Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:56 PM GMT

PDB ID	:	4GQ2
Title	:	S. pombe Nup120-Nup37 complex
Authors	:	Liu, X.; Mitchell, J.; Wozniak, R.; Blobel, G.; Fan, J.
Deposited on	:	2012-08-22
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

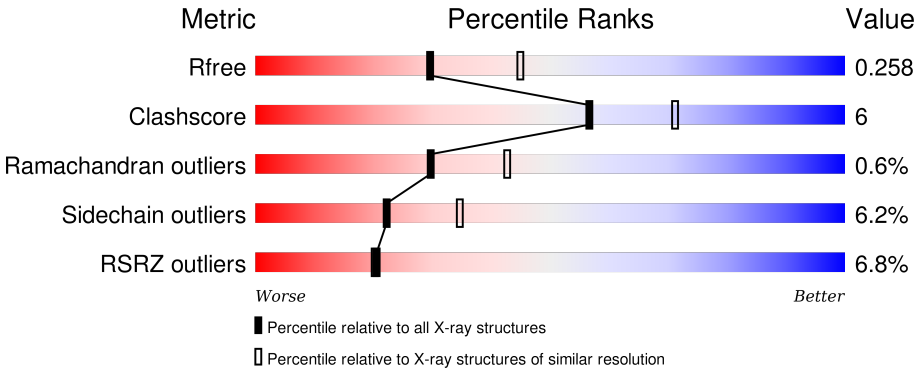
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	M	950	5% 80% 13% • 5%
2	P	393	10% 74% 17% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10236 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 Nucleoporin nup120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	904	Total	C	N	O	S	0	0	0
			7274	4701	1149	1397	27			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	ARG	-	EXPRESSION TAG	UNP O43044

- Molecule 2 is a protein called Nup37.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	371	Total	C	N	O	S	0	0	0
			2840	1794	484	546	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-1	GLY	-	EXPRESSION TAG	UNP O36030
P	0	SER	-	EXPRESSION TAG	UNP O36030

- Molecule 3 is water.

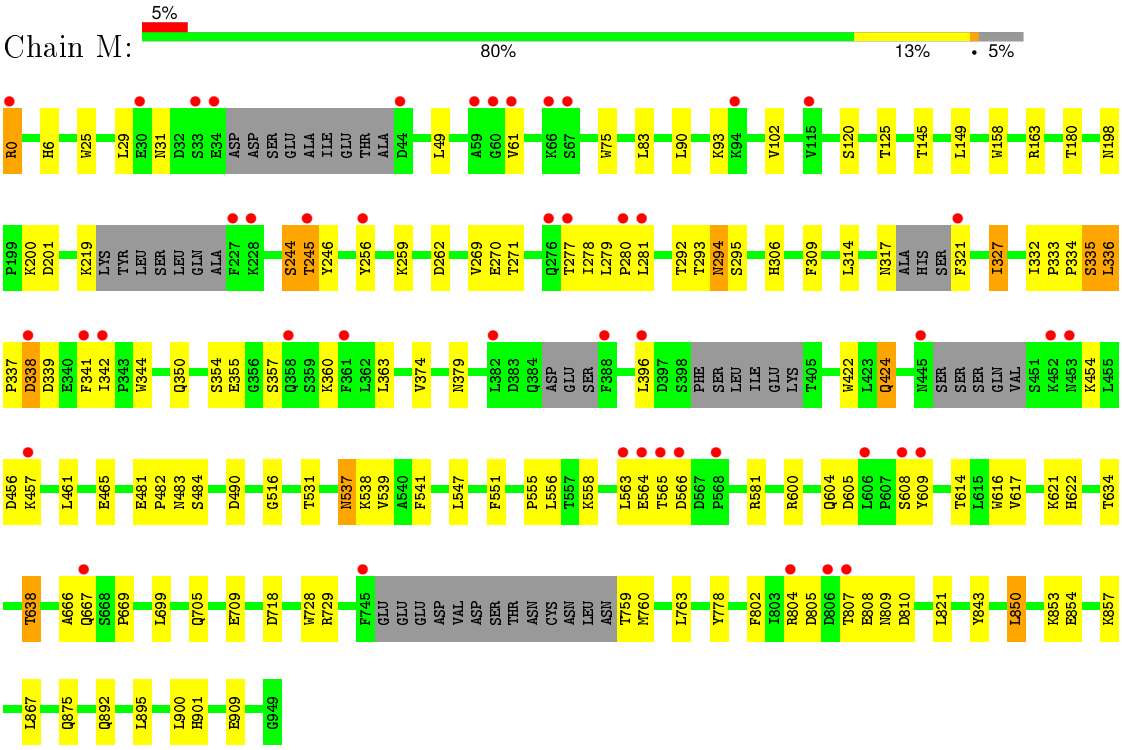
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	M	97	Total	O	0	0
			97	97		
3	P	25	Total	O	0	0
			25	25		

