wwPDB X-ray Structure Validation Summary Report (i)

Oct 7, 2026 – 07:05 pm BST

PDB ID	:	9TUY / pdb_00009tuy
Title	:	PfRIPR EGF5 and 6 bound to monoclonal antibody MAD8-739
Authors	:	Farrell, B.; Higgins, M.K.
Deposited on	:	2026-01-10
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

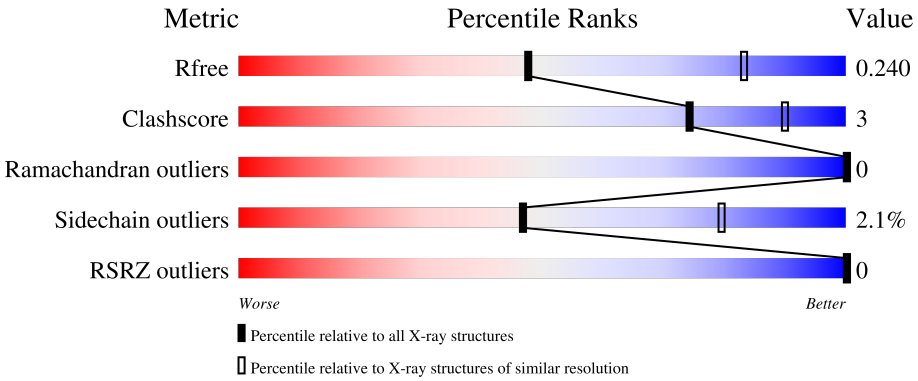
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 of 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	288	74% 9% 17%
1	C	288	73% 10% 17%
2	B	359	25% · 73%
2	D	359	25% · 73%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5143 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 MAD8-739 scFv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1768	1103	303	356	6			
1	C	239	Total	C	N	O	S	0	0	0
			1768	1103	303	356	6			

