Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2026 – 11:24 AM UTC

PDB ID	:	3RSW / pdb_00003rsw
Title	:	Crystal Structure of Heart Fatty Acid Binding Protein (FABP3)
Authors	:	Carney, D.F.; Shankaran, B.; Zwart, P.H.; Stebbins, J.W.; Prasad, G.S.
Deposited on	:	2011-05-02
Resolution	:	2.60 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 (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:

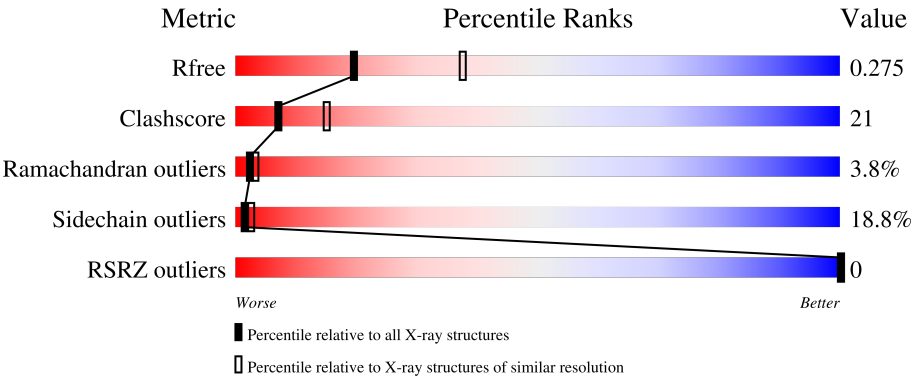
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	158	39% 37% 7% • 16%
1	B	158	47% 28% 9% 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2123 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 Fatty acid-binding protein, heart.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1043	662	173	204	4			
1	B	133	Total	C	N	O	S	0	0	0
			1043	662	173	204	4			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	expression tag	UNP P05413
A	-23	GLY	-	expression tag	UNP P05413
A	-22	SER	-	expression tag	UNP P05413
A	-21	SER	-	expression tag	UNP P05413
A	-20	HIS	-	expression tag	UNP P05413
A	-19	HIS	-	expression tag	UNP P05413
A	-18	HIS	-	expression tag	UNP P05413
A	-17	HIS	-	expression tag	UNP P05413
A	-16	HIS	-	expression tag	UNP P05413
A	-15	HIS	-	expression tag	UNP P05413
A	-14	SER	-	expression tag	UNP P05413
A	-13	SER	-	expression tag	UNP P05413
A	-12	GLY	-	expression tag	UNP P05413
A	-11	LEU	-	expression tag	UNP P05413
A	-10	VAL	-	expression tag	UNP P05413
A	-9	PRO	-	expression tag	UNP P05413
A	-8	ARG	-	expression tag	UNP P05413
A	-7	GLY	-	expression tag	UNP P05413
A	-6	SER	-	expression tag	UNP P05413
A	-5	HIS	-	expression tag	UNP P05413
A	-4	MET	-	expression tag	UNP P05413
A	-3	LEU	-	expression tag	UNP P05413
A	-2	GLN	-	expression tag	UNP P05413
A	-1	ASP	-	expression tag	UNP P05413
A	0	LEU	-	expression tag	UNP P05413

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	MET	-	expression tag	UNP P05413
B	-23	GLY	-	expression tag	UNP P05413
B	-22	SER	-	expression tag	UNP P05413
B	-21	SER	-	expression tag	UNP P05413
B	-20	HIS	-	expression tag	UNP P05413
B	-19	HIS	-	expression tag	UNP P05413
B	-18	HIS	-	expression tag	UNP P05413
B	-17	HIS	-	expression tag	UNP P05413
B	-16	HIS	-	expression tag	UNP P05413
B	-15	HIS	-	expression tag	UNP P05413
B	-14	SER	-	expression tag	UNP P05413
B	-13	SER	-	expression tag	UNP P05413
B	-12	GLY	-	expression tag	UNP P05413
B	-11	LEU	-	expression tag	UNP P05413
B	-10	VAL	-	expression tag	UNP P05413
B	-9	PRO	-	expression tag	UNP P05413
B	-8	ARG	-	expression tag	UNP P05413
B	-7	GLY	-	expression tag	UNP P05413
B	-6	SER	-	expression tag	UNP P05413
B	-5	HIS	-	expression tag	UNP P05413
B	-4	MET	-	expression tag	UNP P05413
B	-3	LEU	-	expression tag	UNP P05413
B	-2	GLN	-	expression tag	UNP P05413
B	-1	ASP	-	expression tag	UNP P05413
B	0	LEU	-	expression tag	UNP P05413

- Molecule 2 is water.

