Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2016 – 01:40 PM EST

PDB ID	:	5L0O
Title	:	IQGAP1 calponin homology domain fragment (CHDF) mutant K161C under oxidizing conditions
Authors	:	Liu, J.; Worthylake, D.
Deposited on	:	2016-07-27
Resolution	:	2.36 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 (i) symbol.

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

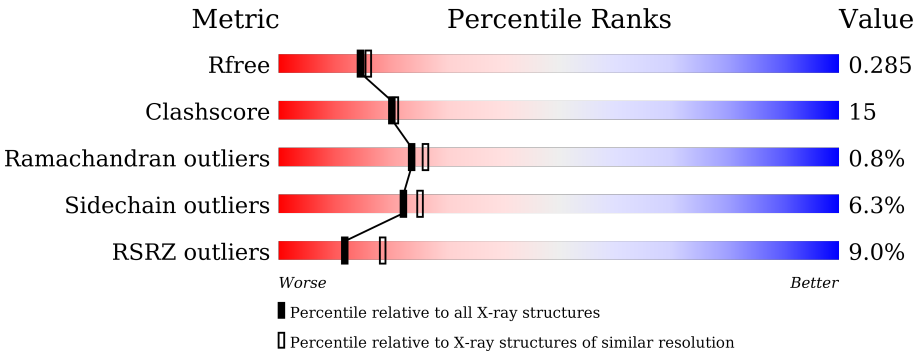
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.36 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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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 <=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	193	8% 60% 21% • 15%
1	B	193	7% 60% 22% • 15%
1	C	193	8% 62% 20% • 15%
1	D	193	8% 60% 22% • 15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5436 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-like protein IQGAP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1359	865	228	256	10			
1	B	164	Total	C	N	O	S	0	0	0
			1359	865	228	256	10			
1	C	164	Total	C	N	O	S	0	0	0
			1359	865	228	256	10			
1	D	164	Total	C	N	O	S	0	0	0
			1359	865	228	256	10			

There are 12 discrepancies between the modelled and reference sequences:

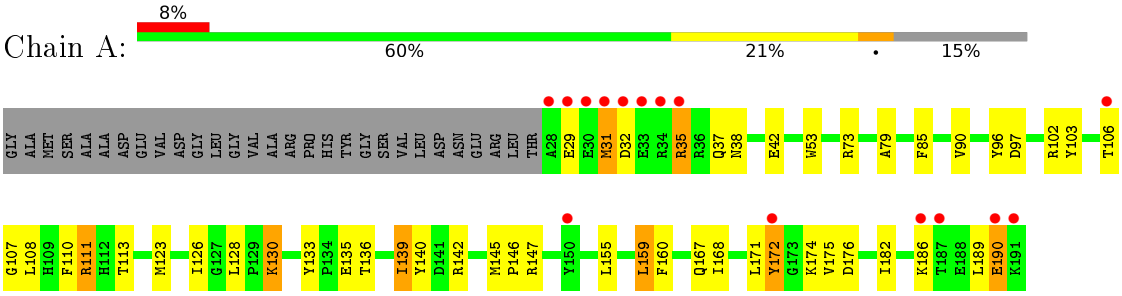
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P46940
A	0	ALA	-	expression tag	UNP P46940
A	161	CYS	LYS	engineered mutation	UNP P46940
B	-1	GLY	-	expression tag	UNP P46940
B	0	ALA	-	expression tag	UNP P46940
B	161	CYS	LYS	engineered mutation	UNP P46940
C	-1	GLY	-	expression tag	UNP P46940
C	0	ALA	-	expression tag	UNP P46940
C	161	CYS	LYS	engineered mutation	UNP P46940
D	-1	GLY	-	expression tag	UNP P46940
D	0	ALA	-	expression tag	UNP P46940
D	161	CYS	LYS	engineered mutation	UNP P46940

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 errors 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.

