Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:27 am BST

PDB ID	:	4BSM
Title	:	Crystal structure of the Nuclear Export Receptor CRM1 (exportin-1) lacking the C-terminal helical extension at 4.5A
Authors	:	Dian, C.; Bernaudat, F.; Langer, K.; Oliva, M.F.; Fornerod, M.; Schoehn, G.; Muller, C.W.; Petosa, C.
Deposited on	:	2013-06-10
Resolution	:	4.50 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 following versions of software and data (see references ①) were used in the production of this report:

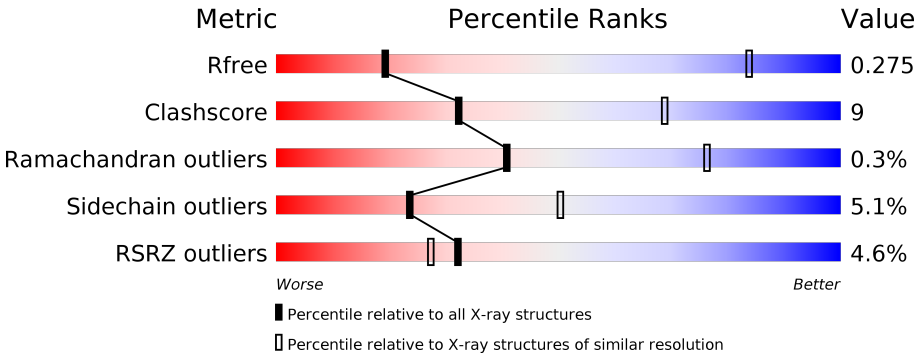
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 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	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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 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	1032	4% 67% 19% • 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6854 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-1.

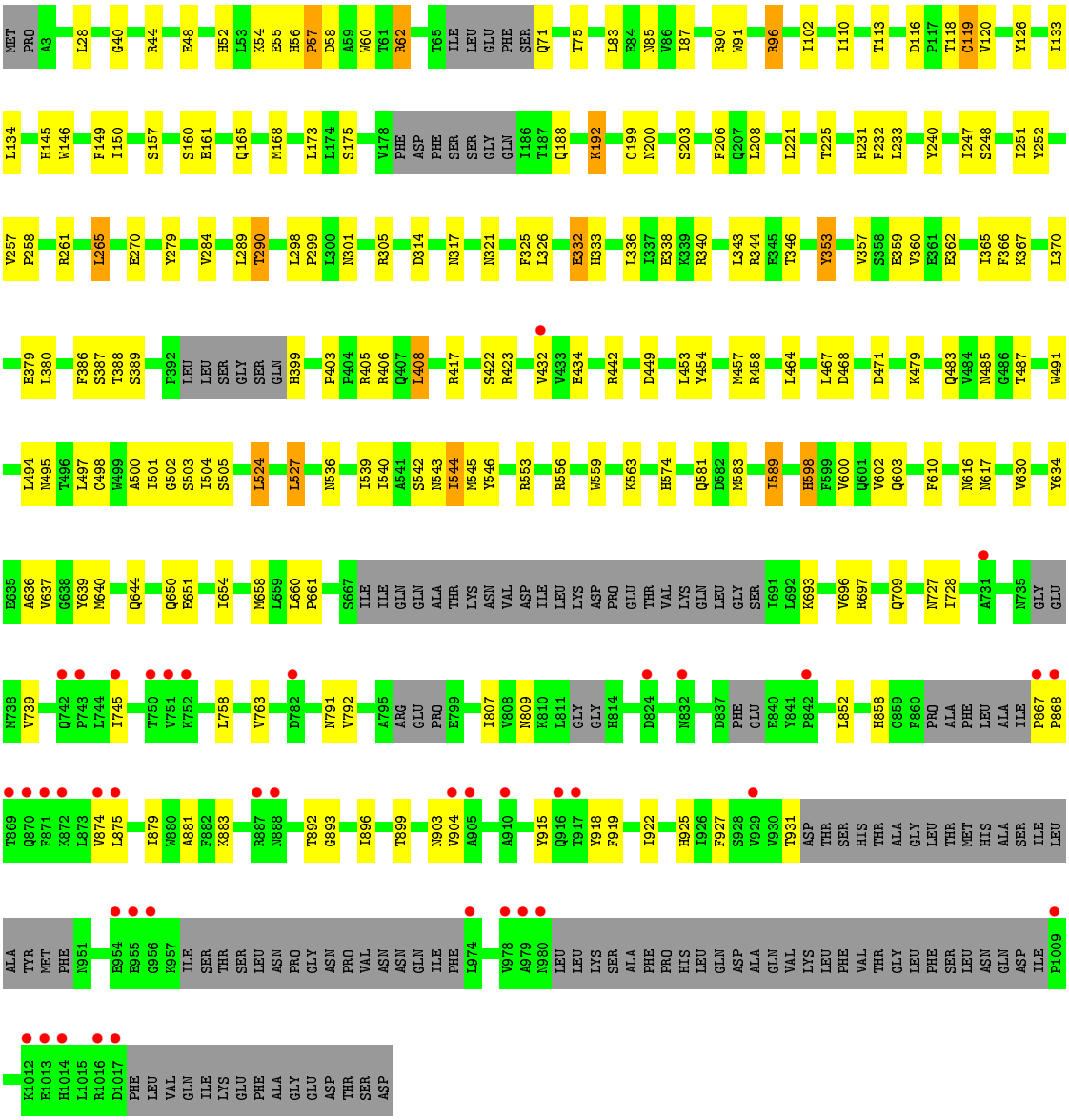
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	896	6854	4379	1169	1262	44	0	0	0

