Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 01:43 AM JST

PDB ID	:	5YU7
Title	:	CRYSTAL STRUCTURE OF EXPORTIN-5
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Deposited on	:	2017-11-20
Resolution	:	3.30 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:

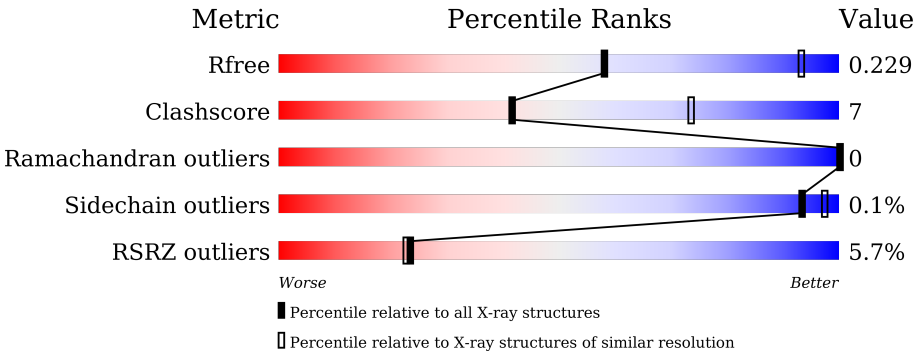
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	1204	5% 76% 17% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8937 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 Exportin-5.

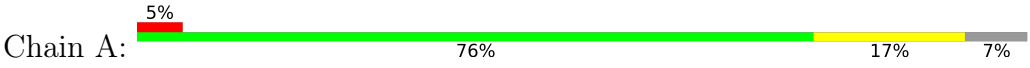
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1118	8937	5714	1513	1635	75	0	0	0

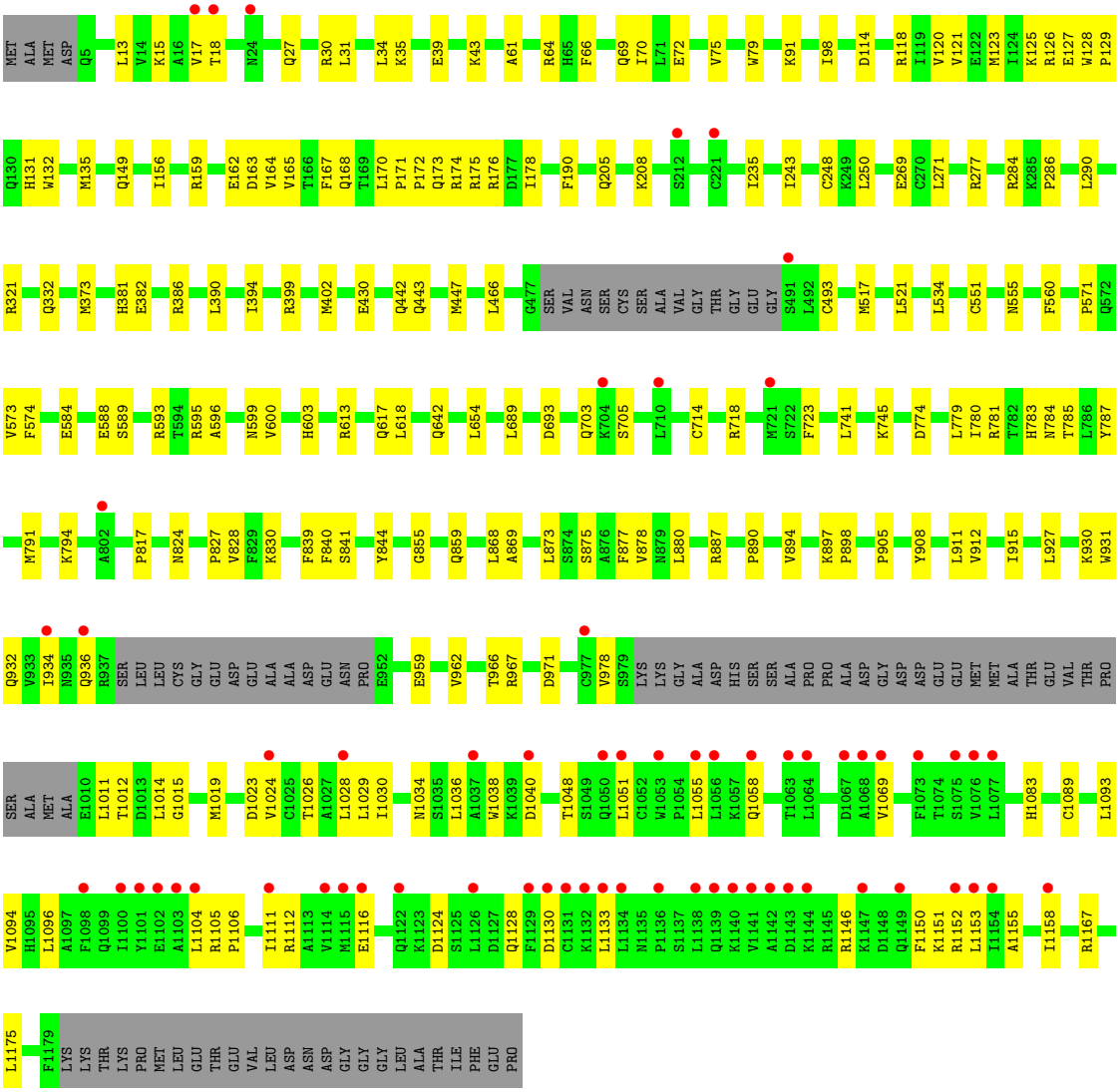
3 Residue-property plots (i)

