Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:21 AM GMT

PDB ID	:	3EAP
Title	:	Crystal structure of the RhoGAP domain of ARHGAP11A
Authors	:	Shen, Y.; Shen, L.; Tong, Y.; Tempel, W.; MacKenzie, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Bochkarev, A.; Park, H.; Structural Genomics Consortium; Structural Genomics Consortium (SGC)
Deposited on	:	2008-08-26
Resolution	:	2.30 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:

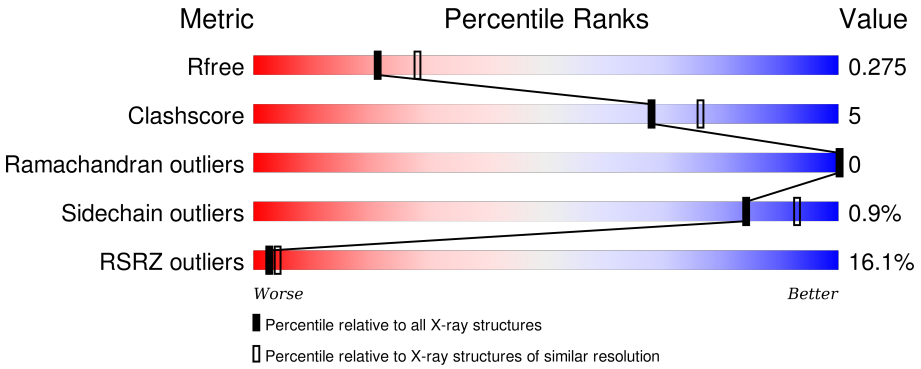
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	271	17%, 75%, 8%, 17%
1	B	271	11%, 71%, 7%, 21%
1	C	271	11%, 70%, 10%, 20%
1	D	271	12%, 66%, 12%, 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNX	A	254	-	-	-	X
2	UNX	B	254	-	-	-	X
2	UNX	B	255	-	-	-	X
2	UNX	B	256	-	-	-	X
2	UNX	B	257	-	-	-	X
2	UNX	C	254	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6525 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 Rho GTPase-activating protein 11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1665	1079	281	299	6			
1	B	213	Total	C	N	O	S	0	0	0
			1606	1041	275	286	4			
1	C	216	Total	C	N	O	S	0	0	0
			1613	1049	273	285	6			
1	D	212	Total	C	N	O	S	0	0	0
			1577	1026	266	280	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	EXPRESSION TAG	UNP Q6P4F7
A	-16	HIS	-	EXPRESSION TAG	UNP Q6P4F7
A	-15	HIS	-	EXPRESSION TAG	UNP Q6P4F7
A	-14	HIS	-	EXPRESSION TAG	UNP Q6P4F7
A	-13	HIS	-	EXPRESSION TAG	UNP Q6P4F7
A	-12	HIS	-	EXPRESSION TAG	UNP Q6P4F7
A	-11	HIS	-	EXPRESSION TAG	UNP Q6P4F7
A	-10	SER	-	EXPRESSION TAG	UNP Q6P4F7
A	-9	SER	-	EXPRESSION TAG	UNP Q6P4F7
A	-8	GLY	-	EXPRESSION TAG	UNP Q6P4F7
A	-7	ARG	-	EXPRESSION TAG	UNP Q6P4F7
A	-6	GLU	-	EXPRESSION TAG	UNP Q6P4F7
A	-5	ASN	-	EXPRESSION TAG	UNP Q6P4F7
A	-4	LEU	-	EXPRESSION TAG	UNP Q6P4F7
A	-3	TYR	-	EXPRESSION TAG	UNP Q6P4F7
A	-2	PHE	-	EXPRESSION TAG	UNP Q6P4F7
A	-1	GLN	-	EXPRESSION TAG	UNP Q6P4F7
A	0	GLY	-	EXPRESSION TAG	UNP Q6P4F7
B	-17	MET	-	EXPRESSION TAG	UNP Q6P4F7
B	-16	HIS	-	EXPRESSION TAG	UNP Q6P4F7
B	-15	HIS	-	EXPRESSION TAG	UNP Q6P4F7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q6P4F7
