



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 10:03 pm GMT

PDB ID : 4HRG  
Title : Crystal Structure of p11-Annexin A2(N-terminal) Fusion Protein in Complex with AHNAK1 Peptide  
Authors : Gao, P.; Patel, D.J.  
Deposited on : 2012-10-27  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

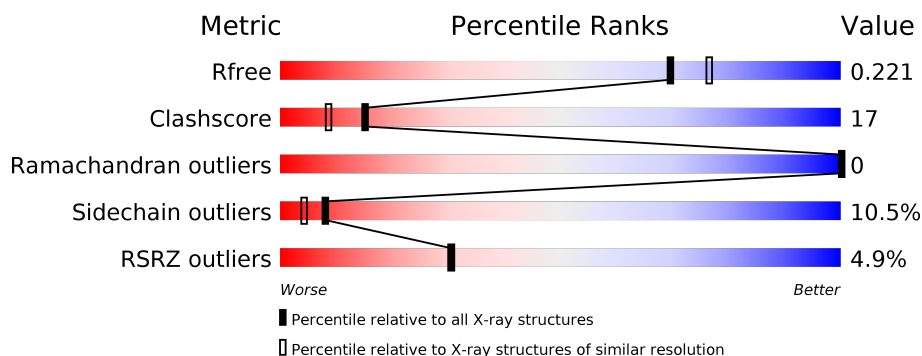
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	115	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>• •</div> </div> </div>
1	B	115	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>5%</div> <div>• •</div> </div> </div>
2	C	15	<div> <div>27%</div> <div>20%</div> <div>7%</div> <div>47%</div> </div>
2	D	15	<div> <div>33%</div> <div>13%</div> <div>7%</div> <div>47%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2101 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 S100-A10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			920	590	147	173	10			
1	B	113	Total	C	N	O	S	0	0	0
			912	585	146	172	9			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P60903
A	93	GLU	-	EXPRESSION TAG	UNP P60903
A	94	ASN	-	EXPRESSION TAG	UNP P60903
A	95	LEU	-	EXPRESSION TAG	UNP P60903
A	96	TYR	-	EXPRESSION TAG	UNP P60903
A	97	PHE	-	EXPRESSION TAG	UNP P60903
A	98	GLN	-	EXPRESSION TAG	UNP P60903
A	99	GLY	-	EXPRESSION TAG	UNP P60903
A	100	ASP	-	EXPRESSION TAG	UNP P60903
A	101	SER	-	EXPRESSION TAG	UNP P60903
A	102	THR	-	EXPRESSION TAG	UNP P60903
A	103	VAL	-	EXPRESSION TAG	UNP P60903
A	104	HIS	-	EXPRESSION TAG	UNP P60903
A	105	GLU	-	EXPRESSION TAG	UNP P60903
A	106	ILE	-	EXPRESSION TAG	UNP P60903
A	107	LEU	-	EXPRESSION TAG	UNP P60903
A	108	SER	-	EXPRESSION TAG	UNP P60903
A	110	LEU	-	EXPRESSION TAG	UNP P60903
A	111	SER	-	EXPRESSION TAG	UNP P60903
A	112	LEU	-	EXPRESSION TAG	UNP P60903
A	113	GLU	-	EXPRESSION TAG	UNP P60903
B	-1	SER	-	EXPRESSION TAG	UNP P60903
B	93	GLU	-	EXPRESSION TAG	UNP P60903
B	94	ASN	-	EXPRESSION TAG	UNP P60903
B	95	LEU	-	EXPRESSION TAG	UNP P60903

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Chain	Residue	Modelled	Actual	Comment	Reference
B	96	TYR	-	EXPRESSION TAG	UNP P60903
B	97	PHE	-	EXPRESSION TAG	UNP P60903
B	98	GLN	-	EXPRESSION TAG	UNP P60903
B	99	GLY	-	EXPRESSION TAG	UNP P60903
B	100	ASP	-	EXPRESSION TAG	UNP P60903
B	101	SER	-	EXPRESSION TAG	UNP P60903
B	102	THR	-	EXPRESSION TAG	UNP P60903
B	103	VAL	-	EXPRESSION TAG	UNP P60903
B	104	HIS	-	EXPRESSION TAG	UNP P60903
B	105	GLU	-	EXPRESSION TAG	UNP P60903
B	106	ILE	-	EXPRESSION TAG	UNP P60903
B	107	LEU	-	EXPRESSION TAG	UNP P60903
B	108	SER	-	EXPRESSION TAG	UNP P60903
B	110	LEU	-	EXPRESSION TAG	UNP P60903
B	111	SER	-	EXPRESSION TAG	UNP P60903
B	112	LEU	-	EXPRESSION TAG	UNP P60903
B	113	GLU	-	EXPRESSION TAG	UNP P60903