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: Exportin-5

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	286.16Å 286.16Å 59.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.30 – 3.30 41.30 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.30-3.30) 99.5 (41.30-3.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.200 , 0.229 0.199 , 0.229	Depositor DCC
R_{free} test set	2156 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	123.2	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 97.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8937	wwPDB-VP
Average B, all atoms (Å^2)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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

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	0.24	0/9112	0.38	0/12330

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	8937	0	9063	126	0
All	All	8937	0	9063	126	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 7.

All (126) 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:170:LEU:HD12	1:A:171:PRO:HD2	1.67	0.77
1:A:125:LYS:HB3	1:A:170:LEU:HD13	1.67	0.76
1:A:1104:LEU:HB2	1:A:1111:ILE:HD11	1.69	0.74
1:A:1089:CYS:O	1:A:1093:LEU:HB2	1.88	0.73
1:A:595:ARG:HG3	1:A:828:VAL:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:VAL:O	1:A:1028:LEU:HB2	1.94	0.67
1:A:787:TYR:OH	1:A:887:ARG:NH1	2.28	0.67
1:A:1024:VAL:O	1:A:1028:LEU:CB	2.43	0.67
1:A:173:GLN:HG2	1:A:1152:ARG:HD2	1.75	0.66
1:A:1012:THR:HG23	1:A:1015:GLY:H	1.63	0.64
1:A:642:GLN:HG3	1:A:723:PHE:HB2	1.80	0.64
1:A:1112:ARG:NH1	1:A:1116:GLU:OE2	2.31	0.64
1:A:176:ARG:HD3	1:A:1152:ARG:HD3	1.80	0.63
1:A:1030:ILE:O	1:A:1034:ASN:HB2	2.00	0.62
1:A:132:TRP:HB3	1:A:135:MET:HB2	1.82	0.61
1:A:121:VAL:HG12	1:A:125:LYS:HE3	1.82	0.60
1:A:551:CYS:O	1:A:555:ASN:ND2	2.35	0.59
1:A:235:ILE:O	1:A:277:ARG:NH2	2.30	0.59
1:A:703:GLN:NE2	1:A:705:SER:O	2.36	0.59
1:A:599:ASN:O	1:A:603:HIS:ND1	2.34	0.59
1:A:1011:LEU:HD13	1:A:1058:GLN:HG3	1.85	0.58
1:A:517:MET:HG3	1:A:521:LEU:HD12	1.85	0.58
1:A:905:PRO:HA	1:A:908:TYR:HB2	1.86	0.58
1:A:75:VAL:HG21	1:A:123:MET:HG2	1.86	0.57
1:A:1105:ARG:NH2	1:A:1130:ASP:OD2	2.37	0.57
1:A:114:ASP:OD1	1:A:159:ARG:NH2	2.36	0.57
1:A:79:TRP:CE2	1:A:126:ARG:HG2	2.40	0.57
1:A:443:GLN:O	1:A:447:MET:HB2	2.05	0.56
