Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 10:19 PM EDT

PDB ID	:	1Y2A
Title	:	Structure of mammalian importin bound to the non-classical PLSCR1-NLS
Authors	:	Chen, M.-H.; Ben-Efraim, I.; Mitrousis, G.; Walker-Kopp, N.; Sims, P.J.; Cingolani, G.
Deposited on	:	2004-11-22
Resolution	:	2.20 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 (i) 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 (1)) were used in the production of this report:

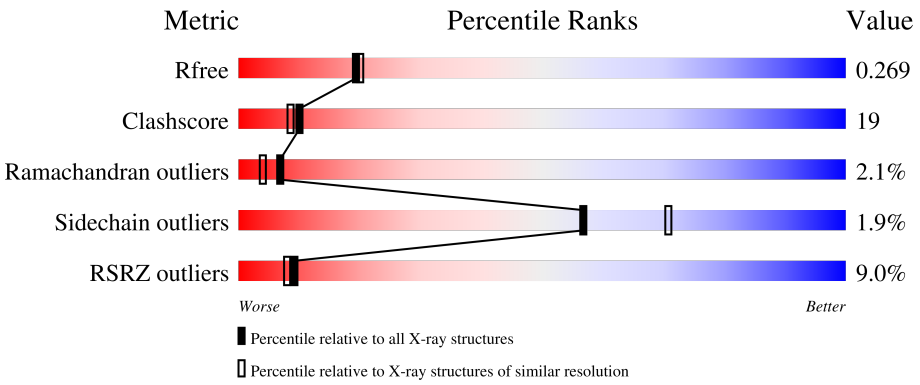
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	C	428	8%, 68%, 29%, • •
2	P	10	50%, 30%, 50%, 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3441 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 Importin alpha-2 Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	423	3227	2055	547	615	10	0	0	0

- Molecule 2 is a protein called decamer fragment of Phospholipid scramblase 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	P	10	80	52	15	13	0	0	0

- Molecule 3 is water.

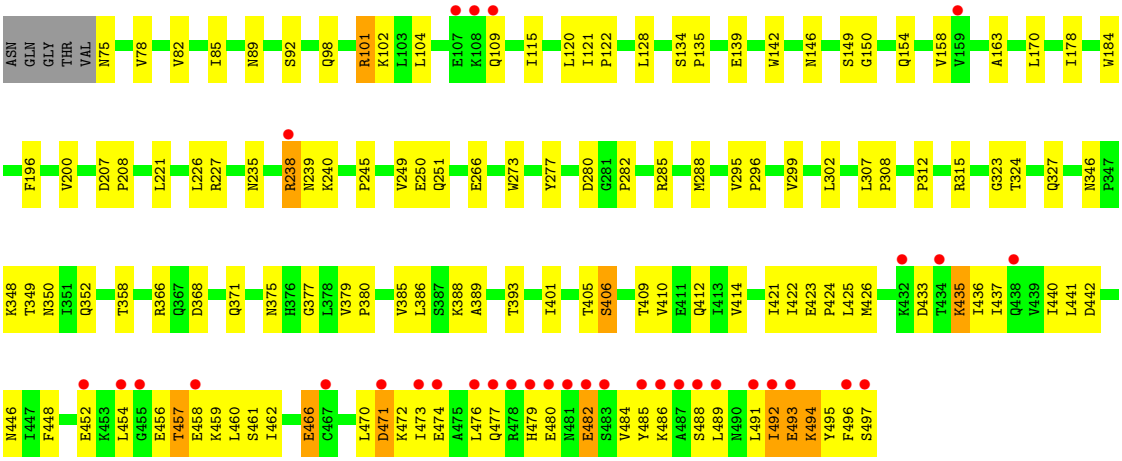
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	C	134	134	134	0	0

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.

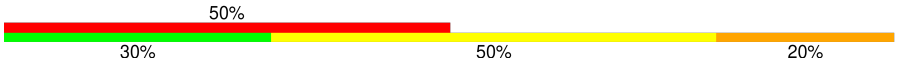
• Molecule 1: Importin alpha-2 Subunit

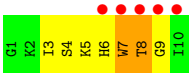
Chain C:



• Molecule 2: decamer fragment of Phospholipid scramblase 1

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.24Å 91.10Å 97.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 42.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 89.4 (42.90-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.15 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.258 0.272 , 0.269	Depositor DCC
R_{free} test set	3377 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 19.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	3441	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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 (i)

5.1 Standard geometry (i)

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	C	0.37	0/3285	0.67	3/4475 (0.1%)
2	P	0.65	0/82	0.63	0/107
All	All	0.38	0/3367	0.67	3/4582 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	238	ARG	N-CA-C	18.45	160.82	111.00
1	C	238	ARG	CB-CA-C	-11.35	87.70	110.40
1	C	239	ASN	N-CA-CB	-10.60	91.53	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	238	ARG	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

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	C	3227	0	3301	123	0
2	P	80	0	85	14	0
3	C	134	0	0	2	0
All	All	3441	0	3386	127	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 19.

