Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 02:38 AM EDT

PDB ID	:	6PXB
Title	:	N-Terminal SH2 domain of the p120RasGAP
Authors	:	Jaber Chehayeb, R.; Stiegler, A.L.; Boggon, T.J.
Deposited on	:	2019-07-25
Resolution	:	1.75 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:

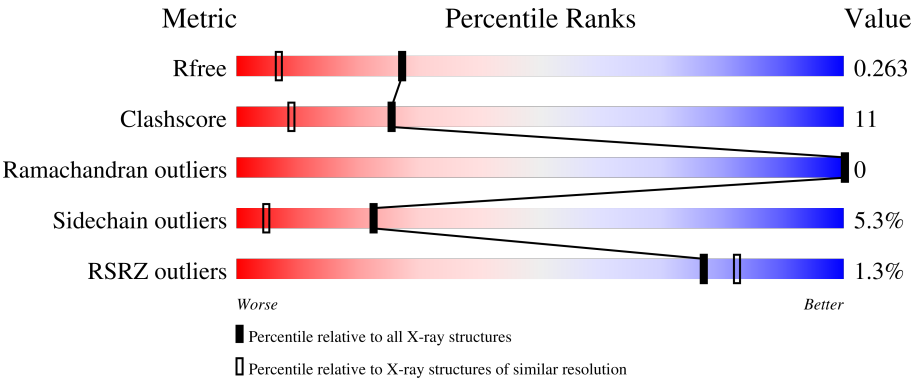
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.75 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	A	109	79% 14% • 6%
1	B	109	% 78% 12% • 7%
1	C	109	% 78% 13% • 6%
1	D	109	3% 83% 6% • 7%
1	E	109	% 66% 25% • 6%

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Mol	Chain	Length	Quality of chain
1	F	109	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5192 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 Ras GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	101	Total	C	N	O	S	0	0	0
			812	515	144	151	2			
1	C	103	Total	C	N	O	S	0	0	0
			829	527	147	153	2			
1	A	103	Total	C	N	O	S	0	0	0
			829	527	147	153	2			
1	D	101	Total	C	N	O	S	0	0	0
			814	519	144	149	2			
1	E	102	Total	C	N	O	S	0	0	0
			822	523	146	151	2			
1	B	101	Total	C	N	O	S	0	0	0
			814	519	144	149	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	172	GLY	-	expression tag	UNP P20936
F	173	SER	-	expression tag	UNP P20936
F	236	SER	CYS	engineered mutation	UNP P20936
F	261	SER	CYS	engineered mutation	UNP P20936
C	172	GLY	-	expression tag	UNP P20936
C	173	SER	-	expression tag	UNP P20936
C	236	SER	CYS	engineered mutation	UNP P20936
C	261	SER	CYS	engineered mutation	UNP P20936
A	172	GLY	-	expression tag	UNP P20936
A	173	SER	-	expression tag	UNP P20936
A	236	SER	CYS	engineered mutation	UNP P20936
A	261	SER	CYS	engineered mutation	UNP P20936
D	172	GLY	-	expression tag	UNP P20936
D	173	SER	-	expression tag	UNP P20936
D	236	SER	CYS	engineered mutation	UNP P20936
D	261	SER	CYS	engineered mutation	UNP P20936
E	172	GLY	-	expression tag	UNP P20936

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Chain	Residue	Modelled	Actual	Comment	Reference
E	173	SER	-	expression tag	UNP P20936
E	236	SER	CYS	engineered mutation	UNP P20936
E	261	SER	CYS	engineered mutation	UNP P20936
B	172	GLY	-	expression tag	UNP P20936
B	173	SER	-	expression tag	UNP P20936
B	236	SER	CYS	engineered mutation	UNP P20936
B	261	SER	CYS	engineered mutation	UNP P20936

- Molecule 2 is water.