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 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.

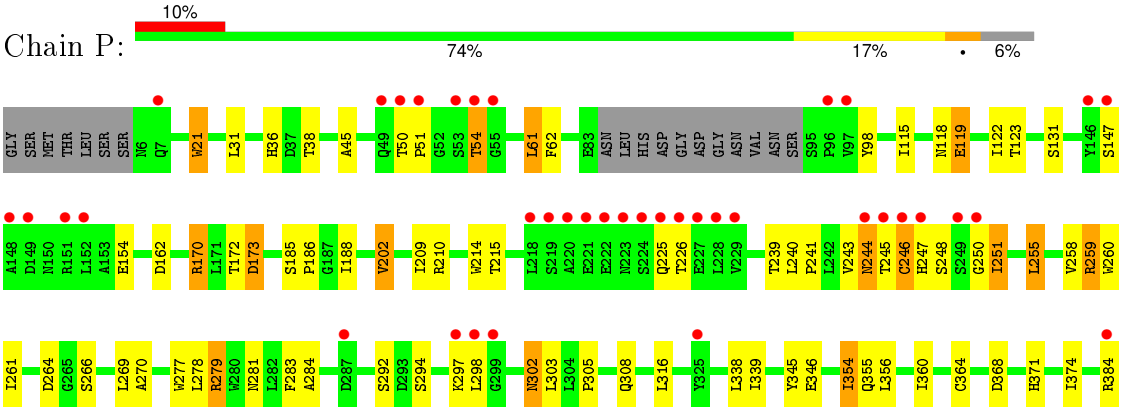
- Molecule 1: Nucleoporin nup120

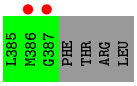
Chain M:



- Molecule 2: Nup37

Chain P:




L385
M386
G387
PHE
THR
ARG
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.47Å 123.02Å 172.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.40 34.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.00-2.40) 99.8 (34.72-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.210 , 0.258 0.210 , 0.258	Depositor DCC
R_{free} test set	2996 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 59341 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10236	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	M	0.47	7/7437 (0.1%)	0.60	3/10091 (0.0%)
2	P	0.52	3/2906 (0.1%)	0.64	1/3971 (0.0%)
All	All	0.48	10/10343 (0.1%)	0.61	4/14062 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	321	PHE	C-N	6.36	1.48	1.34
1	M	728	TRP	CD2-CE2	5.61	1.48	1.41
2	P	260	TRP	CD2-CE2	5.45	1.47	1.41
1	M	616	TRP	CD2-CE2	5.28	1.47	1.41
1	M	75	TRP	CD2-CE2	5.25	1.47	1.41
2	P	21	TRP	CD2-CE2	5.17	1.47	1.41
2	P	277	TRP	CD2-CE2	5.17	1.47	1.41
1	M	25	TRP	CD2-CE2	5.15	1.47	1.41
1	M	422	TRP	CD2-CE2	5.15	1.47	1.41
1	M	158	TRP	CD2-CE2	5.02	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	321	PHE	O-C-N	16.48	149.07	122.70
1	M	321	PHE	CA-C-N	-12.35	90.04	117.20
1	M	321	PHE	C-N-CA	-8.74	99.86	121.70
2	P	345	TYR	N-CA-C	8.07	132.80	111.00

There are no chirality outliers.

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	M	7274	0	7170	73	0
2	P	2840	0	2773	49	0
3	M	97	0	0	2	0
3	P	25	0	0	0	0
All	All	10236	0	9943	122	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 6.

