Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:04 PM GMT

PDB ID	:	1NDM
Title	:	Crystal structure of Fab fragment of antibody HyHEL-26 complexed with lysozyme
Authors	:	Mariuzza, R.A.; Li, Y.; Li, H.
Deposited on	:	2002-12-09
Resolution	:	2.10 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:

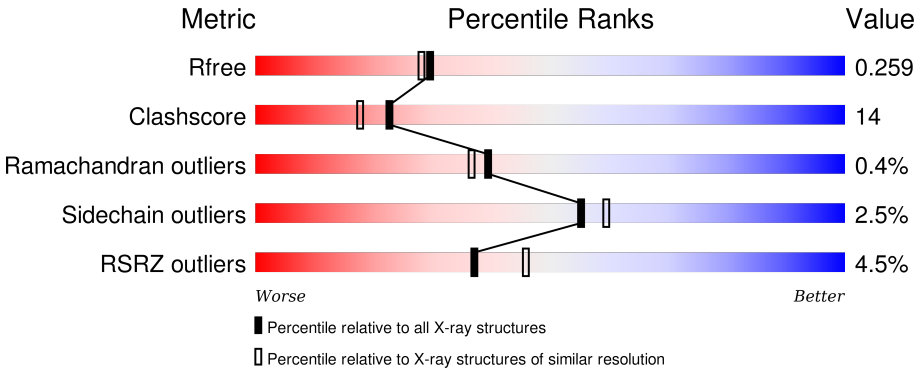
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	214	% 78% 21% ·
2	B	210	5% 70% 30% ·
3	C	129	9% 74% 25% ·

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4856 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 antibody kappa light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1647	1021	277	342	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASP	GLU	CLONING ARTIFACT	UNP P01837
A	2	ILE	LEU	CLONING ARTIFACT	UNP P01837
A	4	LEU	MET	CLONING ARTIFACT	UNP P01837

- Molecule 2 is a protein called immunoglobulin gamma 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1610	1017	257	329	7			

- Molecule 3 is a protein called Lysozyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			

- Molecule 4 is water.

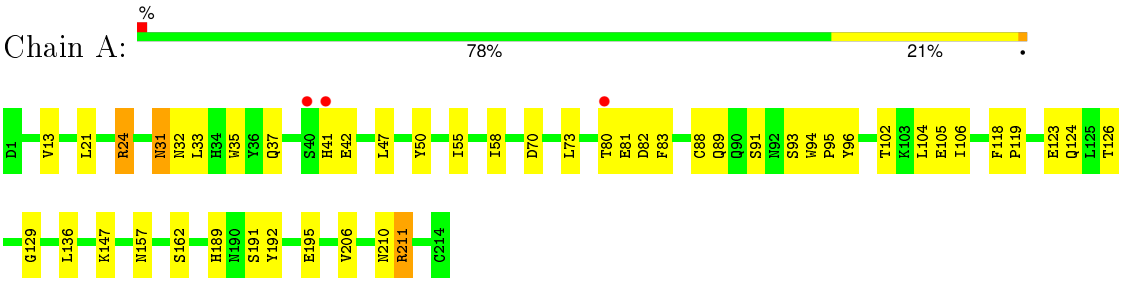
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	249	Total	O	0	0
			249	249		
4	B	239	Total	O	0	0
			239	239		
4	C	110	Total	O	0	0
			110	110		

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.

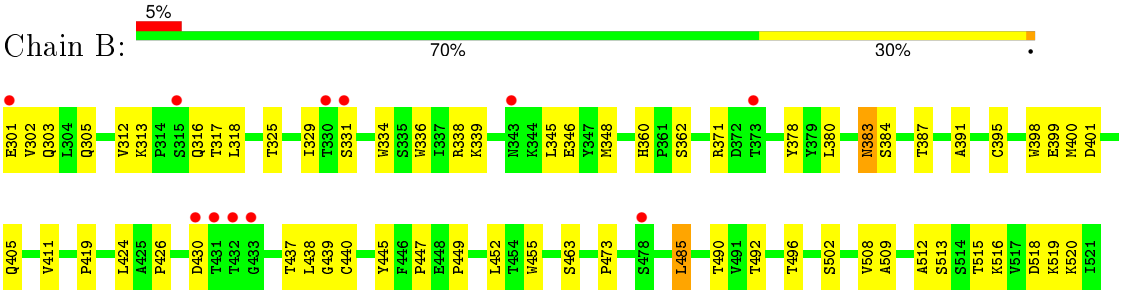
- Molecule 1: antibody kappa light chain

Chain A:



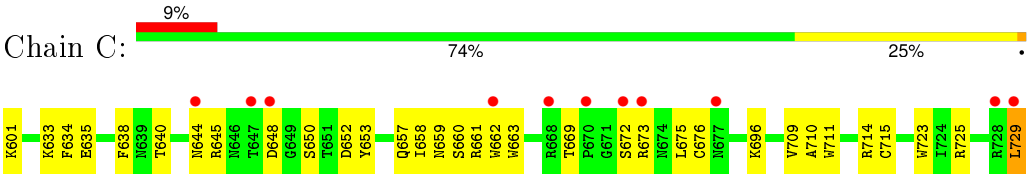
- Molecule 2: immunoglobulin gamma 1 chain

Chain B:



- Molecule 3: Lysozyme C

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	90.68Å 164.02Å 40.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.45 – 2.10 8.45 – 2.02	Depositor EDS
% Data completeness (in resolution range)	89.5 (8.45-2.10) 85.5 (8.45-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.02Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.258 0.208 , 0.259	Depositor DCC
R_{free} test set	1564 reflections (4.97%)	DCC
Wilson B-factor (Å^2)	13.3	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.48 , 68.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 33802 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4856	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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	0.38	0/1684	0.64	0/2286
2	B	0.38	0/1653	0.69	0/2263
3	C	0.33	0/1021	0.60	0/1379
All	All	0.37	0/4358	0.65	0/5928

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	1647	0	1556	40	0
2	B	1610	0	1553	49	0
3	C	1001	0	956	30	0
4	A	249	0	0	4	0
4	B	239	0	0	4	0
4	C	110	0	0	3	0
All	All	4856	0	4065	113	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 14.