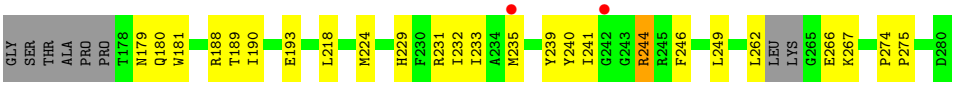
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	43	Total O 43 43	0	0
2	C	50	Total O 50 50	0	0
2	A	51	Total O 51 51	0	0
2	D	39	Total O 39 39	0	0
2	E	39	Total O 39 39	0	0
2	B	50	Total O 50 50	0	0

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.

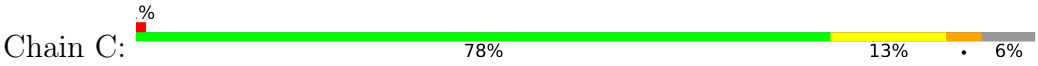
• Molecule 1: Ras GTPase-activating protein 1

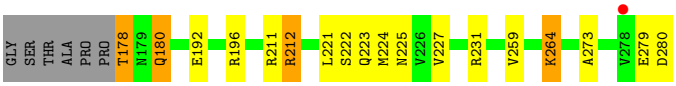
Chain F:



• Molecule 1: Ras GTPase-activating protein 1

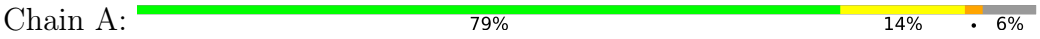
Chain C:





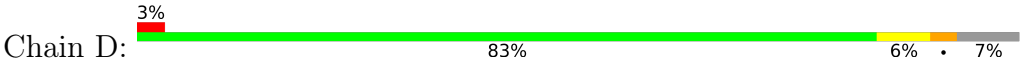
• Molecule 1: Ras GTPase-activating protein 1

Chain A:



• Molecule 1: Ras GTPase-activating protein 1

Chain D:

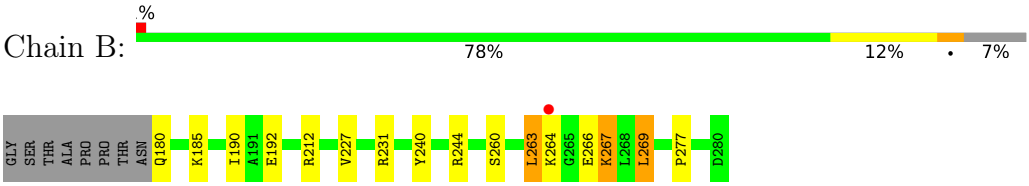


• Molecule 1: Ras GTPase-activating protein 1

Chain E:

• Molecule 1: Ras GTPase-activating protein 1

Chain B:


%
78%
12%
7%
GLY
SER
THR
ALA
PRO
PRO
THR
ASN
Q180
K185
I190
A191
E192
R212
V227
R231
Y240
R244
S260
L263
K264
G265
E266
K267
L268
L269
P277
D280

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	64.02Å 64.02Å 119.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.82 – 1.75 39.82 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.82-1.75) 99.3 (39.82-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.220 , 0.263 0.220 , 0.263	Depositor DCC
R_{free} test set	2810 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l 0.043 for h,-h-k,-l 0.480 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5192	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3391e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.87	1/849 (0.1%)	0.77	0/1145
1	B	0.74	1/834 (0.1%)	0.69	0/1124
1	C	0.65	0/849	0.76	0/1145
1	D	0.64	2/834 (0.2%)	0.72	0/1124
1	E	0.69	0/842	0.72	0/1135
1	F	0.68	0/831	0.75	0/1120
All	All	0.72	4/5039 (0.1%)	0.73	0/6793

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	266	GLU	CD-OE2	-6.12	1.19	1.25
1	A	208	GLU	CD-OE2	-5.17	1.20	1.25
1	D	266	GLU	CD-OE1	-5.13	1.20	1.25
1	B	266	GLU	CD-OE2	-5.11	1.20	1.25

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	829	0	816	16	0
1	B	814	0	803	11	0
1	C	829	0	816	19	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	814	0	803	17	0
1	E	822	0	809	28	0
1	F	812	0	791	27	1
2	A	51	0	0	4	0
2	B	50	0	0	3	0
2	C	50	0	0	3	0
2	D	39	0	0	3	0
2	E	39	0	0	6	0
2	F	43	0	0	2	0
All	All	5192	0	4838	103	1

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 11.

