Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 01:31 am BST

PDB ID	:	2X3V
Title	:	Structure of The F-BAR Domain of Mouse Syndapin I
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Deposited on	:	2010-01-27
Resolution	:	2.45 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	:	2.11
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)	:	2.11

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 2.45 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.
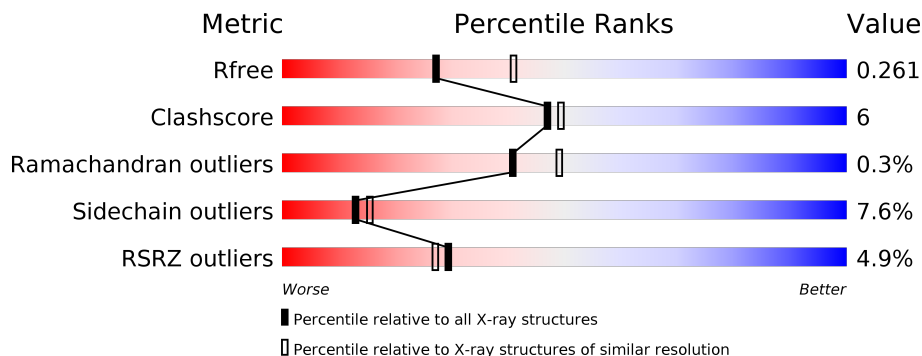
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 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	337	4% / 70% / 14% · 14%
1	B	337	4% / 70% / 15% · 13%
1	C	337	5% / 73% / 12% · 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7419 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 PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total 2418	C 1514	N 430	O 457	S 17	0	0	0
1	B	292	Total 2425	C 1518	N 431	O 459	S 17	0	0	0
1	C	291	Total 2418	C 1514	N 430	O 457	S 17	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total 61	O 61	0	0
2	B	72	Total 72	O 72	0	0
2	C	25	Total 25	O 25	0	0

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: PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1
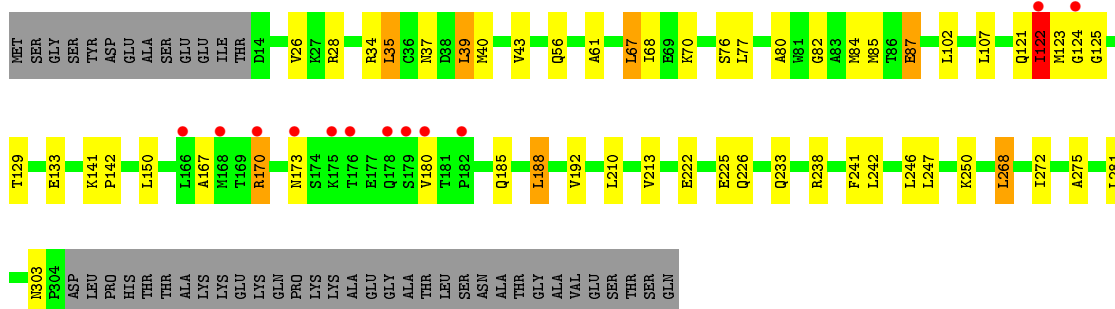
● Molecule 1: PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1
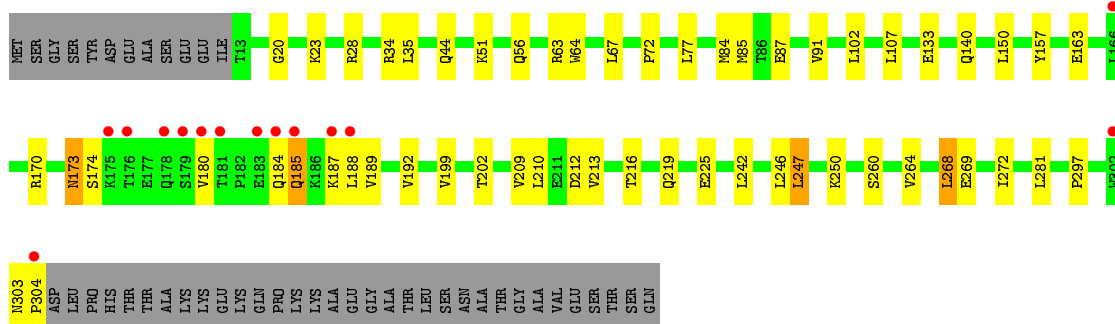
● Molecule 1: PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1
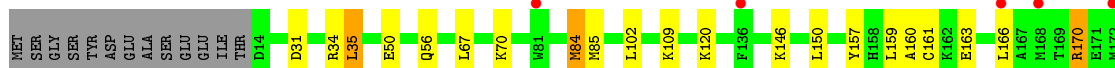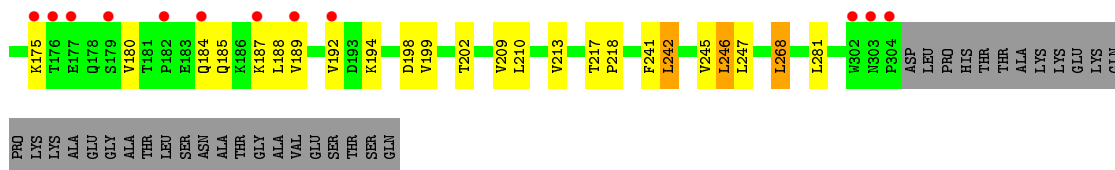
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	85.06Å 153.49Å 213.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.70 – 2.45 76.75 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (76.70-2.45) 95.7 (76.75-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.212 , 0.260 0.217 , 0.261	Depositor DCC
R_{free} test set	2795 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.019 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.032 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7419	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.37	0/2466	0.53	0/3305
1	B	0.39	0/2473	0.52	0/3315
1	C	0.36	0/2466	0.48	0/3305
All	All	0.37	0/7405	0.51	0/9925