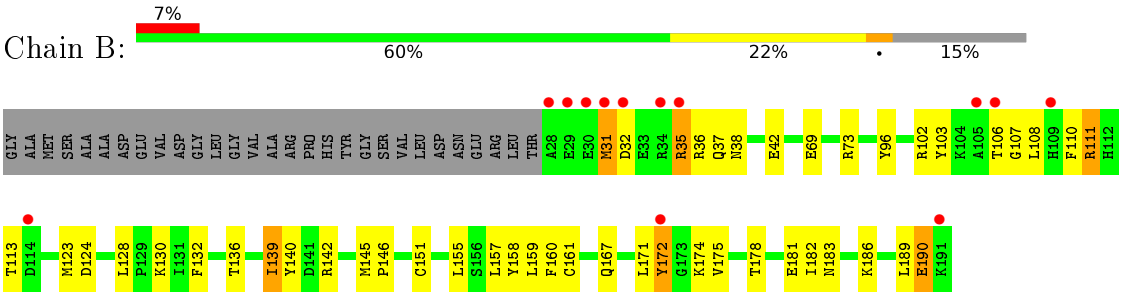
- Molecule 1: Ras GTPase-activating-like protein IQGAP1

Chain A:



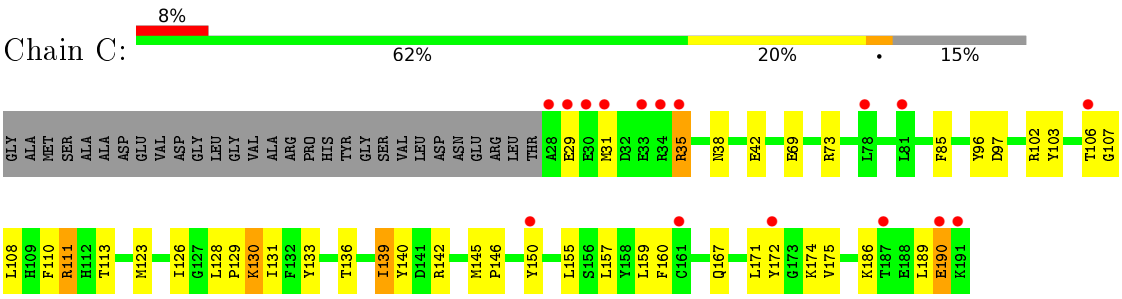
- Molecule 1: Ras GTPase-activating-like protein IQGAP1

Chain B:



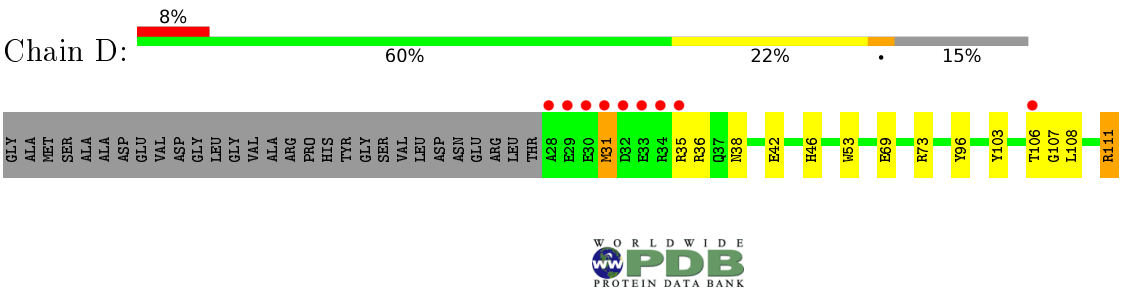
- Molecule 1: Ras GTPase-activating-like protein IQGAP1

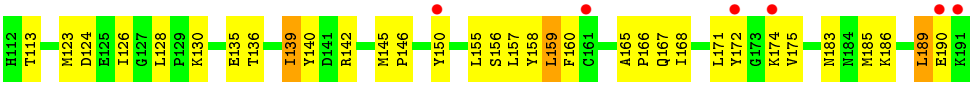
Chain C:



