Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:35 AM GMT

PDB ID	:	3FB2
Title	:	Crystal structure of the human brain alpha spectrin repeats 15 and 16. Northeast Structural Genomics Consortium target HR5563a.
Authors	:	Vorobiev, S.M.; Su, M.; Seetharaman, J.; Shastry, R.; Foote, E.L.; Ciccosanti, C.; Janjua, H.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2008-11-18
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:

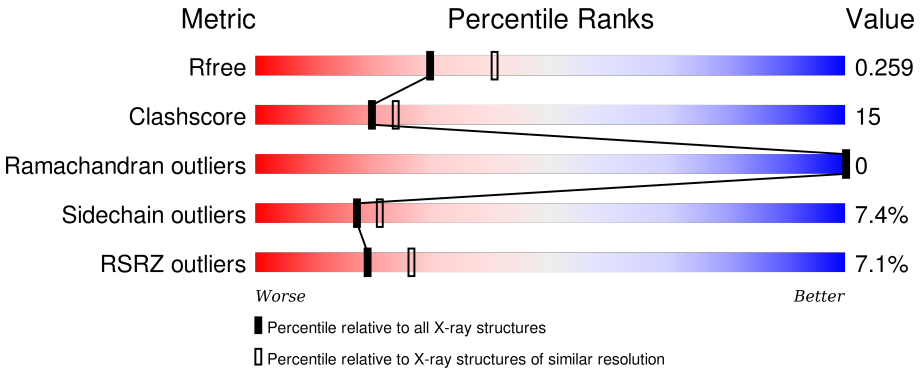
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	218	10%, 56%, 28%, ·, 14%
1	B	218	2%, 75%, 16%, ·, 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3459 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 Spectrin alpha chain, brain spectrin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	Se	0	0	0
			1533	952	284	290	2	5			
1	B	202	Total	C	N	O	S	Se	0	0	0
			1646	1022	305	312	2	5			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1327	MSE	-	expression tag	UNP Q13813
A	1328	GLY	-	expression tag	UNP Q13813
A	1329	HIS	-	expression tag	UNP Q13813
A	1330	HIS	-	expression tag	UNP Q13813
A	1331	HIS	-	expression tag	UNP Q13813
A	1332	HIS	-	expression tag	UNP Q13813
A	1333	HIS	-	expression tag	UNP Q13813
A	1334	HIS	-	expression tag	UNP Q13813
A	1335	SER	-	expression tag	UNP Q13813
A	1336	HIS	-	expression tag	UNP Q13813
B	1327	MSE	-	expression tag	UNP Q13813
B	1328	GLY	-	expression tag	UNP Q13813
B	1329	HIS	-	expression tag	UNP Q13813
B	1330	HIS	-	expression tag	UNP Q13813
B	1331	HIS	-	expression tag	UNP Q13813
B	1332	HIS	-	expression tag	UNP Q13813
B	1333	HIS	-	expression tag	UNP Q13813
B	1334	HIS	-	expression tag	UNP Q13813
B	1335	SER	-	expression tag	UNP Q13813
B	1336	HIS	-	expression tag	UNP Q13813

- Molecule 2 is water.

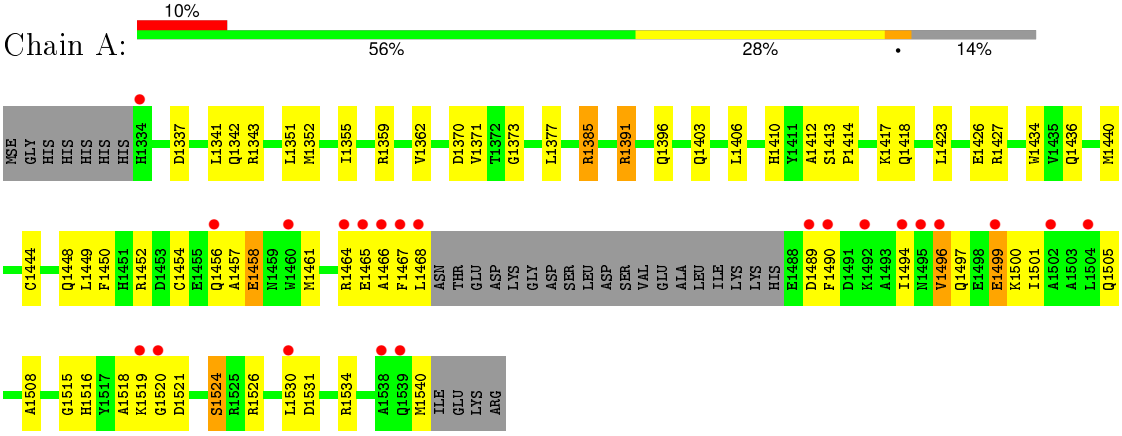
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	120	Total O 120 120	0	0
2	B	160	Total O 160 160	0	0

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.