All (122) 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:M:564:GLU:H	1:M:565:THR:HA	1.14	1.08
1:M:564:GLU:N	1:M:565:THR:HA	1.71	1.03
1:M:634:THR:O	1:M:638:THR:HG23	1.75	0.87
1:M:31:ASN:H	1:M:163:ARG:HH22	1.32	0.78
1:M:843:TYR:OH	1:M:901:HIS:HE1	1.68	0.76
1:M:279:LEU:H	1:M:280:PRO:HD3	1.52	0.75
1:M:565:THR:H	1:M:566:ASP:HA	1.52	0.74
2:P:339:ILE:HB	2:P:354:ILE:HG23	1.71	0.72
1:M:565:THR:N	1:M:566:ASP:HA	2.05	0.72
2:P:243:VAL:HG12	2:P:244:ASN:N	2.06	0.70
1:M:120:SER:HB3	1:M:180:THR:HG21	1.78	0.66
1:M:563:LEU:HB3	1:M:564:GLU:HG3	1.79	0.65
2:P:36:HIS:HD2	2:P:38:THR:H	1.44	0.64
2:P:302:ASN:HD22	2:P:302:ASN:C	2.01	0.64
1:M:0:ARG:HH21	1:M:563:LEU:HD21	1.63	0.62
1:M:621:LYS:HG3	1:M:622:HIS:CD2	2.35	0.61
2:P:278:LEU:HD23	2:P:305:PRO:HG3	1.81	0.61
1:M:547:LEU:HD22	1:M:551:PHE:HE1	1.65	0.61
1:M:634:THR:O	1:M:638:THR:CG2	2.48	0.61
1:M:279:LEU:N	1:M:280:PRO:HD3	2.15	0.60
2:P:243:VAL:HG12	2:P:244:ASN:H	1.67	0.59
2:P:245:THR:OG1	2:P:308:GLN:CD	2.41	0.59
2:P:245:THR:OG1	2:P:308:GLN:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:284:ALA:HB2	2:P:292:SER:HA	1.85	0.59
1:M:759:THR:HG23	1:M:760:MET:H	1.68	0.58
2:P:356:LEU:HD12	2:P:360:ILE:HD11	1.87	0.57
1:M:854:GLU:HG2	1:M:857:LYS:HD2	1.87	0.57
1:M:279:LEU:N	1:M:280:PRO:CD	2.67	0.57
2:P:21:TRP:HH2	2:P:45:ALA:HB2	1.72	0.55
1:M:854:GLU:CG	1:M:857:LYS:HD2	2.37	0.55
1:M:483:ASN:HB2	1:M:490:ASP:HB2	1.87	0.55
2:P:61:LEU:HB3	2:P:62:PHE:CD2	2.42	0.55
1:M:145:THR:HG23	1:M:149:LEU:HD12	1.89	0.55
1:M:31:ASN:N	1:M:163:ARG:HH22	2.03	0.54
1:M:537:ASN:HD21	1:M:538:LYS:HZ2	1.55	0.54
2:P:266:SER:HA	2:P:283:PHE:HB2	1.88	0.54
2:P:258:VAL:O	2:P:259:ARG:HD3	2.08	0.54
2:P:294:SER:O	2:P:298:LEU:HG	2.07	0.54
2:P:170:ARG:HD2	2:P:214:TRP:CZ3	2.42	0.53
2:P:239:THR:HG23	2:P:278:LEU:HD13	1.89	0.53
1:M:244:SER:O	1:M:294:ASN:HB2	2.08	0.53
1:M:339:ASP:O	1:M:342:ILE:HG13	2.08	0.53
2:P:54:THR:HB	2:P:384:ARG:HH22	1.73	0.53
1:M:843:TYR:OH	1:M:901:HIS:CE1	2.55	0.52
1:M:306:HIS:CD2	1:M:337:PRO:HD2	2.45	0.52
2:P:243:VAL:CG1	2:P:244:ASN:N	2.71	0.52
1:M:609:TYR:HB2	1:M:614:THR:HG23	1.92	0.51
2:P:243:VAL:CG1	2:P:244:ASN:H	2.24	0.51
1:M:198:ASN:HB3	1:M:201:ASP:OD1	2.11	0.51
2:P:261:ILE:HD11	2:P:269:LEU:HB2	1.91	0.50
1:M:262:ASP:HB2	1:M:269:VAL:CG2	2.41	0.50
2:P:243:VAL:O	2:P:244:ASN:CB	2.59	0.50
2:P:154:GLU:HG2	2:P:172:THR:HG22	1.93	0.50
1:M:600:ARG:HD2	3:M:1035:HOH:O	2.11	0.49
1:M:309:PHE:HB2	1:M:332:ILE:HB	1.93	0.49
1:M:555:PRO:HD2	1:M:558:LYS:HB3	1.93	0.49
2:P:266:SER:HB2	2:P:283:PHE:O	2.13	0.49
1:M:729:ARG:HD2	3:M:1037:HOH:O	2.12	0.49
2:P:50:THR:N	2:P:51:PRO:HD2	2.28	0.48
2:P:279:ARG:NH1	2:P:281:ASN:OD1	2.46	0.48
2:P:21:TRP:HD1	2:P:364:CYS:HG	1.56	0.48
1:M:335:SER:O	1:M:337:PRO:HD3	2.13	0.48
1:M:244:SER:HA	1:M:246:TYR:N	2.29	0.48
