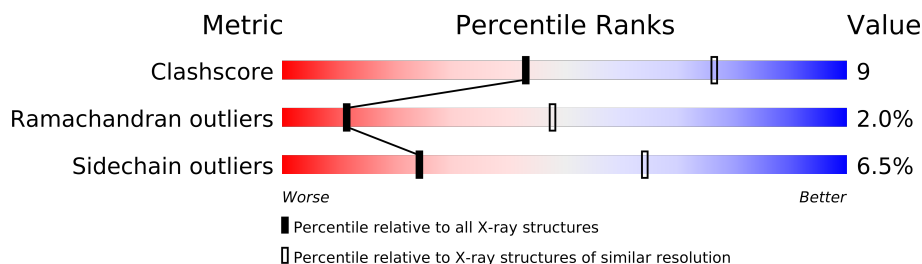
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.05 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))
Clashscore	79885	2629 (3.12-3.00)
Ramachandran outliers	78287	2536 (3.12-3.00)
Sidechain outliers	78261	2539 (3.12-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	865	
1	B	865	
2	C	49	
2	D	49	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12740 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	827	Total	C	N	O	S	0	0	0
			6253	4009	1046	1147	51			
1	B	810	Total	C	N	O	S	4	0	0
			6133	3933	1025	1124	51			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	GLY	-	SEE REMARK 999	UNP Q92973
A	338	GLY	-	SEE REMARK 999	UNP Q92973
A	339	SER	-	SEE REMARK 999	UNP Q92973
A	340	GLY	-	SEE REMARK 999	UNP Q92973
A	341	GLY	-	SEE REMARK 999	UNP Q92973
A	342	SER	-	SEE REMARK 999	UNP Q92973
A	343	GLY	-	SEE REMARK 999	UNP Q92973
B	337	GLY	-	SEE REMARK 999	UNP Q92973
B	338	GLY	-	SEE REMARK 999	UNP Q92973
B	339	SER	-	SEE REMARK 999	UNP Q92973
B	340	GLY	-	SEE REMARK 999	UNP Q92973
B	341	GLY	-	SEE REMARK 999	UNP Q92973
B	342	SER	-	SEE REMARK 999	UNP Q92973
B	343	GLY	-	SEE REMARK 999	UNP Q92973

- Molecule 2 is a protein called HNRPA1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	23	Total	C	N	O	S	0	0	0
			161	96	31	33	1			
2	D	27	Total	C	N	O	S	0	0	0
			193	119	35	38	1			

