



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:54 AM UTC

PDB ID : 4GQ2 / pdb_00004gq2
Title : S. pombe Nup120-Nup37 complex
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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

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

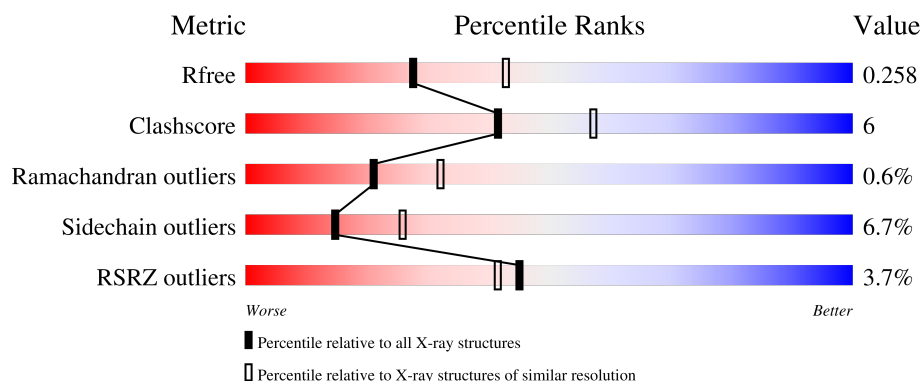
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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 $\leq 5\%$. 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	 3% 79% 15% • 5%
2	P	393	 5% 73% 18% • 6%

2 Entry composition [i](#)

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

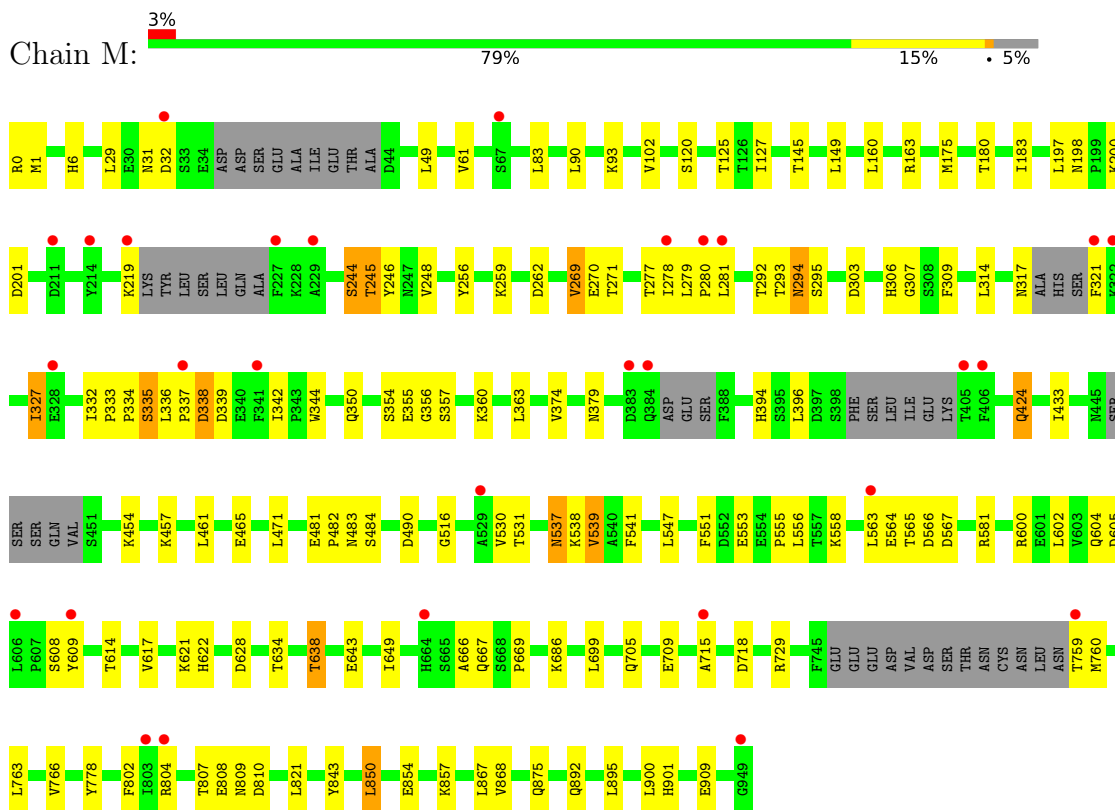
- Molecule 3 is water.