1:M:424:GLN:HB3	1:M:424:GLN:HE21	1.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:802:PHE:O	1:M:804:ARG:HG3	2.14	0.47
1:M:565:THR:N	1:M:566:ASP:CA	2.77	0.47
1:M:31:ASN:H	1:M:163:ARG:NH2	2.08	0.47
2:P:371:HIS:CE1	2:P:384:ARG:HD3	2.49	0.47
2:P:122:ILE:HG13	2:P:123:THR:HG22	1.96	0.47
2:P:173:ASP:N	2:P:173:ASP:OD1	2.48	0.47
1:M:729:ARG:NH2	1:M:810:ASP:OD1	2.48	0.47
2:P:356:LEU:HD12	2:P:360:ILE:CD1	2.45	0.47
1:M:564:GLU:N	1:M:565:THR:CA	2.60	0.46
1:M:547:LEU:O	1:M:551:PHE:HD1	1.98	0.46
1:M:327:ILE:HG13	1:M:327:ILE:H	1.49	0.46
1:M:809:ASN:HD22	1:M:875:GLN:NE2	2.14	0.46
2:P:338:LEU:HD23	2:P:355:GLN:HG2	1.98	0.46
1:M:617:VAL:O	1:M:621:LYS:HG2	2.15	0.45
1:M:293:THR:O	1:M:295:SER:N	2.49	0.45
2:P:225:GLN:CB	2:P:226:THR:HA	2.45	0.45
1:M:344:TRP:CH2	1:M:374:VAL:HG23	2.52	0.45
1:M:29:LEU:HB3	1:M:163:ARG:NH2	2.31	0.45
1:M:729:ARG:HH22	1:M:810:ASP:CG	2.20	0.45
2:P:188:ILE:HD11	2:P:255:LEU:CD1	2.47	0.45
1:M:666:ALA:HA	1:M:667:GLN:HA	1.54	0.45
1:M:516:GLY:HA3	1:M:537:ASN:ND2	2.32	0.44
2:P:243:VAL:O	2:P:244:ASN:HB3	2.18	0.44
1:M:262:ASP:HB2	1:M:269:VAL:HG21	1.99	0.44
1:M:350:GLN:O	1:M:363:LEU:HD12	2.17	0.44
1:M:336:LEU:H	1:M:336:LEU:HD23	1.83	0.44
2:P:162:ASP:HA	2:P:186:PRO:HB3	2.00	0.43
2:P:259:ARG:HD2	2:P:259:ARG:HA	1.82	0.43
1:M:760:MET:HG2	1:M:763:LEU:HG	2.01	0.43
1:M:759:THR:HG23	1:M:760:MET:N	2.32	0.43
2:P:115:ILE:HD12	2:P:123:THR:HG23	1.99	0.43
1:M:259:LYS:HG2	1:M:271:THR:HG23	2.00	0.43
1:M:551:PHE:O	1:M:581:ARG:HD3	2.19	0.43
2:P:185:SER:HB2	2:P:186:PRO:CD	2.49	0.42
1:M:563:LEU:HA	1:M:564:GLU:HA	1.74	0.42
2:P:188:ILE:HD11	2:P:255:LEU:HD13	2.02	0.42
1:M:454:LYS:HA	1:M:457:LYS:HD3	2.01	0.42
1:M:461:LEU:HG	1:M:465:GLU:HB3	2.01	0.42
1:M:280:PRO:CB	1:M:281:LEU:HA	2.50	0.41
2:P:98:TYR:H	2:P:118:ASN:HD21	1.68	0.41
2:P:360:ILE:HD12	2:P:374:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:537:ASN:ND2	1:M:538:LYS:HG3	2.35	0.41
1:M:355:GLU:C	1:M:357:SER:HA	2.40	0.41
2:P:62:PHE:HB2	2:P:119:GLU:HG3	2.01	0.41
2:P:209:ILE:HD11	2:P:270:ALA:HB2	2.03	0.41
2:P:202:VAL:HG13	2:P:210:ARG:HB2	2.02	0.41
1:M:850:LEU:HD13	1:M:909:GLU:HG3	2.02	0.41
1:M:354:SER:OG	1:M:360:LYS:HB3	2.20	0.41
1:M:600:ARG:HG2	1:M:604:GLN:NE2	2.36	0.41
2:P:240:LEU:HB2	2:P:241:PRO:HD3	2.02	0.41
1:M:481:GLU:HA	1:M:482:PRO:HD2	1.85	0.41
1:M:669:PRO:HB3	1:M:778:TYR:CD1	2.56	0.41
2:P:98:TYR:H	2:P:118:ASN:ND2	2.19	0.40
1:M:244:SER:CB	1:M:245:THR:HA	2.52	0.40
1:M:333:PRO:HA	1:M:334:PRO:HD3	1.93	0.40
2:P:251:ILE:HG23	2:P:251:ILE:O	2.21	0.40
1:M:483:ASN:HA	1:M:484:SER:HA	1.82	0.40
2:P:246:CYS:HA	2:P:247:HIS:HB2	2.02	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	M	888/950 (94%)	840 (95%)	45 (5%)	3 (0%)	46	63
2	P	367/393 (93%)	338 (92%)	25 (7%)	4 (1%)	17	25
All	All	1255/1343 (93%)	1178 (94%)	70 (6%)	7 (1%)	30	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	338	ASP