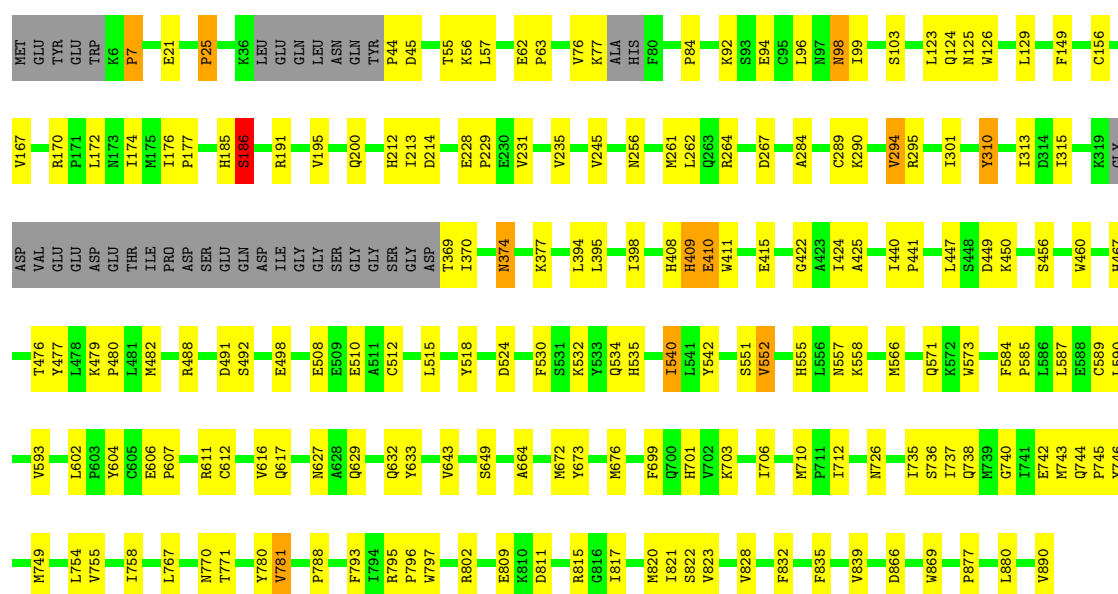
3 Residue-property plots

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.

Note EDS was not executed.

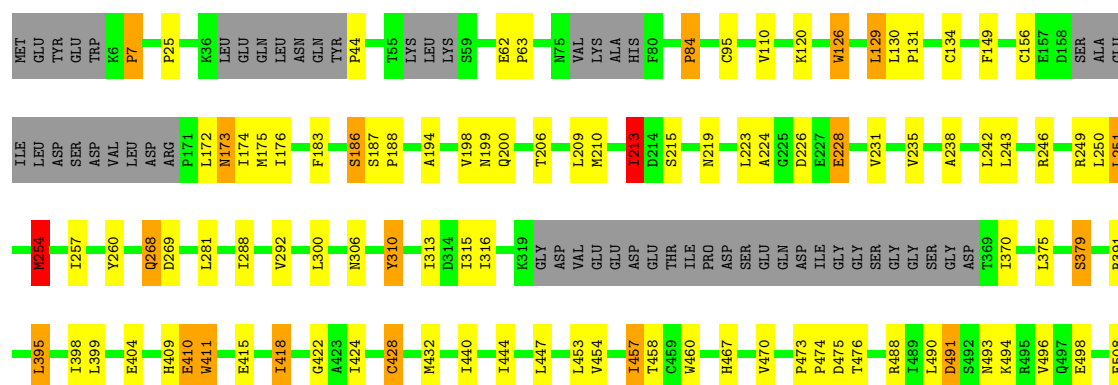
• Molecule 1: Transportin-1

Chain A:



• Molecule 1: Transportin-1

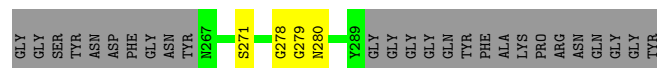
Chain B:





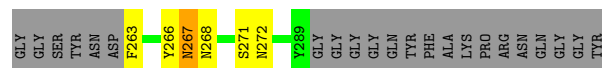
- Molecule 2: HNRPA1 protein

Chain C:



- Molecule 2: HNRPA1 protein

Chain D:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.01Å 154.09Å 141.67Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	50.00 – 3.05	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12740	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

