Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 12:28 AM EDT

PDB ID	:	5MGX
Title	:	The structure of FKBP38 in complex with the MEEVD tetratricopeptide binding-motif of Hsp90
Authors	:	Roe, S.M.; Blundell, K.L.; Prodromou, C.
Deposited on	:	2016-11-22
Resolution	:	2.18 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 ⓘ 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 ⓘ) were used in the production of this report:

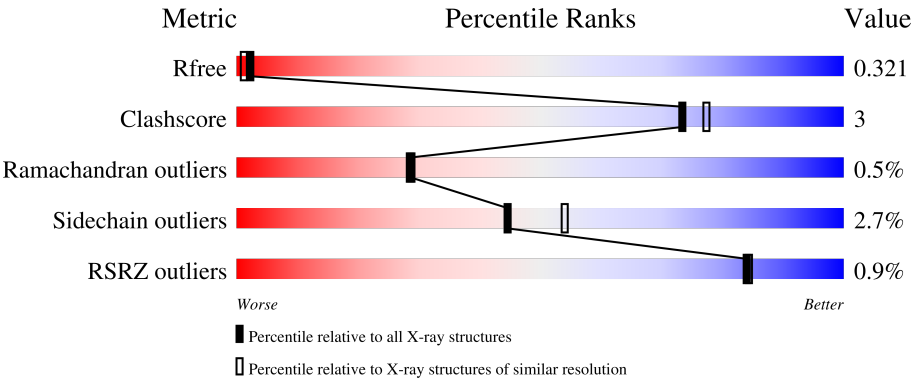
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	8	62% 12% 25%
1	B	8	88% 12%
1	C	8	75% 25%
1	D	8	50% 50%
2	E	290	81% 10% 9%

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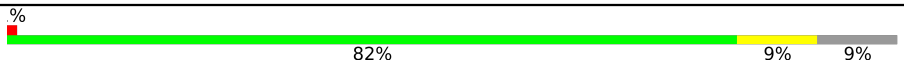
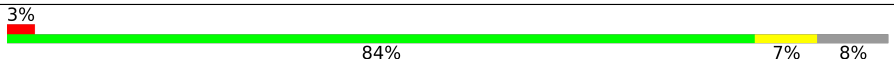
Mol	Chain	Length	Quality of chain
2	F	290	
2	G	290	
2	H	290	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9225 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 yeast HSP90 C-terminus.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	8	Total	C	N	O	S	0	0	0
			62	35	8	18	1			
1	B	8	Total	C	N	O	S	0	0	0
			66	37	8	20	1			
1	C	6	Total	C	N	O	S	0	0	0
			50	29	5	15	1			
1	D	4	Total	C	N	O	S	0	0	0
			31	18	4	8	1			

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	265	Total	C	N	O	S	0	0	0
			2006	1268	352	376	10			
2	F	265	Total	C	N	O	S	3	0	0
			1996	1260	349	377	10			
2	G	266	Total	C	N	O	S	0	0	0
			2016	1276	346	384	10			
2	H	266	Total	C	N	O	S	2	0	0
			1940	1229	334	368	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	24	Total	O	0	0
			24	24		
3	C	20	Total	O	0	0
			20	20		
3	D	3	Total	O	0	0
			3	3		

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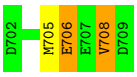
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	332	Total O 332 332	0	0
3	F	211	Total O 211 211	0	0
3	G	289	Total O 289 289	0	0
3	H	167	Total O 167 167	0	0

3 Residue-property plots

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: yeast HSP90 C-terminus

Chain A:



• Molecule 1: yeast HSP90 C-terminus

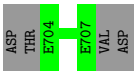
Chain B:

• Molecule 1: yeast HSP90 C-terminus

Chain C:

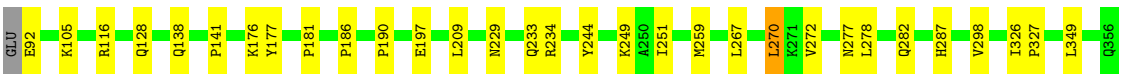
• Molecule 1: yeast HSP90 C-terminus

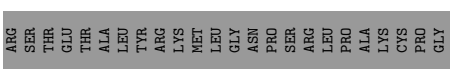
Chain D:



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP8

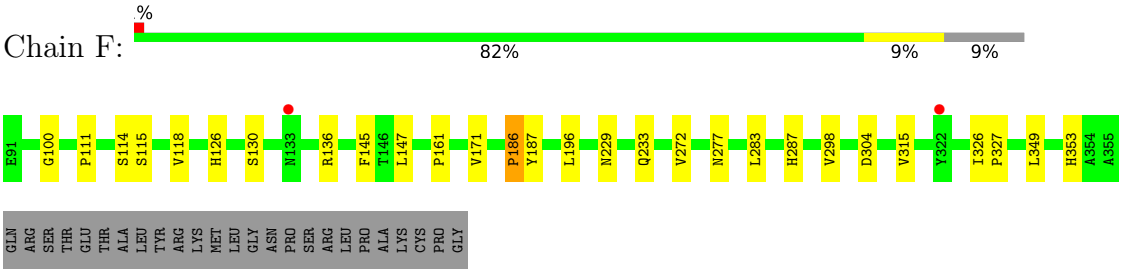
Chain E:





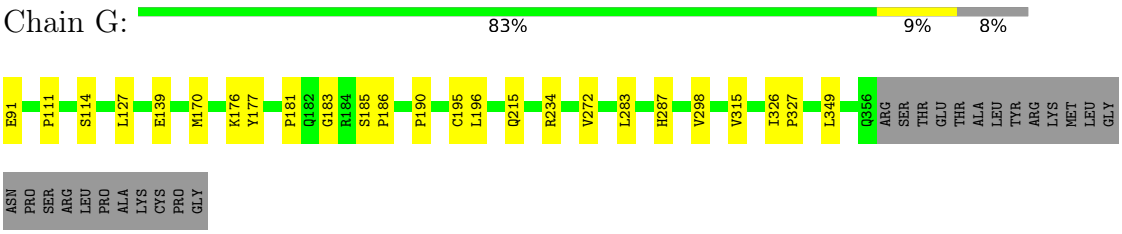
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP8

Chain F:



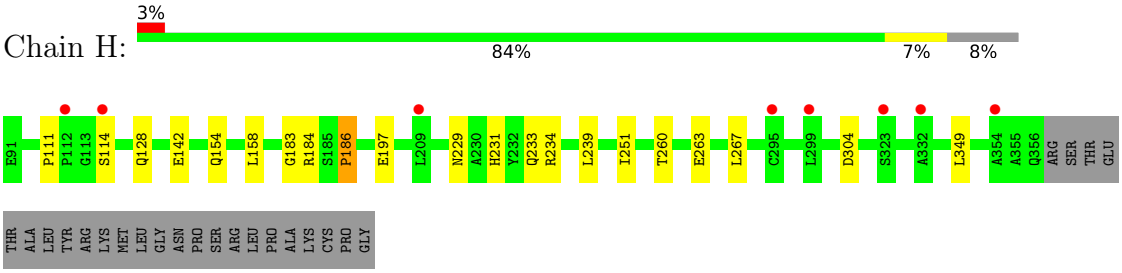
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP8

Chain G:



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP8

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.29Å 105.64Å 100.19Å 90.00° 93.10° 90.00°	Depositor
Resolution (Å)	100.00 – 2.18 100.04 – 2.18	Depositor EDS
% Data completeness (in resolution range)	94.7 (100.00-2.18) 80.6 (100.04-2.18)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.18Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.246 , 0.308 0.255 , 0.321	Depositor DCC
R_{free} test set	3525 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.977	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9225	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.1936e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.56	0/61	1.10	0/80
1	B	0.51	0/65	0.94	0/85
1	C	0.58	0/49	0.81	0/62
1	D	0.59	0/30	0.79	0/38
2	E	0.46	0/2039	0.65	1/2766 (0.0%)
2	F	0.42	0/2029	0.64	1/2756 (0.0%)
2	G	0.45	0/2049	0.66	1/2780 (0.0%)
2	H	0.44	0/1971	0.67	1/2687 (0.0%)
All	All	0.45	0/8293	0.66	4/11254 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	186	PRO	C-N-CA	6.62	138.24	121.70
2	G	186	PRO	C-N-CA	6.03	136.76	121.70
2	H	186	PRO	C-N-CA	5.98	136.65	121.70
2	F	186	PRO	C-N-CA	5.67	135.87	121.70

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	62	0	46	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	66	0	50	0	0
1	C	50	0	38	0	0
1	D	31	0	22	0	0
2	E	2006	0	2050	17	0
2	F	1996	0	2013	11	0
2	G	2016	0	2044	13	0
2	H	1940	0	1905	12	0
3	A	12	0	0	0	0
3	B	24	0	0	0	0
3	C	20	0	0	0	0
3	D	3	0	0	0	0
3	E	332	0	0	2	0
3	F	211	0	0	0	0
3	G	289	0	0	0	0
3	H	167	0	0	0	0
All	All	9225	0	8168	54	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.