B	-13	HIS	-	EXPRESSION TAG	UNP Q6P4F7
B	-12	HIS	-	EXPRESSION TAG	UNP Q6P4F7
B	-11	HIS	-	EXPRESSION TAG	UNP Q6P4F7
B	-10	SER	-	EXPRESSION TAG	UNP Q6P4F7
B	-9	SER	-	EXPRESSION TAG	UNP Q6P4F7
B	-8	GLY	-	EXPRESSION TAG	UNP Q6P4F7
B	-7	ARG	-	EXPRESSION TAG	UNP Q6P4F7
B	-6	GLU	-	EXPRESSION TAG	UNP Q6P4F7
B	-5	ASN	-	EXPRESSION TAG	UNP Q6P4F7
B	-4	LEU	-	EXPRESSION TAG	UNP Q6P4F7
B	-3	TYR	-	EXPRESSION TAG	UNP Q6P4F7
B	-2	PHE	-	EXPRESSION TAG	UNP Q6P4F7
B	-1	GLN	-	EXPRESSION TAG	UNP Q6P4F7
B	0	GLY	-	EXPRESSION TAG	UNP Q6P4F7
C	-17	MET	-	EXPRESSION TAG	UNP Q6P4F7
C	-16	HIS	-	EXPRESSION TAG	UNP Q6P4F7
C	-15	HIS	-	EXPRESSION TAG	UNP Q6P4F7
C	-14	HIS	-	EXPRESSION TAG	UNP Q6P4F7
C	-13	HIS	-	EXPRESSION TAG	UNP Q6P4F7
C	-12	HIS	-	EXPRESSION TAG	UNP Q6P4F7
C	-11	HIS	-	EXPRESSION TAG	UNP Q6P4F7
C	-10	SER	-	EXPRESSION TAG	UNP Q6P4F7
C	-9	SER	-	EXPRESSION TAG	UNP Q6P4F7
C	-8	GLY	-	EXPRESSION TAG	UNP Q6P4F7
C	-7	ARG	-	EXPRESSION TAG	UNP Q6P4F7
C	-6	GLU	-	EXPRESSION TAG	UNP Q6P4F7
C	-5	ASN	-	EXPRESSION TAG	UNP Q6P4F7
C	-4	LEU	-	EXPRESSION TAG	UNP Q6P4F7
C	-3	TYR	-	EXPRESSION TAG	UNP Q6P4F7
C	-2	PHE	-	EXPRESSION TAG	UNP Q6P4F7
C	-1	GLN	-	EXPRESSION TAG	UNP Q6P4F7
C	0	GLY	-	EXPRESSION TAG	UNP Q6P4F7
D	-17	MET	-	EXPRESSION TAG	UNP Q6P4F7
D	-16	HIS	-	EXPRESSION TAG	UNP Q6P4F7
D	-15	HIS	-	EXPRESSION TAG	UNP Q6P4F7
D	-14	HIS	-	EXPRESSION TAG	UNP Q6P4F7
D	-13	HIS	-	EXPRESSION TAG	UNP Q6P4F7
D	-12	HIS	-	EXPRESSION TAG	UNP Q6P4F7
D	-11	HIS	-	EXPRESSION TAG	UNP Q6P4F7
D	-10	SER	-	EXPRESSION TAG	UNP Q6P4F7
D	-9	SER	-	EXPRESSION TAG	UNP Q6P4F7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	GLY	-	EXPRESSION TAG	UNP Q6P4F7
D	-7	ARG	-	EXPRESSION TAG	UNP Q6P4F7
D	-6	GLU	-	EXPRESSION TAG	UNP Q6P4F7
D	-5	ASN	-	EXPRESSION TAG	UNP Q6P4F7
D	-4	LEU	-	EXPRESSION TAG	UNP Q6P4F7
D	-3	TYR	-	EXPRESSION TAG	UNP Q6P4F7
D	-2	PHE	-	EXPRESSION TAG	UNP Q6P4F7
D	-1	GLN	-	EXPRESSION TAG	UNP Q6P4F7
D	0	GLY	-	EXPRESSION TAG	UNP Q6P4F7

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	4	Total X 4 4	0	0
2	A	1	Total X 1 1	0	0
2	C	1	Total X 1 1	0	0

- Molecule 3 is water.