- Molecule 1: Ras GTPase-activating-like protein IQGAP1

Chain D:




H112
T113
M123
D124
E125
I126
G127
L128
P129
K130
E135
T136
I139
Y140
D141
R142
M145
P146
Y150
L155
S156
L157
Y158
L159
F160
C161
A165
P166
Q167
I168
L171
Y172
G173
K174
V175
N183
N184
M185
K186
L189
E190
K191

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.75Å 72.46Å 73.27Å 77.15° 72.07° 86.80°	Depositor
Resolution (Å)	15.00 – 2.36 24.94 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.6 (15.00-2.36) 91.0 (24.94-2.36)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.36Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.262 , 0.286 0.260 , 0.285	Depositor DCC
R_{free} test set	2056 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5436	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 5.87% 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	0.38	0/1389	0.58	0/1874
1	B	0.38	0/1389	0.59	0/1874
1	C	0.38	0/1389	0.57	0/1874
1	D	0.38	0/1389	0.58	0/1874
All	All	0.38	0/5556	0.58	0/7496

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	1359	0	1329	40	0
1	B	1359	0	1329	41	0
1	C	1359	0	1329	38	0
1	D	1359	0	1329	42	0
All	All	5436	0	5316	158	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 15.

All (158) 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:42:GLU:HG2	1:C:172:TYR:HE1	1.24	1.01
1:A:42:GLU:HG2	1:A:172:TYR:HE1	1.34	0.89
1:D:73:ARG:HD3	1:D:142:ARG:HB2	1.56	0.88
1:A:37:GLN:HE21	1:A:182:ILE:HG22	1.40	0.87
1:B:42:GLU:HG2	1:B:172:TYR:HE1	1.40	0.86
1:A:73:ARG:HD3	1:A:142:ARG:HB2	1.58	0.86
1:D:42:GLU:HG2	1:D:172:TYR:HE1	1.41	0.86
1:C:73:ARG:HD3	1:C:142:ARG:HB2	1.58	0.85
1:A:123:MET:HE2	1:A:155:LEU:HD13	1.59	0.82
1:C:42:GLU:HG2	1:C:172:TYR:CE1	2.14	0.82
1:A:96:TYR:CD1	1:A:111:ARG:HG2	2.15	0.80
1:B:73:ARG:HA	1:B:139:ILE:HD12	1.64	0.79
1:C:123:MET:HE2	1:C:155:LEU:HD13	1.63	0.78
1:B:31:MET:HE1	1:B:32:ASP:HA	1.65	0.78
1:B:73:ARG:HD3	1:B:142:ARG:HB2	1.66	0.76
1:A:35:ARG:HA	1:A:35:ARG:HH11	1.51	0.75
1:D:73:ARG:HA	1:D:139:ILE:HD12	1.68	0.75
1:A:35:ARG:HA	1:A:35:ARG:NH1	2.01	0.75
1:A:42:GLU:HG2	1:A:172:TYR:CE1	2.22	0.75
1:C:96:TYR:CD1	1:C:111:ARG:HG2	2.22	0.74
1:B:35:ARG:HH11	1:B:35:ARG:HA	1.52	0.72
1:B:113:THR:HG23	1:B:136:THR:HG21	1.70	0.72
1:C:73:ARG:HA	1:C:139:ILE:HD12	1.71	0.71
1:B:42:GLU:HG2	1:B:172:TYR:CE1	2.25	0.71
1:D:96:TYR:CD1	1:D:111:ARG:HG2	2.26	0.70
1:C:150:TYR:HB3	1:D:150:TYR:OH	1.92	0.70
1:A:73:ARG:HA	1:A:139:ILE:HD12	1.75	0.69
1:B:123:MET:HE2	1:B:155:LEU:HD13	1.75	0.68
1:B:124:ASP:OD2	1:B:130:LYS:HE3	1.93	0.68
1:C:113:THR:HG23	1:C:136:THR:HG21	1.77	0.67
1:C:35:ARG:NH1	1:C:35:ARG:HA	2.10	0.66
1:D:113:THR:HG23	1:D:136:THR:HG21	1.77	0.64
1:D:123:MET:HE1	1:D:128:LEU:HD22	1.80	0.63
1:C:123:MET:HE3	1:C:155:LEU:HD22	1.79	0.63
1:B:158:TYR:O	1:B:161:CYS:HB3	1.99	0.62
1:A:186:LYS:O	1:A:190:GLU:HG3	1.99	0.62