All (113) 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)
2:B:492:THR:O	2:B:496:THR:HG22	1.75	0.85
2:B:317:THR:HG22	2:B:383:ASN:HA	1.59	0.85
1:A:24:ARG:HD2	1:A:70:ASP:OD1	1.84	0.77
3:C:645:ARG:NH1	3:C:645:ARG:HB3	2.01	0.75
1:A:191:SER:HB3	1:A:210:ASN:OD1	1.86	0.74
2:B:419:PRO:HB3	2:B:445:TYR:HB3	1.70	0.72
3:C:645:ARG:HH11	3:C:645:ARG:HB3	1.55	0.71
2:B:437:THR:HG22	2:B:490:THR:HG23	1.73	0.69
2:B:338:ARG:HD3	2:B:346:GLU:OE1	1.95	0.66
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.78	0.66
3:C:633:LYS:HG2	3:C:723:TRP:CH2	2.30	0.66
1:A:55:ILE:HB	1:A:58:ILE:HG13	1.78	0.66
3:C:673:ARG:HD3	3:C:675:LEU:HD11	1.79	0.65
1:A:94:TRP:CD2	1:A:95:PRO:HA	2.33	0.64
3:C:673:ARG:HB3	3:C:675:LEU:CD1	2.29	0.63
2:B:360:HIS:CD2	2:B:362:SER:H	2.17	0.63
3:C:673:ARG:HB3	3:C:675:LEU:HD13	1.81	0.62
1:A:21:LEU:HD22	1:A:102:THR:HG21	1.82	0.62
3:C:634:PHE:CD1	3:C:714:ARG:HD3	2.37	0.59
1:A:124:GLN:HG2	1:A:129:GLY:O	2.03	0.58
1:A:189:HIS:O	1:A:211:ARG:NH2	2.37	0.58
1:A:89:GLN:HE22	2:B:400:MET:CE	2.18	0.57
2:B:518:ASP:O	2:B:519:LYS:HD2	2.05	0.57
3:C:645:ARG:CB	3:C:645:ARG:HH11	2.17	0.56
3:C:661:ARG:HD3	3:C:661:ARG:O	2.05	0.56
1:A:136:LEU:HD12	1:A:136:LEU:N	2.21	0.56
1:A:211:ARG:HH21	1:A:211:ARG:HG3	1.71	0.56
1:A:89:GLN:HE22	2:B:400:MET:HE2	1.71	0.56
2:B:509:ALA:HB2	2:B:516:LYS:HG3	1.88	0.55
2:B:502:SER:OG	2:B:520:LYS:HE3	2.07	0.55
2:B:303:GLN:HG3	4:B:1022:HOH:O	2.06	0.54
1:A:162:SER:OG	2:B:473:PRO:HD2	2.07	0.54
2:B:437:THR:HG22	2:B:490:THR:CG2	2.36	0.54
1:A:24:ARG:HB3	4:A:1227:HOH:O	2.08	0.54
2:B:452:LEU:C	2:B:452:LEU:HD23	2.28	0.54
1:A:31:ASN:C	1:A:31:ASN:ND2	2.62	0.54
2:B:447:PRO:HD2	2:B:512:ALA:CB	2.38	0.53
2:B:387:THR:HG22	2:B:411:VAL:O	2.08	0.53
1:A:13:VAL:HG11	1:A:104:LEU:HD21	1.92	0.52
1:A:195:GLU:HG3	1:A:206:VAL:HG22	1.90	0.52
2:B:318:LEU:HD23	2:B:318:LEU:C	2.30	0.52
3:C:650:SER:CB	3:C:659:ASN:HD21	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:THR:HG23	2:B:496:THR:HB	1.92	0.52
2:B:426:PRO:HD3	2:B:438:LEU:CD1	2.41	0.51
1:A:33:LEU:HD21	1:A:88:CYS:HB2	1.92	0.51
2:B:485:LEU:HD23	2:B:485:LEU:C	2.31	0.51
2:B:426:PRO:HD3	2:B:438:LEU:HD12	1.93	0.51
1:A:83:PHE:CD2	1:A:106:ILE:HG13	2.46	0.51
4:A:935:HOH:O	2:B:437:THR:HG21	2.10	0.50
2:B:339:LYS:O	2:B:391:ALA:HB1	2.11	0.50
1:A:31:ASN:HD21	3:C:696:LYS:NZ	2.10	0.50
3:C:729:LEU:HD23	3:C:729:LEU:H	1.76	0.50
1:A:55:ILE:HB	1:A:58:ILE:CG1	2.40	0.50
1:A:31:ASN:C	1:A:31:ASN:HD22	2.14	0.50
1:A:32:ASN:HD21	3:C:696:LYS:NZ	2.10	0.50
2:B:339:LYS:HB2	2:B:345:LEU:HD23	1.93	0.49
3:C:650:SER:HB2	3:C:659:ASN:HD21	1.77	0.48
1:A:123:GLU:O	1:A:126:THR:HB	2.13	0.48
3:C:652:ASP:HB3	3:C:657:GLN:HB3	1.95	0.48
2:B:334:TRP:HB3	2:B:378:TYR:CZ	2.49	0.48
2:B:509:ALA:HB2	2:B:516:LYS:HE2	1.96	0.48
3:C:711:TRP:CD1	3:C:715:CYS:HB2	2.49	0.48
1:A:32:ASN:HD22	1:A:50:TYR:HE1	1.62	0.48
1:A:189:HIS:HB2	1:A:192:TYR:OH	2.14	0.47
1:A:41:HIS:O	1:A:42:GLU:HG3	2.14	0.47
1:A:80:THR:O	1:A:83:PHE:HD1	1.98	0.47
2:B:303:GLN:HB2	2:B:325:THR:OG1	2.15	0.47
1:A:81:GLU:N	1:A:81:GLU:OE2	2.37	0.47
2:B:305:GLN:OE1	2:B:405:GLN:NE2	2.48	0.46
3:C:658:ILE:CG2	3:C:663:TRP:HB2	2.45	0.46
2:B:360:HIS:HD2	2:B:362:SER:H	1.60	0.46
1:A:13:VAL:CG1	1:A:104:LEU:HD21	2.46	0.46
2:B:312:VAL:O	2:B:411:VAL:HA	2.15	0.45
2:B:378:TYR:OH	2:B:395:CYS:HB2	2.17	0.45
3:C:601:LYS:N	3:C:640:THR:HG1	2.15	0.45
3:C:669:THR:HB	3:C:672:SER:OG	2.17	0.45
3:C:663:TRP:O	3:C:676:CYS:HB2	2.16	0.45
2:B:336:TRP:CE2	2:B:380:LEU:HB2	2.51	0.45
1:A:147:LYS:HE3	1:A:147:LYS:HB2	1.70	0.44
2:B:302:VAL:HG23	2:B:325:THR:O	2.17	0.44
1:A:31:ASN:O	1:A:50:TYR:HA	2.17	0.44
3:C:645:ARG:HD2	4:C:1059:HOH:O	2.17	0.44
3:C:633:LYS:HB2	3:C:638:PHE:CZ	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:513:SER:O	2:B:515:THR:HG23	2.17	0.44
3:C:725:ARG:HG2	3:C:725:ARG:HH21	1.82	0.44
2:B:437:THR:HG22	2:B:490:THR:OG1	2.18	0.44
1:A:35:TRP:CD2	1:A:73:LEU:HB2	2.53	0.44
1:A:91:SER:HA	1:A:96:TYR:CD2	2.53	0.44
2:B:399:GLU:HB2	2:B:401:ASP:OD2	2.18	0.43
2:B:508:VAL:O	2:B:516:LYS:HA	2.18	0.43
2:B:387:THR:HG21	4:B:937:HOH:O	2.18	0.43
2:B:419:PRO:CB	2:B:445:TYR:HB3	2.44	0.43
2:B:398:TRP:O	2:B:400:MET:HG3	2.18	0.43
1:A:80:THR:HG23	1:A:81:GLU:OE2	2.19	0.43
3:C:635:GLU:OE2	3:C:710:ALA:HB3	2.19	0.43
1:A:42:GLU:HA	4:B:897:HOH:O	2.18	0.42
3:C:662:TRP:CZ3	3:C:673:ARG:HD2	2.54	0.42
3:C:635:GLU:CD	3:C:710:ALA:HB3	2.39	0.42
2:B:331:SER:HA	3:C:673:ARG:HE	1.84	0.42
2:B:313:LYS:HB2	2:B:316:GLN:HG2	2.01	0.42
3:C:709:VAL:HG23	4:C:1180:HOH:O	2.18	0.41
1:A:118:PHE:HA	1:A:119:PRO:HD3	1.87	0.41
3:C:644:ASN:HB2	4:C:982:HOH:O	2.19	0.41
3:C:653:TYR:HE1	3:C:660:SER:HB3	1.84	0.41
1:A:211:ARG:HH21	1:A:211:ARG:CG	2.32	0.41
1:A:21:LEU:HB3	4:A:823:HOH:O	2.20	0.41
2:B:336:TRP:O	2:B:348:MET:HB2	2.21	0.41
2:B:329:ILE:HG23	2:B:371:ARG:HH11	1.86	0.41
4:A:858:HOH:O	2:B:400:MET:HG2	2.21	0.40
1:A:82:ASP:O	1:A:104:LEU:HD13	2.20	0.40
2:B:424:LEU:HB2	2:B:439:GLY:C	2.42	0.40
2:B:440:CYS:HB2	2:B:455:TRP:CH2	2.57	0.40
2:B:301:GLU:HA	4:B:1217:HOH:O	2.22	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	212/214 (99%)	204 (96%)	8 (4%)	0	100 100
2	B	208/210 (99%)	192 (92%)	15 (7%)	1 (0%)	34 30
3	C	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	24 17
All	All	547/553 (99%)	514 (94%)	31 (6%)	2 (0%)	39 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	430	ASP
3	C	648	ASP