All (127) 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)
2:P:8:THR:HG22	2:P:9:GLY:H	1.27	0.99
1:C:457:THR:HG23	1:C:458:GLU:H	1.47	0.80
1:C:477:GLN:NE2	1:C:492:ILE:HG13	1.95	0.80
1:C:493:GLU:O	1:C:494:LYS:HB2	1.87	0.75
2:P:5:LYS:HE3	2:P:7:TRP:CZ2	2.22	0.75
1:C:207:ASP:HB2	1:C:208:PRO:HD3	1.69	0.74
1:C:101:ARG:HD3	1:C:139:GLU:OE1	1.89	0.72
1:C:221:LEU:HD12	1:C:226:LEU:HD13	1.72	0.71
1:C:346:ASN:HD22	1:C:348:LYS:H	1.39	0.71
1:C:346:ASN:ND2	1:C:348:LYS:HB2	2.06	0.70
1:C:479:HIS:CG	1:C:480:GLU:H	2.11	0.68
2:P:8:THR:HG22	2:P:9:GLY:N	2.06	0.68
1:C:282:PRO:HD2	1:C:285:ARG:HG3	1.75	0.67
1:C:101:ARG:HH22	2:P:9:GLY:N	1.92	0.66
1:C:346:ASN:ND2	1:C:348:LYS:H	1.93	0.66
1:C:435:LYS:HB2	1:C:435:LYS:NZ	2.10	0.66
1:C:472:LYS:O	1:C:476:LEU:HG	1.95	0.66
1:C:98:GLN:HA	1:C:139:GLU:OE1	1.95	0.66
1:C:482:GLU:HG2	1:C:486:LYS:HD2	1.78	0.65
1:C:448:PHE:CE1	1:C:460:LEU:HD23	2.33	0.64
1:C:482:GLU:O	1:C:486:LYS:HG3	1.97	0.63
1:C:146:ASN:HD21	2:P:5:LYS:H	1.46	0.63
1:C:435:LYS:HB2	1:C:435:LYS:HZ3	1.61	0.63
1:C:470:LEU:O	1:C:474:GLU:HB2	1.99	0.62
1:C:207:ASP:OD2	1:C:251:GLN:NE2	2.35	0.60
1:C:115:ILE:HG23	1:C:120:LEU:HD12	1.84	0.59
1:C:315:ARG:HH11	1:C:315:ARG:HG2	1.67	0.59
1:C:477:GLN:NE2	1:C:489:LEU:HD12	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:TRP:CE2	1:C:312:PRO:HB3	2.39	0.58
1:C:184:TRP:CH2	2:P:5:LYS:HB2	2.40	0.57
1:C:437:ILE:O	1:C:441:LEU:HG	2.04	0.57
1:C:456:GLU:OE2	1:C:459:LYS:HD3	2.05	0.56
1:C:101:ARG:HD2	1:C:142:TRP:CE3	2.41	0.56
1:C:295:VAL:HB	1:C:296:PRO:HD3	1.88	0.55
1:C:452:GLU:OE2	1:C:495:TYR:HE1	1.90	0.54
1:C:128:LEU:HD22	1:C:170:LEU:HD11	1.90	0.54
1:C:101:ARG:HH22	2:P:9:GLY:CA	2.20	0.54
1:C:458:GLU:O	1:C:462:ILE:HG13	2.08	0.53
1:C:346:ASN:HD22	1:C:348:LYS:N	2.06	0.53
1:C:352:GLN:HG2	1:C:393:THR:HG21	1.90	0.53
1:C:435:LYS:NZ	1:C:435:LYS:CB	2.72	0.53
1:C:121:ILE:HB	1:C:122:PRO:HD3	1.89	0.53
1:C:409:THR:H	1:C:412:GLN:NE2	2.06	0.53
1:C:457:THR:HG23	1:C:458:GLU:N	2.21	0.53
1:C:477:GLN:O	1:C:485:TYR:HB2	2.08	0.53
1:C:85:ILE:HD12	1:C:120:LEU:HD22	1.91	0.52
1:C:448:PHE:CD1	1:C:460:LEU:HD23	2.45	0.52
1:C:89:ASN:HB3	1:C:92:SER:HB2	1.91	0.52
1:C:433:ASP:OD1	1:C:435:LYS:HB3	2.11	0.51
1:C:235:ASN:HA	1:C:238:ARG:HG2	1.92	0.51
1:C:479:HIS:CG	1:C:480:GLU:N	2.77	0.51
1:C:78:VAL:O	1:C:82:VAL:HG23	2.11	0.50
1:C:315:ARG:HG2	1:C:315:ARG:NH1	2.27	0.50
1:C:479:HIS:CD2	1:C:480:GLU:H	2.28	0.50
1:C:423:GLU:HB3	1:C:424:PRO:CD	2.42	0.50
1:C:250:GLU:HG2	1:C:288:MET:CE	2.41	0.49
1:C:422:ILE:O	1:C:426:MET:HG2	2.11	0.49
1:C:477:GLN:CD	1:C:492:ILE:HG13	2.32	0.49
1:C:482:GLU:C	1:C:486:LYS:HG3	2.32	0.49
1:C:101:ARG:HH22	2:P:8:THR:C	2.15	0.49
1:C:102:LYS:HE2	2:P:9:GLY:HA2	1.93	0.49
1:C:150:GLY:HA3	1:C:154:GLN:OE1	2.12	0.48
1:C:482:GLU:CG	1:C:486:LYS:HD2	2.44	0.48
1:C:307:LEU:N	1:C:308:PRO:CD	2.77	0.48
1:C:421:ILE:O	1:C:425:LEU:HB2	2.13	0.48
1:C:146:ASN:ND2	2:P:5:LYS:H	2.11	0.48