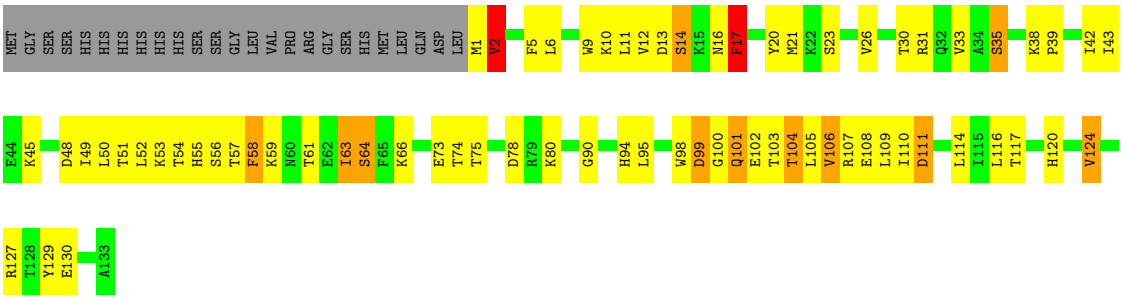
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	21	Total O 21 21	0	0
2	B	16	Total O 16 16	0	0

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.

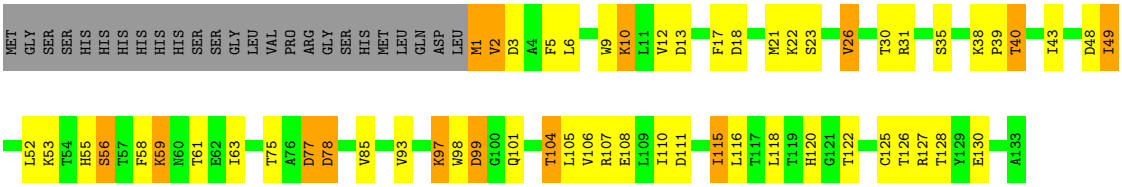
• Molecule 1: Fatty acid-binding protein, heart

Chain A:



• Molecule 1: Fatty acid-binding protein, heart

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	42.47Å 42.47Å 168.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.48 – 2.60 42.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.48-2.60) 99.9 (42.47-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.273 0.230 , 0.275	Depositor DCC
R_{free} test set	437 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	54.9	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
Reported twinning fraction	0.513 for H, K, L 0.487 for K, H, -L	Depositor
Outliers	0 of 9186 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2123	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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	0.97	1/1058 (0.1%)	1.12	4/1427 (0.3%)
1	B	1.02	0/1058	1.23	2/1427 (0.1%)
All	All	1.00	1/2116 (0.0%)	1.18	6/2854 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	VAL	CA-CB	5.62	1.62	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	49	ILE	N-CA-C	6.22	116.58	107.37
1	A	74	THR	N-CA-C	-5.52	100.18	109.07
1	A	78	ASP	N-CA-C	5.45	119.23	112.58
1	A	102	GLU	N-CA-C	5.28	116.17	108.14
1	B	18	ASP	N-CA-C	-5.19	105.54	111.14
1	A	106	VAL	CB-CA-C	-5.17	104.71	110.96

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	1043	0	1066	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1043	0	1066	41	1
2	A	21	0	0	5	1
2	B	16	0	0	2	0
All	All	2123	0	2132	88	1

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 21.