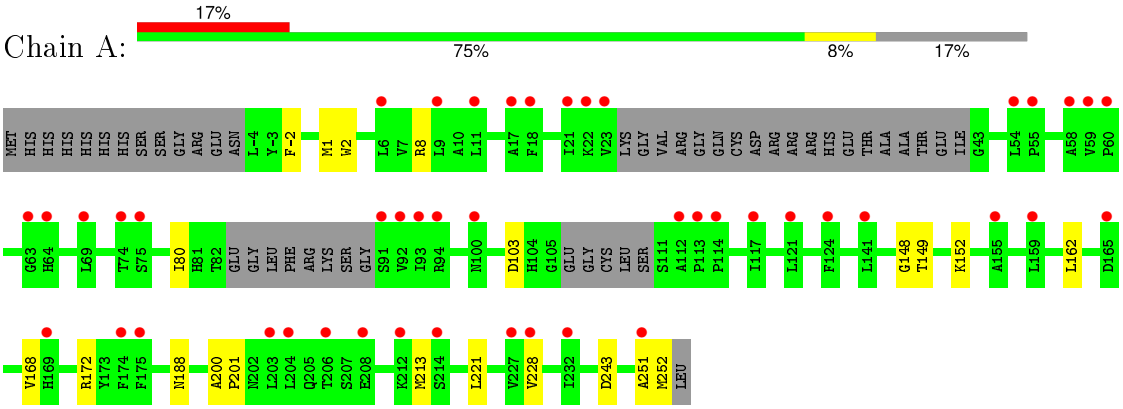
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	19	Total O 19 19	0	0
3	C	15	Total O 15 15	0	0
3	D	14	Total O 14 14	0	0

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.

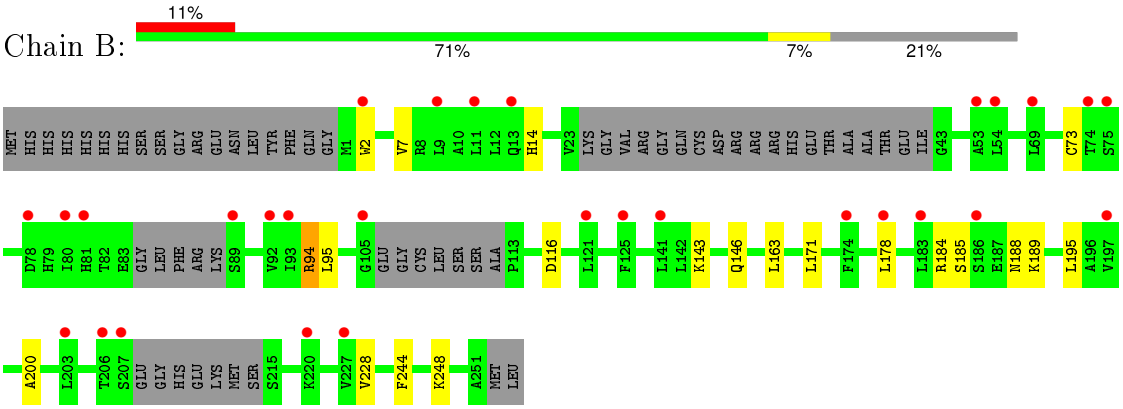
- Molecule 1: Rho GTPase-activating protein 11A

Chain A:



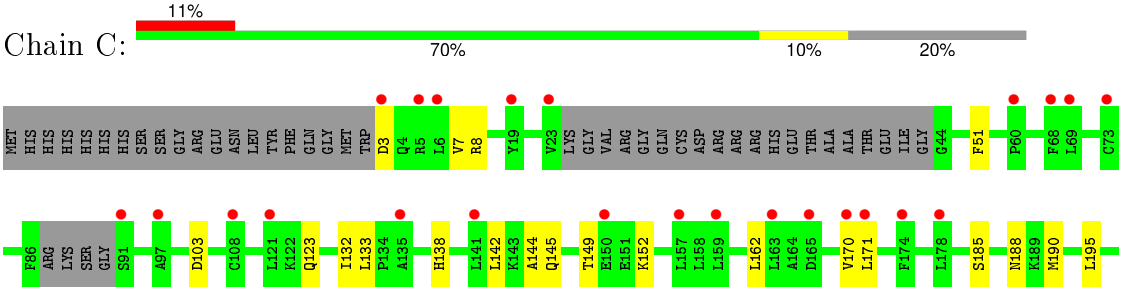
- Molecule 1: Rho GTPase-activating protein 11A