1:A:613:ARG:HB2	1:A:654:LEU:HD13	1.87	0.56
1:A:382:GLU:O	1:A:386:ARG:NH1	2.38	0.56
1:A:284:ARG:HE	1:A:332:GLN:HE22	1.52	0.55
1:A:1155:ALA:HA	1:A:1158:ILE:HG13	1.89	0.54
1:A:868:LEU:HD12	1:A:911:LEU:HD22	1.90	0.54
1:A:927:LEU:O	1:A:931:TRP:HB2	2.09	0.54
1:A:781:ARG:HG2	1:A:878:VAL:HG21	1.89	0.53
1:A:781:ARG:HG3	1:A:875:SER:HA	1.91	0.53
1:A:1133:LEU:HD21	1:A:1146:ARG:HD3	1.91	0.53
1:A:373:MET:SD	1:A:442:GLN:NE2	2.82	0.53
1:A:1038:TRP:O	1:A:1083:HIS:NE2	2.42	0.53
1:A:430:GLU:HB3	1:A:817:PRO:HB2	1.90	0.53
1:A:190:PHE:HZ	1:A:250:LEU:HD22	1.73	0.52
1:A:128:TRP:N	1:A:129:PRO:HD2	2.25	0.52
1:A:890:PRO:O	1:A:894:VAL:HB	2.10	0.52
1:A:932:GLN:NE2	1:A:936:GLN:OE1	2.43	0.51
1:A:163:ASP:OD1	1:A:1167:ARG:NH2	2.44	0.51
1:A:584:GLU:HG3	1:A:593:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLU:HB2	1:A:131:HIS:HB2	1.91	0.51
1:A:780:ILE:O	1:A:784:ASN:ND2	2.43	0.50
1:A:98:ILE:HD11	1:A:120:VAL:HG21	1.94	0.50
1:A:783:HIS:HE1	1:A:840:PHE:HD1	1.58	0.50
1:A:79:TRP:HH2	1:A:91:LYS:NZ	2.09	0.50
1:A:66:PHE:CE2	1:A:70:ILE:HD11	2.47	0.50
1:A:908:TYR:O	1:A:912:VAL:HB	2.12	0.50
1:A:978:VAL:HG21	1:A:1051:LEU:HA	1.93	0.50
1:A:61:ALA:HA	1:A:64:ARG:HD3	1.94	0.50
1:A:841:SER:OG	1:A:887:ARG:NH2	2.45	0.50
1:A:66:PHE:O	1:A:69:GLN:HB3	2.11	0.49
1:A:399:ARG:HA	1:A:402:MET:HE2	1.93	0.49
1:A:1015:GLY:O	1:A:1019:MET:HG2	2.13	0.49
1:A:930:LYS:HD3	1:A:962:VAL:HG22	1.94	0.49
1:A:126:ARG:HD3	1:A:174:ARG:NH2	2.28	0.48
1:A:39:GLU:O	1:A:43:LYS:HB2	2.14	0.48
1:A:120:VAL:HG11	1:A:156:ILE:HD13	1.95	0.48
1:A:596:ALA:O	1:A:600:VAL:HG23	2.14	0.48
1:A:35:LYS:O	1:A:39:GLU:HB2	2.14	0.48
1:A:693:ASP:OD1	1:A:794:LYS:NZ	2.43	0.47
1:A:269:GLU:HG2	1:A:321:ARG:HD2	1.95	0.47
1:A:205:GLN:HA	1:A:208:LYS:HG3	1.97	0.47
1:A:443:GLN:O	1:A:447:MET:CB	2.63	0.47
1:A:1094:VAL:HG11	1:A:1151:LYS:HE2	1.97	0.47
1:A:1024:VAL:O	1:A:1028:LEU:HB3	2.13	0.46
1:A:855:GLY:O	1:A:859:GLN:HA	2.15	0.46
1:A:897:LYS:HB3	1:A:898:PRO:HD3	1.97	0.46
1:A:689:LEU:HD22	1:A:779:LEU:HD13	1.96	0.46
1:A:126:ARG:HD3	1:A:174:ARG:HH22	1.81	0.46
1:A:284:ARG:HE	1:A:332:GLN:NE2	2.14	0.45
1:A:783:HIS:NE2	1:A:844:TYR:HB2	2.32	0.45
1:A:560:PHE:HE2	1:A:573:VAL:HG11	1.82	0.45
1:A:1175:LEU:HD23	1:A:1175:LEU:HA	1.89	0.45
1:A:897:LYS:NZ	1:A:971:ASP:OD2	2.49	0.44
1:A:205:GLN:HA	1:A:208:LYS:HE3	1.99	0.44