- Molecule 2 is a protein called Neuroblast differentiation-associated protein AHNAK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	S	0	0	0
			70	50	10	9	1			
2	D	8	Total	C	N	O	S	0	0	0
			70	50	10	9	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5654	GLN	-	EXPRESSION TAG	UNP Q09666
D	5654	GLN	-	EXPRESSION TAG	UNP Q09666

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	62	Total	O	0	0
			62	62		
3	C	2	Total	O	0	0
			2	2		

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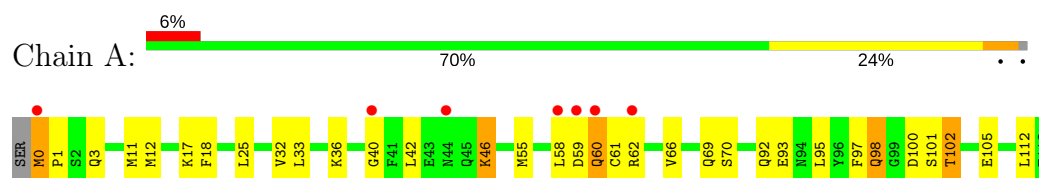
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total	O	0	0
			3	3		

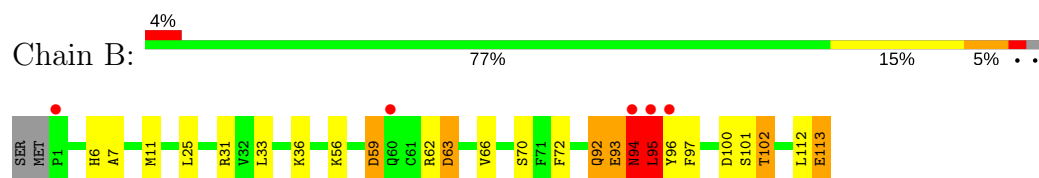
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

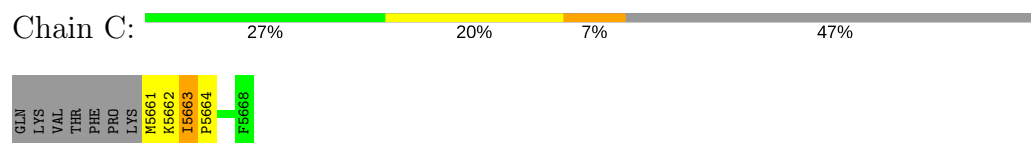
- Molecule 1: Protein S100-A10



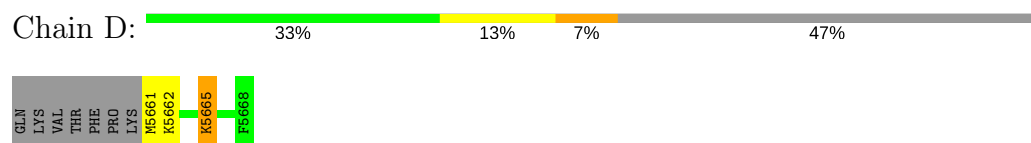
- Molecule 1: Protein S100-A10



- Molecule 2: Neuroblast differentiation-associated protein AHNAK



- Molecule 2: Neuroblast differentiation-associated protein AHNAK



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.28Å 55.65Å 60.62Å 90.00° 105.98° 90.00°	Depositor
Resolution (Å)	14.99 – 2.00 33.14 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (14.99-2.00) 99.7 (33.14-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.191 , 0.217 0.201 , 0.221	Depositor DCC
$R_{free}$ test set	1014 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.67	0/939	0.77	2/1257 (0.2%)
1	B	0.64	0/931	0.79	3/1246 (0.2%)
2	C	0.53	0/72	0.51	0/94
2	D	0.43	0/72	0.47	0/94
All	All	0.64	0/2014	0.76	5/2691 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	4
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ASP	CB-CG-OD2	8.56	126.01	118.30
1	B	95	LEU	CA-CB-CG	6.97	131.33	115.30
1	A	100	ASP	CB-CG-OD1	-5.79	113.08	118.30
1	B	93	GLU	N-CA-C	5.25	125.18	111.00
1	B	59	ASP	CB-CA-C	-5.22	99.96	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	GLY	Peptide
1	B	92	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	B	93	GLU	Peptide
1	B	94	ASN	Peptide
1	B	95	LEU	Peptide