1:C:479:HIS:HB3	1:C:485:TYR:HB3	1.95	0.48
1:C:149:SER:OG	2:P:4:SER:HB3	2.14	0.48
1:C:462:ILE:O	1:C:466:GLU:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:TRP:CD2	1:C:312:PRO:HB3	2.49	0.47
1:C:250:GLU:CD	1:C:288:MET:HE3	2.35	0.47
1:C:238:ARG:HB3	1:C:277:TYR:CD2	2.50	0.47
1:C:349:THR:HG23	1:C:350:ASN:N	2.29	0.47
1:C:379:VAL:HB	1:C:380:PRO:HD3	1.97	0.47
1:C:406:SER:HA	1:C:446:ASN:ND2	2.30	0.47
1:C:371:GLN:HE21	1:C:375:ASN:HD21	1.62	0.46
1:C:386:LEU:HD21	1:C:425:LEU:HD13	1.96	0.46
1:C:425:LEU:HG	1:C:440:ILE:HG23	1.96	0.46
1:C:184:TRP:HE1	2:P:3:ILE:HG13	1.81	0.46
1:C:250:GLU:HG2	1:C:288:MET:HE1	1.97	0.46
1:C:410:VAL:O	1:C:414:VAL:HG23	2.16	0.46
1:C:238:ARG:HB3	1:C:277:TYR:CE2	2.51	0.46
1:C:240:LYS:HD3	1:C:280:ASP:O	2.16	0.46
1:C:385:VAL:CG1	1:C:393:THR:HG22	2.46	0.46
1:C:448:PHE:O	1:C:452:GLU:HG3	2.16	0.45
1:C:282:PRO:HD2	1:C:285:ARG:CG	2.46	0.45
1:C:346:ASN:HD21	1:C:348:LYS:HB2	1.79	0.44
1:C:406:SER:CA	1:C:446:ASN:ND2	2.81	0.44
1:C:482:GLU:HG2	1:C:486:LYS:CD	2.44	0.44
1:C:227:ARG:NH1	1:C:266:GLU:OE2	2.51	0.44
1:C:307:LEU:HB3	1:C:308:PRO:HD3	1.98	0.44
1:C:366:ARG:HB2	1:C:368:ASP:OD1	2.18	0.44
1:C:496:PHE:O	1:C:497:SER:C	2.56	0.44
1:C:85:ILE:CD1	1:C:120:LEU:HD22	2.48	0.43
1:C:406:SER:N	1:C:446:ASN:HD22	2.16	0.43
1:C:423:GLU:HB3	1:C:424:PRO:HD3	1.98	0.43
1:C:470:LEU:HD13	1:C:496:PHE:CD1	2.53	0.43
1:C:477:GLN:HE21	1:C:489:LEU:HA	1.83	0.43
1:C:401:ILE:O	1:C:405:THR:HG23	2.19	0.43
1:C:435:LYS:HA	1:C:435:LYS:HZ2	1.83	0.43
1:C:98:GLN:HG2	1:C:102:LYS:HE3	2.00	0.42
1:C:377:GLY:O	1:C:380:PRO:HD2	2.19	0.42
1:C:488:SER:O	1:C:491:LEU:HB2	2.19	0.42
1:C:134:SER:OG	1:C:135:PRO:HD3	2.19	0.42
1:C:207:ASP:CB	1:C:208:PRO:HD3	2.45	0.42
1:C:299:VAL:O	1:C:302:LEU:HB3	2.20	0.42
1:C:436:ILE:O	1:C:440:ILE:HG13	2.19	0.42
1:C:388:LYS:O	1:C:389:ALA:HB2	2.20	0.42
1:C:461:SER:O	1:C:496:PHE:HE1	2.03	0.42
1:C:349:THR:HG22	3:C:535:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:THR:HA	3:C:499:HOH:O	2.18	0.41
1:C:473:ILE:HG22	1:C:473:ILE:O	2.20	0.41
1:C:104:LEU:HD21	1:C:115:ILE:HG13	2.02	0.41
1:C:134:SER:HB2	1:C:178:ILE:HD11	2.02	0.41
1:C:196:PHE:O	1:C:200:VAL:HG23	2.20	0.41
1:C:385:VAL:HG11	1:C:393:THR:HG22	2.02	0.41
1:C:134:SER:N	1:C:135:PRO:CD	2.84	0.41
1:C:324:THR:OG1	1:C:327:GLN:HG3	2.20	0.41
1:C:184:TRP:CZ2	2:P:5:LYS:HB2	2.56	0.41
1:C:158:VAL:HG12	1:C:163:ALA:HB3	2.03	0.41
1:C:471:ASP:O	1:C:474:GLU:N	2.51	0.41
1:C:476:LEU:HD23	1:C:476:LEU:HA	1.88	0.41
1:C:454:LEU:O	1:C:456:GLU:N	2.54	0.41
1:C:245:PRO:O	1:C:249:VAL:HG23	2.21	0.40
1:C:323:GLY:HA3	1:C:327:GLN:OE1	2.21	0.40
1:C:75:ASN:OD1	1:C:75:ASN:N	2.54	0.40
2:P:3:ILE:HG13	2:P:3:ILE:O	2.22	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	C	421/428 (98%)	394 (94%)	20 (5%)	7 (2%)	9 6
2	P	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0 0
All	All	429/438 (98%)	398 (93%)	22 (5%)	9 (2%)	7 4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	494	LYS

