



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:12 am GMT

PDB ID : 2FDB
Title : Crystal Structure of Fibroblast growth factor (FGF)8b in complex with FGF Receptor (FGFR) 2c
Authors : Mohammadi, M.; Olsen, S.K.
Deposited on : 2005-12-13
Resolution : 2.28 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

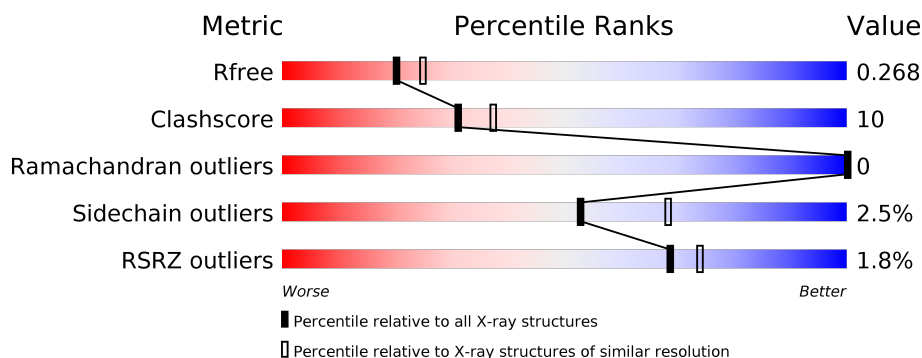
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	100719	5609 (2.30-2.26)
Clashscore	112137	6364 (2.30-2.26)
Ramachandran outliers	110173	6281 (2.30-2.26)
Sidechain outliers	110143	6281 (2.30-2.26)
RSRZ outliers	101464	5639 (2.30-2.26)

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 $\leq 5\%$. 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	164	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>
1	N	164	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>•</div> <div>10%</div> </div> </div>
2	P	220	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>•</div> <div>10%</div> </div> </div>
2	R	220	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5345 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 fibroblast growth factor 8 isoform B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	149	Total	C	N	O	S	0	0	0
			1161	727	220	208	6			
1	N	148	Total	C	N	O	S	0	0	0
			1128	708	209	205	6			

- Molecule 2 is a protein called Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	197	Total	C	N	O	S	0	0	0
			1506	957	272	269	8			
2	R	191	Total	C	N	O	S	0	0	0
			1425	910	254	253	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	2253	ARG	PRO	ENGINEERED	UNP Q9UQH9
R	3253	ARG	PRO	ENGINEERED	UNP Q9UQH9

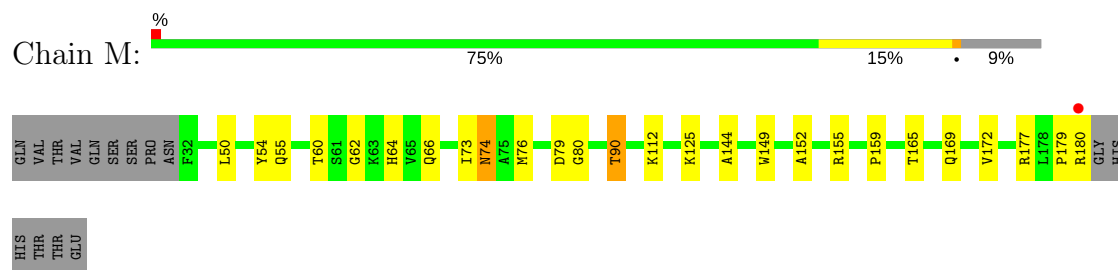
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	M	34	Total	O	0	0
			34	34		
3	N	21	Total	O	0	0
			21	21		
3	P	39	Total	O	0	0
			39	39		
3	R	31	Total	O	0	0
			31	31		