1:A:390:LEU:O	1:A:394:ILE:HG13	2.17	0.44
1:A:617:GLN:HG2	1:A:618:LEU:HD12	1.98	0.44
1:A:1069:VAL:HG23	1:A:1104:LEU:HD13	1.99	0.44
1:A:1029:LEU:HD12	1:A:1055:LEU:HD23	2.00	0.44
1:A:827:PRO:HG2	1:A:830:LYS:HB2	1.99	0.44
1:A:75:VAL:O	1:A:126:ARG:NH2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:VAL:HG13	1:A:165:VAL:HG23	2.00	0.43
1:A:493:CYS:HB3	1:A:824:ASN:CG	2.39	0.43
1:A:571:PRO:O	1:A:574:PHE:HB2	2.18	0.43
1:A:15:LYS:HA	1:A:18:THR:HG22	2.00	0.43
1:A:13:LEU:O	1:A:17:VAL:HG23	2.18	0.43
1:A:114:ASP:O	1:A:118:ARG:HG3	2.18	0.43
1:A:162:GLU:HB3	1:A:167:PHE:HE2	1.83	0.43
1:A:967:ARG:HG3	1:A:1040:ASP:OD2	2.19	0.43
1:A:1048:THR:HA	1:A:1096:LEU:HD11	2.00	0.43
1:A:1124:ASP:O	1:A:1128:GLN:HB2	2.19	0.43
1:A:271:LEU:HD11	1:A:290:LEU:HD11	2.00	0.42
1:A:927:LEU:HD21	1:A:966:THR:HA	2.00	0.42
1:A:1105:ARG:HB3	1:A:1106:PRO:HD3	2.01	0.42
1:A:1150:PHE:HB2	1:A:1153:LEU:HD12	2.01	0.42
1:A:171:PRO:HA	1:A:172:PRO:HD3	1.89	0.42
1:A:248:CYS:SG	1:A:286:PRO:HB2	2.60	0.42
1:A:908:TYR:CZ	1:A:1014:LEU:HB3	2.55	0.42
1:A:774:ASP:OD1	1:A:774:ASP:N	2.52	0.42
1:A:27:GLN:HG2	1:A:30:ARG:HH21	1.84	0.42
1:A:31:LEU:HA	1:A:34:LEU:HD12	2.02	0.42
1:A:1036:LEU:HD13	1:A:1093:LEU:HD21	2.02	0.42
1:A:718:ARG:HB2	1:A:839:PHE:CZ	2.56	0.41
1:A:877:PHE:HD2	1:A:880:LEU:HD11	1.85	0.41
1:A:934:ILE:HD13	1:A:959:GLU:HG3	2.02	0.41
1:A:149:GLN:OE1	1:A:149:GLN:N	2.47	0.41
1:A:168:GLN:HG2	1:A:175:ARG:HD2	2.02	0.41
1:A:714:CYS:O	1:A:718:ARG:HG2	2.20	0.41
1:A:72:GLU:O	1:A:75:VAL:HG12	2.20	0.41
1:A:243:ILE:HG23	1:A:250:LEU:HD23	2.03	0.41
1:A:873:LEU:HA	1:A:877:PHE:HD1	1.86	0.41
1:A:466:LEU:HD23	1:A:534:LEU:HD22	2.03	0.41
1:A:205:GLN:HG2	1:A:208:LYS:HE3	2.03	0.41
1:A:284:ARG:HB3	1:A:332:GLN:HE22	1.87	0.40
1:A:588:GLU:HG3	1:A:589:SER:H	1.85	0.40
1:A:869:ALA:HA	1:A:915:ILE:HD11	2.03	0.40
1:A:741:LEU:O	1:A:745:LYS:HG3	2.22	0.40
1:A:785:THR:HG22	1:A:791:MET:HG3	2.02	0.40
1:A:129:PRO:HD3	1:A:178:ILE:HG12	2.04	0.40
1:A:1023:ASP:HA	1:A:1026:THR:HG22	2.04	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	1110/1204 (92%)	1086 (98%)	24 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	1007/1073 (94%)	1006 (100%)	1 (0%)	93 97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	GLN
1	A	783	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)