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	0.39	0/6378	0.56	4/8691 (0.0%)
1	B	0.37	0/6257	0.57	5/8526 (0.1%)
2	C	0.42	0/165	0.46	0/220
2	D	0.41	0/199	0.47	0/266
All	All	0.38	0/12999	0.56	9/17703 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	PRO	N-CA-CB	6.18	110.71	103.30
1	A	7	PRO	N-CA-CB	6.17	110.70	103.30
1	A	44	PRO	N-CA-CB	6.09	110.61	103.30
1	B	25	PRO	N-CA-CB	5.99	110.49	103.30
1	B	44	PRO	N-CA-CB	5.96	110.45	103.30
1	B	84	PRO	N-CA-CB	5.94	110.42	103.30
1	B	7	PRO	N-CA-CB	5.86	110.34	103.30
1	A	25	PRO	N-CA-CB	5.83	110.30	103.30
1	B	268	GLN	CA-CB-CG	-5.71	100.84	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6253	0	6073	98	0
1	B	6133	0	5931	123	0
2	C	161	0	134	1	0
2	D	193	0	157	5	0
All	All	12740	0	12295	219	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (219) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:627:ASN:HD22	1:B:617:GLN:HE22	1.18	0.91
1:B:679:LYS:H	1:B:679:LYS:HD3	1.44	0.82
1:A:735:ILE:HG22	1:A:743:MET:HE3	1.66	0.77
1:B:798:CYS:O	1:B:802:ARG:HB2	1.84	0.76
1:A:498:GLU:HG3	1:A:540:ILE:HD12	1.67	0.75
1:A:409:HIS:CG	1:A:410:GLU:H	2.03	0.75
1:B:310:TYR:HB2	1:B:313:ILE:HG13	1.66	0.74
1:A:606:GLU:HB3	1:A:607:PRO:HD3	1.67	0.74
1:A:398:ILE:HG12	1:A:424:ILE:HD11	1.70	0.74
1:A:450:LYS:HD2	1:A:450:LYS:H	1.52	0.73
1:B:609:TYR:OH	1:B:668:ILE:HG12	1.90	0.72
1:B:793:PHE:HZ	1:B:820:MET:HE1	1.55	0.71
1:A:313:ILE:HG23	1:A:370:ILE:HG21	1.72	0.71
1:A:795:ARG:HB3	1:A:796:PRO:HD3	1.73	0.71
1:B:842:TRP:HB3	1:B:845:PRO:HG3	1.74	0.69
1:B:552:VAL:HG13	1:B:555:HIS:HB2	1.74	0.69
1:A:735:ILE:HG22	1:A:743:MET:CE	2.22	0.68
1:B:717:LEU:HD11	1:B:750:VAL:HG22	1.76	0.68
1:B:130:LEU:HB2	1:B:131:PRO:HD3	1.77	0.67
1:A:310:TYR:HB3	1:A:313:ILE:HD12	1.75	0.67
1:B:424:ILE:HG23	1:B:428:CYS:SG	2.34	0.67
1:A:374:ASN:HD21	1:A:377:LYS:HG3	1.60	0.66
1:B:710:MET:HG2	1:B:746:TYR:HB3	1.79	0.65
1:B:744:GLN:HA	1:B:747:ILE:HD12	1.77	0.65
1:B:467:HIS:HA	1:B:510:GLU:HG2	1.78	0.65
1:B:559:PRO:O	1:B:563:GLN:HB2	1.96	0.64
1:A:374:ASN:ND2	1:A:377:LYS:HG3	2.13	0.64
1:A:185:HIS:O	1:A:186:SER:O	2.17	0.63
1:B:418:ILE:HD11	1:B:458:THR:HA	1.82	0.62