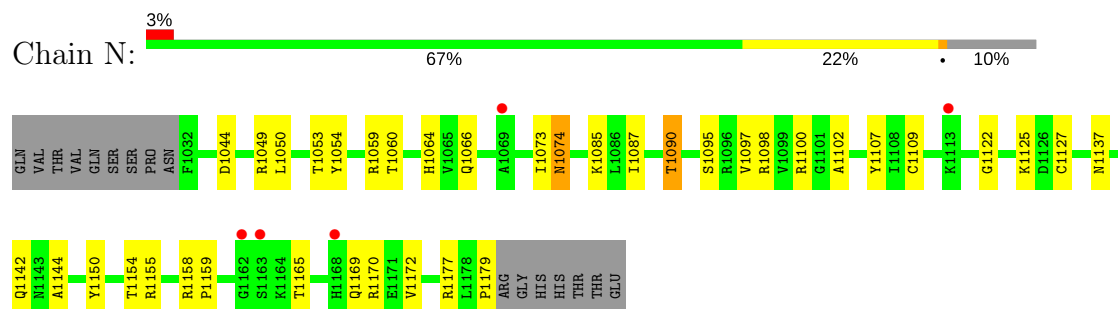
3 Residue-property plots

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.

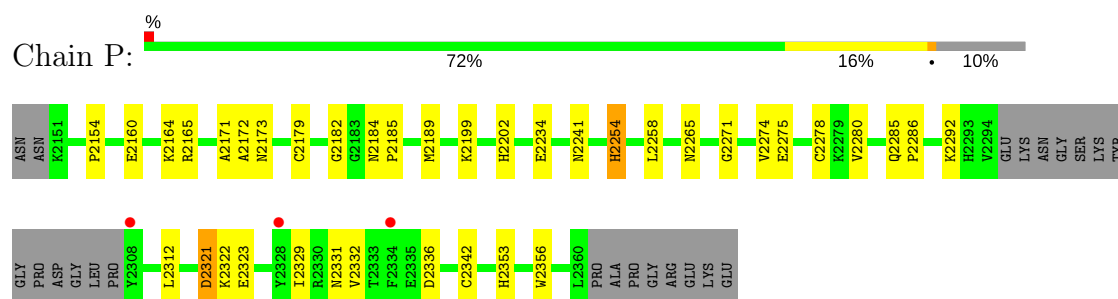
- Molecule 1: fibroblast growth factor 8 isoform B



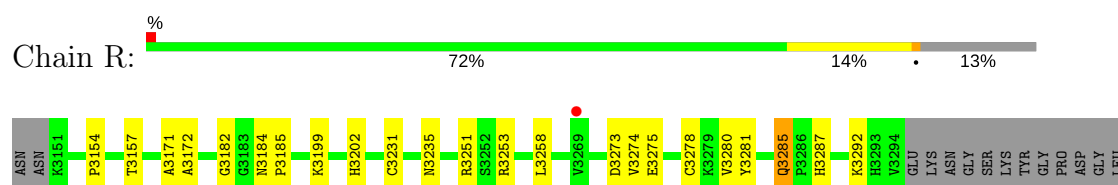
- Molecule 1: fibroblast growth factor 8 isoform B

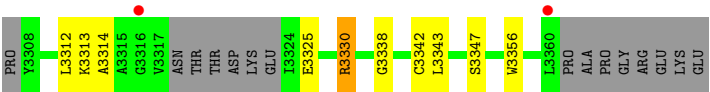


- Molecule 2: Fibroblast growth factor receptor 2



- Molecule 2: Fibroblast growth factor receptor 2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.85Å 46.91Å 109.62Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	25.00 – 2.28 29.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (25.00-2.28) 97.6 (29.95-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.58 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.272 0.238 , 0.268	Depositor DCC
R_{free} test set	6011 reflections (15.23%)	DCC
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5345	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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	0.37	0/1181	0.64	0/1592
1	N	0.35	0/1148	0.63	0/1553
2	P	0.37	0/1543	0.63	0/2099
2	R	0.34	0/1461	0.65	0/1993
All	All	0.36	0/5333	0.64	0/7237

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
2	R	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	R	3281	TYR	Sidechain

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	1161	0	1130	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1128	0	1072	34	0
2	P	1506	0	1454	31	0
2	R	1425	0	1340	24	0
3	M	34	0	0	0	0
3	N	21	0	0	0	0
3	P	39	0	0	0	0
3	R	31	0	0	1	0
All	All	5345	0	4996	99	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 10.

