Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 07:50 AM EDT

PDB ID	:	2PJU
Title	:	Crystal structure of propionate catabolism operon regulatory protein prpR
Authors	:	Ramagopal, U.A.; Toro, R.; Gilmore, M.; Wu, B.; Koss, J.; Groshong, C.; Gheyi, T.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-04-16
Resolution	:	2.10 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 (i) symbol.

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

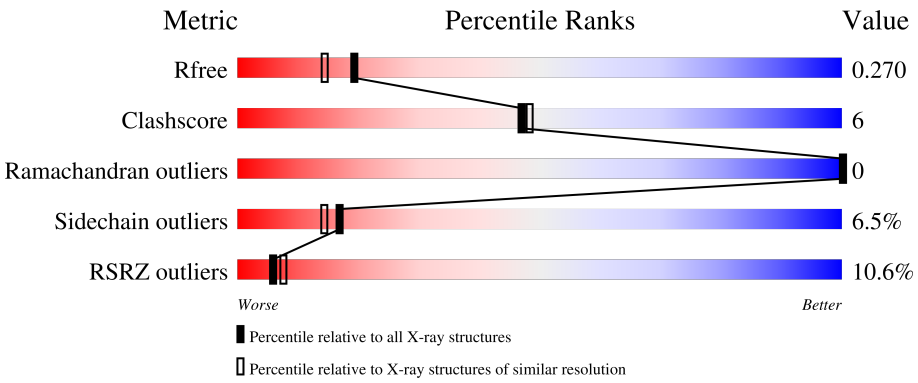
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	225	12% 72% 9% • 17%
1	B	225	8% 74% 6% • 18%
1	C	225	8% 69% 12% • 16%
1	D	225	9% 76% 14% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6218 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 Propionate catabolism operon regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1440	920	242	274	4	0	1	0
1	B	184	1417	906	239	268	4	0	0	0
1	C	188	1462	936	248	274	4	0	1	0
1	D	208	1627	1033	287	303	4	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP P77743
A	0	SER	-	cloning artifact	UNP P77743
A	1	LEU	-	cloning artifact	UNP P77743
A	96	PHE	ALA	engineered mutation	UNP P77743
A	216	GLU	-	cloning artifact	UNP P77743
A	217	GLY	-	cloning artifact	UNP P77743
A	218	HIS	-	cloning artifact	UNP P77743
A	219	HIS	-	cloning artifact	UNP P77743
A	220	HIS	-	cloning artifact	UNP P77743
A	221	HIS	-	cloning artifact	UNP P77743
A	222	HIS	-	cloning artifact	UNP P77743
A	223	HIS	-	cloning artifact	UNP P77743
B	-1	MET	-	cloning artifact	UNP P77743
B	0	SER	-	cloning artifact	UNP P77743
B	1	LEU	-	cloning artifact	UNP P77743
B	96	PHE	ALA	engineered mutation	UNP P77743
B	216	GLU	-	cloning artifact	UNP P77743
B	217	GLY	-	cloning artifact	UNP P77743
B	218	HIS	-	cloning artifact	UNP P77743
B	219	HIS	-	cloning artifact	UNP P77743
B	220	HIS	-	cloning artifact	UNP P77743

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Chain	Residue	Modelled	Actual	Comment	Reference
B	221	HIS	-	cloning artifact	UNP P77743
B	222	HIS	-	cloning artifact	UNP P77743
B	223	HIS	-	cloning artifact	UNP P77743
C	-1	MET	-	cloning artifact	UNP P77743
C	0	SER	-	cloning artifact	UNP P77743
C	1	LEU	-	cloning artifact	UNP P77743
C	96	PHE	ALA	engineered mutation	UNP P77743
C	216	GLU	-	cloning artifact	UNP P77743
C	217	GLY	-	cloning artifact	UNP P77743
C	218	HIS	-	cloning artifact	UNP P77743
C	219	HIS	-	cloning artifact	UNP P77743
C	220	HIS	-	cloning artifact	UNP P77743
C	221	HIS	-	cloning artifact	UNP P77743
C	222	HIS	-	cloning artifact	UNP P77743
C	223	HIS	-	cloning artifact	UNP P77743
D	-1	MET	-	cloning artifact	UNP P77743
D	0	SER	-	cloning artifact	UNP P77743
D	1	LEU	-	cloning artifact	UNP P77743
D	96	PHE	ALA	engineered mutation	UNP P77743
D	216	GLU	-	cloning artifact	UNP P77743
D	217	GLY	-	cloning artifact	UNP P77743
D	218	HIS	-	cloning artifact	UNP P77743
D	219	HIS	-	cloning artifact	UNP P77743
D	220	HIS	-	cloning artifact	UNP P77743
D	221	HIS	-	cloning artifact	UNP P77743
D	222	HIS	-	cloning artifact	UNP P77743
D	223	HIS	-	cloning artifact	UNP P77743

- Molecule 2 is water.