1:B:96:TYR:CD1	1:B:111:ARG:HG2	2.35	0.61
1:A:113:THR:HG23	1:A:136:THR:HG21	1.84	0.60
1:A:139:ILE:HG13	1:A:140:TYR:N	2.17	0.59
1:D:123:MET:HE1	1:D:128:LEU:CD2	2.32	0.59
1:A:85:PHE:HD1	1:A:126:ILE:HG21	1.68	0.59
1:B:123:MET:CE	1:B:155:LEU:HB2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:ILE:HG13	1:D:140:TYR:N	2.18	0.58
1:D:123:MET:HE2	1:D:155:LEU:HD13	1.84	0.58
1:A:106:THR:HG22	1:A:107:GLY:H	1.69	0.58
1:B:123:MET:HE1	1:B:128:LEU:CD2	2.34	0.57
1:D:106:THR:HG22	1:D:107:GLY:H	1.69	0.57
1:D:69:GLU:HB3	1:D:145:MET:HG2	1.86	0.57
1:C:123:MET:HE1	1:C:128:LEU:CD2	2.33	0.57
1:C:139:ILE:HG13	1:C:140:TYR:N	2.19	0.57
1:B:106:THR:HG22	1:B:107:GLY:H	1.70	0.57
1:C:186:LYS:O	1:C:190:GLU:HG3	2.04	0.57
1:B:139:ILE:HG13	1:B:140:TYR:N	2.19	0.56
1:C:106:THR:HG22	1:C:107:GLY:H	1.69	0.56
1:D:36:ARG:HD2	1:D:190:GLU:OE1	2.06	0.55
1:B:69:GLU:HB3	1:B:145:MET:HG2	1.87	0.55
1:B:132:PHE:O	1:B:151:CYS:HB2	2.07	0.54
1:B:186:LYS:O	1:B:190:GLU:HG3	2.08	0.54
1:A:29:GLU:N	1:A:29:GLU:OE2	2.41	0.53
1:C:123:MET:CE	1:C:155:LEU:HD22	2.39	0.53
1:B:35:ARG:CA	1:B:35:ARG:HH11	2.21	0.53
1:D:157:LEU:HD23	1:D:157:LEU:C	2.30	0.52
1:B:123:MET:HE1	1:B:128:LEU:HD22	1.92	0.52
1:B:142:ARG:O	1:B:142:ARG:HG2	2.11	0.51
1:C:142:ARG:O	1:C:142:ARG:HG2	2.11	0.51
1:B:73:ARG:HA	1:B:139:ILE:CD1	2.36	0.50
1:A:97:ASP:CG	1:A:102:ARG:HB3	2.32	0.50
1:D:160:PHE:CE1	1:D:167:GLN:HB2	2.47	0.50
1:B:178:THR:OG1	1:B:181:GLU:HG3	2.12	0.50
1:D:123:MET:CE	1:D:155:LEU:HB2	2.41	0.50
1:A:96:TYR:CE2	1:A:111:ARG:HB3	2.46	0.49
1:D:123:MET:CE	1:D:155:LEU:HD22	2.42	0.49
1:A:123:MET:HE1	1:A:128:LEU:CD2	2.43	0.49
1:A:142:ARG:HG2	1:A:142:ARG:O	2.12	0.49
1:C:85:PHE:HD1	1:C:126:ILE:HG21	1.78	0.49
1:C:160:PHE:CE1	1:C:167:GLN:HB2	2.48	0.49
1:D:142:ARG:O	1:D:142:ARG:HG2	2.12	0.49
1:A:85:PHE:CE2	1:A:155:LEU:HD21	2.47	0.48
1:B:123:MET:HE3	1:B:155:LEU:HD22	1.95	0.48
1:C:123:MET:CE	1:C:155:LEU:HB2	2.43	0.48
1:D:186:LYS:O	1:D:190:GLU:HG3	2.13	0.48
1:D:36:ARG:HD2	1:D:190:GLU:CD	2.34	0.48
1:B:171:LEU:HB3	1:B:175:VAL:HG23	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLN:HE21	1:B:182:ILE:HG22	1.79	0.48
1:D:124:ASP:OD2	1:D:130:LYS:HE3	2.13	0.48
1:D:171:LEU:HB3	1:D:175:VAL:HG23	1.95	0.48
1:A:53:TRP:HB2	1:A:168:ILE:HG13	1.95	0.48
1:C:128:LEU:HD12	1:C:129:PRO:HD2	1.96	0.48
1:A:123:MET:CE	1:A:155:LEU:HB2	2.43	0.48
1:A:130:LYS:HD2	1:A:130:LYS:H	1.78	0.47
1:C:96:TYR:CE2	1:C:111:ARG:HB3	2.49	0.47
1:B:157:LEU:C	1:B:157:LEU:HD23	2.35	0.47
1:D:42:GLU:HG2	1:D:172:TYR:CE1	2.33	0.47
1:A:171:LEU:HB3	1:A:175:VAL:HG23	1.96	0.47
1:B:96:TYR:CE2	1:B:111:ARG:HB3	2.50	0.47
1:B:123:MET:CE	1:B:128:LEU:HD22	2.45	0.47
1:B:103:TYR:O	1:B:106:THR:O	2.33	0.47
1:B:35:ARG:HB2	1:B:35:ARG:NH1	2.30	0.47
1:C:133:TYR:CD1	1:C:133:TYR:N	2.82	0.47
1:C:97:ASP:CG	1:C:102:ARG:HB3	2.36	0.47
1:D:165:ALA:HB1	1:D:166:PRO:HD2	1.98	0.46