All (99) 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:60:THR:HG22	1:M:155:ARG:HA	1.44	0.96
2:P:2265:ASN:ND2	2:P:2356:TRP:H	1.69	0.91
1:M:55:GLN:HE22	1:M:80:GLY:H	1.21	0.88
2:R:3199:LYS:H	2:R:3202:HIS:CD2	1.92	0.87
1:N:1066:GLN:HE21	1:N:1074:ASN:HD21	1.24	0.86
2:P:2199:LYS:H	2:P:2202:HIS:CD2	1.94	0.84
2:R:3258:LEU:HD22	2:R:3280:VAL:HG22	1.60	0.84
1:N:1060:THR:HG22	1:N:1155:ARG:HA	1.62	0.80
2:P:2258:LEU:HD22	2:P:2280:VAL:HG22	1.65	0.77
1:N:1170:ARG:HG2	1:N:1170:ARG:HH11	1.49	0.77
2:P:2265:ASN:HD22	2:P:2356:TRP:H	1.32	0.75
2:P:2199:LYS:H	2:P:2202:HIS:HD2	1.37	0.73
1:N:1109:CYS:HG	1:N:1127:CYS:HG	0.73	0.72
1:M:60:THR:HG22	1:M:155:ARG:CA	2.20	0.71
1:M:90:THR:HG22	2:P:2285:GLN:HE21	1.54	0.71
1:M:66:GLN:HE21	1:M:74:ASN:HD21	1.34	0.71
1:N:1169:GLN:O	1:N:1172:VAL:HG12	1.92	0.69
1:N:1064:HIS:CE1	1:N:1177:ARG:HH11	2.11	0.69
1:M:50:LEU:HD11	2:P:2323:GLU:HG3	1.74	0.69
1:N:1137:ASN:O	2:R:3251:ARG:HG3	1.92	0.69
1:M:79:ASP:OD2	1:M:180:ARG:HD3	1.94	0.68
2:P:2254:HIS:HE1	2:R:3253:ARG:H	1.44	0.65
1:N:1064:HIS:HE1	1:N:1177:ARG:HH11	1.45	0.64
1:N:1050:LEU:HD22	2:R:3285:GLN:HE22	1.63	0.64
1:M:64:HIS:HE1	1:M:177:ARG:HH11	1.47	0.62
1:N:1150:TYR:HB3	1:N:1172:VAL:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:2254:HIS:CE1	2:R:3253:ARG:H	2.20	0.59
1:N:1064:HIS:HE1	1:N:1177:ARG:HD3	1.68	0.59
1:N:1125:LYS:HE2	1:N:1144:ALA:O	2.05	0.56
1:M:74:ASN:HD22	1:M:74:ASN:C	2.10	0.55
2:R:3278:CYS:CB	2:R:3342:CYS:HG	2.21	0.54
1:M:62:GLY:HA3	2:P:2164:LYS:HG3	1.89	0.54
1:N:1060:THR:HG22	1:N:1155:ARG:CA	2.34	0.54
1:M:50:LEU:CD1	2:P:2323:GLU:HG3	2.38	0.54
1:N:1050:LEU:HD22	2:R:3285:GLN:NE2	2.25	0.52
1:N:1049:ARG:HD2	1:N:1090:THR:O	2.09	0.52
2:R:3313:LYS:HG2	2:R:3314:ALA:O	2.10	0.52
2:P:2258:LEU:HD13	2:P:2278:CYS:SG	2.50	0.52
2:P:2278:CYS:HG	2:P:2342:CYS:HG	0.54	0.51
1:M:55:GLN:NE2	1:M:80:GLY:H	1.99	0.51
1:N:1074:ASN:C	1:N:1074:ASN:HD22	2.13	0.51
1:N:1100:ARG:HD2	1:N:1107:TYR:CZ	2.45	0.51
2:R:3274:VAL:HG22	2:R:3275:GLU:N	2.26	0.50
1:N:1170:ARG:HG2	1:N:1170:ARG:NH1	2.21	0.50
2:R:3157:THR:O	2:R:3157:THR:HG22	2.11	0.50
2:P:2171:ALA:O	2:P:2172:ALA:HB3	2.12	0.50
2:P:2271:GLY:HA2	2:P:2331:ASN:ND2	2.26	0.50
2:P:2271:GLY:HA2	2:P:2331:ASN:HD22	1.78	0.49
1:M:112:LYS:O	1:M:149:TRP:HH2	1.94	0.49
1:N:1090:THR:HA	1:N:1097:VAL:HG12	1.95	0.49
2:P:2321:ASP:O	2:P:2322:LYS:HB3	2.13	0.49
1:N:1142:GLN:HB2	1:N:1150:TYR:CE1	2.49	0.48
2:P:2179:CYS:HB2	2:P:2189:MET:CE	2.43	0.48
1:M:165:THR:HA	1:M:169:GLN:OE1	2.14	0.48
