Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:39 pm BST

PDB ID	:	4R4Z
Title	:	Structure of PNGF-II in P21 space group
Authors	:	Sun, G.; Yu, X.; Celimuge; Wang, L.; Li, M.; Gan, J.; Qu, D.; Ma, J.; Chen, L.
Deposited on	:	2014-08-20
Resolution	:	2.81 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 ⓘ) were used in the production of this report:

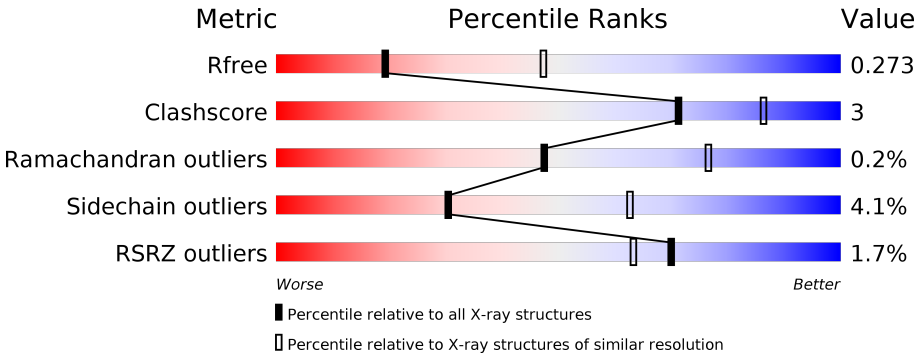
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	544	88% 10%
1	B	544	87% 12%
1	C	544	4% 88% 11%
1	D	544	89% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17034 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 PNGF-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4256	2705	725	819	7			
1	B	539	Total	C	N	O	S	0	0	0
			4259	2707	725	820	7			
1	C	539	Total	C	N	O	S	0	0	0
			4259	2707	725	820	7			
1	D	538	Total	C	N	O	S	0	0	0
			4249	2701	722	819	7			

- Molecule 2 is water.

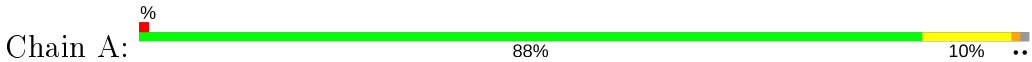
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	2	Total	O	0	0
			2	2		
2	C	2	Total	O	0	0
			2	2		
2	D	4	Total	O	0	0
			4	4		

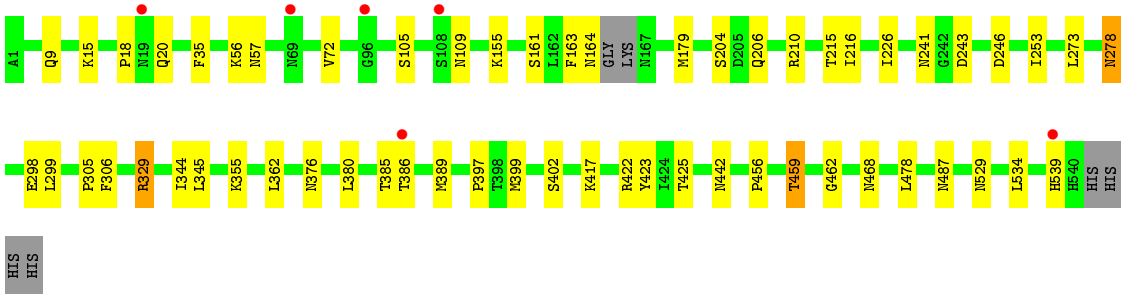
3 Residue-property plots (i)

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: PNGF-II

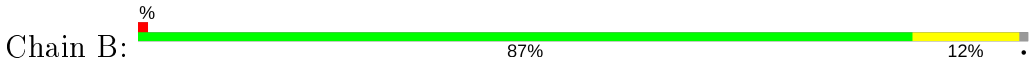
Chain A:

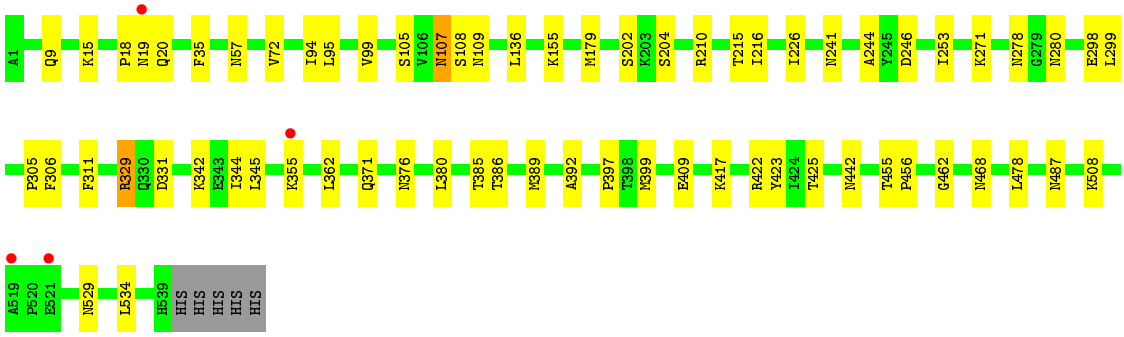




- Molecule 1: PNGF-II

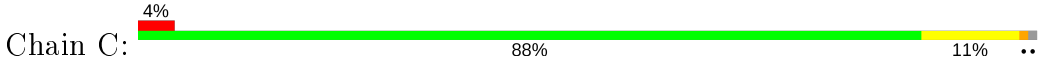
Chain B:

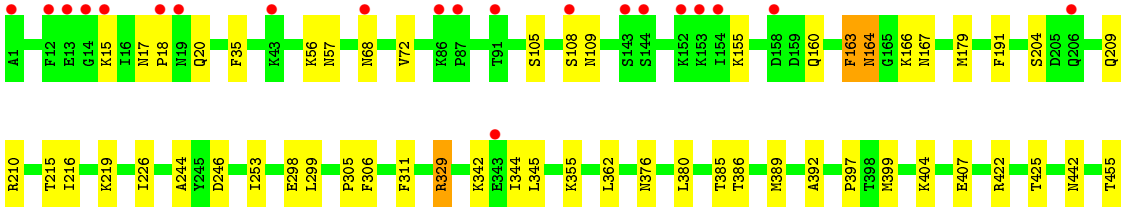


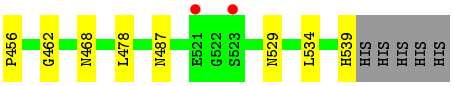


- Molecule 1: PNGF-II

Chain C:

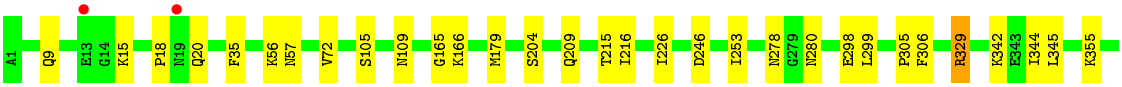


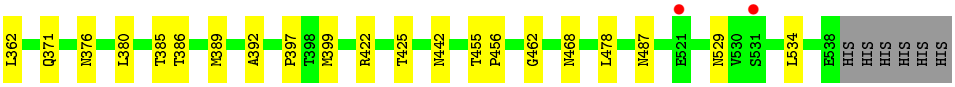




- Molecule 1: PNGF-II

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.80Å 94.20Å 165.80Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	29.50 – 2.81 29.47 – 2.82	Depositor EDS
% Data completeness (in resolution range)	91.0 (29.50-2.81) 91.2 (29.47-2.82)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.199 , 0.257 0.214 , 0.273	Depositor DCC
R_{free} test set	2856 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 16.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	17034	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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	0.47	0/4348	0.63	0/5887
1	B	0.46	0/4351	0.63	0/5891
1	C	0.45	0/4351	0.62	0/5891
1	D	0.46	0/4340	0.62	0/5876
All	All	0.46	0/17390	0.63	0/23545

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	4256	0	4201	27	0
1	B	4259	0	4211	47	0
1	C	4259	0	4211	30	0
1	D	4249	0	4204	21	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	4	0	0	0	0
All	All	17034	0	16827	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 3.