## 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	920	0	903	44	0
1	B	912	0	894	26	0
2	C	70	0	77	6	0
2	D	70	0	77	3	0
3	A	62	0	0	8	0
3	B	62	0	0	4	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
All	All	2101	0	1951	66	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 17.

All (66) 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:0:MET:CE	1:B:100:ASP:HB2	1.59	1.33
1:A:0:MET:HE1	1:B:100:ASP:CB	1.60	1.29
1:A:0:MET:H3	1:A:0:MET:HE3	1.16	1.09
1:A:0:MET:H3	1:A:0:MET:CE	1.67	1.06
1:A:60:GLN:HG3	1:A:70:SER:OG	1.65	0.96
1:A:0:MET:CE	1:A:0:MET:N	2.30	0.95
1:A:59:ASP:HB2	2:C:5662:LYS:HB3	1.51	0.93
1:B:95:LEU:HD22	1:B:97:PHE:H	1.35	0.92
1:A:0:MET:CE	1:B:100:ASP:CB	2.32	0.91
1:A:0:MET:HE3	1:A:1:PRO:HD3	1.55	0.85
1:B:94:ASN:H	1:B:94:ASN:ND2	1.78	0.77
1:B:95:LEU:CD2	1:B:97:PHE:H	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:MET:HE2	1:A:0:MET:N	2.00	0.76
1:A:105:GLU:CG	3:A:262:HOH:O	2.36	0.74
2:C:5661:MET:N	2:D:5661:MET:O	2.23	0.70
1:B:63:ASP:OD1	1:B:63:ASP:N	2.24	0.70
1:B:112:LEU:HD12	2:D:5665:LYS:O	1.94	0.67
1:A:0:MET:H1	1:A:0:MET:HE2	1.60	0.67
1:A:59:ASP:O	1:A:60:GLN:HG3	1.95	0.66
1:B:36:LYS:HG2	3:B:259:HOH:O	1.95	0.65
1:B:95:LEU:HD22	1:B:97:PHE:N	2.11	0.65
1:A:98:GLN:HG2	1:A:101:SER:CB	2.27	0.64
1:B:113:GLU:C	3:B:257:HOH:O	2.34	0.64
1:A:105:GLU:CD	3:A:262:HOH:O	2.37	0.62
1:A:105:GLU:HG3	3:A:262:HOH:O	1.99	0.60
1:A:25:LEU:HB2	1:A:66:VAL:HB	1.82	0.59
1:A:32:VAL:O	1:A:36:LYS:HG2	2.03	0.59
1:B:95:LEU:O	1:B:96:TYR:CG	2.56	0.59
1:A:98:GLN:HG2	1:A:101:SER:HB2	1.85	0.58
1:A:97:PHE:HB3	1:A:102:THR:HG21	1.84	0.58
1:A:0:MET:H3	1:A:1:PRO:CD	2.17	0.58
1:A:60:GLN:CG	1:A:70:SER:OG	2.45	0.57
2:C:5661:MET:O	2:D:5661:MET:N	2.38	0.57
1:A:0:MET:N	1:A:1:PRO:CD	2.68	0.57
3:A:220:HOH:O	1:B:102:THR:HG23	2.05	0.57
1:A:59:ASP:HB2	2:C:5662:LYS:CB	2.33	0.55
1:A:98:GLN:O	1:A:102:THR:HG23	2.08	0.54
1:A:92:GLN:HG2	3:A:214:HOH:O	2.09	0.52
1:B:95:LEU:HD22	1:B:96:TYR:HA	1.92	0.52
1:B:11:MET:HE3	1:B:72:PHE:HE1	1.72	0.52
1:B:25:LEU:HB2	1:B:66:VAL:HB	1.92	0.51
1:B:7:ALA:HA	3:B:258:HOH:O	2.10	0.51
1:B:56:LYS:HB3	1:B:56:LYS:NZ	2.26	0.51
1:A:0:MET:HE1	1:B:100:ASP:HB2	0.70	0.49
1:A:0:MET:H3	1:A:1:PRO:HD3	1.77	0.49
1:A:58:LEU:O	1:A:61:CYS:HB3	2.13	0.47
1:A:0:MET:HE3	1:A:1:PRO:CD	2.37	0.47
1:B:6:HIS:HD2	3:B:258:HOH:O	1.97	0.47
1:A:60:GLN:O	1:A:70:SER:OG	2.31	0.47
1:A:0:MET:CE	1:B:100:ASP:HB3	2.38	0.47
1:A:1:PRO:HB3	1:B:101:SER:HB2	1.98	0.46
1:A:46:LYS:HA	1:A:46:LYS:HD3	1.54	0.45
2:C:5663:ILE:HG12	2:C:5664:PRO:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LYS:HD3	1:A:18:PHE:CE2	2.52	0.45
1:A:93:GLU:OE2	3:A:253:HOH:O	2.21	0.44
1:A:0:MET:C	1:A:0:MET:SD	2.97	0.43
1:A:33:LEU:C	1:A:33:LEU:HD23	2.39	0.43
1:A:69:GLN:OE1	3:A:210:HOH:O	2.21	0.43
1:A:59:ASP:CB	2:C:5662:LYS:HB3	2.34	0.43
1:B:94:ASN:H	1:B:94:ASN:HD22	1.63	0.43
1:B:33:LEU:HD23	1:B:33:LEU:C	2.40	0.42
1:A:11:MET:HE1	1:B:11:MET:CE	2.50	0.41
1:A:98:GLN:HG2	1:A:101:SER:HB3	1.99	0.41
1:A:60:GLN:HG3	1:A:60:GLN:O	2.19	0.41
1:B:59:ASP:O	1:B:70:SER:OG	2.22	0.41
1:A:102:THR:HB	3:A:260:HOH:O	2.20	0.41