All (103) 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:E:222:SER:OG	1:E:266:GLU:OE2	1.65	1.14
1:F:188:ARG:NH2	1:D:280:ASP:O	1.80	1.14
1:C:224:MET:CE	1:D:280:ASP:HB3	1.81	1.10
1:F:188:ARG:HH22	1:D:280:ASP:C	1.68	0.96
1:E:280:ASP:OD2	2:E:301:HOH:O	1.84	0.95
1:E:244:ARG:NH1	1:E:255:TYR:OH	1.99	0.95
1:C:212:ARG:HG2	1:C:212:ARG:HH11	1.33	0.93
1:C:224:MET:HE2	1:D:280:ASP:HB3	1.51	0.90
1:C:224:MET:HE1	1:D:280:ASP:HB3	1.55	0.88
1:A:189:THR:HG22	1:B:190:ILE:HD11	1.62	0.81
1:B:263:LEU:HG	1:B:264:LYS:HG3	1.63	0.81
1:E:210:ASP:CB	2:E:315:HOH:O	2.34	0.74
1:C:279:GLU:HB3	2:C:318:HOH:O	1.86	0.73
1:C:212:ARG:HH11	1:C:212:ARG:CG	2.02	0.72
1:C:279:GLU:OE1	1:D:200:LYS:HG2	1.89	0.72
1:F:190:ILE:HD11	1:E:189:THR:HG22	1.73	0.70
1:C:264:LYS:NZ	1:C:264:LYS:HB3	2.06	0.69
1:E:216:PHE:O	1:E:232:ILE:N	2.24	0.69
1:F:235:MET:HB2	1:F:240:TYR:CE2	2.28	0.68
1:E:244:ARG:NH1	1:E:255:TYR:CZ	2.61	0.68
1:A:264:LYS:O	1:A:264:LYS:HG3	1.93	0.66
1:A:262:LEU:HD12	1:A:262:LEU:N	2.10	0.66
1:E:210:ASP:HB3	2:E:315:HOH:O	1.94	0.64
1:E:240:TYR:HA	1:E:244:ARG:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:ARG:HB3	2:D:311:HOH:O	1.98	0.63
1:A:182:TYR:OH	2:A:301:HOH:O	2.12	0.62
1:D:263:LEU:HG	1:D:264:LYS:HE3	1.82	0.61
1:E:240:TYR:CE1	1:E:245:ARG:HG3	2.35	0.61
1:C:180:GLN:O	1:C:273:ALA:HA	2.01	0.60
1:A:276:GLU:OE2	1:A:276:GLU:HA	2.02	0.59
1:A:262:LEU:HB3	2:A:322:HOH:O	2.00	0.59
1:F:229:HIS:O	1:D:279:GLU:HB2	2.03	0.59
1:A:190:ILE:HD13	1:B:190:ILE:HD13	1.84	0.58
1:D:180:GLN:HA	1:D:180:GLN:OE1	2.03	0.58
1:E:210:ASP:HB2	2:E:315:HOH:O	1.98	0.58
1:B:277:PRO:HG2	2:B:330:HOH:O	2.02	0.58
1:C:224:MET:HE1	1:D:280:ASP:CB	2.32	0.57
1:A:180:GLN:HA	1:A:180:GLN:OE1	2.04	0.57
1:A:267:LYS:HG3	1:A:268:LEU:N	2.20	0.57
1:F:241:ILE:HA	2:F:332:HOH:O	2.04	0.57
1:F:233:ILE:O	1:F:240:TYR:N	2.32	0.57
1:F:190:ILE:HD13	1:E:190:ILE:HD13	1.87	0.57
1:D:279:GLU:HB3	2:D:337:HOH:O	2.04	0.56
1:F:224:MET:HE1	2:A:320:HOH:O	2.06	0.56
1:F:180:GLN:O	1:F:274:PRO:HD3	2.06	0.55
1:B:231:ARG:HD3	2:B:342:HOH:O	2.07	0.54
1:F:235:MET:HB2	1:F:240:TYR:CD2	2.43	0.54
1:F:235:MET:HB2	1:F:240:TYR:HE2	1.72	0.54
1:F:189:THR:HG22	1:E:190:ILE:HD11	1.90	0.54
1:E:241:ILE:O	1:E:241:ILE:HG23	2.07	0.54
1:D:264:LYS:O	1:D:264:LYS:HG3	2.09	0.53
1:C:264:LYS:HB3	1:C:264:LYS:HZ3	1.74	0.52