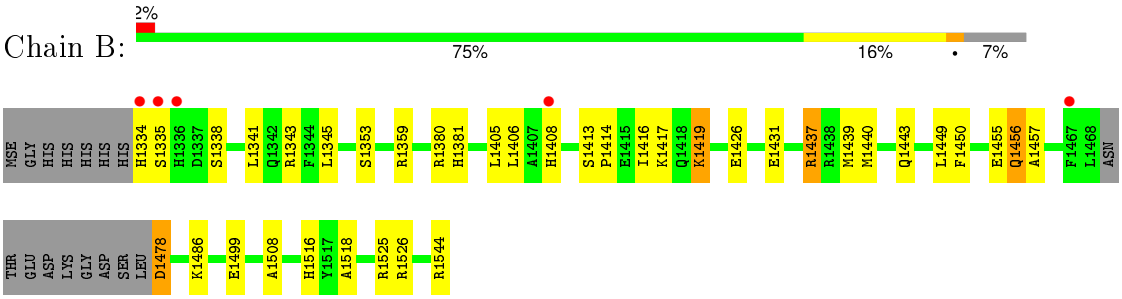
- Molecule 1: Spectrin alpha chain, brain spectrin

Chain A:



- Molecule 1: Spectrin alpha chain, brain spectrin

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.61Å 96.38Å 111.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.41 – 2.30 36.41 – 2.29	Depositor EDS
% Data completeness (in resolution range)	81.7 (36.41-2.30) 90.2 (36.41-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.58 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.248 0.233 , 0.259	Depositor DCC
R_{free} test set	1529 reflections (5.68%)	DCC
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	1.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 58852 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3459	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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

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	0.32	0/1554	0.49	0/2078
1	B	0.35	0/1668	0.47	0/2229
All	All	0.33	0/3222	0.48	0/4307