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Mol	Chain	Res	Type
1	M	294	ASN
2	P	244	ASN
2	P	250	GLY
1	M	608	SER
2	P	147	SER
2	P	251	ILE

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	M	831/876 (95%)	781 (94%)	50 (6%)	24	37
2	P	321/344 (93%)	299 (93%)	22 (7%)	19	30
All	All	1152/1220 (94%)	1080 (94%)	72 (6%)	22	35

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	0	ARG
1	M	6	HIS
1	M	49	LEU
1	M	61	VAL
1	M	83	LEU
1	M	90	LEU
1	M	93	LYS
1	M	102	VAL
1	M	125	THR
1	M	200	LYS
1	M	219	LYS
1	M	244	SER
1	M	245	THR
1	M	256	TYR
1	M	270	GLU
1	M	277	THR
1	M	278	ILE

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Mol	Chain	Res	Type
1	M	292	THR
1	M	314	LEU
1	M	317	ASN
1	M	327	ILE
1	M	335	SER
1	M	336	LEU
1	M	338	ASP
1	M	341	PHE
1	M	379	ASN
1	M	396	LEU
1	M	424	GLN
1	M	456	ASP
1	M	531	THR
1	M	537	ASN
1	M	539	VAL
1	M	541	PHE
1	M	556	LEU
1	M	605	ASP
1	M	638	THR
1	M	699	LEU
1	M	705	GLN
1	M	709	GLU
1	M	718	ASP
1	M	805	ASP
1	M	807	THR
1	M	808	GLU
1	M	821	LEU
1	M	850	LEU
1	M	853	LYS
1	M	867	LEU
1	M	892	GLN
1	M	895	LEU
1	M	900	LEU
2	P	31	LEU
2	P	54	THR
2	P	61	LEU
2	P	119	GLU
2	P	131	SER
2	P	170	ARG
2	P	173	ASP
2	P	202	VAL
2	P	215	THR