1:A:175:VAL:HG12	1:A:176:ASP:N	2.31	0.46
1:D:103:TYR:O	1:D:106:THR:O	2.33	0.46
1:A:85:PHE:CD1	1:A:126:ILE:HG21	2.48	0.46
1:C:69:GLU:HB3	1:C:145:MET:HG2	1.98	0.46
1:C:130:LYS:HB2	1:C:130:LYS:NZ	2.31	0.46
1:C:131:ILE:HG13	1:D:46:HIS:CD2	2.51	0.46
1:A:135:GLU:HG3	1:A:147:ARG:HH12	1.81	0.45
1:A:31:MET:CE	1:A:32:ASP:HB2	2.46	0.45
1:A:110:PHE:O	1:A:113:THR:HB	2.16	0.45
1:A:160:PHE:CE1	1:A:167:GLN:HB2	2.51	0.45
1:A:103:TYR:O	1:A:106:THR:O	2.35	0.45
1:C:29:GLU:N	1:C:29:GLU:OE2	2.50	0.45
1:D:73:ARG:HA	1:D:139:ILE:CD1	2.44	0.44
1:D:126:ILE:HD12	1:D:158:TYR:CE2	2.52	0.44
1:C:96:TYR:CG	1:C:111:ARG:HG2	2.52	0.44
1:B:35:ARG:HB2	1:B:35:ARG:CZ	2.48	0.44
1:C:171:LEU:HB3	1:C:175:VAL:HG23	1.98	0.44
1:B:110:PHE:O	1:B:113:THR:HB	2.17	0.44
1:A:155:LEU:HG	1:A:159:LEU:HD22	2.00	0.44
1:D:123:MET:CE	1:D:128:LEU:HD22	2.46	0.44
1:D:69:GLU:CB	1:D:145:MET:HG2	2.48	0.43
1:B:103:TYR:HE1	1:B:108:LEU:HD22	1.83	0.43
1:C:123:MET:HE1	1:C:128:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HD11	1:A:155:LEU:HD11	2.00	0.43
1:C:103:TYR:HE1	1:C:108:LEU:HD22	1.84	0.43
1:A:96:TYR:CE1	1:A:111:ARG:HG2	2.52	0.43
1:D:123:MET:HE2	1:D:155:LEU:HD22	2.01	0.43
1:A:96:TYR:CG	1:A:111:ARG:HG2	2.52	0.42
1:A:103:TYR:HE1	1:A:108:LEU:HD22	1.84	0.42
1:B:145:MET:N	1:B:146:PRO:CD	2.82	0.42
1:B:160:PHE:CE1	1:B:167:GLN:HB2	2.55	0.42
1:D:142:ARG:O	1:D:142:ARG:CG	2.67	0.42
1:D:53:TRP:HB2	1:D:168:ILE:HG13	2.00	0.42
1:C:157:LEU:HD11	1:D:158:TYR:CD1	2.54	0.42
1:B:36:ARG:HD2	1:B:190:GLU:OE1	2.20	0.41
1:C:123:MET:CE	1:C:128:LEU:CD2	2.96	0.41
1:B:123:MET:CE	1:B:155:LEU:HD22	2.49	0.41
1:C:103:TYR:O	1:C:106:THR:O	2.38	0.41
1:C:145:MET:N	1:C:146:PRO:CD	2.84	0.41
1:D:156:SER:OG	1:D:168:ILE:HB	2.21	0.41
1:A:133:TYR:N	1:A:133:TYR:CD1	2.88	0.41
1:B:142:ARG:O	1:B:142:ARG:CG	2.66	0.41
1:D:96:TYR:CG	1:D:111:ARG:HG2	2.55	0.41
1:C:110:PHE:O	1:C:113:THR:HB	2.21	0.41
1:C:133:TYR:HD1	1:C:133:TYR:N	2.19	0.41
1:C:142:ARG:O	1:C:142:ARG:CG	2.67	0.41
1:D:145:MET:N	1:D:146:PRO:CD	2.83	0.41
1:B:171:LEU:O	1:B:172:TYR:C	2.60	0.41
1:D:103:TYR:HE1	1:D:108:LEU:HD22	1.84	0.41
1:B:36:ARG:HD2	1:B:190:GLU:CD	2.42	0.40
1:D:185:MET:SD	1:D:189:LEU:HD13	2.61	0.40
1:A:79:ALA:O	1:A:90:VAL:HG11	2.21	0.40
1:D:171:LEU:O	1:D:172:TYR:C	2.59	0.40
1:D:31:MET:HE2	1:D:35:ARG:HB2	2.02	0.40
1:A:145:MET:N	1:A:146:PRO:CD	2.85	0.40
1:D:155:LEU:HG	1:D:159:LEU:HD22	2.04	0.40
1:A:142:ARG:CG	1:A:142:ARG:O	2.70	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	162/193 (84%)	157 (97%)	3 (2%)	2 (1%)	16	15
1	B	162/193 (84%)	157 (97%)	3 (2%)	2 (1%)	16	15
1	C	162/193 (84%)	157 (97%)	4 (2%)	1 (1%)	30	34
1	D	162/193 (84%)	157 (97%)	5 (3%)	0	100	100
All	All	648/772 (84%)	628 (97%)	15 (2%)	5 (1%)	24	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	190	GLU
1	A	190	GLU
1	B	172	TYR
1	B	190	GLU
1	A	172	TYR