1:B:415:GLU:OE2	1:B:457:ILE:HG12	2.01	0.61
1:B:188:PRO:HB3	1:B:228:GLU:HG3	1.83	0.60
1:B:498:GLU:HG2	1:B:540:ILE:HD12	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:795:ARG:HB3	1:B:796:PRO:HD3	1.82	0.60
1:A:573:TRP:CZ2	1:A:611:ARG:HD3	2.37	0.59
1:B:769:GLU:OE1	2:D:271:SER:HB2	2.02	0.59
1:B:176:ILE:HD13	1:B:209:LEU:HB2	1.83	0.59
1:B:877:PRO:HG2	2:D:263:PHE:HB2	1.84	0.59
1:A:284:ALA:HA	1:A:289:CYS:SG	2.43	0.59
1:A:758:ILE:HG12	1:A:796:PRO:HB2	1.85	0.58
1:A:409:HIS:CG	1:A:410:GLU:N	2.71	0.58
1:B:710:MET:HE1	1:B:735:ILE:HG21	1.84	0.58
1:A:508:GLU:HA	1:A:515:LEU:HD11	1.85	0.57
1:A:447:LEU:O	1:A:488:ARG:HD2	2.03	0.57
1:B:804:ILE:HD12	1:B:807:ASN:HD21	1.70	0.57
1:B:840:ALA:HB3	2:D:266:TYR:OH	2.06	0.55
1:A:797:TRP:CZ2	1:A:817:ILE:HG13	2.42	0.55
1:B:156:CYS:HB3	1:B:200:GLN:HG3	1.88	0.55
1:A:821:ILE:HG12	1:A:828:VAL:HG21	1.88	0.55
1:A:96:LEU:HD23	1:A:99:ILE:HD11	1.88	0.55
1:A:409:HIS:ND1	1:A:410:GLU:N	2.51	0.54
1:B:779:GLY:HA3	1:B:820:MET:SD	2.47	0.54
1:B:398:ILE:HG21	1:B:424:ILE:HD11	1.89	0.54
1:A:877:PRO:HD2	1:A:880:LEU:HD23	1.89	0.54
1:A:395:LEU:HA	1:A:398:ILE:HG22	1.89	0.54
1:A:664:ALA:HB2	1:A:701:HIS:CE1	2.43	0.54
1:B:587:LEU:HB2	1:B:643:VAL:HG13	1.89	0.54
1:B:573:TRP:HZ3	1:B:587:LEU:HD22	1.73	0.54
1:A:726:ASN:HD21	1:A:770:ASN:HD22	1.56	0.54
1:A:156:CYS:HB3	1:A:200:GLN:HG3	1.88	0.54
1:B:793:PHE:HZ	1:B:820:MET:CE	2.20	0.54
1:B:288:ILE:HD12	1:B:288:ILE:H	1.73	0.54
1:A:811:ASP:OD1	1:A:815:ARG:NH1	2.36	0.53
1:B:183:PHE:HD2	1:B:219:ASN:HB3	1.72	0.53
1:A:612:CYS:O	1:A:616:VAL:HG23	2.08	0.53
1:A:754:LEU:HD22	1:A:771:THR:HG23	1.91	0.53
1:B:62:GLU:N	1:B:63:PRO:HD2	2.24	0.53
1:B:418:ILE:CD1	1:B:458:THR:HA	2.39	0.53
1:B:183:PHE:CD2	1:B:219:ASN:HB3	2.44	0.53
1:B:411:TRP:C	1:B:411:TRP:CD1	2.81	0.53
1:A:672:MET:O	1:A:676:MET:HG3	2.09	0.52
1:A:552:VAL:HG13	1:A:555:HIS:HB2	1.90	0.52
1:B:310:TYR:N	1:B:310:TYR:CD1	2.78	0.52
1:A:710:MET:HE1	1:A:735:ILE:HG21	1.91	0.52
1:A:699:PHE:CG	1:A:738:GLN:HG2	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:95:CYS:HB2	1:B:110:VAL:HG13	1.91	0.52
1:B:415:GLU:HG2	1:B:457:ILE:HD11	1.90	0.52
1:A:604:TYR:O	1:A:607:PRO:HD2	2.11	0.51