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 (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	2418	0	2377	45	0
1	B	2425	0	2384	36	0
1	C	2418	0	2377	21	0
2	A	61	0	0	1	0
2	B	72	0	0	2	0
2	C	25	0	0	1	1
All	All	7419	0	7138	89	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 6.

All (89) 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:A:247:LEU:HD22	1:B:272:ILE:HG21	1.59	0.83
1:A:272:ILE:HG21	1:B:247:LEU:HD13	1.63	0.81
1:B:150:LEU:HD21	1:B:210:LEU:HD13	1.66	0.75
1:A:170:ARG:HG3	1:A:188:LEU:HD11	1.74	0.68
1:C:109:LYS:HD3	1:C:245:VAL:HG22	1.77	0.67
1:C:150:LEU:HD21	1:C:210:LEU:HD13	1.80	0.64
1:A:272:ILE:CG2	1:B:247:LEU:HD13	2.28	0.64
1:A:82:GLY:HA2	1:A:85:MET:CE	2.33	0.58
1:A:247:LEU:CD2	1:B:272:ILE:HG21	2.32	0.57
1:A:61:ALA:HA	1:A:85:MET:HG3	1.85	0.56
1:C:241:PHE:CE1	1:C:245:VAL:HG21	2.41	0.56
1:A:82:GLY:HA2	1:A:85:MET:HE2	1.87	0.56
1:A:123:MET:HE2	1:A:124:GLY:O	2.07	0.55
1:B:189:VAL:O	1:B:192:VAL:HG22	2.07	0.55
1:B:173:ASN:HD22	1:B:174:SER:N	2.05	0.54
1:A:247:LEU:HD22	1:B:272:ILE:CG2	2.34	0.54
1:A:122:ILE:CG1	1:A:123:MET:HB3	2.37	0.54
1:C:159:LEU:HD12	1:C:160:ALA:N	2.22	0.54
1:A:68:ILE:CD1	1:A:85:MET:HE1	2.38	0.54
1:A:68:ILE:HD12	1:A:85:MET:CE	2.38	0.53
1:A:77:LEU:HD12	1:B:242:LEU:CD1	2.40	0.52
1:A:247:LEU:CD2	1:B:272:ILE:CG2	2.87	0.52
1:B:56:GLN:NE2	2:B:2025:HOH:O	2.42	0.52
1:A:35:LEU:HD23	1:A:238:ARG:NH1	2.23	0.52
1:A:222:GLU:HG2	1:A:226:GLN:HE21	1.74	0.52
1:C:180:VAL:HG13	1:C:184:GLN:HB3	1.92	0.52
1:C:242:LEU:HD22	1:C:246:LEU:HD22	1.91	0.52
1:A:122:ILE:CB	1:A:123:MET:HB3	2.40	0.52
1:B:20:GLY:H	1:B:140:GLN:HE22	1.58	0.51
1:B:170:ARG:HG2	1:B:188:LEU:HD11	1.93	0.51
1:C:31:ASP:O	1:C:35:LEU:HD22	2.10	0.51
1:C:157:TYR:HA	1:C:202:THR:CG2	2.41	0.51
1:A:180:VAL:HG12	1:A:185:GLN:NE2	2.26	0.51
1:C:170:ARG:HD2	1:C:188:LEU:HD23	1.93	0.51
1:A:84:MET:O	1:A:87:GLU:HG3	2.11	0.51
1:A:26:VAL:HG12	1:A:129:THR:HG23	1.93	0.50
1:A:238:ARG:O	1:A:242:LEU:HD23	2.12	0.49
1:C:209:VAL:O	1:C:213:VAL:HG23	2.13	0.49
1:C:84:MET:HE2	1:C:268:LEU:HD11	1.94	0.49
1:A:122:ILE:HB	1:A:123:MET:HB3	1.94	0.48
1:A:43:VAL:CG2	1:A:107:LEU:HD23	2.43	0.48