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	147/168 (88%)	138 (94%)	9 (6%)	23	27
1	B	147/168 (88%)	137 (93%)	10 (7%)	20	22
1	C	147/168 (88%)	138 (94%)	9 (6%)	23	27
1	D	147/168 (88%)	138 (94%)	9 (6%)	23	27
All	All	588/672 (88%)	551 (94%)	37 (6%)	22	25

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	MET
1	A	35	ARG
1	A	38	ASN
1	A	111	ARG
1	A	130	LYS
1	A	139	ILE
1	A	159	LEU
1	A	174	LYS
1	A	189	LEU
1	B	31	MET
1	B	35	ARG
1	B	38	ASN
1	B	102	ARG
1	B	111	ARG
1	B	139	ILE
1	B	159	LEU
1	B	174	LYS
1	B	183	ASN
1	B	189	LEU
1	C	31	MET
1	C	35	ARG
1	C	38	ASN
1	C	111	ARG
1	C	130	LYS
1	C	139	ILE
1	C	159	LEU
1	C	174	LYS
1	C	189	LEU
1	D	31	MET
1	D	38	ASN
1	D	111	ARG
1	D	135	GLU
1	D	139	ILE
1	D	159	LEU
1	D	174	LYS
1	D	183	ASN
1	D	189	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	83	ASN
1	A	118	GLN
1	B	37	GLN
1	B	83	ASN
1	B	118	GLN
1	C	37	GLN
1	C	83	ASN
1	C	118	GLN
1	D	83	ASN