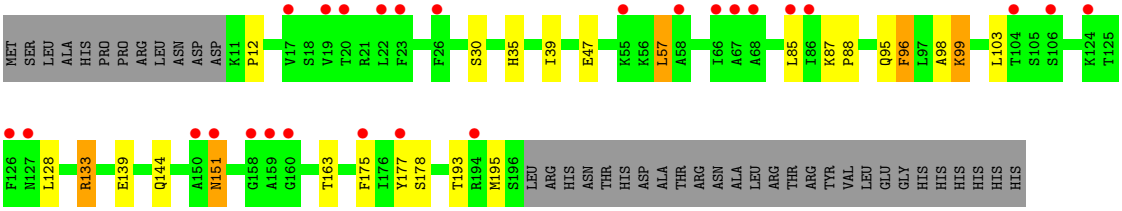
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	68	68	68	0	0
			Total	O		
2	B	68	68	68	0	0
			Total	O		
2	C	95	95	95	0	0
			Total	O		
2	D	41	41	41	0	0

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.

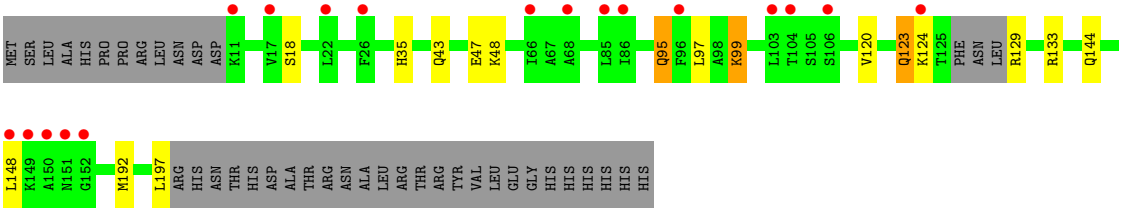
• Molecule 1: Propionate catabolism operon regulatory protein

Chain A:



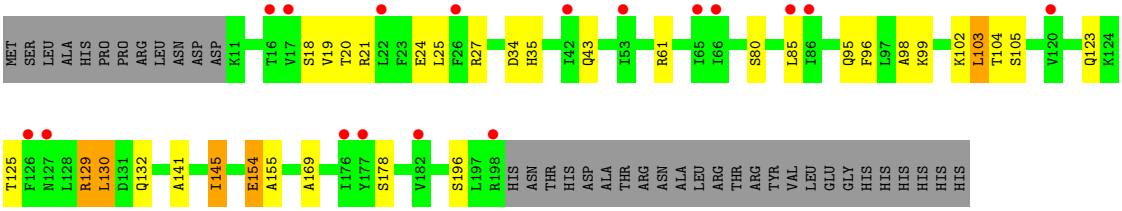
• Molecule 1: Propionate catabolism operon regulatory protein

Chain B:



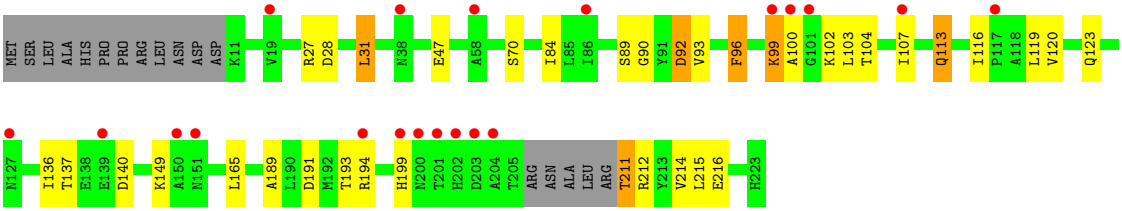
• Molecule 1: Propionate catabolism operon regulatory protein

Chain C:



• Molecule 1: Propionate catabolism operon regulatory protein

Chain D:


MET
SER
LEU
ALA
HIS
PRO
PRO
ARG
LEU
ASN
ASP
ASP
K11
V19
R27
D28
L31
N38
E47
A58
S70
I84
L85
I86
S89
G90
Y91
D92
V93
F96
K99
A100
G101
K102
L103
T104
I107
Q113
I116
P117
A118
L119
V120
Q123