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Mol	Chain	Res	Type
1	C	492	ILE
2	P	7	TRP
2	P	8	THR
1	C	466	GLU
1	C	482	GLU
1	C	484	VAL
1	C	493	GLU
1	C	109	GLN

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	C	355/359 (99%)	349 (98%)	6 (2%)	60	74
2	P	8/8 (100%)	7 (88%)	1 (12%)	4	4
All	All	363/367 (99%)	356 (98%)	7 (2%)	57	71

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	101	ARG
1	C	406	SER
1	C	435	LYS
1	C	442	ASP
1	C	457	THR
1	C	471	ASP
2	P	6	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	75	ASN
1	C	86	ASN
1	C	88	ASN

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Mol	Chain	Res	Type
1	C	109	GLN
1	C	146	ASN
1	C	228	ASN
1	C	261	HIS
1	C	283	ASN
1	C	346	ASN
1	C	352	GLN
1	C	375	ASN
1	C	412	GLN
1	C	438	GLN
1	C	446	ASN
1	C	449	GLN
1	C	477	GLN
1	C	479	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 (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	C	423/428 (98%)	0.66	34 (8%)	12	11	20, 20, 20, 20	0
2	P	10/10 (100%)	3.44	5 (50%)	0	0	20, 20, 20, 20	0
All	All	433/438 (98%)	0.72	39 (9%)	9	8	20, 20, 20, 20	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	7	TRP	10.1
2	P	8	THR	9.0
1	C	485	TYR	6.1
1	C	497	SER	5.9
1	C	432	LYS	5.4
2	P	6	HIS	5.2
1	C	479	HIS	5.0
2	P	9	GLY	5.0
1	C	489	LEU	5.0
1	C	478	ARG	4.7
1	C	482	GLU	4.1
1	C	496	PHE	4.0
1	C	493	GLU	3.8
1	C	477	GLN	3.8
1	C	480	GLU	3.7
1	C	476	LEU	3.6
2	P	10	ILE	3.4
1	C	481	ASN	3.3
1	C	486	LYS	3.3
1	C	492	ILE	3.2
1	C	109	GLN	3.0
1	C	108	LYS	3.0
1	C	491	LEU	2.9
1	C	473	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	483	SER	2.8
1	C	434	THR	2.7
1	C	107	GLU	2.6
1	C	454	LEU	2.6
1	C	474	GLU	2.6
1	C	458	GLU	2.5
1	C	452	GLU	2.4
1	C	488	SER	2.3
1	C	487	ALA	2.3
1	C	159	VAL	2.2
1	C	438	GLN	2.2
1	C	471	ASP	2.2
1	C	467	CYS	2.1
1	C	455	GLY	2.1
1	C	238	ARG	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.