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

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	164/193 (84%)	0.49	15 (9%)	11	18	12, 26, 76, 122	0
1	B	164/193 (84%)	0.51	13 (7%)	15	24	11, 26, 72, 120	0
1	C	164/193 (84%)	0.55	16 (9%)	10	16	13, 29, 74, 106	0
1	D	164/193 (84%)	0.56	15 (9%)	11	18	13, 25, 81, 122	0
All	All	656/772 (84%)	0.53	59 (8%)	12	18	11, 26, 80, 122	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	31	MET	9.1
1	A	31	MET	7.5
1	B	31	MET	6.4
1	A	28	ALA	6.2
1	D	28	ALA	5.8
1	C	28	ALA	5.1
1	B	28	ALA	4.9
1	C	31	MET	4.8
1	A	29	GLU	4.6
1	D	191	LYS	4.4
1	B	30	GLU	4.3
1	A	172	TYR	4.2
1	B	191	LYS	3.9
1	C	150	TYR	3.8
1	D	172	TYR	3.8
1	D	150	TYR	3.7
1	A	191	LYS	3.7
1	A	35	ARG	3.6
1	C	161	CYS	3.6
1	B	106	THR	3.6
1	A	190	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	29	GLU	3.5
1	A	106	THR	3.5
1	C	35	ARG	3.4
1	D	35	ARG	3.4
1	A	187	THR	3.4
1	B	29	GLU	3.4
1	B	172	TYR	3.3
1	D	34	ARG	3.3
1	D	32	ASP	3.2
1	B	109	HIS	3.2
1	C	191	LYS	3.1
1	D	106	THR	3.0
1	A	34	ARG	3.0
1	B	105	ALA	2.9
1	B	35	ARG	2.9
1	C	29	GLU	2.9
1	D	30	GLU	2.8
1	D	33	GLU	2.7
1	D	161	CYS	2.7
1	C	34	ARG	2.6
1	C	81	LEU	2.6
1	C	30	GLU	2.5
1	C	172	TYR	2.5
1	C	106	THR	2.5
1	B	34	ARG	2.5
1	D	190	GLU	2.4
1	B	32	ASP	2.4
1	B	114	ASP	2.3
1	C	190	GLU	2.3
1	A	150	TYR	2.3
1	C	78	LEU	2.3
1	A	186	LYS	2.2
1	C	187	THR	2.2
1	A	33	GLU	2.1
1	C	33	GLU	2.1
1	A	32	ASP	2.1
1	A	30	GLU	2.1
1	D	174	LYS	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

There are no carbohydrates 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.