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

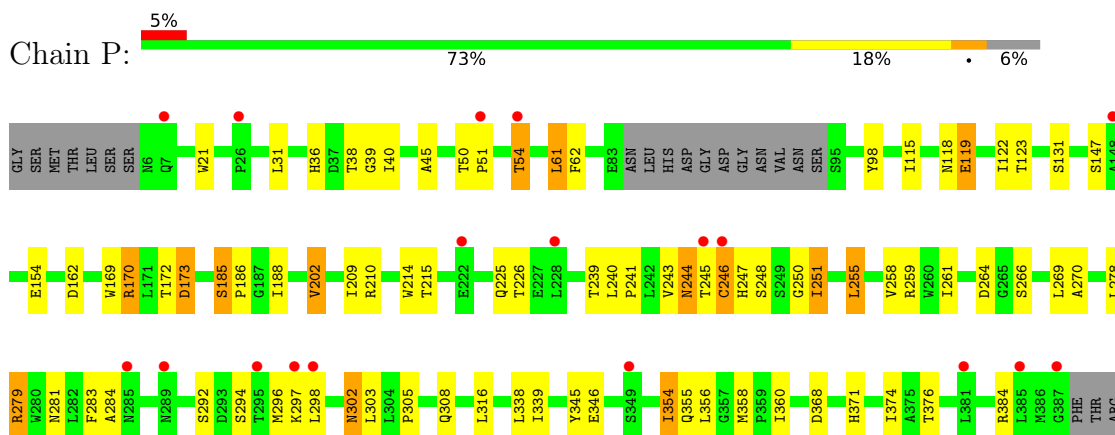
3 Residue-property plots

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: Nucleoporin nup120



• Molecule 2: Nup37



LEU

4 Data and refinement statistics

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 35.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.00-2.40) 99.8 (35.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	M	0.60	2/7437 (0.0%)	0.85	10/10091 (0.1%)
2	P	0.66	0/2906	0.88	5/3971 (0.1%)
All	All	0.62	2/10343 (0.0%)	0.86	15/14062 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	321	PHE	C-N	10.49	1.48	1.33
1	M	686	LYS	C-O	-5.01	1.18	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	321	PHE	O-C-N	16.29	149.07	123.00
2	P	345	TYR	N-CA-C	15.28	132.80	113.55
1	M	321	PHE	CA-C-N	-15.02	99.86	122.09
1	M	321	PHE	C-N-CA	-15.02	99.86	122.09
1	M	32	ASP	N-CA-C	7.96	119.59	111.07
2	P	345	TYR	CA-C-N	5.99	132.48	121.70
2	P	345	TYR	C-N-CA	5.99	132.48	121.70
1	M	628	ASP	CA-C-N	5.74	125.86	119.32
1	M	628	ASP	C-N-CA	5.74	125.86	119.32
1	M	530	VAL	N-CA-C	5.58	117.03	108.71
2	P	185	SER	CA-C-N	-5.52	114.07	119.76
2	P	185	SER	C-N-CA	-5.52	114.07	119.76
1	M	715	ALA	N-CA-C	5.33	122.15	110.80
1	M	539	VAL	CB-CA-C	-5.27	102.47	110.95
1	M	567	ASP	N-CA-C	5.16	114.76	108.11