1:A:37:ASN:HA	1:A:40:MET:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLN:NE2	2:A:2013:HOH:O	2.45	0.48
1:A:67:LEU:HD12	1:A:70:LYS:NZ	2.29	0.48
1:A:35:LEU:HD11	1:B:72:PRO:HD2	1.95	0.47
1:B:180:VAL:HG13	1:B:185:GLN:NE2	2.30	0.47
1:A:122:ILE:HG13	1:A:123:MET:HB3	1.97	0.47
1:B:84:MET:O	1:B:87:GLU:HG3	2.15	0.46
1:B:242:LEU:HD22	1:B:246:LEU:HD13	1.98	0.46
1:B:268:LEU:HD22	1:B:272:ILE:HD11	1.97	0.46
1:A:26:VAL:HG11	1:A:133:GLU:HG2	1.98	0.45
1:C:84:MET:CE	1:C:268:LEU:HD11	2.46	0.45
1:C:56:GLN:NE2	2:C:2008:HOH:O	2.47	0.45
1:C:189:VAL:O	1:C:192:VAL:HG22	2.16	0.45
1:A:68:ILE:HD12	1:A:85:MET:HE1	1.98	0.45
1:A:141:LYS:HB3	1:A:142:PRO:HD3	1.99	0.44
1:B:268:LEU:HD22	1:B:272:ILE:CD1	2.47	0.44
1:C:241:PHE:O	1:C:245:VAL:HG23	2.17	0.44
1:A:76:SER:HB2	1:A:275:ALA:HA	1.99	0.44
1:B:260:SER:O	1:B:264:VAL:HG23	2.18	0.44
1:A:167:ALA:HB1	1:A:192:VAL:HG12	2.00	0.43
1:A:268:LEU:HD13	1:B:250:LYS:CG	2.48	0.43
1:B:51:LYS:NZ	2:B:2023:HOH:O	2.51	0.43
1:B:44:GLN:HG3	1:B:107:LEU:CD1	2.49	0.43
1:C:199:VAL:O	1:C:202:THR:HG22	2.19	0.43
1:C:84:MET:CE	1:C:268:LEU:HD21	2.49	0.43
1:B:303:ASN:CG	1:B:304:PRO:HA	2.39	0.42
1:A:268:LEU:HD13	1:B:250:LYS:HG3	2.00	0.42
1:B:150:LEU:CD2	1:B:210:LEU:HD13	2.42	0.42
1:B:87:GLU:O	1:B:91:VAL:HG23	2.19	0.42
1:C:185:GLN:HA	1:C:188:LEU:HD12	2.01	0.42
1:A:77:LEU:HD12	1:B:242:LEU:HD13	2.01	0.42
1:B:157:TYR:HA	1:B:202:THR:CG2	2.49	0.42
1:B:216:THR:HA	1:B:219:GLN:NE2	2.35	0.42
1:A:213:VAL:HG11	1:B:297:PRO:HG2	2.01	0.42
1:A:39:LEU:O	1:A:43:VAL:HG13	2.20	0.41
1:C:217:THR:HB	1:C:218:PRO:HD3	2.02	0.41
1:A:238:ARG:HG2	1:A:242:LEU:HD23	2.02	0.41
1:B:64:TRP:CZ3	1:B:67:LEU:HD23	2.55	0.41
1:C:159:LEU:HD12	1:C:159:LEU:C	2.41	0.41
1:A:67:LEU:HD12	1:A:70:LYS:HZ2	1.86	0.41
1:C:198:ASP:O	1:C:202:THR:HG22	2.20	0.41
1:A:250:LYS:HE3	1:B:269:GLU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:HG12	1:A:185:GLN:CG	2.51	0.41
1:A:241:PHE:HD1	1:A:242:LEU:HD22	1.86	0.41
1:B:77:LEU:HA	1:B:77:LEU:HD13	1.98	0.41
1:B:199:VAL:HA	1:B:202:THR:HG22	2.04	0.40
1:A:80:ALA:HB2	1:A:275:ALA:HB2	2.03	0.40
1:B:209:VAL:O	1:B:213:VAL:HG23	2.21	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)
2:C:2006:HOH:O	2:C:2006:HOH:O[4_555]	2.15	0.05