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Mol	Chain	Res	Type
2	P	246	CYS
2	P	248	SER
2	P	255	LEU
2	P	259	ARG
2	P	264	ASP
2	P	279	ARG
2	P	297	LYS
2	P	302	ASN
2	P	303	LEU
2	P	316	LEU
2	P	346	GLU
2	P	354	ILE
2	P	368	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	91	ASN
1	M	204	HIS
1	M	317	ASN
1	M	394	HIS
1	M	424	GLN
1	M	444	GLN
1	M	537	ASN
1	M	705	GLN
1	M	875	GLN
1	M	901	HIS
2	P	36	HIS
2	P	118	ASN
2	P	286	ASN
2	P	302	ASN
2	P	308	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	M	904/950 (95%)	0.02	46 (5%) 32 32	26, 56, 112, 159	0
2	P	371/393 (94%)	0.36	41 (11%) 7 7	30, 56, 128, 184	0
All	All	1275/1343 (94%)	0.12	87 (6%) 20 20	26, 56, 118, 184	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	321	PHE	8.6
2	P	54	THR	8.4
2	P	224	SER	7.1
2	P	226	THR	6.6
2	P	220	ALA	6.4
2	P	229	VAL	6.2
1	M	281	LEU	6.0
2	P	223	ASN	5.9
2	P	222	GLU	5.8
2	P	225	GLN	5.5
2	P	297	LYS	5.3
2	P	221	GLU	5.3
2	P	228	LEU	5.2
2	P	49	GLN	5.0
2	P	387	GLY	4.8
2	P	50	THR	4.7
2	P	152	LEU	4.4
2	P	219	SER	4.3
2	P	148	ALA	4.3
2	P	246	CYS	4.3
1	M	609	TYR	4.2
1	M	44	ASP	4.1
1	M	227	PHE	3.9
1	M	565	THR	3.9

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Mol	Chain	Res	Type	RSRZ
2	P	51	PRO	3.9
1	M	457	LYS	3.7
2	P	53	SER	3.7
1	M	804	ARG	3.6
2	P	298	LEU	3.5
2	P	55	GLY	3.4
1	M	0	ARG	3.3
2	P	384	ARG	3.2
1	M	30	GLU	3.2
2	P	97	VAL	3.2
1	M	745	PHE	3.2
2	P	249	SER	3.2
2	P	245	THR	3.2
1	M	67	SER	3.1
1	M	564	GLU	3.1
1	M	60	GLY	3.1
1	M	245	THR	3.1
1	M	228	LYS	3.0
2	P	227	GLU	3.0
1	M	66	LYS	3.0
1	M	606	LEU	3.0
2	P	147	SER	3.0
2	P	247	HIS	3.0
1	M	277	THR	2.9
2	P	386	MET	2.9
1	M	276	GLN	2.9
1	M	338	ASP	2.8
2	P	146	TYR	2.8
1	M	59	ALA	2.8
2	P	244	ASN	2.8
1	M	33	SER	2.6
2	P	7	GLN	2.6
1	M	452	LYS	2.6
2	P	96	PRO	2.6
2	P	325	TYR	2.6
1	M	445	ASN	2.5
2	P	218	LEU	2.5
2	P	287	ASP	2.5
2	P	151	ARG	2.5
1	M	566	ASP	2.5
1	M	667	GLN	2.5
1	M	807	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	361	PHE	2.4
2	P	299	GLY	2.4
1	M	358	GLN	2.3
1	M	563	LEU	2.3
1	M	388	PHE	2.3
2	P	250	GLY	2.3
1	M	396	LEU	2.3
1	M	61	VAL	2.3
1	M	34	GLU	2.3
1	M	115	VAL	2.3
1	M	453	ASN	2.2
1	M	568	PRO	2.2
1	M	382	LEU	2.2
1	M	342	ILE	2.2
2	P	149	ASP	2.2
1	M	608	SER	2.2
1	M	341	PHE	2.2
1	M	256	TYR	2.1
1	M	806	ASP	2.1
1	M	94	LYS	2.1
1	M	280	PRO	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.