



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2017 – 02:23 PM EST

PDB ID : 5WTT
Title : Structure of the 093G9 Fab in complex with the epitope peptide
Authors : Zhong, C.; Hu, K.; Shen, J.; Ding, J.
Deposited on : unknown
Resolution : 2.70 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

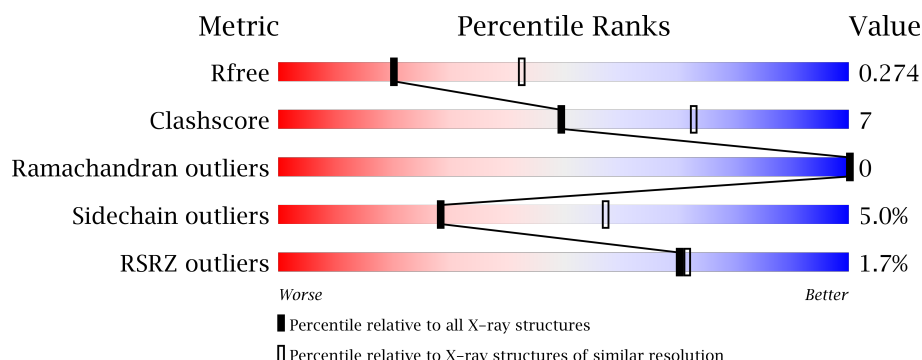
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



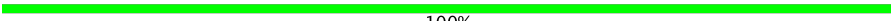
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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 $\leq 5\%$. 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	241	
1	H	241	
2	B	239	
2	L	239	
3	C	8	

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Mol	Chain	Length	Quality of chain
3	P	8	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6801 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 Heavy chain of 093G9 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	214	Total	C	N	O	S	0	0	0
			1644	1044	265	329	6			
1	A	216	Total	C	N	O	S	0	0	0
			1660	1052	268	333	7			

- Molecule 2 is a protein called Light chain of 093G9 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	216	Total	C	N	O	S	0	0	0
			1676	1054	282	334	6			
2	B	216	Total	C	N	O	S	0	1	0
			1685	1059	283	337	6			

- Molecule 3 is a protein called Epitope peptide of Cyr61.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	8	Total	C	N	O	S	0	0	0
			56	34	9	11	2			
3	C	8	Total	C	N	O	S	0	0	0
			56	34	9	11	2			

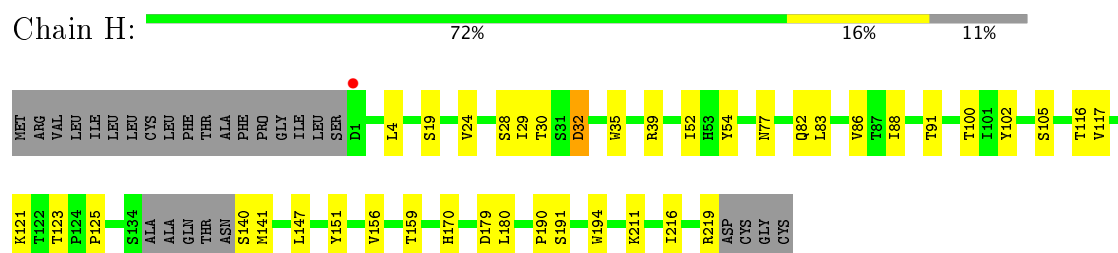
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	7	Total	O	0	0
			7	7		
4	L	9	Total	O	0	0
			9	9		
4	A	4	Total	O	0	0
			4	4		
4	B	4	Total	O	0	0
			4	4		

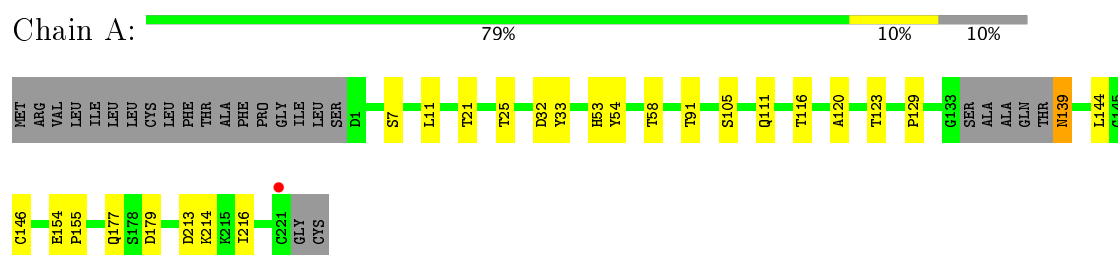
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