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	M	7274	0	7170	77	0
2	P	2840	0	2773	52	0
3	M	97	0	0	2	0
3	P	25	0	0	0	0
All	All	10236	0	9943	129	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 (129) 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:302:ASN:C	2:P:302:ASN:HD22	2.01	0.69
2:P:243:VAL:HG12	2:P:244:ASN:N	2.06	0.68
2:P:358:MET:HE3	2:P:376:THR:HG21	1.75	0.68
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:245:THR:OG1	2:P:308:GLN:CD	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:245:THR:OG1	2:P:308:GLN:NE2	2.36	0.59
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:483:ASN:HB2	1:M:490:ASP:HB2	1.87	0.55
1:M:854:GLU:CG	1:M:857:LYS:HD2	2.37	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
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
2:P:296:MET:HA	2:P:296:MET:HE3	1.90	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
1:M:198:ASN:HB3	1:M:201:ASP:OD1	2.11	0.51
2:P:243:VAL:CG1	2:P:244:ASN:H	2.24	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
1:M:729:ARG:HH22	1:M:810:ASP:CG	2.20	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
1:M:729:ARG:HD2	3:M:1037:HOH:O	2.12	0.49
2:P:266:SER:HB2	2:P:283:PHE:O	2.13	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:424:GLN:HE21	1:M:424:GLN:HB3	1.54	0.48
1:M:802:PHE:O	1:M:804:ARG:HG3	2.14	0.47
1:M:31:ASN:H	1:M:163:ARG:NH2	2.08	0.47
1:M:565:THR:N	1:M:566:ASP:CA	2.77	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:327:ILE:H	1:M:327:ILE:HG13	1.49	0.46
1:M:547:LEU:O	1:M:551:PHE:HD1	1.98	0.46
1:M:564:GLU:N	1:M:565:THR:CA	2.60	0.46
1:M:355:GLU:C	1:M:357:SER:HA	2.40	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:293:THR:O	1:M:295:SER:N	2.49	0.45
1:M:617:VAL:O	1:M:621:LYS:HG2	2.15	0.45
1:M:344:TRP:CH2	1:M:374:VAL:HG23	2.52	0.45
2:P:225:GLN:CB	2:P:226:THR:HA	2.45	0.45
1:M:29:LEU:HB3	1:M:163:ARG:NH2	2.31	0.45
1:M:303:ASP:CG	1:M:307:GLY:HA2	2.41	0.45
1:M:1:MET:HE2	1:M:394:HIS:HD2	1.82	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:336:LEU:H	1:M:336:LEU:HD23	1.83	0.44
1:M:350:GLN:O	1:M:363:LEU:HD12	2.17	0.44
2:P:162:ASP:HA	2:P:186:PRO:HB3	2.00	0.43
2:P:39:GLY:C	2:P:40:ILE:HG13	2.42	0.43
2:P:259:ARG:HA	2:P:259:ARG:HD2	1.82	0.43
1:M:354:SER:C	1:M:356:GLY:H	2.26	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:471:LEU:C	1:M:471:LEU:HD23	2.45	0.42
1:M:563:LEU:HA	1:M:564:GLU:HA	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:454:LYS:HA	1:M:457:LYS:HD3	2.01	0.42
2:P:188:ILE:HD11	2:P:255:LEU:HD13	2.02	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
1:M:537:ASN:ND2	1:M:538:LYS:HG3	2.35	0.41
2:P:360:ILE:HD12	2:P:374:ILE:HG21	2.02	0.41
1:M:354:SER:OG	1:M:360:LYS:HB3	2.20	0.41
1:M:850:LEU:HD13	1:M:909:GLU:HG3	2.02	0.41
2:P:62:PHE:HB2	2:P:119:GLU:HG3	2.01	0.41
2:P:202:VAL:HG13	2:P:210:ARG:HB2	2.02	0.41
2:P:209:ILE:HD11	2:P:270:ALA:HB2	2.03	0.41
1:M:175:MET:HE2	1:M:183:ILE:HD11	2.03	0.41
1:M:600:ARG:HG2	1:M:604:GLN:NE2	2.36	0.41
1:M:481:GLU:HA	1:M:482:PRO:HD2	1.85	0.41
2:P:240:LEU:HB2	2:P:241:PRO:HD3	2.02	0.41
1:M:669:PRO:HB3	1:M:778:TYR:CD1	2.56	0.41
2:P:169:TRP:CD1	2:P:169:TRP:C	2.98	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:O	2:P:251:ILE:HG23	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%)	36 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	367/393 (93%)	338 (92%)	25 (7%)	4 (1%)	11	18
All	All	1255/1343 (93%)	1178 (94%)	70 (6%)	7 (1%)	21	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	338	ASP
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%)	775 (93%)	56 (7%)	15	26
2	P	321/344 (93%)	300 (94%)	21 (6%)	15	27
All	All	1152/1220 (94%)	1075 (93%)	77 (7%)	15	26