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 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-1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	148.64Å 248.33Å 107.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 4.50 48.59 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.59-4.50) 99.9 (48.59-4.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 4.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1056)	Depositor
R, R_{free}	0.229 , 0.269 0.233 , 0.275	Depositor DCC
R_{free} test set	1213 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å^2)	145.8	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 154.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.086 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.074 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6854	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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	0.25	0/6978	0.42	0/9473

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	6854	0	6542	118	0
All	All	6854	0	6542	118	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 (118) 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:387:SER:HB3	1:A:468:ASP:HA	1.61	0.82
1:A:483:GLN:HG2	1:A:494:LEU:HD13	1.71	0.71
1:A:616:ASN:ND2	1:A:617:ASN:OD1	2.29	0.65
1:A:524:LEU:HD13	1:A:544:ILE:HG12	1.78	0.65
1:A:55:GLU:HG3	1:A:90:ARG:HH22	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:ASN:OD1	1:A:858:HIS:NE2	2.33	0.62
1:A:600:VAL:HG11	1:A:644:GLN:HB2	1.82	0.61
1:A:56:HIS:N	1:A:57:PRO:HD2	2.16	0.61
1:A:406:ARG:NH2	1:A:467:LEU:HA	2.15	0.60
1:A:454:TYR:OH	1:A:546:TYR:OH	2.18	0.60
1:A:338:GLU:HG2	1:A:408:LEU:HD13	1.84	0.60
1:A:62:ARG:NH1	1:A:75:THR:O	2.33	0.60
1:A:696:VAL:HG12	1:A:758:LEU:HD13	1.83	0.59
1:A:370:LEU:HD11	1:A:457:MET:HG2	1.86	0.58
1:A:485:ASN:OD1	1:A:487:THR:OG1	2.19	0.58
1:A:298:LEU:O	1:A:353:TYR:OH	2.22	0.57
1:A:417:ARG:NH1	1:A:471:ASP:OD2	2.38	0.57
1:A:422:SER:OG	1:A:479:LYS:NZ	2.36	0.57
1:A:388:THR:HG22	1:A:406:ARG:NH1	2.21	0.56
1:A:879:ILE:HG22	1:A:883:LYS:HE3	1.88	0.56
1:A:157:SER:HB2	1:A:208:LEU:HD11	1.87	0.55
1:A:233:LEU:HD23	1:A:270:GLU:HB3	1.89	0.55
1:A:563:LYS:HG3	1:A:610:PHE:HE1	1.72	0.55
1:A:852:LEU:HD11	1:A:874:VAL:HG13	1.89	0.54
1:A:453:LEU:O	1:A:457:MET:HG3	2.08	0.54
1:A:28:LEU:HD13	1:A:71:GLN:HA	1.89	0.54
1:A:458:ARG:HG3	1:A:503:SER:HB2	1.88	0.54
1:A:388:THR:HG23	1:A:467:LEU:O	2.07	0.54
1:A:362:GLU:HB3	1:A:365:ILE:HG22	1.90	0.54
1:A:495:ASN:ND2	1:A:543:ASN:OD1	2.42	0.53
1:A:892:THR:O	1:A:896:ILE:HG13	2.10	0.52
1:A:464:LEU:HA	1:A:467:LEU:HD12	1.91	0.51
1:A:251:ILE:HG21	1:A:289:LEU:HB3	1.93	0.51
1:A:763:VAL:HG11	1:A:807:ILE:HG22	1.93	0.51
1:A:728:ILE:HG23	1:A:745:ILE:HD12	1.93	0.50
1:A:113:THR:HG21	1:A:126:TYR:HE2	1.75	0.50
1:A:559:TRP:HH2	1:A:610:PHE:HB2	1.77	0.50
1:A:116:ASP:OD2	1:A:118:THR:OG1	2.28	0.50
1:A:146:TRP:HB3	1:A:149:PHE:HB2	1.94	0.49
1:A:536:ASN:O	1:A:540:ILE:HG12	2.12	0.49
1:A:199:CYS:SG	1:A:200:ASN:N	2.85	0.49
1:A:360:VAL:HB	1:A:365:ILE:HD13	1.94	0.49
1:A:325:PHE:HD2	1:A:326:LEU:HD22	1.77	0.49
1:A:56:HIS:O	1:A:58:ASP:N	2.46	0.48
1:A:160:SER:OG	1:A:161:GLU:N	2.46	0.48
1:A:495:ASN:HA	1:A:543:ASN:HD21	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:PRO:HG2	1:A:406:ARG:HD2	1.94	0.48