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	289/337 (86%)	281 (97%)	6 (2%)	2 (1%)	22	25
1	B	290/337 (86%)	284 (98%)	5 (2%)	1 (0%)	41	49
1	C	289/337 (86%)	285 (99%)	4 (1%)	0	100	100
All	All	868/1011 (86%)	850 (98%)	15 (2%)	3 (0%)	41	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	185	GLN
1	A	122	ILE
1	A	125	GLY

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	258/295 (88%)	238 (92%)	20 (8%)	12	15
1	B	259/295 (88%)	242 (93%)	17 (7%)	16	20
1	C	258/295 (88%)	236 (92%)	22 (8%)	10	12
All	All	775/885 (88%)	716 (92%)	59 (8%)	13	15

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	34	ARG
1	A	35	LEU
1	A	39	LEU
1	A	67	LEU
1	A	87	GLU
1	A	102	LEU
1	A	121	GLN
1	A	122	ILE
1	A	150	LEU
1	A	170	ARG
1	A	173	ASN
1	A	188	LEU
1	A	210	LEU
1	A	225	GLU
1	A	233	GLN
1	A	246	LEU
1	A	268	LEU
1	A	281	LEU
1	A	303	ASN
1	B	23	LYS
1	B	28	ARG
1	B	34	ARG
1	B	35	LEU
1	B	63	ARG
1	B	85	MET

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Mol	Chain	Res	Type
1	B	102	LEU
1	B	133	GLU
1	B	163	GLU
1	B	173	ASN
1	B	184	GLN
1	B	187	LYS
1	B	212	ASP
1	B	225	GLU
1	B	247	LEU
1	B	268	LEU
1	B	281	LEU
1	C	34	ARG
1	C	35	LEU
1	C	50	GLU
1	C	67	LEU
1	C	70	LYS
1	C	84	MET
1	C	85	MET
1	C	102	LEU
1	C	120	LYS
1	C	146	LYS
1	C	161	CYS
1	C	163	GLU
1	C	166	LEU
1	C	170	ARG
1	C	175	LYS
1	C	187	LYS
1	C	194	LYS
1	C	242	LEU
1	C	246	LEU
1	C	247	LEU
1	C	268	LEU
1	C	281	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	173	ASN
1	A	185	GLN
1	A	200	GLN
1	A	226	GLN

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Mol	Chain	Res	Type
1	A	233	GLN
1	A	303	ASN
1	B	56	GLN
1	B	66	GLN
1	B	121	GLN
1	B	140	GLN
1	B	173	ASN
1	B	185	GLN
1	B	219	GLN
1	B	226	GLN
1	B	295	ASN
1	C	197	GLN

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 carbohydrates 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(Å²)	Q<0.9
1	A	291/337 (86%)	0.34	12 (4%)	37	34	20, 32, 74, 84	0
1	B	292/337 (86%)	0.34	14 (4%)	30	28	14, 31, 72, 84	0
1	C	291/337 (86%)	0.32	17 (5%)	23	20	25, 39, 68, 72	0
All	All	874/1011 (86%)	0.33	43 (4%)	29	27	14, 35, 70, 84	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	SER	5.1
1	C	304	PRO	5.1
1	B	180	VAL	4.7
1	B	178	GLN	4.7
1	A	176	THR	4.6
1	C	189	VAL	4.6
1	C	176	THR	3.8
1	C	182	PRO	3.7
1	B	166	LEU	3.5
1	B	181	THR	3.5
1	C	184	GLN	3.5
1	C	303	ASN	3.4
1	B	187	LYS	3.3
1	A	178	GLN	3.2
1	A	180	VAL	3.1
1	B	183	GLU	3.0
1	C	166	LEU	3.0
1	B	176	THR	2.9
1	B	175	LYS	2.9
1	A	166	LEU	2.9
1	A	124	GLY	2.9
1	B	184	GLN	2.8
1	B	188	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	182	PRO	2.8
1	C	187	LYS	2.7
1	A	170	ARG	2.7
1	C	175	LYS	2.7
1	A	122	ILE	2.6
1	C	177	GLU	2.6
1	A	168	MET	2.6
1	C	179	SER	2.6
1	B	302	TRP	2.5
1	C	192	VAL	2.4
1	B	179	SER	2.4
1	A	175	LYS	2.3
1	C	81	TRP	2.3
1	B	304	PRO	2.3
1	B	185	GLN	2.2
1	C	302	TRP	2.2
1	C	168	MET	2.1
1	C	172	MET	2.1
1	A	173	ASN	2.1
1	C	136	PHE	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.