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	127	ILE

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Mol	Chain	Res	Type
1	M	160	LEU
1	M	197	LEU
1	M	200	LYS
1	M	219	LYS
1	M	244	SER
1	M	245	THR
1	M	248	VAL
1	M	256	TYR
1	M	269	VAL
1	M	270	GLU
1	M	277	THR
1	M	278	ILE
1	M	292	THR
1	M	314	LEU
1	M	317	ASN
1	M	327	ILE
1	M	335	SER
1	M	338	ASP
1	M	379	ASN
1	M	396	LEU
1	M	424	GLN
1	M	433	ILE
1	M	531	THR
1	M	537	ASN
1	M	539	VAL
1	M	541	PHE
1	M	553	GLU
1	M	556	LEU
1	M	602	LEU
1	M	605	ASP
1	M	638	THR
1	M	643	GLU
1	M	649	ILE
1	M	699	LEU
1	M	705	GLN
1	M	709	GLU
1	M	718	ASP
1	M	766	VAL
1	M	807	THR
1	M	808	GLU
1	M	821	LEU
1	M	850	LEU

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Mol	Chain	Res	Type
1	M	867	LEU
1	M	868	VAL
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
2	P	246	CYS
2	P	248	SER
2	P	255	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	91	ASN
1	M	133	HIS
1	M	170	GLN
1	M	204	HIS
1	M	294	ASN
1	M	315	ASN
1	M	317	ASN
1	M	394	HIS
1	M	424	GLN
1	M	537	ASN
1	M	872	HIS
1	M	875	GLN

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Mol	Chain	Res	Type
1	M	901	HIS
2	P	36	HIS
2	P	118	ASN
2	P	150	ASN
2	P	199	GLN
2	P	208	ASN
2	P	238	ASN
2	P	286	ASN
2	P	302	ASN

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 oligosaccharides 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, 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	M	904/950 (95%)	0.01	29 (3%)	50 46	26, 56, 112, 159	0
2	P	371/393 (94%)	0.13	18 (4%)	35 31	30, 56, 128, 184	0
All	All	1275/1343 (94%)	0.05	47 (3%)	45 41	26, 56, 118, 184	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	321	PHE	7.4
2	P	387	GLY	4.8
1	M	606	LEU	4.8
1	M	227	PHE	4.1
2	P	246	CYS	3.9
1	M	804	ARG	3.5
1	M	563	LEU	3.3
2	P	245	THR	3.2
1	M	383	ASP	3.0
2	P	222	GLU	2.9
1	M	280	PRO	2.8
2	P	228	LEU	2.8
1	M	281	LEU	2.8
1	M	341	PHE	2.8
2	P	385	LEU	2.7
1	M	384	GLN	2.7
1	M	609	TYR	2.6
2	P	297	LYS	2.6
1	M	278	ILE	2.6
1	M	406	PHE	2.5
1	M	715	ALA	2.4
2	P	54	THR	2.4
1	M	219	LYS	2.4
1	M	405	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	P	295	THR	2.3
2	P	349	SER	2.3
2	P	285	ASN	2.3
2	P	7	GLN	2.3
2	P	51	PRO	2.3
1	M	803	ILE	2.3
2	P	289	ASN	2.2
1	M	949	GLY	2.2
1	M	211	ASP	2.2
1	M	322	LYS	2.2
2	P	381	LEU	2.2
1	M	337	PRO	2.2
2	P	148	ALA	2.2
1	M	759	THR	2.1
1	M	664	HIS	2.1
1	M	229	ALA	2.1
2	P	298	LEU	2.1
1	M	32	ASP	2.1
1	M	67	SER	2.1
2	P	26	PRO	2.1
1	M	328	GLU	2.1
1	M	214	TYR	2.1
1	M	529	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 oligosaccharides 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.