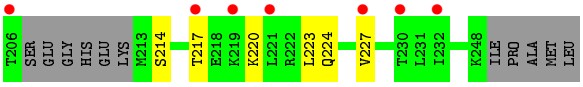
Chain B:



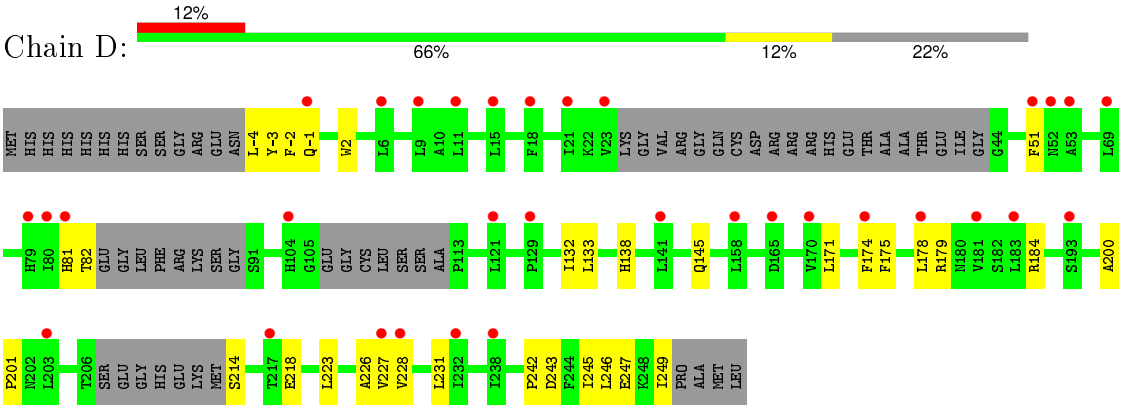
- Molecule 1: Rho GTPase-activating protein 11A

Chain C:





- Molecule 1: Rho GTPase-activating protein 11A



4 Data and refinement statistics (i)

Property	Value
Space group	P 1 21 1
Cell constants a, b, c, α, β, γ	46.07Å 106.15Å 107.33Å 90.00° 97.16° 90.00°
Resolution (Å)	20.00 – 2.30 19.94 – 2.30
% Data completeness (in resolution range)	98.1 (20.00-2.30) 98.1 (19.94-2.30)
R_{merge}	0.06
R_{sym}	(Not available)
$< I/\sigma(I) >$ [1]	2.24 (at 2.30Å)
Refinement program	REFMAC 5.4.0069, resolve, tlsmd, FFAS03/SCWRL, coot, molprobity
R, R_{free}	0.227 , 0.277 0.232 , 0.275
R_{free} test set	2233 reflections (5.27%)
Wilson B-factor (Å^2)	44.5
Anisotropy	0.028
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 88.5
Estimated twinning fraction	No twinning to report.
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$
Outliers	0 of 44568 reflections
F_o,F_c correlation	0.93
Total number of atoms	6525
Average B, all atoms (Å^2)	60.0

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNX

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	0.70	0/1701	0.69	0/2321
1	B	0.72	1/1639 (0.1%)	0.69	0/2230
1	C	0.80	0/1645	0.69	0/2235
1	D	0.71	0/1610	0.72	1/2192 (0.0%)
All	All	0.73	1/6595 (0.0%)	0.70	1/8978 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	CYS	CB-SG	-5.37	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	179	ARG	NE-CZ-NH1	-5.43	117.58	120.30

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	1665	0	1583	14	0
1	B	1606	0	1567	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1613	0	1569	14	0
1	D	1577	0	1511	23	0
2	A	1	0	0	0	0
2	B	4	0	0	0	0
2	C	1	0	0	0	0
3	A	10	0	0	0	0
3	B	19	0	0	1	0
3	C	15	0	0	0	0
3	D	14	0	0	0	0
All	All	6525	0	6230	60	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 5.