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:B:94:ILE:CD1	1:B:136:LEU:HB2	1.59	1.33
1:B:94:ILE:HD12	1:B:136:LEU:HB2	1.29	1.07
1:B:94:ILE:HD13	1:B:136:LEU:HB2	1.47	0.96
1:B:94:ILE:CD1	1:B:136:LEU:CB	2.43	0.96
1:B:94:ILE:HD12	1:B:136:LEU:HD12	1.50	0.94
1:B:94:ILE:HD12	1:B:136:LEU:CB	1.99	0.92
1:B:94:ILE:HD12	1:B:136:LEU:CD1	2.08	0.83
1:C:160:GLN:HG2	1:C:164:ASN:ND2	1.93	0.82
1:B:107:ASN:N	1:B:107:ASN:HD22	1.80	0.79
1:B:94:ILE:HD13	1:B:136:LEU:CB	2.13	0.76
1:B:386:THR:HG22	1:B:529:ASN:HB3	1.69	0.75
1:B:94:ILE:CD1	1:B:99:VAL:HG11	2.17	0.74
1:D:386:THR:HG22	1:D:529:ASN:HB3	1.69	0.74
1:A:386:THR:HG22	1:A:529:ASN:HB3	1.70	0.73
1:A:163:PHE:O	1:A:164:ASN:C	2.25	0.73
1:A:243:ASP:HA	1:B:108:SER:OG	1.88	0.73
1:B:94:ILE:HG13	1:B:99:VAL:HG11	1.69	0.73
1:B:107:ASN:N	1:B:107:ASN:ND2	2.35	0.72
1:C:386:THR:HG22	1:C:529:ASN:HB3	1.70	0.72
1:C:160:GLN:HG2	1:C:164:ASN:HD21	1.53	0.71
1:B:94:ILE:CG1	1:B:99:VAL:HG11	2.28	0.64
1:B:298:GLU:O	1:B:422:ARG:NH2	2.32	0.63
1:B:107:ASN:H	1:B:107:ASN:HD22	1.46	0.63
1:A:298:GLU:O	1:A:422:ARG:NH2	2.33	0.62
1:B:456:PRO:HB2	1:B:487:ASN:HB2	1.82	0.62
1:D:72:VAL:HG11	1:D:179:MET:CE	2.30	0.61
1:C:456:PRO:HB2	1:C:487:ASN:HB2	1.82	0.61
1:C:298:GLU:O	1:C:422:ARG:NH2	2.33	0.61
1:D:298:GLU:O	1:D:422:ARG:NH2	2.33	0.61
1:C:389:MET:HB3	1:C:392:ALA:HB3	1.82	0.61
1:A:456:PRO:HB2	1:A:487:ASN:HB2	1.82	0.60
1:B:389:MET:HB3	1:B:392:ALA:HB3	1.83	0.60
1:D:456:PRO:HB2	1:D:487:ASN:HB2	1.84	0.60
1:B:72:VAL:HG11	1:B:179:MET:CE	2.32	0.60
1:B:94:ILE:HG13	1:B:99:VAL:CG1	2.32	0.60
1:D:389:MET:HB3	1:D:392:ALA:HB3	1.84	0.59
1:A:72:VAL:HG11	1:A:179:MET:CE	2.32	0.59
1:B:409:GLU:OE2	1:B:508:LYS:HE3	2.03	0.59
1:A:459:THR:HG22	1:B:331:ASP:HB3	1.85	0.59
1:C:72:VAL:HG11	1:C:179:MET:CE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:HG21	1:B:136:LEU:HB3	1.86	0.57
1:B:94:ILE:HD12	1:B:136:LEU:CG	2.35	0.56
1:C:204:SER:HB3	1:C:210:ARG:H	1.71	0.55
1:B:202:SER:OG	1:B:202:SER:O	2.21	0.54
1:B:204:SER:HB3	1:B:210:ARG:H	1.72	0.54
1:C:160:GLN:CG	1:C:164:ASN:HD21	2.19	0.54
1:A:305:PRO:CB	1:A:468:ASN:OD1	2.56	0.54
1:C:305:PRO:CB	1:C:468:ASN:OD1	2.56	0.53
1:D:305:PRO:CB	1:D:468:ASN:OD1	2.56	0.53
1:B:105:SER:HA	1:B:109:ASN:O	2.08	0.53
1:A:204:SER:HB3	1:A:210:ARG:H	1.73	0.53
1:C:105:SER:HA	1:C:109:ASN:O	2.09	0.52
1:A:105:SER:HA	1:A:109:ASN:O	2.10	0.52
1:C:344:ILE:HG13	1:C:345:LEU:N	2.25	0.51
1:D:344:ILE:HG13	1:D:345:LEU:N	2.25	0.51
1:D:105:SER:HA	1:D:109:ASN:O	2.10	0.51
1:B:386:THR:HG22	1:B:529:ASN:CB	2.41	0.50
1:A:386:THR:HG22	1:A:529:ASN:CB	2.40	0.50
1:B:305:PRO:CB	1:B:468:ASN:OD1	2.60	0.50
1:B:344:ILE:HG13	1:B:345:LEU:N	2.27	0.50
1:C:386:THR:HG22	1:C:529:ASN:CB	2.41	0.49
1:A:462:GLY:HA3	1:B:329:ARG:HD3	1.95	0.49
1:B:271:LYS:N	1:B:271:LYS:HD3	2.28	0.48