1:A:262:LEU:N	1:A:262:LEU:CD1	2.72	0.52
1:C:212:ARG:HG2	1:C:212:ARG:NH1	2.13	0.52
1:F:188:ARG:NH2	1:D:280:ASP:C	2.45	0.52
1:C:192:GLU:HG2	1:C:227:VAL:HG11	1.92	0.52
1:F:262:LEU:HD13	1:F:266:GLU:O	2.11	0.51
1:C:259:VAL:O	2:C:301:HOH:O	2.19	0.51
1:C:264:LYS:NZ	1:C:264:LYS:CB	2.72	0.51
1:A:231:ARG:HG2	2:E:301:HOH:O	2.10	0.51
1:E:180:GLN:HG3	2:E:302:HOH:O	2.11	0.50
1:A:252:LEU:C	1:A:252:LEU:HD23	2.33	0.49
1:F:262:LEU:HD12	1:F:262:LEU:N	2.29	0.48
1:B:240:TYR:HA	1:B:244:ARG:O	2.14	0.48
1:A:279:GLU:HB3	2:A:316:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLU:HG2	1:B:227:VAL:HG11	1.97	0.47
1:E:180:GLN:HB3	1:E:273:ALA:CB	2.45	0.47
1:F:275:PRO:HB3	1:E:197:GLN:NE2	2.30	0.46
1:D:257:SER:HA	1:D:267:LYS:HD3	1.98	0.46
1:F:239:TYR:N	1:F:246:PHE:O	2.45	0.46
1:C:221:LEU:HD11	2:C:315:HOH:O	2.15	0.46
1:F:179:ASN:HA	1:F:181:TRP:NE1	2.31	0.46
1:B:267:LYS:HE3	1:B:269:LEU:CD2	2.46	0.46
1:C:222:SER:OG	1:C:223:GLN:N	2.49	0.45
1:C:180:GLN:OE1	1:C:180:GLN:HA	2.11	0.45
1:A:262:LEU:HD13	1:A:266:GLU:O	2.16	0.45
1:C:196:ARG:NE	1:C:225:ASN:OD1	2.26	0.45
1:E:180:GLN:HB3	1:E:273:ALA:HB2	1.98	0.44
1:F:249:LEU:HD23	1:F:249:LEU:HA	1.79	0.44
1:B:267:LYS:HE3	1:B:269:LEU:HD23	1.99	0.44
1:A:211:ARG:NH2	1:A:211:ARG:HG3	2.33	0.44
1:D:263:LEU:HD23	1:D:266:GLU:HB2	1.99	0.44
1:E:211:ARG:HA	1:E:211:ARG:HD2	1.59	0.44
1:F:233:ILE:O	1:F:239:TYR:HA	2.18	0.44
1:F:235:MET:CB	1:F:240:TYR:HE2	2.30	0.43
1:F:241:ILE:HG23	1:F:241:ILE:O	2.18	0.43
1:F:244:ARG:CG	1:F:244:ARG:HH11	2.33	0.42
1:D:250:SER:OG	2:D:301:HOH:O	2.22	0.42
1:E:185:LYS:HB2	1:E:185:LYS:HE2	1.79	0.42
1:E:217:VAL:HA	1:E:230:PHE:O	2.20	0.42
1:B:267:LYS:HG3	1:B:269:LEU:HD23	2.02	0.42
1:B:244:ARG:NE	2:B:301:HOH:O	2.23	0.42
1:F:193:GLU:HG3	2:F:328:HOH:O	2.19	0.42
1:E:203:SER:HA	1:E:270:TYR:O	2.19	0.42
1:E:262:LEU:O	1:E:262:LEU:HD23	2.19	0.42
1:E:216:PHE:HB2	1:E:232:ILE:HB	2.02	0.41
1:A:211:ARG:HG3	1:A:211:ARG:HH21	1.85	0.41
1:E:186:LEU:HD11	1:E:190:ILE:HG21	2.02	0.41
1:E:204:TYR:CE2	1:E:268:LEU:HB3	2.55	0.41
1:F:218:LEU:HB2	1:F:232:ILE:HD11	2.03	0.41
1:D:257:SER:O	1:D:267:LYS:HD3	2.21	0.41
1:E:241:ILE:O	1:E:241:ILE:CG2	2.69	0.41
1:E:187:ASP:OD1	1:E:189:THR:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:ARG:NH2	1:C:178:THR:O[2_754]	2.18	0.02