1:A:617:GLN:HE22	1:B:627:ASN:HD22	1.57	0.51
1:B:268:GLN:O	1:B:269:ASP:HB3	2.09	0.51
1:B:758:ILE:HG12	1:B:796:PRO:HB2	1.92	0.51
1:B:418:ILE:HG12	1:B:457:ILE:HD13	1.93	0.51
1:B:447:LEU:O	1:B:488:ARG:HD2	2.10	0.51
1:A:703:LYS:HA	1:A:706:ILE:HG12	1.91	0.51
1:A:290:LYS:O	1:A:294:VAL:HG23	2.12	0.50
1:A:821:ILE:C	1:A:823:VAL:H	2.14	0.50
1:B:173:ASN:OD1	1:B:173:ASN:N	2.45	0.50
1:A:92:LYS:HD2	1:A:126:TRP:CD2	2.46	0.50
1:A:587:LEU:HB2	1:A:643:VAL:CG1	2.41	0.50
1:B:395:LEU:HD12	1:B:399:LEU:HG	1.93	0.50
1:A:301:ILE:HD11	1:A:394:LEU:HD11	1.94	0.50
1:B:130:LEU:HD22	1:B:172:LEU:HD21	1.94	0.49
1:A:869:TRP:HE1	1:A:890:VAL:HG13	1.77	0.49
1:A:176:ILE:HB	1:A:177:PRO:HD3	1.93	0.49
1:B:663:VAL:HG13	1:B:668:ILE:HD11	1.94	0.49
1:B:215:SER:O	1:B:219:ASN:HB2	2.11	0.49
1:A:793:PHE:O	1:A:796:PRO:HD2	2.13	0.49
1:B:409:HIS:ND1	1:B:410:GLU:N	2.50	0.49
1:B:391:ARG:O	1:B:428:CYS:HB3	2.13	0.49
1:B:313:ILE:HB	1:B:370:ILE:HG21	1.94	0.48
1:B:587:LEU:HB2	1:B:643:VAL:CG1	2.42	0.48
1:A:755:VAL:HG13	1:A:793:PHE:HB3	1.94	0.48
1:A:699:PHE:CD2	1:A:738:GLN:HG3	2.47	0.48
1:B:493:ASN:OD1	1:B:496:VAL:HG23	2.13	0.48
1:B:226:ASP:OD1	1:B:228:GLU:HB2	2.14	0.48
1:A:213:ILE:HG23	1:A:214:ASP:N	2.29	0.48
1:A:744:GLN:HB3	1:A:745:PRO:HD3	1.96	0.48
1:A:261:MET:HA	1:A:261:MET:HE2	1.95	0.48
1:B:254:MET:HA	1:B:254:MET:HE2	1.95	0.48
1:A:512:CYS:HA	1:A:551:SER:O	2.13	0.47
1:A:191:ARG:O	1:A:195:VAL:HG23	2.14	0.47
1:A:710:MET:HG2	1:A:746:TYR:HB3	1.96	0.47
1:B:488:ARG:NE	1:B:488:ARG:HA	2.29	0.47
1:B:861:LYS:HD2	1:B:869:TRP:CD1	2.49	0.47
1:B:673:TYR:O	1:B:677:GLN:HG3	2.14	0.47
1:B:134:CYS:SG	1:B:175:MET:SD	3.12	0.47
1:A:566:MET:CE	1:A:593:VAL:HG11	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:584:PHE:N	1:A:584:PHE:CD1	2.81	0.47
1:A:440:ILE:HB	1:A:441:PRO:HD3	1.96	0.47
1:A:746:TYR:O	1:A:749:MET:HG2	2.15	0.46
1:B:580:ASP:O	1:B:583:LEU:HB2	2.14	0.46
1:B:805:ARG:HB3	2:D:268:ASN:OD1	2.14	0.46
1:A:467:HIS:HA	1:A:510:GLU:HG2	1.97	0.46
1:A:835:PHE:O	1:A:839:VAL:HG23	2.15	0.46
1:A:742:GLU:O	1:A:745:PRO:HD2	2.15	0.46
1:B:787:ALA:N	1:B:788:PRO:HD2	2.30	0.46
1:A:557:ASN:O	1:A:558:LYS:HG2	2.16	0.46
1:B:490:LEU:O	1:B:491:ASP:O	2.33	0.46