All (88) 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:101:GLN:HE21	1:B:120:HIS:CE1	1.74	1.06
1:B:101:GLN:HE21	1:B:120:HIS:HE1	0.98	0.97
1:A:52:LEU:HD12	1:A:63:ILE:HD11	1.54	0.89
1:B:107:ARG:HG3	1:B:116:LEU:HD13	1.58	0.84
1:B:10:LYS:HE2	1:B:40:THR:HB	1.60	0.83
1:A:104:THR:HG23	1:A:106:VAL:HG23	1.59	0.83
1:A:2:VAL:HA	2:A:144:HOH:O	1.78	0.81
1:A:14:SER:HB2	1:A:127:ARG:HG2	1.64	0.80
1:B:104:THR:HG23	1:B:106:VAL:HG23	1.62	0.80
1:B:1:MET:O	1:B:2:VAL:HG12	1.83	0.78
1:A:11:LEU:HD11	1:A:13:ASP:O	1.83	0.77
1:B:12:VAL:HG21	1:B:130:GLU:HG3	1.68	0.75
1:A:23:SER:OG	1:A:120:HIS:HD2	1.71	0.74
1:B:1:MET:O	1:B:1:MET:HG2	1.88	0.73
1:B:3:ASP:HA	1:B:6:LEU:HD13	1.71	0.72
1:A:107:ARG:HG2	1:A:116:LEU:HD13	1.72	0.71
1:B:101:GLN:NE2	1:B:120:HIS:HE1	1.81	0.71
1:B:21:MET:O	1:B:26:VAL:HG23	1.90	0.71
1:B:10:LYS:CE	1:B:40:THR:HB	2.21	0.70
1:A:104:THR:HG22	2:A:137:HOH:O	1.94	0.68
1:B:101:GLN:NE2	1:B:120:HIS:CE1	2.57	0.68
1:A:6:LEU:HD11	1:A:45:LYS:HB2	1.77	0.67
1:A:104:THR:CG2	1:A:106:VAL:HG23	2.25	0.67
1:A:39:PRO:HB3	1:A:56:SER:HB3	1.77	0.65
1:A:12:VAL:HG11	1:A:130:GLU:HG3	1.77	0.65
1:B:12:VAL:CG2	1:B:130:GLU:HG3	2.27	0.64
1:A:9:TRP:HB3	1:A:129:TYR:HB3	1.79	0.64
1:B:105:LEU:HG	1:B:118:LEU:HD22	1.82	0.62
1:A:17:PHE:N	1:A:17:PHE:HD2	1.97	0.62
1:A:17:PHE:N	1:A:17:PHE:CD2	2.69	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:C	1:B:2:VAL:HG12	2.28	0.59
1:B:110:ILE:HB	1:B:115:ILE:HG13	1.85	0.59
1:A:31:ARG:O	1:A:35:SER:HB3	2.02	0.58
1:B:5:PHE:O	1:B:9:TRP:CZ3	2.58	0.56
1:A:98:TRP:O	1:A:99:ASP:C	2.47	0.56
1:A:101:GLN:HE21	1:A:120:HIS:HE1	1.53	0.55
1:A:12:VAL:CG1	1:A:130:GLU:HG3	2.36	0.55
1:B:43:ILE:HG12	1:B:52:LEU:HD22	1.88	0.55
1:B:10:LYS:HE2	1:B:40:THR:CB	2.36	0.55
1:A:48:ASP:HB3	1:A:66:LYS:HE3	1.90	0.54
1:B:55:HIS:O	1:B:56:SER:HB3	2.08	0.54
1:A:54:THR:HB	1:A:61:THR:OG1	2.08	0.52
1:B:106:VAL:O	1:B:116:LEU:HA	2.10	0.52
1:B:12:VAL:HG21	1:B:130:GLU:CG	2.40	0.51
1:A:52:LEU:HD13	1:A:107:ARG:HH21	1.76	0.51
1:A:107:ARG:CG	1:A:116:LEU:HD13	2.40	0.51
1:B:127:ARG:NH1	2:B:134:HOH:O	2.44	0.51
1:B:53:LYS:HA	1:B:61:THR:O	2.12	0.49
1:A:107:ARG:HB3	1:A:114:LEU:HD21	1.95	0.49
1:A:53:LYS:NZ	2:A:150:HOH:O	2.46	0.48
1:A:12:VAL:O	1:A:13:ASP:HB2	2.13	0.48
1:A:53:LYS:HA	1:A:61:THR:O	2.13	0.48
1:B:13:ASP:CG	2:B:141:HOH:O	2.57	0.48
1:B:104:THR:CG2	1:B:106:VAL:HG23	2.38	0.47
1:A:110:ILE:O	1:A:111:ASP:CG	2.57	0.47
1:B:75:THR:C	1:B:77:ASP:N	2.72	0.47
1:B:59:LYS:HD3	1:B:59:LYS:HA	1.40	0.47
1:A:42:ILE:HB	1:A:53:LYS:HB2	1.98	0.46
1:A:20:TYR:HE1	1:A:120:HIS:HB2	1.81	0.46
1:B:97:LYS:HB2	1:B:97:LYS:HE3	1.66	0.46
1:A:90:GLY:O	2:A:136:HOH:O	2.21	0.45
1:A:51:THR:HA	1:A:63:ILE:O	2.16	0.45
1:A:94:HIS:HB3	1:A:105:LEU:HB2	1.98	0.45
1:B:1:MET:O	1:B:2:VAL:CG1	2.59	0.45
1:A:100:GLY:O	1:A:101:GLN:HB2	2.16	0.45
1:B:1:MET:HG2	1:B:2:VAL:HG12	1.99	0.44
1:B:5:PHE:O	1:B:9:TRP:HZ3	2.00	0.44
1:B:23:SER:OG	1:B:120:HIS:HD2	2.01	0.44
1:A:2:VAL:N	2:A:142:HOH:O	2.51	0.43
1:B:77:ASP:O	1:B:78:ASP:HB2	2.18	0.43
1:A:98:TRP:HZ3	1:A:103:THR:HG22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:VAL:HA	1:B:93:VAL:O	2.18	0.43
1:A:12:VAL:HG11	1:A:130:GLU:CG	2.45	0.43
1:B:98:TRP:O	1:B:99:ASP:C	2.62	0.43
1:A:5:PHE:O	1:A:9:TRP:CH2	2.71	0.43
1:B:38:LYS:HA	1:B:39:PRO:HD3	1.63	0.43
1:A:23:SER:CB	1:A:120:HIS:HD2	2.31	0.43
1:A:21:MET:HB3	1:A:26:VAL:HB	2.01	0.42
1:A:5:PHE:O	1:A:43:ILE:HB	2.19	0.42
1:A:52:LEU:HD13	1:A:107:ARG:NH2	2.35	0.42
1:B:22:LYS:HE3	1:B:31:ARG:HH12	1.85	0.41
1:A:16:ASN:HB3	1:A:124:VAL:O	2.20	0.41
1:A:50:LEU:O	1:A:64:SER:HA	2.20	0.41
1:A:54:THR:O	1:A:55:HIS:HD2	2.04	0.41
1:A:58:PHE:CE2	1:A:59:LYS:HB2	2.56	0.41
1:B:1:MET:HE2	1:B:2:VAL:CG1	2.51	0.41
1:B:21:MET:HB3	1:B:26:VAL:HG21	2.03	0.41
1:A:23:SER:OG	1:A:120:HIS:CD2	2.61	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LYS:NZ	2:A:150:HOH:O[3_454]	1.90	0.30