N127
I136
T137
E138
E139
D140
K149
A150
N151
L165
A169
L190
D191
M192
T193
R194
H199
N200
T201
H202
D203
A204
T205
ARG
ASN
ALA
LEU
ARG
T211
R212
Y213
V214
L215
E216
H223

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	35.66Å 58.55Å 103.58Å 85.03° 88.56° 86.94°	Depositor
Resolution (Å)	37.06 – 2.10 30.31 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (37.06-2.10) 97.8 (30.31-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.252 0.229 , 0.270	Depositor DCC
R_{free} test set	2436 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6218	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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 26.78 % 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 2.4748e-03. 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 (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	A	0.65	0/1462	0.69	1/1981 (0.1%)
1	B	0.62	2/1437 (0.1%)	0.73	2/1944 (0.1%)
1	C	0.65	0/1484	0.72	0/2010
1	D	0.56	0/1657	0.66	0/2242
All	All	0.62	2/6040 (0.0%)	0.70	3/8177 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	ARG	NE-CZ	5.44	1.40	1.33
1	B	129	ARG	CZ-NH1	5.26	1.39	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	129	ARG	NE-CZ-NH2	-10.75	114.93	120.30
1	B	129	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	57	LEU	CA-CB-CG	5.04	126.89	115.30

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	A	1440	0	1465	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1417	0	1457	10	0
1	C	1462	0	1506	24	0
1	D	1627	0	1632	28	0
2	A	68	0	0	2	0
2	B	68	0	0	0	0
2	C	95	0	0	1	0
2	D	41	0	0	2	0
All	All	6218	0	6060	74	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 (74) 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:C:20:THR:HG23	1:C:21:ARG:H	1.36	0.90
1:C:21:ARG:HD3	2:C:303:HOH:O	1.82	0.79
1:D:90:GLY:HA2	1:D:119:LEU:HG	1.67	0.76
1:D:27:ARG:HG2	1:D:27:ARG:HH11	1.51	0.75
1:A:95:GLN:O	1:A:99:LYS:HD2	1.86	0.73
1:B:95:GLN:HE21	1:B:95:GLN:HA	1.55	0.71
1:B:35:HIS:CD2	1:B:35:HIS:H	2.08	0.71
1:B:133:ARG:HB3	1:B:144:GLN:HE21	1.56	0.71
1:C:27:ARG:HH11	1:C:27:ARG:HG2	1.55	0.70
1:D:116:ILE:O	1:D:120:VAL:HG23	1.92	0.70
1:A:96:PHE:CE1	1:A:178:SER:HB2	2.28	0.69
1:D:96:PHE:CE1	2:D:237:HOH:O	2.47	0.67
1:C:98:ALA:HA	1:C:103:LEU:CD2	2.25	0.67
1:D:137:THR:HG23	1:D:140:ASP:H	1.61	0.65
1:A:12:PRO:HB3	1:A:193:THR:HG21	1.79	0.64
1:C:20:THR:HG23	1:C:21:ARG:N	2.12	0.63
1:C:35:HIS:H	1:C:35:HIS:CD2	2.16	0.63
1:D:84:ILE:HD13	1:D:189:ALA:HB2	1.81	0.62
1:B:133:ARG:HB3	1:B:144:GLN:NE2	2.14	0.62
1:D:99:LYS:HG3	1:D:100:ALA:N	2.16	0.60
1:A:47:GLU:HB2	2:A:235:HOH:O	2.00	0.60
1:C:105:SER:HB3	1:C:154:GLU:HG3	1.84	0.60
1:C:19:VAL:HG23	1:C:20:THR:HG22	1.84	0.59