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	1533	0	1471	58	0
1	B	1646	0	1587	39	0
2	A	120	0	0	6	0
2	B	160	0	0	7	0
All	All	3459	0	3058	93	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 (93) 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:1439:MSE:HE3	1:B:1440:MSE:HE3	1.38	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1381:HIS:CE1	1:B:1437:ARG:HG2	1.98	0.99
1:B:1405:LEU:HA	1:B:1408:HIS:CE1	2.00	0.97
1:B:1516:HIS:HD2	1:B:1518:ALA:H	1.19	0.89
1:A:1464:ARG:HA	1:A:1467:PHE:CZ	2.10	0.87
1:A:1508:ALA:HB3	1:A:1526:ARG:HD3	1.57	0.86
1:A:1464:ARG:HA	1:A:1467:PHE:CE2	2.13	0.84
1:A:1505:GLN:HG3	1:A:1530:LEU:HD11	1.60	0.83
1:B:1439:MSE:CE	1:B:1440:MSE:HE3	2.09	0.81
1:B:1405:LEU:HD12	1:B:1408:HIS:HE1	1.46	0.80
1:B:1508:ALA:HB3	1:B:1526:ARG:HD3	1.67	0.76
1:A:1396:GLN:HE21	1:B:1380:ARG:HH21	1.33	0.76
1:A:1352:MSE:HE1	1:A:1426:GLU:HG3	1.70	0.73
1:B:1431:GLU:HG3	2:B:2327:HOH:O	1.88	0.72
1:A:1464:ARG:HG3	1:A:1467:PHE:HZ	1.55	0.72
1:A:1454:CYS:O	1:A:1458:GLU:HB2	1.89	0.71
1:B:1405:LEU:HD12	1:B:1408:HIS:CE1	2.24	0.71
1:B:1516:HIS:CD2	1:B:1518:ALA:H	2.08	0.71
1:A:1490:PHE:CZ	1:A:1540:MSE:HE2	2.28	0.69
1:A:1410:HIS:HD2	1:A:1412:ALA:H	1.39	0.69
1:B:1440:MSE:HE2	1:B:1440:MSE:HA	1.77	0.66
1:B:1405:LEU:HA	1:B:1408:HIS:NE2	2.11	0.66
1:A:1396:GLN:NE2	1:B:1380:ARG:HH21	1.93	0.65
1:A:1516:HIS:HD2	1:A:1518:ALA:H	1.43	0.65
1:B:1486:LYS:HE2	1:B:1544:ARG:O	1.97	0.65
1:A:1436:GLN:HE21	1:A:1440:MSE:CE	2.10	0.64
1:A:1515:GLY:HA2	1:A:1519:LYS:HE2	1.79	0.64
1:B:1439:MSE:HE3	1:B:1440:MSE:CE	2.22	0.63
1:A:1490:PHE:O	1:A:1494:ILE:HG12	1.99	0.63
1:A:1452:ARG:O	1:A:1456:GLN:HG3	1.99	0.63
1:A:1417:LYS:HE2	2:A:2360:HOH:O	1.98	0.62
1:A:1370:ASP:O	1:A:1448:GLN:HG3	1.99	0.62
1:A:1516:HIS:CD2	1:A:1518:ALA:H	2.18	0.61
1:A:1440:MSE:HE3	2:A:2267:HOH:O	2.00	0.60
1:B:1456:GLN:NE2	2:B:2227:HOH:O	2.34	0.60
1:A:1508:ALA:CB	1:A:1526:ARG:HD3	2.31	0.59
1:A:1449:LEU:HD23	1:A:1452:ARG:HD3	1.83	0.59
1:A:1410:HIS:CD2	1:A:1412:ALA:H	2.22	0.57
1:A:1490:PHE:CE1	1:A:1540:MSE:HE2	2.40	0.57
1:B:1413:SER:N	1:B:1414:PRO:HD2	2.19	0.57
1:A:1464:ARG:HG3	1:A:1467:PHE:CZ	2.37	0.56
1:B:1359:ARG:NH1	2:B:2321:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1456:GLN:NE2	1:B:1457:ALA:N	2.54	0.56
1:A:1337:ASP:O	1:A:1410:HIS:HE1	1.90	0.55
1:B:1443:GLN:O	1:B:1516:HIS:HE1	1.89	0.55
1:B:1478:ASP:N	2:B:2202:HOH:O	2.40	0.54
1:A:1371:VAL:HG21	1:A:1452:ARG:HD2	1.88	0.54
1:A:1461:MSE:O	1:A:1465:GLU:HG3	2.08	0.53
1:A:1436:GLN:NE2	1:A:1440:MSE:CE	2.72	0.52
1:A:1352:MSE:CE	1:A:1426:GLU:HG3	2.38	0.52
1:A:1450:PHE:CE1	1:A:1508:ALA:HB2	2.45	0.51
1:A:1496:VAL:HG12	1:A:1497:GLN:N	2.24	0.51
1:A:1457:ALA:O	1:A:1461:MSE:HG3	2.10	0.51
1:B:1414:PRO:HG2	2:B:2152:HOH:O	2.12	0.49
1:A:1352:MSE:SE	1:A:1426:GLU:HG3	2.62	0.49
1:B:1406:LEU:HD21	1:B:1417:LYS:HG2	1.94	0.49
1:B:1450:PHE:CE1	1:B:1508:ALA:HB2	2.48	0.48
1:B:1508:ALA:CB	1:B:1526:ARG:HD3	2.40	0.47
1:B:1334:HIS:O	1:B:1338:SER:HB2	2.14	0.47
1:A:1464:ARG:CG	1:A:1467:PHE:HZ	2.26	0.47
1:A:1342:GLN:NE2	2:A:2201:HOH:O	2.45	0.47
1:A:1355:ILE:O	1:A:1359:ARG:HB2	2.15	0.46
1:B:1437:ARG:HD3	2:B:2144:HOH:O	2.15	0.46
1:A:1444:CYS:O	1:A:1448:GLN:HG2	2.15	0.46
1:B:1334:HIS:O	1:B:1338:SER:CB	2.64	0.46
1:A:1499:GLU:HG2	1:A:1500:LYS:N	2.30	0.45
1:B:1419:LYS:HE3	2:B:2299:HOH:O	2.16	0.45
1:A:1436:GLN:HE21	1:A:1440:MSE:HE2	1.81	0.45
1:A:1440:MSE:HE1	2:A:2333:HOH:O	2.17	0.45
1:A:1362:VAL:O	1:A:1362:VAL:CG1	2.65	0.45
1:A:1418:GLN:NE2	2:A:2332:HOH:O	2.49	0.44
1:B:1359:ARG:NH2	1:B:1426:GLU:OE1	2.44	0.44
1:A:1520:GLY:O	1:A:1524:SER:HB2	2.17	0.44
1:B:1525:ARG:HH11	1:B:1525:ARG:HG3	1.83	0.43
1:A:1466:ALA:C	1:A:1468:LEU:H	2.22	0.43
1:A:1413:SER:HB2	1:A:1414:PRO:HD3	2.00	0.43
1:B:1437:ARG:O	1:B:1437:ARG:HG3	2.17	0.43
1:A:1521:ASP:HB3	2:A:2337:HOH:O	2.18	0.43
1:A:1531:ASP:HA	1:A:1534:ARG:NH1	2.34	0.43
1:B:1443:GLN:O	1:B:1516:HIS:CE1	2.71	0.42
1:A:1516:HIS:HD2	1:A:1518:ALA:N	2.14	0.42
1:A:1403:GLN:NE2	1:B:1380:ARG:HH11	2.18	0.42
1:A:1370:ASP:HB3	1:A:1373:GLY:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1385:ARG:HB2	1:A:1434:TRP:CZ2	2.54	0.42
1:B:1406:LEU:HD13	1:B:1416:ILE:HG21	2.01	0.42
1:A:1423:LEU:O	1:A:1427:ARG:HG3	2.21	0.41
1:A:1359:ARG:HA	1:A:1359:ARG:HD2	1.85	0.41
1:A:1391:ARG:HD3	1:A:1391:ARG:HA	1.81	0.41
1:B:1405:LEU:HB3	1:B:1416:ILE:HD13	2.02	0.41
1:B:1413:SER:O	1:B:1417:LYS:HG3	2.21	0.41
1:A:1403:GLN:HE21	1:B:1380:ARG:HB2	1.86	0.40
1:A:1371:VAL:HG21	1:A:1452:ARG:CD	2.50	0.40
1:A:1457:ALA:HB1	1:A:1501:ILE:HD11	2.03	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	184/218 (84%)	181 (98%)	3 (2%)	0	100	100
1	B	198/218 (91%)	197 (100%)	1 (0%)	0	100	100
All	All	382/436 (88%)	378 (99%)	4 (1%)	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	156/178 (88%)	144 (92%)	12 (8%)	16	20
1	B	168/178 (94%)	156 (93%)	12 (7%)	18	23
All	All	324/356 (91%)	300 (93%)	24 (7%)	17	21