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	131/158 (83%)	113 (86%)	12 (9%)	6 (5%)	2	2
1	B	131/158 (83%)	114 (87%)	13 (10%)	4 (3%)	3	5
All	All	262/316 (83%)	227 (87%)	25 (10%)	10 (4%)	2	3

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	17	PHE
1	B	2	VAL
1	B	99	ASP
1	A	99	ASP
1	A	111	ASP
1	B	58	PHE
1	A	101	GLN
1	B	56	SER
1	A	57	THR

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	117/139 (84%)	95 (81%)	22 (19%)	1 2
1	B	117/139 (84%)	95 (81%)	22 (19%)	1 2
All	All	234/278 (84%)	190 (81%)	44 (19%)	1 2

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	VAL
1	A	10	LYS
1	A	14	SER
1	A	17	PHE
1	A	30	THR
1	A	33	VAL
1	A	35	SER
1	A	38	LYS
1	A	49	ILE
1	A	58	PHE
1	A	63	ILE
1	A	64	SER

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Mol	Chain	Res	Type
1	A	73	GLU
1	A	75	THR
1	A	80	LYS
1	A	95	LEU
1	A	104	THR
1	A	108	GLU
1	A	109	LEU
1	A	117	THR
1	A	124	VAL
1	B	1	MET
1	B	10	LYS
1	B	17	PHE
1	B	26	VAL
1	B	30	THR
1	B	35	SER
1	B	40	THR
1	B	48	ASP
1	B	49	ILE
1	B	59	LYS
1	B	63	ILE
1	B	77	ASP
1	B	78	ASP
1	B	97	LYS
1	B	104	THR
1	B	108	GLU
1	B	111	ASP
1	B	115	ILE
1	B	122	THR
1	B	125	CYS
1	B	126	THR
1	B	128	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	101	GLN
1	A	120	HIS
1	B	32	GLN
1	B	46	ASN
1	B	60	ASN
1	B	120	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 oligosaccharides 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	133/158 (84%)	-1.17	0	100	100	33, 53, 72, 77	0
1	B	133/158 (84%)	-1.16	0	100	100	29, 50, 66, 74	0
All	All	266/316 (84%)	-1.17	0	100	100	29, 52, 69, 77	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.