1:M:64:HIS:CE1	1:M:177:ARG:HH11	2.29	0.48
2:R:3292:LYS:NZ	2:R:3338:GLY:HA3	2.29	0.47
1:N:1172:VAL:O	1:N:1172:VAL:HG22	2.14	0.47
2:P:2154:PRO:HA	2:P:2182:GLY:O	2.15	0.47
2:P:2258:LEU:HB2	2:P:2353:HIS:CE1	2.51	0.46
1:N:1150:TYR:HB3	1:N:1172:VAL:CG2	2.43	0.46
2:P:2292:LYS:HB2	2:P:2312:LEU:HD11	1.97	0.46
1:N:1054:TYR:HA	1:N:1179:PRO:HG3	1.98	0.45
2:P:2154:PRO:HG2	2:P:2234:GLU:HA	1.98	0.45
2:R:3171:ALA:O	2:R:3172:ALA:HB3	2.15	0.45
1:M:125:LYS:HE2	1:M:144:ALA:O	2.17	0.45
1:M:74:ASN:HD22	1:M:76:MET:H	1.64	0.45
1:N:1165:THR:HA	1:N:1169:GLN:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:74:ASN:ND2	1:M:76:MET:H	2.14	0.45
1:N:1095:SER:HB2	2:R:3347:SER:HB3	1.99	0.44
1:M:90:THR:CG2	2:P:2285:GLN:HE21	2.28	0.44
1:N:1098:ARG:NE	1:N:1122:GLY:O	2.49	0.44
1:N:1044:ASP:OD2	2:R:3287:HIS:HE1	2.00	0.44
1:M:54:TYR:HA	1:M:179:PRO:HG3	2.00	0.44
1:M:50:LEU:HD11	2:P:2323:GLU:CG	2.46	0.44
2:R:3154:PRO:HA	2:R:3182:GLY:O	2.18	0.44
1:M:74:ASN:ND2	1:M:74:ASN:C	2.71	0.44
1:N:1090:THR:HG22	2:R:3285:GLN:NE2	2.33	0.43
1:M:155:ARG:NH2	2:P:2160:GLU:O	2.51	0.43
1:M:90:THR:HG21	2:P:2286:PRO:O	2.18	0.43
2:P:2179:CYS:HB2	2:P:2189:MET:HE3	2.00	0.43
2:R:3325:GLU:HB3	3:R:4104:HOH:O	2.18	0.43
2:P:2274:VAL:HG22	2:P:2275:GLU:N	2.34	0.43
2:P:2332:VAL:HG13	2:P:2336:ASP:HB2	2.01	0.42
1:N:1073:ILE:O	1:N:1159:PRO:HG3	2.19	0.42
2:R:3273:ASP:OD2	2:R:3330:ARG:HG2	2.19	0.42
2:P:2184:ASN:HA	2:P:2185:PRO:C	2.39	0.42
1:N:1054:TYR:HB2	1:N:1177:ARG:O	2.20	0.41
1:N:1154:THR:HG23	1:N:1158:ARG:O	2.20	0.41
2:R:3231:CYS:SG	2:R:3231:CYS:O	2.77	0.41
2:R:3154:PRO:HD3	2:R:3235:ASN:CG	2.40	0.41
2:R:3199:LYS:H	2:R:3202:HIS:HD2	1.59	0.41
2:R:3292:LYS:HB2	2:R:3312:LEU:HD11	2.03	0.41
1:N:1087:ILE:HG13	1:N:1102:ALA:HB2	2.02	0.41
1:N:1059:ARG:CZ	1:N:1170:ARG:NH1	2.84	0.41
2:R:3184:ASN:HA	2:R:3185:PRO:C	2.41	0.41
1:M:152:ALA:HB2	1:M:172:VAL:HG12	2.02	0.41
1:N:1053:THR:HG21	1:N:1085:LYS:HE2	2.02	0.41
2:P:2274:VAL:HG12	2:P:2329:ILE:HB	2.03	0.41
1:M:73:ILE:O	1:M:159:PRO:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	147/164 (90%)	142 (97%)	5 (3%)	0	100	100
1	N	146/164 (89%)	141 (97%)	5 (3%)	0	100	100
2	P	193/220 (88%)	185 (96%)	8 (4%)	0	100	100
2	R	185/220 (84%)	177 (96%)	8 (4%)	0	100	100
All	All	671/768 (87%)	645 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	116/143 (81%)	114 (98%)	2 (2%)	66	79
1	N	110/143 (77%)	108 (98%)	2 (2%)	64	78
2	P	154/187 (82%)	149 (97%)	5 (3%)	44	58
2	R	140/187 (75%)	136 (97%)	4 (3%)	48	62
All	All	520/660 (79%)	507 (98%)	13 (2%)	53	68