1:A:163:THR:HG21	1:A:175:PHE:HA	1.87	0.56
1:A:98:ALA:HB2	1:A:103:LEU:HD22	1.86	0.56
1:A:133:ARG:HD2	1:A:144:GLN:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ALA:HA	1:C:103:LEU:HD22	1.89	0.54
1:D:137:THR:HG22	1:D:140:ASP:CG	2.27	0.54
1:C:99:LYS:NZ	1:C:99:LYS:HB2	2.24	0.52
1:D:189:ALA:O	1:D:193:THR:HG23	2.09	0.52
1:A:30:SER:HB2	1:A:39:ILE:HD13	1.92	0.52
1:D:93:VAL:HG11	1:D:119:LEU:HD11	1.92	0.52
1:D:137:THR:CG2	1:D:140:ASP:H	2.23	0.51
1:C:141:ALA:O	1:C:145:ILE:HG23	2.11	0.50
1:D:89:SER:OG	1:D:92:ASP:HB2	2.11	0.50
1:C:20:THR:O	1:C:24:GLU:HG2	2.12	0.49
1:C:35:HIS:H	1:C:35:HIS:HD2	1.61	0.49
1:C:145:ILE:HD11	1:C:169:ALA:HB2	1.94	0.49
1:D:96:PHE:O	1:D:99:LYS:HG3	2.13	0.49
1:B:18:SER:O	1:B:43:GLN:HA	2.13	0.49
1:C:98:ALA:HB2	1:C:103:LEU:HD21	1.96	0.48
1:D:211:THR:HG23	1:D:214:VAL:H	1.78	0.48
1:C:196:SER:OG	1:D:199:HIS:HE1	1.96	0.48
1:D:28:ASP:O	1:D:31:LEU:HB2	2.14	0.48
1:C:130:LEU:HD22	1:C:132:GLN:HG2	1.96	0.47
1:C:125:THR:HG21	1:D:103:LEU:HB3	1.96	0.47
1:D:211:THR:CG2	1:D:214:VAL:HG23	2.45	0.47
1:B:95:GLN:HA	1:B:95:GLN:NE2	2.26	0.47
1:B:35:HIS:H	1:B:35:HIS:HD2	1.58	0.46
1:C:27:ARG:HH11	1:C:27:ARG:CG	2.26	0.46
1:D:104:THR:O	1:D:104:THR:HG22	2.16	0.46
1:A:96:PHE:HE1	2:A:246:HOH:O	1.98	0.45
1:C:130:LEU:HD22	1:C:132:GLN:CG	2.46	0.45
1:D:96:PHE:O	1:D:99:LYS:CG	2.64	0.45
1:C:96:PHE:CE2	1:C:178:SER:HB3	2.53	0.44
1:D:99:LYS:HG3	1:D:100:ALA:H	1.82	0.44
1:D:27:ARG:HH11	1:D:27:ARG:CG	2.26	0.43
1:A:195:MET:SD	1:B:192:MET:HG2	2.57	0.43
1:C:102:LYS:HG2	1:C:155:ALA:HB2	2.01	0.43
1:C:104:THR:O	1:C:129:ARG:NH1	2.52	0.42
1:D:96:PHE:HA	1:D:99:LYS:HG2	2.01	0.42
1:D:212:ARG:O	1:D:216:GLU:HB2	2.19	0.42
1:D:113:GLN:HG3	1:D:136:ILE:HD11	2.02	0.42
1:A:88:PRO:HG3	1:A:177:TYR:CD1	2.55	0.42
1:A:35:HIS:H	1:A:35:HIS:CD2	2.38	0.42
1:A:151:ASN:HD22	1:A:151:ASN:C	2.23	0.42
1:C:18:SER:O	1:C:43:GLN:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PRO:HG3	1:A:177:TYR:CE1	2.55	0.41
1:B:123:GLN:HE21	1:B:123:GLN:HB3	1.59	0.41
1:D:96:PHE:HE1	2:D:237:HOH:O	1.93	0.41
1:A:85:LEU:CD2	1:A:87:LYS:HE2	2.50	0.41
1:D:102:LYS:O	1:D:107:ILE:HD11	2.20	0.41
1:D:191:ASP:OD1	1:D:194:ARG:NH2	2.52	0.41
1:B:99:LYS:HD3	1:B:99:LYS:HA	1.93	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	185/225 (82%)	180 (97%)	5 (3%)	0	100	100
1	B	180/225 (80%)	176 (98%)	4 (2%)	0	100	100
1	C	187/225 (83%)	182 (97%)	5 (3%)	0	100	100
1	D	204/225 (91%)	196 (96%)	8 (4%)	0	100	100
All	All	756/900 (84%)	734 (97%)	22 (3%)	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	153/188 (81%)	146 (95%)	7 (5%)	27	26
1	B	151/188 (80%)	141 (93%)	10 (7%)	16	14
1	C	156/188 (83%)	144 (92%)	12 (8%)	13	9
1	D	172/188 (92%)	160 (93%)	12 (7%)	15	12
All	All	632/752 (84%)	591 (94%)	41 (6%)	17	14