1:A:545:MET:HG3	1:A:583:MET:SD	2.53	0.48
1:A:379:GLU:OE1	1:A:405:ARG:NH1	2.47	0.47
1:A:500:ALA:O	1:A:504:ILE:HG12	2.14	0.47
1:A:559:TRP:CD2	1:A:603:GLN:HG3	2.49	0.47
1:A:497:LEU:O	1:A:501:ILE:HG12	2.15	0.47
1:A:57:PRO:O	1:A:60:TRP:NE1	2.48	0.47
1:A:340:ARG:HD2	1:A:343:LEU:HD23	1.97	0.46
1:A:406:ARG:HH21	1:A:467:LEU:HD23	1.80	0.46
1:A:52:HIS:CE1	1:A:85:ASN:HB3	2.49	0.46
1:A:344:ARG:HG3	1:A:408:LEU:HD21	1.97	0.46
1:A:498:CYS:SG	1:A:543:ASN:HB3	2.55	0.46
1:A:333:HIS:HB3	1:A:336:LEU:HD12	1.97	0.46
1:A:284:VAL:HG21	1:A:340:ARG:HH21	1.80	0.46
1:A:87:ILE:O	1:A:91:TRP:HB2	2.16	0.46
1:A:357:VAL:HG12	1:A:365:ILE:HD11	1.98	0.46
1:A:388:THR:HG22	1:A:406:ARG:HH11	1.81	0.46
1:A:491:TRP:NE1	1:A:536:ASN:OD1	2.49	0.46
1:A:261:ARG:NH1	1:A:314:ASP:OD2	2.49	0.45
1:A:502:GLY:HA3	1:A:546:TYR:CE2	2.51	0.45
1:A:881:ALA:HB3	1:A:893:GLY:HA3	1.98	0.45
1:A:206:PHE:CE2	1:A:240:TYR:HB3	2.51	0.45
1:A:298:LEU:HA	1:A:299:PRO:HD3	1.79	0.45
1:A:739:VAL:HG12	1:A:745:ILE:HG13	1.99	0.45
1:A:491:TRP:CD1	1:A:539:ILE:HG13	2.52	0.45
1:A:879:ILE:HG21	1:A:925:HIS:HB3	1.99	0.45
1:A:353:TYR:O	1:A:357:VAL:HG23	2.17	0.44
1:A:660:LEU:HB2	1:A:661:PRO:HD3	2.00	0.44
1:A:150:ILE:HD12	1:A:150:ILE:H	1.82	0.44
1:A:556:ARG:O	1:A:598:HIS:NE2	2.51	0.44
1:A:119:CYS:SG	1:A:120:VAL:N	2.91	0.44
1:A:388:THR:OG1	1:A:389:SER:N	2.51	0.44
1:A:367:LYS:NZ	1:A:449:ASP:OD1	2.48	0.44
1:A:203:SER:HG	1:A:240:TYR:HE2	1.65	0.44
1:A:247:ILE:HG13	1:A:248:SER:H	1.83	0.44
1:A:40:GLY:O	1:A:44:ARG:HB2	2.17	0.43
1:A:658:MET:SD	1:A:709:GLN:HG2	2.57	0.43
1:A:175:SER:OG	1:A:231:ARG:HG2	2.19	0.43
1:A:317:ASN:O	1:A:321:ASN:ND2	2.51	0.43
1:A:581:GLN:H	1:A:581:GLN:HG2	1.67	0.43
1:A:650:GLN:HG3	1:A:651:GLU:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ILE:HG22	1:A:252:TYR:CD1	2.54	0.43
1:A:693:LYS:O	1:A:697:ARG:HG2	2.19	0.43
1:A:96:ARG:HG3	1:A:145:HIS:CE1	2.53	0.42
1:A:257:VAL:HA	1:A:258:PRO:HD3	1.87	0.42
1:A:284:VAL:HG21	1:A:340:ARG:NH2	2.34	0.42
1:A:168:MET:HE3	1:A:225:THR:HA	2.02	0.42
1:A:55:GLU:HB3	1:A:57:PRO:HD2	2.01	0.42
1:A:589:ILE:HG12	1:A:636:ALA:HB2	2.01	0.42
1:A:637:VAL:HA	1:A:640:MET:HE2	2.00	0.42
1:A:165:GLN:HB3	1:A:221:LEU:HD13	2.02	0.42
1:A:305:ARG:HD3	1:A:359:GLU:O	2.19	0.42
1:A:251:ILE:HD11	1:A:290:THR:HG23	2.02	0.42
1:A:527:LEU:HD22	1:A:527:LEU:HA	1.90	0.41
1:A:359:GLU:OE1	1:A:423:ARG:NH2	2.47	0.41
1:A:918:TYR:O	1:A:922:ILE:HG13	2.20	0.41
1:A:899:THR:HG22	1:A:903:ASN:ND2	2.35	0.41
1:A:332:GLU:HB3	1:A:333:HIS:CE1	2.56	0.41
1:A:791:ASN:OD1	1:A:792:VAL:N	2.53	0.41
1:A:915:TYR:O	1:A:919:PHE:HB3	2.21	0.41
1:A:175:SER:HB3	1:A:232:PHE:CE1	2.56	0.41
1:A:44:ARG:HD3	1:A:44:ARG:N	2.36	0.41
1:A:110:ILE:HD11	1:A:134:LEU:HB2	2.02	0.41
1:A:83:LEU:HD23	1:A:133:ILE:HD13	2.02	0.41
1:A:403:PRO:HB2	1:A:406:ARG:HB2	2.02	0.41
1:A:343:LEU:O	1:A:346:THR:OG1	2.31	0.41
1:A:650:GLN:O	1:A:654:ILE:HG13	2.21	0.41
1:A:192:LYS:HA	1:A:192:LYS:HD2	1.89	0.40
1:A:265:LEU:HD22	1:A:265:LEU:HA	1.95	0.40
1:A:188:GLN:O	1:A:192:LYS:HG2	2.21	0.40
1:A:432:VAL:HG21	1:A:542:SER:HB2	2.01	0.40
1:A:867:PRO:HA	1:A:868:PRO:HD3	1.90	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	870/1032 (84%)	834 (96%)	33 (4%)	3 (0%)	41 76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	57	PRO
1	A	505	SER