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	74	ASN
1	M	90	THR
2	P	2165	ARG
2	P	2173	ASN
2	P	2241	ASN
2	P	2254	HIS
2	P	2321	ASP
1	N	1074	ASN

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Mol	Chain	Res	Type
1	N	1090	THR
2	R	3285	GLN
2	R	3330	ARG
2	R	3343	LEU
2	R	3356	TRP

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	55	GLN
1	M	64	HIS
1	M	74	ASN
2	P	2202	HIS
2	P	2241	ASN
2	P	2265	ASN
2	P	2285	GLN
2	P	2287	HIS
2	P	2331	ASN
1	N	1064	HIS
1	N	1074	ASN
2	R	3202	HIS
2	R	3245	HIS
2	R	3285	GLN
2	R	3287	HIS

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 [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	M	149/164 (90%)	-0.10	1 (0%) 87 90	7, 21, 33, 38	0
1	N	148/164 (90%)	0.12	5 (3%) 46 52	6, 23, 34, 40	0
2	P	197/220 (89%)	-0.03	3 (1%) 74 78	6, 20, 39, 47	0
2	R	191/220 (86%)	-0.10	3 (1%) 72 77	7, 21, 38, 47	0
All	All	685/768 (89%)	-0.03	12 (1%) 69 74	6, 22, 38, 47	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	1163	SER	4.6
1	N	1113	LYS	4.3
2	P	2334	PHE	3.5
2	P	2308	TYR	3.2
2	R	3269	VAL	3.2
1	N	1162	GLY	3.2
2	R	3316	GLY	2.5
2	P	2328	TYR	2.3
1	N	1069	ALA	2.2
2	R	3360	LEU	2.2
1	N	1168	HIS	2.2
1	M	180	ARG	2.1

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.