All (54) 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:H:184:ARG:HG3	2:H:186:PRO:HD2	1.25	1.11
2:E:278:LEU:O	2:E:282:GLN:HG3	1.75	0.87
2:F:147:LEU:HD21	2:F:161:PRO:HG3	1.58	0.83
2:F:171:VAL:HG23	2:F:196:LEU:HB2	1.62	0.82
2:H:184:ARG:CG	2:H:186:PRO:HD2	2.07	0.82
2:G:181:PRO:O	2:G:190:PRO:HB3	1.91	0.69
2:H:184:ARG:HG3	2:H:186:PRO:CD	2.17	0.63
2:H:183:GLY:O	2:H:234:ARG:HG3	2.00	0.61
2:E:259:MET:CE	2:E:267:LEU:HD12	2.31	0.60
2:F:171:VAL:CG2	2:F:196:LEU:HB2	2.31	0.60
2:H:128:GLN:HB2	2:H:197:GLU:HB2	1.84	0.59
2:E:259:MET:HE1	2:E:267:LEU:HD12	1.85	0.57
2:F:229:ASN:O	2:F:233:GLN:HG2	2.06	0.56
2:H:229:ASN:O	2:H:233:GLN:HG2	2.06	0.56
1:A:705:MET:O	1:A:706:GLU:HB2	2.06	0.55
2:E:251:ILE:HD11	2:E:270:LEU:HD22	1.89	0.54
2:E:229:ASN:O	2:E:233:GLN:HG2	2.09	0.53
2:F:272:VAL:HG13	2:F:298:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:272:VAL:HG13	2:E:298:VAL:HG13	1.91	0.52
2:H:154:GLN:O	2:H:158:LEU:HD23	2.09	0.52
2:F:326:ILE:HG23	2:F:327:PRO:HD3	1.92	0.52
2:G:272:VAL:HG13	2:G:298:VAL:HG13	1.92	0.52
2:G:183:GLY:O	2:G:234:ARG:HG3	2.09	0.52
2:F:283:LEU:HD13	2:F:315:VAL:HG22	1.94	0.50
2:E:326:ILE:HG23	2:E:327:PRO:HD3	1.94	0.49
2:G:111:PRO:HG2	2:G:114:SER:HB3	1.95	0.49
2:G:326:ILE:HG23	2:G:327:PRO:HD3	1.94	0.49
2:E:259:MET:HE1	2:E:267:LEU:CD1	2.42	0.49
1:A:708:VAL:HG22	2:F:277:ASN:CG	2.33	0.48
2:E:244:TYR:CZ	2:E:277:ASN:HB3	2.49	0.48
2:G:196:LEU:N	2:G:196:LEU:HD12	2.28	0.47
2:F:130:SER:HB3	2:F:136:ARG:HD2	1.96	0.47
2:F:111:PRO:HG2	2:F:114:SER:HB3	1.98	0.46
2:H:111:PRO:HG2	2:H:114:SER:HB3	1.97	0.46
2:G:127:LEU:HD11	2:G:196:LEU:HB3	1.97	0.46
2:H:231:HIS:CE1	2:H:239:LEU:HD23	2.51	0.46
2:E:259:MET:CE	2:E:267:LEU:CD1	2.95	0.45
2:H:154:GLN:O	2:H:158:LEU:CD2	2.66	0.44
2:G:170:MET:CE	2:G:195:CYS:HB3	2.47	0.44
2:G:283:LEU:HD13	2:G:315:VAL:HG22	2.00	0.44
2:E:92:GLU:HB3	2:E:105:LYS:HE3	2.00	0.43
2:E:128:GLN:HB2	2:E:197:GLU:HB3	2.00	0.43
2:H:251:ILE:HG12	2:H:267:LEU:HD23	2.00	0.43
3:E:520:HOH:O	2:G:287:HIS:HB2	2.18	0.43
2:E:181:PRO:O	2:E:190:PRO:HB3	2.18	0.42
2:E:259:MET:HE3	2:E:267:LEU:HD12	2.00	0.42
2:F:283:LEU:HD13	2:F:315:VAL:CG2	2.49	0.42
2:G:176:LYS:HD2	2:G:177:TYR:CZ	2.55	0.42
2:G:272:VAL:CG1	2:G:298:VAL:HG13	2.50	0.41
2:E:209:LEU:HD11	2:E:249:LYS:HE2	2.03	0.41
2:G:170:MET:HE2	2:G:195:CYS:HB3	2.03	0.40
2:E:116:ARG:HD3	3:E:455:HOH:O	2.22	0.40
2:H:260:THR:HG23	2:H:263:GLU:H	1.85	0.40
2:E:176:LYS:HD2	2:E:177:TYR:CZ	2.57	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	6/8 (75%)	5 (83%)	0	1 (17%)	0 0
1	B	6/8 (75%)	6 (100%)	0	0	100 100
1	C	4/8 (50%)	4 (100%)	0	0	100 100
1	D	2/8 (25%)	0	2 (100%)	0	100 100
2	E	263/290 (91%)	254 (97%)	7 (3%)	2 (1%)	19 17
2	F	263/290 (91%)	250 (95%)	11 (4%)	2 (1%)	19 17
2	G	264/290 (91%)	258 (98%)	6 (2%)	0	100 100
2	H	264/290 (91%)	257 (97%)	7 (3%)	0	100 100
All	All	1072/1192 (90%)	1034 (96%)	33 (3%)	5 (0%)	29 28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	187	TYR
2	E	141	PRO
2	E	138	GLN
1	A	706	GLU
2	F	100	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	7/8 (88%)	6 (86%)	1 (14%)	3 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	8/8 (100%)	7 (88%)	1 (12%)	4 3
1	C	5/8 (62%)	5 (100%)	0	100 100
1	D	3/8 (38%)	3 (100%)	0	100 100
2	E	215/243 (88%)	211 (98%)	4 (2%)	57 68
2	F	211/243 (87%)	202 (96%)	9 (4%)	29 34
2	G	215/243 (88%)	210 (98%)	5 (2%)	50 60
2	H	195/243 (80%)	192 (98%)	3 (2%)	65 76
All	All	859/1004 (86%)	836 (97%)	23 (3%)	44 54