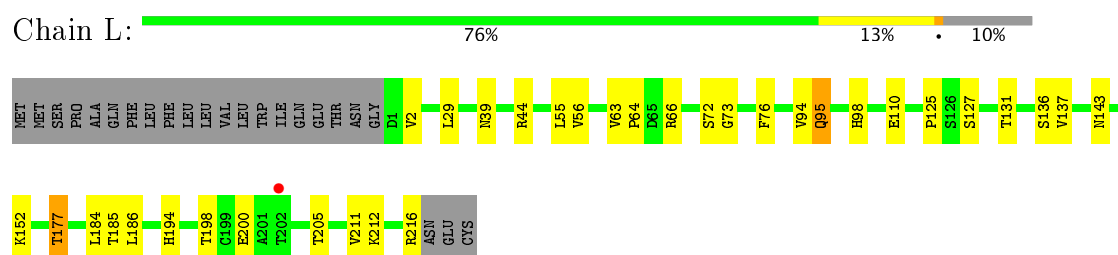
- Molecule 1: Heavy chain of 093G9 Fab



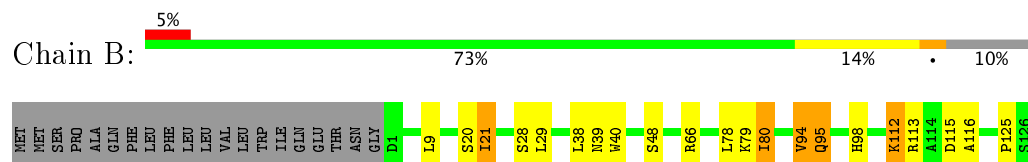
- Molecule 1: Heavy chain of 093G9 Fab

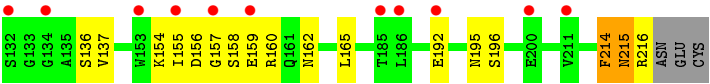


- Molecule 2: Light chain of 093G9 Fab



- Molecule 2: Light chain of 093G9 Fab



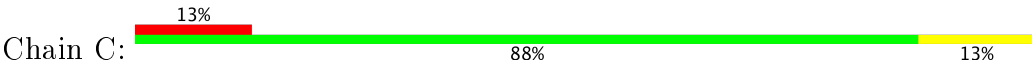


● Molecule 3: Epitope peptide of Cyr61



There are no outlier residues recorded for this chain.

● Molecule 3: Epitope peptide of Cyr61



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.88Å 214.44Å 50.05Å 90.00° 92.81° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 48.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.70) 99.1 (48.68-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.222 , 0.274 0.222 , 0.274	Depositor DCC
R_{free} test set	1221 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6801	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.51	0/1707	0.57	0/2340
1	H	0.48	0/1691	0.60	0/2318
2	B	0.47	0/1722	0.58	0/2335
2	L	0.48	0/1713	0.58	0/2323
3	C	0.71	0/56	0.71	0/73
3	P	0.52	0/56	0.64	0/73
All	All	0.48	0/6945	0.59	0/9462

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	1660	0	1601	13	0
1	H	1644	0	1591	24	0
2	B	1685	0	1649	39	0
2	L	1676	0	1644	20	0
3	C	56	0	48	0	0
3	P	56	0	48	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	H	7	0	0	6	0
4	L	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6801	0	6581	90	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 7.