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

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	1118/1204 (92%)	0.19	64 (5%)	23	23	71, 151, 267, 407	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1068	ALA	10.6
1	A	1101	TYR	9.4
1	A	1129	PHE	6.5
1	A	1075	SER	5.5
1	A	1149	GLN	5.3
1	A	710	LEU	5.0
1	A	1136	PRO	4.6
1	A	1024	VAL	4.6
1	A	934	ILE	4.3
1	A	1133	LEU	4.3
1	A	1116	GLU	4.3
1	A	1028	LEU	4.2
1	A	1143	ASP	4.2
1	A	1115	MET	4.1
1	A	1139	GLN	4.0
1	A	1140	LYS	4.0
1	A	1154	ILE	4.0
1	A	1104	LEU	4.0
1	A	1058	GLN	3.9
1	A	1132	LYS	3.9
1	A	1098	PHE	3.6
1	A	1130	ASP	3.5
1	A	1147	LYS	3.4
1	A	1076	VAL	3.4
1	A	1103	ALA	3.3
1	A	1073	PHE	3.2
1	A	1131	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	936	GLN	3.2
1	A	1055	LEU	3.1
1	A	491	SER	3.1
1	A	1063	THR	3.0
1	A	1102	GLU	3.0
1	A	1144	LYS	3.0
1	A	1050	GLN	3.0
1	A	1069	VAL	2.9
1	A	1158	ILE	2.9
1	A	977	CYS	2.9
1	A	1152	ARG	2.9
1	A	1114	VAL	2.8
1	A	1126	LEU	2.8
1	A	1138	LEU	2.8
1	A	221	CYS	2.8
1	A	1122	GLN	2.8
1	A	1153	LEU	2.7
1	A	18	THR	2.6
1	A	1134	LEU	2.5
1	A	1051	LEU	2.5
1	A	1111	ILE	2.5
1	A	1064	LEU	2.4
1	A	1142	ALA	2.3
1	A	1053	TRP	2.3
1	A	1067	ASP	2.3
1	A	1037	ALA	2.3
1	A	1141	VAL	2.3
1	A	704	LYS	2.1
1	A	17	VAL	2.1
1	A	1077	LEU	2.1
1	A	1100	ILE	2.1
1	A	721	MET	2.1
1	A	1056	LEU	2.1
1	A	24	ASN	2.1
1	A	1040	ASP	2.0
1	A	212	SER	2.0
1	A	802	ALA	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.