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	96	PHE
1	A	99	LYS
1	A	128	LEU
1	A	133	ARG
1	A	139	GLU
1	A	151	ASN
1	B	47	GLU
1	B	48	LYS
1	B	95	GLN
1	B	97	LEU
1	B	99	LYS
1	B	120	VAL
1	B	123	GLN
1	B	124	LYS
1	B	148	LEU
1	B	197	LEU
1	C	25	LEU
1	C	34	ASP
1	C	61	ARG
1	C	80	SER
1	C	85	LEU
1	C	95	GLN
1	C	103	LEU
1	C	123	GLN
1	C	129	ARG
1	C	130	LEU
1	C	145	ILE
1	C	154	GLU
1	D	31	LEU
1	D	47	GLU
1	D	70	SER
1	D	92	ASP

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Mol	Chain	Res	Type
1	D	96	PHE
1	D	99	LYS
1	D	113	GLN
1	D	123	GLN
1	D	149	LYS
1	D	165	LEU
1	D	211	THR
1	D	215	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	151	ASN
1	B	35	HIS
1	B	43	GLN
1	B	95	GLN
1	B	123	GLN
1	B	144	GLN
1	C	35	HIS
1	C	43	GLN
1	C	113	GLN
1	C	123	GLN
1	D	35	HIS
1	D	199	HIS

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 monosaccharides 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 (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	A	186/225 (82%)	0.71	26 (13%)	2	3	31, 38, 48, 55	0
1	B	184/225 (81%)	0.67	18 (9%)	7	10	32, 39, 47, 52	0
1	C	188/225 (83%)	0.69	17 (9%)	9	12	31, 38, 46, 53	0
1	D	208/225 (92%)	0.64	20 (9%)	8	10	30, 39, 51, 58	0
All	All	766/900 (85%)	0.68	81 (10%)	6	7	30, 39, 49, 58	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	THR	4.5
1	A	127	ASN	4.3
1	D	202	HIS	4.3
1	B	124	LYS	4.0
1	C	17	VAL	3.9
1	A	68	ALA	3.8
1	D	150	ALA	3.8
1	C	198	ARG	3.7
1	B	150	ALA	3.5
1	C	66	ILE	3.4
1	A	20	THR	3.4
1	A	86	ILE	3.3
1	A	19	VAL	3.3
1	C	86	ILE	3.3
1	A	17	VAL	3.2
1	B	152	GLY	3.2
1	D	117	PRO	3.1
1	D	199	HIS	3.1
1	A	104	THR	3.0
1	D	19	VAL	3.0
1	C	42	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	126	PHE	2.9
1	A	22	LEU	2.9
1	D	201	THR	2.9
1	C	22	LEU	2.9
1	B	17	VAL	2.8
1	A	58	ALA	2.8
1	D	58	ALA	2.8
1	D	101	GLY	2.7
1	B	151	ASN	2.7
1	D	204	ALA	2.7
1	A	177	TYR	2.7
1	A	150	ALA	2.7
1	D	100	ALA	2.7
1	B	22	LEU	2.6
1	B	66	ILE	2.6
1	A	160	GLY	2.6
1	C	16	THR	2.6
1	B	148	LEU	2.6
1	C	182	VAL	2.6
1	A	194	ARG	2.5
1	A	159	ALA	2.5
1	B	26	PHE	2.5
1	C	26	PHE	2.5
1	D	139	GLU	2.5
1	C	177	TYR	2.5
1	A	124	LYS	2.5
1	B	103	LEU	2.4
1	D	127	ASN	2.4
1	A	67	ALA	2.4
1	B	11	LYS	2.4
1	A	26	PHE	2.4
1	A	106	SER	2.4
1	B	149	LYS	2.4
1	A	23	PHE	2.3
1	D	203	ASP	2.3
1	D	99	LYS	2.3
1	C	176	ILE	2.3
1	A	175	PHE	2.3
1	C	65	ILE	2.3
1	C	127	ASN	2.2
1	D	38	ASN	2.2
1	B	106	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	55	LYS	2.2
1	B	86	ILE	2.1
1	A	151	ASN	2.1
1	B	68	ALA	2.1
1	C	85	LEU	2.1
1	A	66	ILE	2.1
1	D	86	ILE	2.1
1	B	96	PHE	2.1
1	D	151	ASN	2.1
1	C	126	PHE	2.1
1	A	85	LEU	2.1
1	D	194	ARG	2.1
1	C	53	ILE	2.0
1	D	200	ASN	2.0
1	B	85	LEU	2.0
1	D	107	ILE	2.0
1	A	158	GLY	2.0
1	C	120	VAL	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 monosaccharides 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.