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

Mol	Chain	Res	Type
1	A	708	VAL
1	B	708	VAL
2	E	234	ARG
2	E	270	LEU
2	E	287	HIS
2	E	349	LEU
2	F	115	SER
2	F	118	VAL
2	F	126	HIS
2	F	145	PHE
2	F	186	PRO
2	F	287	HIS
2	F	304	ASP
2	F	349	LEU
2	F	353	HIS
2	G	91	GLU
2	G	139	GLU
2	G	185	SER
2	G	215	GLN
2	G	349	LEU
2	H	142	GLU
2	H	304	ASP
2	H	349	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	121	GLN
2	G	231	HIS
2	H	126	HIS
2	H	353	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 monosaccharides 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	8/8 (100%)	-0.02	0 100 100	27, 40, 48, 52	0
1	B	8/8 (100%)	-0.11	0 100 100	26, 31, 42, 44	0
1	C	6/8 (75%)	-0.56	0 100 100	18, 21, 23, 30	0
1	D	4/8 (50%)	-0.02	0 100 100	54, 56, 64, 68	0
2	E	265/290 (91%)	-0.11	0 100 100	7, 23, 48, 67	0
2	F	265/290 (91%)	0.14	2 (0%) 86 86	21, 37, 59, 85	2 (0%)
2	G	266/290 (91%)	-0.07	0 100 100	7, 24, 47, 61	0
2	H	266/290 (91%)	0.32	8 (3%) 50 51	21, 42, 66, 87	2 (0%)
All	All	1088/1192 (91%)	0.06	10 (0%) 84 84	7, 31, 59, 87	4 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	322	TYR	3.3
2	H	299	LEU	2.5
2	F	133	ASN	2.4
2	H	209	LEU	2.3
2	H	323	SER	2.3
2	H	332	ALA	2.2
2	H	114	SER	2.1
2	H	295	CYS	2.1
2	H	354	ALA	2.0
2	H	112	PRO	2.0

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 (i)

There are no monosaccharides 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.