All (60) 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:ARG:CG	1:B:94:ARG:HH21	1.64	1.10
1:B:94:ARG:NH2	1:B:94:ARG:HG2	1.46	1.01
1:A:1:MET:O	1:A:251:ALA:HB1	1.88	0.73
1:C:223:LEU:O	1:C:227:VAL:HG23	2.01	0.61
1:C:3:ASP:O	1:C:7:VAL:HG23	2.04	0.57
1:C:190:MET:HG3	1:C:195:LEU:HG	1.87	0.56
1:B:94:ARG:HG2	1:B:94:ARG:HH21	0.68	0.56
1:A:200:ALA:HB3	1:A:201:PRO:HD3	1.88	0.55
1:B:185:SER:HA	1:B:188:ASN:OD1	2.06	0.55
1:D:223:LEU:O	1:D:227:VAL:HG23	2.06	0.55
1:C:142:LEU:HD21	1:C:224:GLN:HG3	1.88	0.54
1:B:94:ARG:NH2	1:B:94:ARG:CG	2.35	0.54
1:B:244:PHE:O	1:B:248:LYS:HD3	2.09	0.52
1:A:243:ASP:OD1	1:D:-3:TYR:CD2	2.62	0.52
1:C:145:GLN:HB2	1:C:223:LEU:HD22	1.91	0.52
1:B:143:LYS:O	1:B:146:GLN:HG2	2.10	0.52
1:B:163:LEU:HD13	1:B:171:LEU:HD12	1.93	0.51
1:D:-4:LEU:O	1:D:-1:GLN:HG2	2.10	0.51
1:D:171:LEU:HD22	1:D:175:PHE:HE2	1.76	0.50
1:D:145:GLN:HG2	1:D:226:ALA:HB3	1.94	0.50
1:B:14:HIS:HE1	3:B:274:HOH:O	1.94	0.49
1:A:149:THR:HG21	1:D:184:ARG:NH1	2.27	0.49
1:A:-2:PHE:HB2	1:D:-2:PHE:HB2	1.95	0.49
1:D:133:LEU:O	1:D:138:HIS:NE2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:MET:SD	1:A:221:LEU:HD12	2.54	0.48
1:D:81:HIS:O	1:D:82:THR:C	2.51	0.47
1:C:214:SER:OG	1:C:217:THR:HG23	2.14	0.47
1:A:243:ASP:OD1	1:D:-3:TYR:CE2	2.67	0.47
1:C:132:ILE:HD13	1:C:171:LEU:HD21	1.97	0.47
1:D:242:PRO:HD2	1:D:245:ILE:HD13	1.98	0.46
1:B:2:TRP:CD1	1:B:7:VAL:HG21	2.51	0.46
1:D:171:LEU:HD22	1:D:175:PHE:CE2	2.50	0.45
1:A:200:ALA:HA	1:A:228:VAL:HG21	1.98	0.45
1:C:185:SER:HA	1:C:188:ASN:OD1	2.16	0.45
1:A:251:ALA:O	1:A:252:MET:C	2.55	0.45
1:D:171:LEU:HA	1:D:171:LEU:HD23	1.91	0.44
1:D:145:GLN:CG	1:D:226:ALA:HB3	2.48	0.44
1:A:148:GLY:O	1:A:152:LYS:HG3	2.17	0.44
1:A:168:VAL:O	1:A:172:ARG:HG3	2.17	0.44
1:C:144:ALA:O	1:C:152:LYS:HB2	2.18	0.44
1:B:178:LEU:HD22	1:B:195:LEU:HD13	1.99	0.44
1:B:184:ARG:HH11	1:C:149:THR:CB	2.31	0.43
1:D:243:ASP:O	1:D:247:GLU:HG3	2.19	0.43
1:B:95:LEU:HD13	1:B:116:ASP:HA	2.01	0.43
1:B:200:ALA:HA	1:B:228:VAL:HG21	2.01	0.42
1:D:214:SER:O	1:D:218:GLU:N	2.45	0.42
1:C:123:GLN:HE21	1:C:123:GLN:HB2	1.69	0.42
1:D:145:GLN:HB3	1:D:223:LEU:HD22	2.01	0.42
1:C:133:LEU:O	1:C:138:HIS:NE2	2.40	0.41
1:D:246:LEU:HA	1:D:249:ILE:HD12	2.02	0.41
1:D:174:PHE:CE2	1:D:178:LEU:HD11	2.56	0.41
1:C:51:PHE:CE1	1:C:170:VAL:HG21	2.55	0.41
1:D:227:VAL:O	1:D:231:LEU:HG	2.21	0.41
1:A:2:TRP:CE2	1:A:251:ALA:HB2	2.55	0.41
1:A:80:ILE:O	1:A:188:ASN:HB3	2.20	0.41
1:D:200:ALA:HA	1:D:228:VAL:HG21	2.02	0.41
1:C:8:ARG:NH1	1:C:162:LEU:HD22	2.36	0.41
1:A:8:ARG:HD3	1:A:162:LEU:CD2	2.51	0.41
1:D:51:PHE:HZ	1:D:132:ILE:HD12	1.86	0.40
1:D:200:ALA:HB3	1:D:201:PRO:HD3	2.03	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	A	217/271 (80%)	211 (97%)	6 (3%)	0	100	100
1	B	203/271 (75%)	201 (99%)	2 (1%)	0	100	100
1	C	208/271 (77%)	204 (98%)	4 (2%)	0	100	100
1	D	202/271 (74%)	195 (96%)	7 (4%)	0	100	100
All	All	830/1084 (77%)	811 (98%)	19 (2%)	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	A	164/233 (70%)	163 (99%)	1 (1%)	90	96
1	B	163/233 (70%)	161 (99%)	2 (1%)	78	89
1	C	160/233 (69%)	158 (99%)	2 (1%)	76	87
1	D	156/233 (67%)	155 (99%)	1 (1%)	90	96
All	All	643/932 (69%)	637 (99%)	6 (1%)	84	93