- Molecule 2 is a protein called Immunoglobulin gamma-1 heavy chain,Rh5-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			772	466	135	155	16			
2	D	98	Total	C	N	O	S	0	0	0
			772	466	135	155	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	468	MET	-	initiating methionine	UNP P0DOX5
B	469	GLY	-	expression tag	UNP P0DOX5
B	470	TRP	-	expression tag	UNP P0DOX5
B	471	SER	-	expression tag	UNP P0DOX5
B	472	CYS	-	expression tag	UNP P0DOX5
B	473	ILE	-	expression tag	UNP P0DOX5
B	474	ILE	-	expression tag	UNP P0DOX5
B	475	LEU	-	expression tag	UNP P0DOX5
B	476	PHE	-	expression tag	UNP P0DOX5
B	477	LEU	-	expression tag	UNP P0DOX5
B	478	VAL	-	expression tag	UNP P0DOX5
B	479	ALA	-	expression tag	UNP P0DOX5
B	480	THR	-	expression tag	UNP P0DOX5
B	481	ALA	-	expression tag	UNP P0DOX5
B	482	THR	-	expression tag	UNP P0DOX5
B	483	GLY	-	expression tag	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	484	VAL	-	expression tag	UNP P0DOX5
B	485	HIS	-	expression tag	UNP P0DOX5
B	486	SER	-	expression tag	UNP P0DOX5
B	615	ASN	SER	conflict	UNP P0DOX5
B	658	ASN	TYR	conflict	UNP P0DOX5
B	699	GLY	-	linker	UNP P0DOX5
B	700	GLY	-	linker	UNP P0DOX5
B	701	GLY	-	linker	UNP P0DOX5
B	702	GLY	-	linker	UNP P0DOX5
B	703	SER	-	linker	UNP P0DOX5
B	704	GLY	-	linker	UNP P0DOX5
B	705	GLY	-	linker	UNP P0DOX5
B	706	GLY	-	linker	UNP P0DOX5
B	707	SER	-	linker	UNP P0DOX5
B	708	GLU	-	linker	UNP P0DOX5
B	709	ASN	-	linker	UNP P0DOX5
B	710	LEU	-	linker	UNP P0DOX5
B	711	TYR	-	linker	UNP P0DOX5
B	712	PHE	-	linker	UNP P0DOX5
B	713	GLN	-	linker	UNP P0DOX5
B	714	GLY	-	linker	UNP P0DOX5
B	715	SER	-	linker	UNP P0DOX5
B	817	GLY	-	expression tag	UNP O97302
B	818	GLY	-	expression tag	UNP O97302
B	819	THR	-	expression tag	UNP O97302
B	820	GLY	-	expression tag	UNP O97302
B	821	GLY	-	expression tag	UNP O97302
B	822	SER	-	expression tag	UNP O97302
B	823	GLU	-	expression tag	UNP O97302
B	824	PRO	-	expression tag	UNP O97302
B	825	GLU	-	expression tag	UNP O97302
B	826	ALA	-	expression tag	UNP O97302
D	468	MET	-	initiating methionine	UNP P0DOX5
D	469	GLY	-	expression tag	UNP P0DOX5
D	470	TRP	-	expression tag	UNP P0DOX5
D	471	SER	-	expression tag	UNP P0DOX5
D	472	CYS	-	expression tag	UNP P0DOX5
D	473	ILE	-	expression tag	UNP P0DOX5
D	474	ILE	-	expression tag	UNP P0DOX5
D	475	LEU	-	expression tag	UNP P0DOX5
D	476	PHE	-	expression tag	UNP P0DOX5
D	477	LEU	-	expression tag	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	478	VAL	-	expression tag	UNP P0DOX5
D	479	ALA	-	expression tag	UNP P0DOX5
D	480	THR	-	expression tag	UNP P0DOX5
D	481	ALA	-	expression tag	UNP P0DOX5
D	482	THR	-	expression tag	UNP P0DOX5
D	483	GLY	-	expression tag	UNP P0DOX5
D	484	VAL	-	expression tag	UNP P0DOX5
D	485	HIS	-	expression tag	UNP P0DOX5
D	486	SER	-	expression tag	UNP P0DOX5
D	615	ASN	SER	conflict	UNP P0DOX5
D	658	ASN	TYR	conflict	UNP P0DOX5
D	699	GLY	-	linker	UNP P0DOX5
D	700	GLY	-	linker	UNP P0DOX5
D	701	GLY	-	linker	UNP P0DOX5
D	702	GLY	-	linker	UNP P0DOX5
D	703	SER	-	linker	UNP P0DOX5
D	704	GLY	-	linker	UNP P0DOX5
D	705	GLY	-	linker	UNP P0DOX5
D	706	GLY	-	linker	UNP P0DOX5
D	707	SER	-	linker	UNP P0DOX5
D	708	GLU	-	linker	UNP P0DOX5
D	709	ASN	-	linker	UNP P0DOX5
D	710	LEU	-	linker	UNP P0DOX5
D	711	TYR	-	linker	UNP P0DOX5
D	712	PHE	-	linker	UNP P0DOX5
D	713	GLN	-	linker	UNP P0DOX5
D	714	GLY	-	linker	UNP P0DOX5
D	715	SER	-	linker	UNP P0DOX5
D	817	GLY	-	expression tag	UNP O97302
D	818	GLY	-	expression tag	UNP O97302
D	819	THR	-	expression tag	UNP O97302
D	820	GLY	-	expression tag	UNP O97302
D	821	GLY	-	expression tag	UNP O97302
D	822	SER	-	expression tag	UNP O97302
D	823	GLU	-	expression tag	UNP O97302
D	824	PRO	-	expression tag	UNP O97302
D	825	GLU	-	expression tag	UNP O97302
D	826	ALA	-	expression tag	UNP O97302

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	11	Total O 11 11	0	0
3	C	23	Total O 23 23	0	0
3	D	5	Total O 5 5	0	0

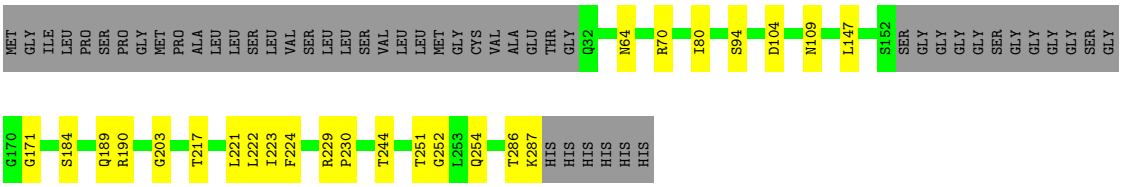
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: MAD8-739 scFv

Chain A:

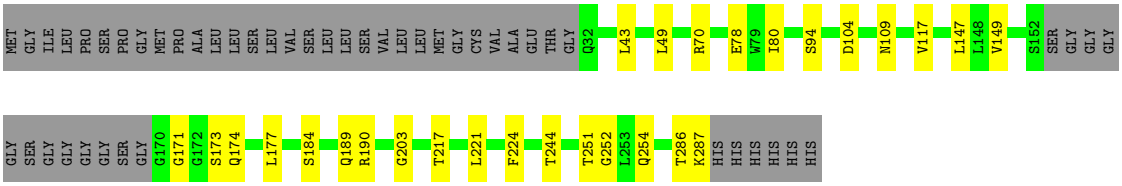




• Molecule 1: MAD8-739 scFv

Chain C:

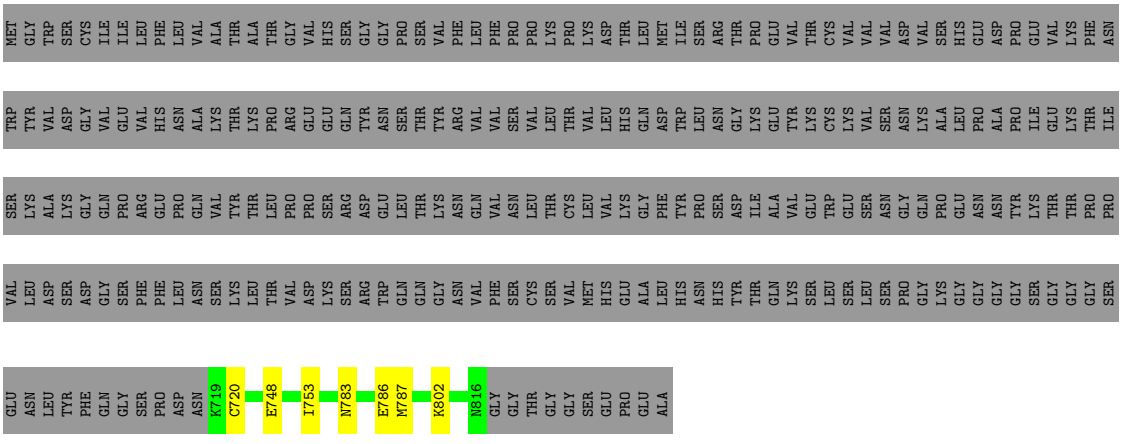




• Molecule 2: Immunoglobulin gamma-1 heavy chain,Rh5-interacting protein

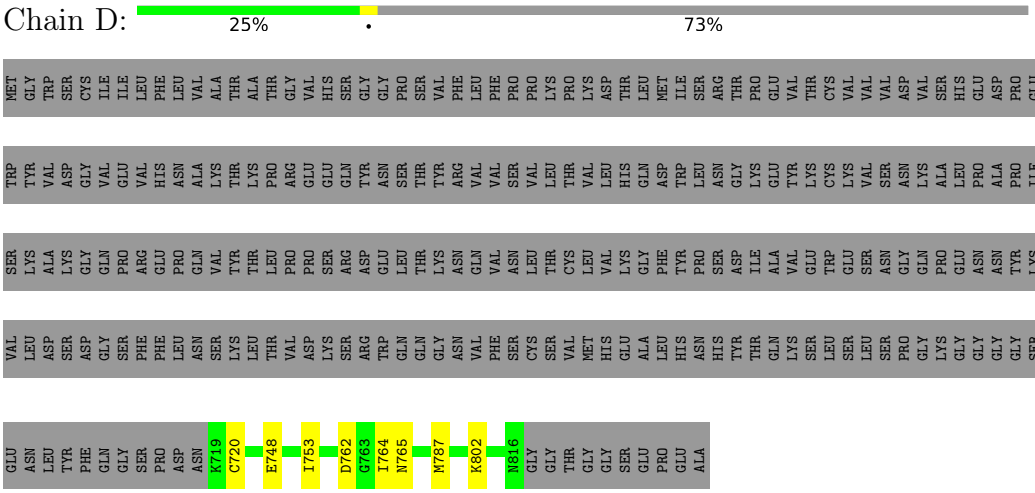
Chain B:





• Molecule 2: Immunoglobulin gamma-1 heavy chain,Rh5-interacting protein

Chain D:


25%
73%
MET GLY TRP SER CYS ILE ILE LEU PHE LEU VAL ALA THR ALA THR GLY VAL HIS SER GLY GLY PRO SER VAL PHE LEU PHE PRO PRO LYS PRO LYS ASP THR LEU MET ILE SER ARG THR PRO GLU VAL THR CYS VAL VAL VAL ASP VAL SER HIS GLU ASP PRO GLU VAL LYS PHE ASN
TRP TYR VAL ASP GLY VAL GLU VAL HIS ASN ALA LYS THR LYS PRO ARG GLU GLU GLN TYR ASN SER THR TYR ARG VAL VAL SER VAL LEU THR VAL LEU HIS GLN ASP TRP LEU ASN GLY LYS GLU TYR LYS CYS LYS VAL SER ASN LYS ALA LEU PRO ALA PRO ILE GLU LYS THR ILE
SER LYS ALA LYS GLY GLN PRO ARG GLU PRO GLN VAL TYR THR LEU PRO PRO SER ARG ASP GLU LEU THR LYS ASN GLN VAL ASN LEU THR CYS LEU VAL LYS GLY PHE TYR PRO SER ASP ILE ALA VAL GLU TRP GLU SER ASN GLY GLN PRO GLU ASN ASN TYR LYS THR THR PRO PRO
VAL LEU ASP SER ASP GLY SER PHE PHE LEU ASN SER LYS LEU THR VAL ASP LYS SER ARG TRP GLN GLN GLY ASN VAL PHE SER CYS SER VAL MET HIS GLU ALA LEU HIS ASN HIS TYR THR GLN LYS SER LEU SER LEU SER PRO GLY LYS GLY GLY GLY GLY SER GLY GLY GLY SER
GLU ASN LEU TYR PHE GLN GLY SER PRO ASP ASN K719 C720 E748 I753 D762 G763 I764 N765 M787 K802 N816 GLY GLY THR GLY GLY SER GLU PRO GLU ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	89.64Å 89.64Å 141.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.02 – 2.80 34.02 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.02-2.80) 100.0 (34.02-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.4 (10-JUL-2024)	Depositor
R, R_{free}	0.228 , 0.255 0.218 , 0.240	Depositor DCC
R_{free} test set	1520 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	68.7	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.460 for h,-h-k,-l 0.001 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5143	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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, 0.333 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	0.66	0/1805	0.95	0/2451
1	C	0.66	0/1805	0.97	0/2451
2	B	0.57	0/780	0.92	0/1043
2	D	0.58	0/780	0.90	0/1043
All	All	0.64	0/5170	0.94	0/6988

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	1768	0	1722	12	0
1	C	1768	0	1722	13	0
2	B	772	0	733	3	0
2	D	772	0	733	3	0
3	A	24	0	0	0	0
3	B	11	0	0	0	0
3	C	23	0	0	0	0
3	D	5	0	0	0	0
All	All	5143	0	4910	31	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 3.

The worst 5 of 31 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:C:78:GLU:HG3	1:C:173:SER:HB3	1.77	0.66
1:A:189:GLN:HG2	1:A:190:ARG:N	2.19	0.58
1:C:43:LEU:HD23	1:C:117:VAL:HG21	1.86	0.58
1:C:189:GLN:HG2	1:C:190:ARG:N	2.19	0.57
1:A:190:ARG:HG3	1:A:251:THR:HG22	1.91	0.53

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	235/288 (82%)	223 (95%)	12 (5%)	0	100	100
1	C	235/288 (82%)	222 (94%)	13 (6%)	0	100	100
2	B	96/359 (27%)	88 (92%)	8 (8%)	0	100	100
2	D	96/359 (27%)	92 (96%)	4 (4%)	0	100	100
All	All	662/1294 (51%)	625 (94%)	37 (6%)	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	195/229 (85%)	191 (98%)	4 (2%)	47 79
1	C	195/229 (85%)	190 (97%)	5 (3%)	40 75
2	B	91/319 (28%)	90 (99%)	1 (1%)	65 87
2	D	91/319 (28%)	89 (98%)	2 (2%)	45 78
All	All	572/1096 (52%)	560 (98%)	12 (2%)	47 79

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	177	LEU
1	C	184	SER
2	D	764	ILE
1	C	217	THR
1	A	217	THR

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

Mol	Chain	Res	Type
2	B	779	ASN
1	C	64	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 oligosaccharides 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

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, 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(Å^2)	Q<0.9
1	A	239/288 (82%)	-1.38	0	100	100	65, 76, 92, 109	0
1	C	239/288 (82%)	-1.39	0	100	100	64, 76, 92, 115	0
2	B	98/359 (27%)	-1.21	0	100	100	76, 100, 131, 150	0
2	D	98/359 (27%)	-1.22	0	100	100	79, 99, 130, 144	0
All	All	674/1294 (52%)	-1.34	0	100	100	64, 80, 119, 150	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.