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	190/193 (98%)	184 (97%)	6 (3%)	46 48
2	B	189/189 (100%)	184 (97%)	5 (3%)	54 58
3	C	105/105 (100%)	104 (99%)	1 (1%)	82 87
All	All	484/487 (99%)	472 (98%)	12 (2%)	55 59

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	31	ASN
1	A	93	SER
1	A	105	GLU
1	A	157	ASN
1	A	211	ARG
2	B	383	ASN
2	B	384	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	449	PRO
2	B	463	SER
2	B	485	LEU
3	C	729	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	32	ASN
1	A	53	GLN
1	A	89	GLN
1	A	92	ASN
2	B	303	GLN
2	B	305	GLN
2	B	360	HIS
2	B	405	GLN
2	B	477	GLN
3	C	615	HIS
3	C	641	GLN
3	C	693	ASN
3	C	713	ASN
3	C	721	GLN

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	214/214 (100%)	0.07	3 (1%)	78	82	7, 16, 30, 43	0
2	B	210/210 (100%)	0.35	11 (5%)	31	39	8, 15, 34, 68	0
3	C	129/129 (100%)	0.45	11 (8%)	13	18	8, 18, 43, 66	0
All	All	553/553 (100%)	0.26	25 (4%)	37	46	7, 16, 39, 68	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	432	THR	10.5
2	B	431	THR	6.5
2	B	478	SER	6.0
1	A	41	HIS	5.9
3	C	647	THR	5.4
3	C	728	ARG	4.6
2	B	331	SER	4.5
3	C	729	LEU	4.1
2	B	430	ASP	3.9
2	B	315	SER	3.7
1	A	40	SER	3.4
3	C	648	ASP	3.2
1	A	80	THR	3.1
2	B	330	THR	2.9
3	C	673	ARG	2.8
3	C	670	PRO	2.7
2	B	373	THR	2.7
3	C	662	TRP	2.6
3	C	672	SER	2.6
3	C	677	ASN	2.3
3	C	644	ASN	2.3
2	B	301	GLU	2.3
3	C	668	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	343	ASN	2.1
2	B	433	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.