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASP
1	B	94	ARG

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Mol	Chain	Res	Type
1	B	189	LYS
1	C	103	ASP
1	C	220	LYS
1	D	2	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	202	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

Of 6 ligands modelled in this entry, 6 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	225/271 (83%)	1.13	46 (20%)	1 2	47, 60, 70, 77	0
1	B	213/271 (78%)	0.86	29 (13%)	4 6	51, 60, 68, 71	0
1	C	216/271 (79%)	0.94	31 (14%)	3 5	52, 60, 70, 77	0
1	D	212/271 (78%)	0.94	33 (15%)	3 4	53, 60, 70, 79	0
All	All	866/1084 (79%)	0.97	139 (16%)	3 4	47, 60, 70, 79	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	23	VAL	5.7
1	A	60	PRO	5.6
1	D	104	HIS	5.6
1	B	53	ALA	5.5
1	B	206	THR	5.4
1	D	121	LEU	5.2
1	D	53	ALA	4.8
1	A	203	LEU	4.6
1	C	219	LYS	4.5
1	D	193	SER	4.5
1	A	6	LEU	4.4
1	A	59	VAL	4.3
1	D	81	HIS	4.3
1	B	203	LEU	4.2
1	D	6	LEU	4.1
1	B	121	LEU	4.1
1	C	150	GLU	4.0
1	A	92	VAL	4.0
1	A	113	PRO	3.9
1	D	80	ILE	3.9
1	A	227	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	89	SER	3.8
1	C	121	LEU	3.8
1	B	207	SER	3.7
1	B	75	SER	3.7
1	D	174	PHE	3.7
1	D	69	LEU	3.6
1	A	112	ALA	3.6
1	A	124	PHE	3.6
1	A	69	LEU	3.5
1	D	227	VAL	3.4
1	A	121	LEU	3.4
1	A	75	SER	3.4
1	A	64	HIS	3.4
1	D	9	LEU	3.3
1	A	212	LYS	3.2
1	D	217	THR	3.2
1	B	125	PHE	3.1
1	C	6	LEU	3.1
1	C	69	LEU	3.1
1	C	60	PRO	3.0
1	B	69	LEU	3.0
1	C	178	LEU	3.0
1	D	158	LEU	3.0
1	C	170	VAL	3.0
1	C	174	PHE	3.0
1	B	220	LYS	3.0
1	A	175	PHE	3.0
1	D	-1	GLN	2.9
1	A	9	LEU	2.9
1	C	171	LEU	2.9
1	C	135	ALA	2.9
1	B	54	LEU	2.9
1	A	63	GLY	2.9
1	D	232	ILE	2.8
1	C	108	CYS	2.8
1	D	165	ASP	2.7
1	B	186	SER	2.7
1	C	221	LEU	2.7
1	D	178	LEU	2.7