1:B:418:ILE:HD11	1:B:458:THR:CA	2.46	0.46
1:B:251:LEU:HA	1:B:254:MET:HG3	1.98	0.46
1:B:740:GLY:HA2	1:B:781:VAL:HG22	1.98	0.46
1:A:587:LEU:HB2	1:A:643:VAL:HG13	1.98	0.45
1:B:498:GLU:CG	1:B:540:ILE:HD12	2.46	0.45
1:A:542:TYR:CD1	1:A:585:PRO:HB2	2.51	0.45
1:B:251:LEU:HA	1:B:254:MET:CG	2.47	0.45
1:A:62:GLU:N	1:A:63:PRO:HD2	2.31	0.45
1:B:231:VAL:O	1:B:235:VAL:HG23	2.16	0.45
1:B:310:TYR:N	1:B:310:TYR:HD1	2.13	0.45
1:A:231:VAL:O	1:A:235:VAL:HG23	2.17	0.45
2:C:278:GLY:O	2:C:280:ASN:N	2.50	0.45
1:A:629:GLN:HB2	1:A:633:TYR:HD1	1.82	0.44
1:B:793:PHE:O	1:B:796:PRO:HD2	2.17	0.44
1:B:609:TYR:CD1	1:B:659:ILE:HD11	2.53	0.44
1:A:264:ARG:O	1:A:267:ASP:HB2	2.17	0.44
1:B:224:ALA:HB1	1:B:260:TYR:CE1	2.51	0.44
1:A:422:GLY:HA3	1:A:460:TRP:CZ3	2.52	0.44
1:B:520:ALA:HB2	1:B:561:TYR:HE1	1.82	0.44
1:A:699:PHE:CG	1:A:738:GLN:CG	3.00	0.44
1:B:254:MET:HE3	1:B:257:ILE:HD12	1.99	0.44
1:B:508:GLU:HA	1:B:515:LEU:HD11	1.99	0.44
1:B:660:GLU:HG2	1:B:701:HIS:NE2	2.33	0.44
1:A:627:ASN:HD22	1:B:617:GLN:NE2	2.00	0.44
1:B:718:ASN:HA	1:B:719:PRO:HD3	1.85	0.44
1:B:310:TYR:HD1	1:B:310:TYR:H	1.66	0.43
1:A:797:TRP:CH2	1:A:817:ILE:HG13	2.53	0.43
1:B:538:LEU:HD22	1:B:542:TYR:CE1	2.54	0.43
1:A:477:TYR:O	1:A:480:PRO:HD2	2.18	0.43
1:A:94:GLU:O	1:A:98:ASN:ND2	2.51	0.43
1:B:766:THR:HG23	2:D:272:ASN:HB3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:479:LYS:HE3	1:A:518:TYR:OH	2.17	0.43
1:B:600:GLY:O	1:B:603:PRO:HD2	2.19	0.43
1:B:310:TYR:CB	1:B:313:ILE:HG13	2.42	0.43
1:B:787:ALA:HA	1:B:820:MET:HE2	2.00	0.43
1:A:228:GLU:HA	1:A:229:PRO:HD3	1.91	0.43
1:A:450:LYS:HD2	1:A:450:LYS:N	2.28	0.43
1:A:477:TYR:C	1:A:480:PRO:HD2	2.38	0.43
1:B:791:GLN:HG3	1:B:791:GLN:O	2.19	0.43
1:B:213:ILE:HD12	1:B:249:ARG:HD2	2.00	0.43
1:B:860:PHE:O	1:B:864:VAL:HG22	2.19	0.43
1:B:454:VAL:HA	1:B:457:ILE:HD11	2.01	0.43
1:B:288:ILE:HG22	1:B:292:VAL:HG21	2.00	0.43
1:B:739:MET:O	1:B:740:GLY:O	2.37	0.43
1:B:718:ASN:HD22	1:B:719:PRO:HD2	1.84	0.43
1:B:310:TYR:HB3	1:B:313:ILE:HD11	2.00	0.43
1:B:606:GLU:HB3	1:B:607:PRO:HD3	2.00	0.43
1:A:310:TYR:CB	1:A:313:ILE:HB	2.49	0.43
1:A:573:TRP:HZ3	1:A:587:LEU:HD22	1.84	0.42