1:A:344:ILE:HG13	1:A:345:LEU:N	2.28	0.48
1:A:253:ILE:HD12	1:A:299:LEU:HD21	1.96	0.48
1:D:72:VAL:HG11	1:D:179:MET:HE1	1.97	0.47
1:B:417:LYS:HE3	1:C:68:ASN:ND2	2.29	0.47
1:D:204:SER:HB3	1:D:209:GLN:HA	1.97	0.47
1:C:253:ILE:HD12	1:C:299:LEU:HD21	1.97	0.47
1:B:253:ILE:HD12	1:B:299:LEU:HD21	1.97	0.47
1:D:253:ILE:HD12	1:D:299:LEU:HD21	1.97	0.47
1:C:68:ASN:O	1:C:166:LYS:NZ	2.38	0.46
1:A:215:THR:HG23	1:A:216:ILE:HG13	1.98	0.46
1:C:385:THR:HB	1:C:397:PRO:HB3	1.98	0.46
1:D:215:THR:HG23	1:D:216:ILE:HG13	1.98	0.46
1:B:246:ASP:HB2	1:B:306:PHE:CE2	2.51	0.46
1:B:94:ILE:HD11	1:B:99:VAL:HG11	1.95	0.46
1:C:329:ARG:HD3	1:D:462:GLY:HA3	1.98	0.45
1:A:72:VAL:HG11	1:A:179:MET:HE1	1.99	0.45
1:A:329:ARG:HD3	1:B:462:GLY:HA3	1.99	0.45
1:D:246:ASP:HB2	1:D:306:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:THR:HG23	1:B:216:ILE:HG13	2.00	0.44
1:C:191:PHE:HE1	1:C:219:LYS:HG3	1.83	0.44
1:C:215:THR:HG23	1:C:216:ILE:HG13	1.98	0.44
1:B:94:ILE:HG22	1:B:95:LEU:HG	2.00	0.44
1:A:273:LEU:HD11	1:A:389:MET:HE1	1.99	0.44
1:D:386:THR:HG22	1:D:529:ASN:CB	2.42	0.43
1:D:385:THR:HB	1:D:397:PRO:HB3	1.99	0.43
1:C:246:ASP:HB2	1:C:306:PHE:CE2	2.53	0.43
1:B:72:VAL:HG11	1:B:179:MET:HE1	1.99	0.43
1:B:385:THR:HB	1:B:397:PRO:HB3	2.00	0.43
1:A:385:THR:HB	1:A:397:PRO:HB3	1.99	0.43
1:C:163:PHE:CD1	1:C:163:PHE:N	2.86	0.43
1:A:206:GLN:OE1	1:A:206:GLN:HA	2.18	0.43
1:D:425:THR:HG21	1:D:442:ASN:OD1	2.18	0.43
1:C:72:VAL:HG11	1:C:179:MET:HE1	2.00	0.42
1:A:417:LYS:HB2	1:A:539:HIS:CE1	2.54	0.42
1:B:425:THR:HG21	1:B:442:ASN:OD1	2.20	0.42
1:A:246:ASP:HB2	1:A:306:PHE:CE2	2.54	0.42
1:C:462:GLY:HA3	1:D:329:ARG:HD3	2.01	0.42
1:C:425:THR:HG21	1:C:442:ASN:OD1	2.20	0.41
1:A:278:ASN:ND2	1:A:402:SER:HB3	2.36	0.41
1:A:425:THR:HG21	1:A:442:ASN:OD1	2.20	0.41
1:A:423:TYR:CE2	1:A:425:THR:OG1	2.73	0.41
1:B:244:ALA:HB2	1:B:311:PHE:CZ	2.56	0.41
1:C:17:ASN:HB2	1:C:20:GLN:HE21	1.86	0.41
1:C:244:ALA:HB2	1:C:311:PHE:CZ	2.56	0.41
1:C:305:PRO:CA	1:C:468:ASN:OD1	2.68	0.41
1:D:165:GLY:C	1:D:166:LYS:HG3	2.41	0.41
1:A:305:PRO:CA	1:A:468:ASN:OD1	2.69	0.41
1:C:404:LYS:HE3	1:C:407:GLU:HB3	2.03	0.41
1:B:423:TYR:CE2	1:B:425:THR:OG1	2.74	0.41
1:A:9:GLN:HG3	1:A:20:GLN:HE22	1.86	0.41
1:D:305:PRO:CA	1:D:468:ASN:OD1	2.69	0.40
1:D:9:GLN:HG3	1:D:20:GLN:HE22	1.86	0.40
1:B:9:GLN:HG3	1:B:20:GLN:HE22	1.87	0.40
1:B:278:ASN:O	1:B:278:ASN:OD1	2.40	0.40
1:C:204:SER:HB2	1:C:209:GLN:HA	2.03	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	534/544 (98%)	506 (95%)	27 (5%)	1 (0%)	47	76
1	B	537/544 (99%)	508 (95%)	28 (5%)	1 (0%)	47	76
1	C	537/544 (99%)	510 (95%)	26 (5%)	1 (0%)	47	76
1	D	536/544 (98%)	509 (95%)	26 (5%)	1 (0%)	47	76
All	All	2144/2176 (98%)	2033 (95%)	107 (5%)	4 (0%)	47	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	18	PRO
1	A	18	PRO
1	C	18	PRO
1	D	18	PRO