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	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
1	B	111/115 (96%)	105 (95%)	6 (5%)	0	100	100
2	C	6/15 (40%)	6 (100%)	0	0	100	100
2	D	6/15 (40%)	6 (100%)	0	0	100	100
All	All	235/260 (90%)	222 (94%)	13 (6%)	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	102/103 (99%)	90 (88%)	12 (12%)	6	3
1	B	101/103 (98%)	93 (92%)	8 (8%)	14	9
2	C	8/15 (53%)	7 (88%)	1 (12%)	5	3
2	D	8/15 (53%)	6 (75%)	2 (25%)	1	0
All	All	219/236 (93%)	196 (90%)	23 (10%)	8	4

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	3	GLN
1	A	12	MET
1	A	42	LEU
1	A	46	LYS
1	A	55	MET
1	A	60	GLN
1	A	62	ARG
1	A	95	LEU
1	A	98	GLN
1	A	102	THR
1	A	112	LEU
1	B	31	ARG
1	B	62	ARG
1	B	63	ASP
1	B	92	GLN
1	B	94	ASN
1	B	95	LEU
1	B	102	THR
1	B	113	GLU
2	C	5663	ILE
2	D	5662	LYS
2	D	5665	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	6	HIS
1	B	94	ASN

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	114/115 (99%)	0.11	7 (6%) 22 22	20, 36, 68, 93	0
1	B	113/115 (98%)	-0.03	5 (4%) 35 35	20, 36, 70, 97	0
2	C	8/15 (53%)	0.14	0 100 100	42, 49, 64, 66	0
2	D	8/15 (53%)	0.30	0 100 100	39, 47, 66, 68	0
All	All	243/260 (93%)	0.05	12 (4%) 30 30	20, 37, 69, 97	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	MET	5.5
1	A	60	GLN	5.4
1	B	1	PRO	4.7
1	B	94	ASN	3.8
1	A	59	ASP	3.4
1	A	58	LEU	3.1
1	B	96	TYR	2.5
1	A	62	ARG	2.4
1	B	95	LEU	2.3
1	B	60	GLN	2.3
1	A	44	ASN	2.1
1	A	40	GLY	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.