1:B:516:VAL:HA	1:B:519:LEU:HD22	2.02	0.42
1:B:663:VAL:HG13	1:B:668:ILE:CD1	2.48	0.42
1:A:264:ARG:NH1	1:A:267:ASP:OD2	2.53	0.42
1:B:422:GLY:HA3	1:B:460:TRP:CZ3	2.54	0.42
1:B:254:MET:HA	1:B:254:MET:CE	2.50	0.42
1:A:482:MET:SD	1:A:518:TYR:CD1	3.12	0.42
1:B:828:VAL:CG1	1:B:832:PHE:HD1	2.32	0.42
1:B:612:CYS:O	1:B:616:VAL:HG23	2.19	0.42
1:B:242:LEU:HB3	1:B:250:LEU:HD11	2.01	0.42
1:A:740:GLY:HA2	1:A:781:VAL:HG22	2.01	0.42
1:A:828:VAL:HG12	1:A:832:PHE:HD1	1.84	0.42
1:A:76:VAL:O	1:A:77:LYS:CB	2.67	0.42
1:A:726:ASN:HD22	1:A:767:LEU:HA	1.84	0.42
1:A:124:GLN:HA	1:A:124:GLN:OE1	2.20	0.42
1:B:692:GLY:HA3	1:B:730:TRP:CZ3	2.55	0.42
1:B:375:LEU:O	1:B:379:SER:OG	2.33	0.42
1:B:706:ILE:HA	1:B:706:ILE:HD13	1.92	0.42
1:A:589:CYS:O	1:A:593:VAL:HG23	2.20	0.41
1:B:186:SER:HB3	1:B:187:SER:H	1.67	0.41
1:A:310:TYR:HB2	1:A:313:ILE:HB	2.02	0.41
1:B:470:VAL:HG11	1:B:510:GLU:O	2.20	0.41
1:A:736:SER:O	1:A:737:ILE:C	2.59	0.41
1:A:55:THR:C	1:A:57:LEU:H	2.24	0.41
1:B:199:ASN:OD1	1:B:238:ALA:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:594:ALA:O	1:B:597:LEU:O	2.37	0.41
1:B:780:TYR:HB2	1:B:816:GLY:CA	2.50	0.41
1:B:194:ALA:O	1:B:198:VAL:HG23	2.20	0.41
1:A:673:TYR:CE1	1:A:712:ILE:CD1	3.03	0.41
1:B:457:ILE:HG13	1:B:457:ILE:H	1.56	0.41
1:A:177:PRO:HG3	1:A:212:HIS:CE1	2.56	0.41
1:B:760:ARG:HA	1:B:761:PRO:HD3	1.90	0.41
1:B:850:ARG:NH1	1:B:887:PHE:O	2.54	0.41
1:B:210:MET:SD	1:B:246:ARG:NH1	2.94	0.41
1:B:440:ILE:O	1:B:444:ILE:HG13	2.21	0.41
1:A:706:ILE:HD13	1:A:706:ILE:HA	1.93	0.41
1:A:98:ASN:N	1:A:98:ASN:ND2	2.69	0.41
1:B:655:LEU:HB3	1:B:658:ASN:HB2	2.04	0.40
1:A:821:ILE:O	1:A:823:VAL:N	2.54	0.40
1:B:828:VAL:HG13	1:B:832:PHE:HD1	1.85	0.40
1:B:473:PRO:HA	1:B:474:PRO:HD3	1.88	0.40
1:B:703:LYS:HB3	1:B:704:PRO:HD3	2.04	0.40
1:A:491:ASP:HA	1:A:532:LYS:NZ	2.37	0.40
1:B:126:TRP:CG	1:B:129:LEU:HB2	2.56	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	819/865 (95%)	748 (91%)	52 (6%)	19 (2%)	10	43
1	B	798/865 (92%)	727 (91%)	58 (7%)	13 (2%)	14	55
2	C	21/49 (43%)	18 (86%)	2 (10%)	1 (5%)	4	21
2	D	25/49 (51%)	22 (88%)	2 (8%)	1 (4%)	5	26
All	All	1663/1828 (91%)	1515 (91%)	114 (7%)	34 (2%)	11	48