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	473/478 (99%)	455 (96%)	18 (4%)	33	65
1	B	473/478 (99%)	453 (96%)	20 (4%)	30	62
1	C	473/478 (99%)	452 (96%)	21 (4%)	28	60
1	D	472/478 (99%)	454 (96%)	18 (4%)	33	65
All	All	1891/1912 (99%)	1814 (96%)	77 (4%)	30	63

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

Mol	Chain	Res	Type
1	A	15	LYS
1	A	35	PHE
1	A	56	LYS
1	A	57	ASN
1	A	155	LYS
1	A	161	SER
1	A	226	ILE
1	A	241	ASN
1	A	278	ASN
1	A	329	ARG
1	A	355	LYS
1	A	362	LEU
1	A	376	ASN
1	A	380	LEU
1	A	399	MET
1	A	459	THR
1	A	478	LEU
1	A	534	LEU
1	B	15	LYS
1	B	19	ASN
1	B	35	PHE
1	B	57	ASN
1	B	107	ASN
1	B	155	LYS
1	B	226	ILE
1	B	241	ASN
1	B	280	ASN
1	B	329	ARG
1	B	342	LYS
1	B	355	LYS
1	B	362	LEU
1	B	371	GLN
1	B	376	ASN
1	B	380	LEU
1	B	399	MET
1	B	455	THR
1	B	478	LEU
1	B	534	LEU
1	C	15	LYS
1	C	35	PHE
1	C	56	LYS
1	C	57	ASN