1	A	18	PHE	2.7
1	D	23	VAL	2.7
1	D	11	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	2	TRP	2.6
1	C	232	ILE	2.6
1	A	169	HIS	2.6
1	C	159	LEU	2.6
1	B	9	LEU	2.6
1	B	93	ILE	2.6
1	C	19	TYR	2.6
1	A	58	ALA	2.6
1	C	73	CYS	2.6
1	A	22	LYS	2.6
1	A	165	ASP	2.6
1	B	78	ASP	2.6
1	C	5	ARG	2.6
1	D	203	LEU	2.6
1	A	93	ILE	2.6
1	A	74	THR	2.5
1	D	183	LEU	2.5
1	A	208	GLU	2.5
1	C	3	ASP	2.5
1	A	91	SER	2.5
1	C	91	SER	2.5
1	A	55	PRO	2.5
1	A	174	PHE	2.5
1	A	141	LEU	2.5
1	B	141	LEU	2.5
1	C	157	LEU	2.5
1	B	92	VAL	2.4
1	B	81	HIS	2.4
1	C	206	THR	2.4
1	A	214	SER	2.4
1	A	228	VAL	2.4
1	D	141	LEU	2.4
1	A	114	PRO	2.4
1	A	21	ILE	2.3
1	A	232	ILE	2.3
1	D	228	VAL	2.3
1	A	206	THR	2.3
1	B	174	PHE	2.3
1	B	11	LEU	2.3
1	A	11	LEU	2.3
1	A	204	LEU	2.3
1	D	129	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	217	THR	2.2
1	C	97	ALA	2.2
1	D	21	ILE	2.2
1	D	52	ASN	2.2
1	B	13	GLN	2.2
1	A	117	ILE	2.2
1	D	181	VAL	2.2
1	A	159	LEU	2.2
1	A	251	ALA	2.2
1	B	178	LEU	2.2
1	B	74	THR	2.2
1	C	68	PHE	2.1
1	C	230	THR	2.1
1	A	23	VAL	2.1
1	D	18	PHE	2.1
1	B	105	GLY	2.1
1	B	227	VAL	2.1
1	C	227	VAL	2.1
1	C	163	LEU	2.1
1	B	197	VAL	2.1
1	D	51	PHE	2.1
1	A	54	LEU	2.1
1	A	100	ASN	2.1
1	B	183	LEU	2.1
1	D	15	LEU	2.1
1	C	165	ASP	2.1
1	B	80	ILE	2.1
1	C	141	LEU	2.0
1	A	17	ALA	2.0
1	A	155	ALA	2.0
1	D	170	VAL	2.0
1	D	79	HIS	2.0
1	A	94	ARG	2.0
1	D	238	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	UNX	B	255	1/1	-0.02	2.40	90.49	2,2,2,2	1
2	UNX	B	254	1/1	-0.44	5.71	85.84	17,17,17,17	1
2	UNX	B	256	1/1	0.37	1.80	67.94	2,2,2,2	1
2	UNX	A	254	1/1	-0.27	2.94	37.37	2,2,2,2	1
2	UNX	C	254	1/1	0.23	1.38	30.95	2,2,2,2	1
2	UNX	B	257	1/1	0.13	1.34	22.44	2,2,2,2	1

6.5 Other polymers (i)

There are no such residues in this entry.