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	101/109 (93%)	99 (98%)	2 (2%)	0	100	100
1	B	99/109 (91%)	98 (99%)	1 (1%)	0	100	100
1	C	101/109 (93%)	100 (99%)	1 (1%)	0	100	100
1	D	99/109 (91%)	99 (100%)	0	0	100	100
1	E	100/109 (92%)	98 (98%)	2 (2%)	0	100	100
1	F	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
All	All	597/654 (91%)	589 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	90/94 (96%)	86 (96%)	4 (4%)	28	8
1	B	88/94 (94%)	81 (92%)	7 (8%)	12	1
1	C	90/94 (96%)	83 (92%)	7 (8%)	12	2
1	D	88/94 (94%)	86 (98%)	2 (2%)	50	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	89/94 (95%)	83 (93%)	6 (7%)	16 3
1	F	88/94 (94%)	86 (98%)	2 (2%)	50 27
All	All	533/564 (94%)	505 (95%)	28 (5%)	22 5

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	244	ARG
1	F	267	LYS
1	C	178	THR
1	C	180	GLN
1	C	211	ARG
1	C	212	ARG
1	C	231	ARG
1	C	264	LYS
1	C	280	ASP
1	A	187	ASP
1	A	263	LEU
1	A	264	LYS
1	A	267	LYS
1	D	263	LEU
1	D	267	LYS
1	E	206	ILE
1	E	209	SER
1	E	241	ILE
1	E	244	ARG
1	E	262	LEU
1	E	264	LYS
1	B	180	GLN
1	B	185	LYS
1	B	212	ARG
1	B	260	SER
1	B	263	LEU
1	B	267	LYS
1	B	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	103/109 (94%)	-0.40	0	100	100	29, 42, 81, 90	0
1	B	101/109 (92%)	-0.39	1 (0%)	82	87	27, 42, 80, 100	0
1	C	103/109 (94%)	-0.36	1 (0%)	82	87	30, 46, 82, 105	0
1	D	101/109 (92%)	-0.29	3 (2%)	50	56	30, 49, 79, 101	0
1	E	102/109 (93%)	-0.26	1 (0%)	82	87	33, 55, 88, 97	0
1	F	101/109 (92%)	-0.25	2 (1%)	65	71	29, 48, 74, 88	0
All	All	611/654 (93%)	-0.33	8 (1%)	77	82	27, 47, 84, 105	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	278	VAL	3.2
1	B	264	LYS	3.0
1	F	242	GLY	2.4
1	E	262	LEU	2.3
1	D	263	LEU	2.3
1	C	278	VAL	2.2
1	F	235	MET	2.2
1	D	265	GLY	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.