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Mol	Chain	Res	Type
1	C	108	SER
1	C	155	LYS
1	C	163	PHE
1	C	164	ASN
1	C	167	ASN
1	C	226	ILE
1	C	329	ARG
1	C	342	LYS
1	C	355	LYS
1	C	362	LEU
1	C	376	ASN
1	C	380	LEU
1	C	399	MET
1	C	455	THR
1	C	478	LEU
1	C	534	LEU
1	C	539	HIS
1	D	15	LYS
1	D	35	PHE
1	D	56	LYS
1	D	57	ASN
1	D	226	ILE
1	D	278	ASN
1	D	280	ASN
1	D	329	ARG
1	D	342	LYS
1	D	355	LYS
1	D	362	LEU
1	D	371	GLN
1	D	376	ASN
1	D	380	LEU
1	D	399	MET
1	D	455	THR
1	D	478	LEU
1	D	534	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	A	278	ASN
1	A	316	GLN

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Mol	Chain	Res	Type
1	A	376	ASN
1	A	418	ASN
1	A	473	ASN
1	A	512	GLN
1	A	539	HIS
1	B	107	ASN
1	B	230	ASN
1	B	280	ASN
1	B	316	GLN
1	B	371	GLN
1	B	376	ASN
1	B	473	ASN
1	B	512	GLN
1	C	68	ASN
1	C	164	ASN
1	C	167	ASN
1	C	230	ASN
1	C	316	GLN
1	C	359	GLN
1	C	376	ASN
1	C	418	ASN
1	C	473	ASN
1	C	512	GLN
1	D	230	ASN
1	D	278	ASN
1	D	280	ASN
1	D	316	GLN
1	D	359	GLN
1	D	371	GLN
1	D	376	ASN
1	D	473	ASN
1	D	512	GLN

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

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	538/544 (98%)	-0.08	6 (1%) 80 75	14, 31, 53, 115	0
1	B	539/544 (99%)	-0.06	4 (0%) 87 84	15, 31, 51, 66	0
1	C	539/544 (99%)	0.09	23 (4%) 35 25	12, 33, 68, 98	0
1	D	538/544 (98%)	-0.18	4 (0%) 87 84	11, 26, 43, 67	0
All	All	2154/2176 (98%)	-0.06	37 (1%) 70 63	11, 30, 59, 115	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	ALA	5.5
1	C	108	SER	5.2
1	C	19	ASN	4.8
1	C	15	LYS	4.4
1	C	14	GLY	4.3
1	C	91	THR	3.5
1	C	12	PHE	3.2
1	C	18	PRO	3.1
1	C	43	LYS	3.0
1	A	539	HIS	2.9
1	C	87	PRO	2.9
1	D	19	ASN	2.9
1	A	96	GLY	2.8
1	C	13	GLU	2.6
1	D	521	GLU	2.6
1	C	343	GLU	2.5
1	C	523	SER	2.5
1	B	19	ASN	2.4
1	B	521	GLU	2.4
1	C	152	LYS	2.4
1	A	69	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	108	SER	2.4
1	A	386	THR	2.3
1	C	143	SER	2.3
1	C	86	LYS	2.3
1	B	355	LYS	2.3
1	C	153	LYS	2.3
1	D	13	GLU	2.3
1	C	144	SER	2.3
1	B	519	ALA	2.2
1	C	206	GLN	2.2
1	C	68	ASN	2.1
1	C	158	ASP	2.1
1	C	521	GLU	2.1
1	A	19	ASN	2.0
1	D	531	SER	2.0
1	C	154	ILE	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.