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1341	LEU
1	A	1343	ARG
1	A	1351	LEU
1	A	1377	LEU
1	A	1385	ARG
1	A	1391	ARG
1	A	1406	LEU
1	A	1458	GLU
1	A	1489	ASP
1	A	1496	VAL
1	A	1499	GLU
1	A	1524	SER
1	B	1335	SER
1	B	1341	LEU
1	B	1343	ARG
1	B	1345	LEU
1	B	1353	SER
1	B	1419	LYS
1	B	1437	ARG
1	B	1449	LEU
1	B	1455	GLU
1	B	1456	GLN
1	B	1478	ASP
1	B	1499	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1382	GLN
1	A	1396	GLN
1	A	1403	GLN
1	A	1410	HIS
1	A	1425	GLN
1	A	1436	GLN

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Mol	Chain	Res	Type
1	A	1459	ASN
1	A	1505	GLN
1	A	1516	HIS
1	B	1403	GLN
1	B	1408	HIS
1	B	1456	GLN
1	B	1459	ASN
1	B	1495	ASN
1	B	1505	GLN
1	B	1516	HIS

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	183/218 (83%)	0.59	22 (12%) 6 9	27, 46, 92, 99	0
1	B	197/218 (90%)	-0.08	5 (2%) 61 70	26, 39, 58, 75	0
All	All	380/436 (87%)	0.24	27 (7%) 19 26	26, 41, 87, 99	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1467	PHE	8.6
1	A	1490	PHE	6.0
1	B	1408	HIS	5.9
1	A	1468	LEU	5.5
1	A	1466	ALA	4.4
1	A	1520	GLY	3.9
1	A	1499	GLU	3.8
1	A	1489	ASP	3.8
1	B	1467	PHE	3.7
1	B	1334	HIS	3.3
1	A	1538	ALA	3.2
1	B	1335	SER	3.1
1	A	1492	LYS	3.1
1	B	1336	HIS	3.1
1	A	1334	HIS	3.0
1	A	1464	ARG	2.8
1	A	1504	LEU	2.6
1	A	1539	GLN	2.5
1	A	1495	ASN	2.5
1	A	1496	VAL	2.5
1	A	1494	ILE	2.4
1	A	1456	GLN	2.3
1	A	1502	ALA	2.2
1	A	1465	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1460	TRP	2.1
1	A	1530	LEU	2.1
1	A	1519	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 (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.