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	711/940 (76%)	675 (95%)	36 (5%)	24 50

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	62	ARG
1	A	96	ARG
1	A	102	ILE
1	A	119	CYS
1	A	173	LEU
1	A	192	LYS
1	A	265	LEU
1	A	279	TYR
1	A	290	THR
1	A	301	ASN
1	A	332	GLU
1	A	353	TYR
1	A	366	PHE
1	A	380	LEU
1	A	386	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	399	HIS
1	A	408	LEU
1	A	434	GLU
1	A	442	ARG
1	A	524	LEU
1	A	527	LEU
1	A	544	ILE
1	A	553	ARG
1	A	574	HIS
1	A	589	ILE
1	A	598	HIS
1	A	602	VAL
1	A	630	VAL
1	A	634	TYR
1	A	639	TYR
1	A	727	ASN
1	A	875	LEU
1	A	904	VAL
1	A	927	PHE
1	A	931	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	166	ASN
1	A	215	ASN
1	A	321	ASN
1	A	495	ASN
1	A	543	ASN
1	A	616	ASN
1	A	870	GLN
1	A	916	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	896/1032 (86%)	0.01	41 (4%) 32 27	27, 133, 293, 328	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	871	PHE	6.1
1	A	888	ASN	5.4
1	A	978	VAL	5.2
1	A	867	PRO	4.9
1	A	752	LYS	3.8
1	A	875	LEU	3.7
1	A	832	ASN	3.7
1	A	872	LYS	3.5
1	A	954	GLU	3.3
1	A	887	ARG	3.3
1	A	1017	ASP	3.2
1	A	980	ASN	3.1
1	A	874	VAL	3.0
1	A	745	ILE	3.0
1	A	910	ALA	2.8
1	A	731	ALA	2.8
1	A	868	PRO	2.7
1	A	824	ASP	2.7
1	A	917	THR	2.7
1	A	916	GLN	2.7
1	A	974	LEU	2.6
1	A	1012	LYS	2.6
1	A	743	PRO	2.6
1	A	1014	HIS	2.5
1	A	979	ALA	2.5
1	A	1013	GLU	2.4
1	A	905	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	842	PRO	2.4
1	A	1009	PRO	2.3
1	A	751	VAL	2.3
1	A	750	THR	2.3
1	A	870	GLN	2.2
1	A	904	VAL	2.2
1	A	782	ASP	2.2
1	A	1016	ARG	2.2
1	A	742	GLN	2.1
1	A	955	GLU	2.1
1	A	432	VAL	2.1
1	A	956	GLY	2.1
1	A	869	THR	2.1
1	A	929	VAL	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 carbohydrates 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.