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	186	SER
1	B	7	PRO
1	B	254	MET
1	B	411	TRP
1	B	491	ASP
1	B	656	GLY
1	B	740	GLY
2	C	279	GLY
1	A	45	ASP
1	A	56	LYS
1	A	409	HIS
1	A	411	TRP
1	A	449	ASP
1	A	822	SER
1	B	84	PRO
1	B	213	ILE
1	B	598	GLN
1	A	21	GLU
1	A	25	PRO
1	A	294	VAL
1	A	408	HIS
1	A	425	ALA
1	A	492	SER
1	A	535	HIS
1	B	186	SER
1	A	123	LEU
1	A	780	TYR
1	B	120	LYS
1	A	129	LEU
1	B	129	LEU
2	D	267	ASN
1	A	788	PRO
1	B	788	PRO

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	655/774 (85%)	619 (94%)	36 (6%)	30	72
1	B	641/774 (83%)	592 (92%)	49 (8%)	19	57
2	C	16/33 (48%)	15 (94%)	1 (6%)	25	66
2	D	18/33 (54%)	17 (94%)	1 (6%)	30	71
All	All	1330/1614 (82%)	1243 (94%)	87 (6%)	24	64

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	103	SER
1	A	125	ASN
1	A	149	PHE
1	A	167	VAL
1	A	170	ARG
1	A	172	LEU
1	A	174	ILE
1	A	186	SER
1	A	245	VAL
1	A	256	ASN
1	A	262	LEU
1	A	295	ARG
1	A	310	TYR
1	A	315	ILE
1	A	369	THR
1	A	374	ASN
1	A	410	GLU
1	A	415	GLU
1	A	456	SER
1	A	476	THR
1	A	524	ASP
1	A	530	PHE
1	A	534	GLN
1	A	540	ILE
1	A	552	VAL
1	A	571	GLN
1	A	590	LEU
1	A	602	LEU
1	A	632	GLN
1	A	649	SER
1	A	781	VAL
1	A	802	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	809	GLU
1	A	820	MET
1	A	866	ASP
1	B	126	TRP
1	B	149	PHE
1	B	173	ASN
1	B	174	ILE
1	B	206	THR
1	B	213	ILE
1	B	223	LEU
1	B	228	GLU
1	B	243	LEU
1	B	251	LEU
1	B	254	MET
1	B	281	LEU
1	B	300	LEU
1	B	306	ASN
1	B	310	TYR
1	B	315	ILE
1	B	316	ILE
1	B	379	SER
1	B	395	LEU
1	B	404	GLU
1	B	410	GLU
1	B	418	ILE
1	B	428	CYS
1	B	432	MET
1	B	453	LEU
1	B	457	ILE
1	B	475	ASP
1	B	476	THR
1	B	494	LYS
1	B	513	THR
1	B	514	GLU
1	B	519	LEU
1	B	538	LEU
1	B	552	VAL
1	B	562	ILE
1	B	611	ARG
1	B	631	ASP
1	B	668	ILE
1	B	679	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	750	VAL
1	B	781	VAL
1	B	799	THR
1	B	811	ASP
1	B	826	SER
1	B	830	GLN
1	B	833	ILE
1	B	850	ARG
1	B	851	ASP
1	B	887	PHE
2	C	271	SER
2	D	267	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	75	ASN
1	A	98	ASN
1	A	143	ASN
1	A	212	HIS
1	A	234	ASN
1	A	374	ASN
1	A	467	HIS
1	A	629	GLN
1	A	632	GLN
1	A	726	ASN
1	A	744	GLN
1	A	858	HIS
1	A	868	ASN
1	B	75	ASN
1	B	207	GLN
1	B	306	ASN
1	B	571	GLN
1	B	614	ASN
1	B	617	GLN
1	B	626	ASN
1	B	627	ASN
1	B	718	ASN
1	B	791	GLN
1	B	868	ASN
2	C	267	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	280	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.