All (90) 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:192[B]:GLU:HA	2:B:216:ARG:NH1	1.61	1.14
2:B:192[A]:GLU:HA	2:B:216:ARG:NH1	1.62	1.14
2:B:192[B]:GLU:HA	2:B:216:ARG:HH12	1.33	0.92
2:B:192[A]:GLU:HA	2:B:216:ARG:HH12	1.33	0.92
1:H:141:MET:HA	4:H:301:HOH:O	1.78	0.83
2:L:95:GLN:HE21	2:L:98:HIS:H	1.34	0.75
1:H:190:PRO:HA	4:H:301:HOH:O	1.88	0.74
2:B:39:ASN:HB2	2:B:94:VAL:HG13	1.72	0.71
2:B:196:SER:HA	2:B:215:ASN:HA	1.73	0.70
1:H:140:SER:O	4:H:301:HOH:O	2.09	0.69
2:B:195:ASN:O	2:B:216:ARG:HB2	1.92	0.68
2:L:136:SER:HB3	2:L:185:THR:HG22	1.78	0.66
1:H:32:ASP:O	1:H:54:TYR:CD1	2.49	0.65
2:B:155:ILE:HD12	2:B:155:ILE:H	1.63	0.64
1:H:141:MET:HE2	4:H:301:HOH:O	1.97	0.63
1:A:32:ASP:O	1:A:54:TYR:CD1	2.55	0.60
2:L:143:ASN:HA	2:L:177:THR:HG21	1.83	0.60
1:H:211:LYS:HE3	4:H:306:HOH:O	2.02	0.58
2:B:20:SER:OG	2:B:79:LYS:HG2	2.04	0.58
2:L:39:ASN:HB2	2:L:94:VAL:HG13	1.87	0.56
2:L:200:GLU:HG2	2:L:211:VAL:HG22	1.88	0.56
2:B:154:LYS:HG2	2:B:157:GLY:C	2.26	0.56
2:B:215:ASN:O	2:B:215:ASN:ND2	2.40	0.55
1:A:105:SER:HB3	2:B:39:ASN:OD1	2.07	0.55
2:B:95:GLN:OE1	2:B:98:HIS:N	2.37	0.54
1:H:91:THR:HG23	1:H:116:THR:HA	1.89	0.54
2:L:143:ASN:HA	2:L:177:THR:CG2	2.38	0.54
1:H:19:SER:OG	1:H:82:GLN:OE1	2.27	0.53
2:B:154:LYS:HG3	2:B:159:GLU:N	2.25	0.52
2:B:113:ARG:HH21	2:B:116:ALA:HB2	1.74	0.52
2:B:129:GLN:HE22	2:B:136:SER:HB2	1.75	0.52
2:B:154:LYS:HG2	2:B:158:SER:N	2.26	0.51
2:B:21:ILE:HD11	2:B:40:TRP:CZ3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:29:LEU:HD22	2:L:95:GLN:HG3	1.93	0.50
2:B:28:SER:O	2:B:98:HIS:HE1	1.96	0.49
2:L:194:HIS:O	2:L:216:ARG:HD3	2.13	0.48
2:B:154:LYS:CG	2:B:159:GLU:H	2.25	0.48
2:L:73:GLY:O	2:L:76:PHE:CE2	2.66	0.48
2:B:154:LYS:HG3	2:B:159:GLU:CA	2.44	0.48
2:L:72:SER:O	2:L:73:GLY:C	2.52	0.48
2:B:195:ASN:O	2:B:216:ARG:N	2.45	0.48
2:B:214:PHE:CD1	2:B:214:PHE:C	2.86	0.48
1:A:177:GLN:HB2	2:B:165:LEU:HD21	1.95	0.47
1:H:121:LYS:O	1:H:123:THR:HG23	2.14	0.47
1:H:125:PRO:HB3	1:H:151:TYR:HB3	1.97	0.47
2:B:154:LYS:HG3	2:B:159:GLU:H	1.79	0.47
1:A:129:PRO:HD3	1:A:214:LYS:HE2	1.97	0.46
1:H:194:TRP:HH2	1:H:216:ILE:O	1.98	0.46
1:H:24:VAL:HG21	1:H:29:ILE:CG2	2.46	0.46
1:H:105:SER:HB3	2:L:39:ASN:OD1	2.16	0.46
2:L:64:PRO:HB2	2:L:66:ARG:HG2	1.98	0.46
1:H:191:SER:N	4:H:301:HOH:O	2.49	0.46
1:H:29:ILE:HA	1:H:35:TRP:CZ2	2.51	0.46
2:B:192[B]:GLU:O	2:B:216:ARG:NH2	2.49	0.45
2:L:125:PRO:HD3	2:L:137:VAL:HG22	1.99	0.44
2:B:154:LYS:CG	2:B:159:GLU:N	2.81	0.44
2:B:127:SER:HA	2:B:130:LEU:HD12	2.00	0.44
2:B:154:LYS:HG3	2:B:159:GLU:HA	1.99	0.44
2:B:192[A]:GLU:O	2:B:216:ARG:NH2	2.50	0.44
2:B:40:TRP:CE2	2:B:78:LEU:HB2	2.53	0.44
1:A:111:GLN:HA	2:B:48:SER:HB3	2.00	0.44
1:A:120:ALA:HB2	1:A:179:ASP:HB3	2.00	0.44
2:B:66:ARG:HH11	2:B:80:ILE:HD11	1.82	0.43
2:B:192[B]:GLU:HA	2:B:216:ARG:CZ	2.40	0.43
2:B:192[A]:GLU:HA	2:B:216:ARG:CZ	2.41	0.43
2:L:44:ARG:HB3	4:L:301:HOH:O	2.18	0.43
1:A:7:SER:HB2	1:A:21:THR:HB	2.01	0.43
1:A:91:THR:HG23	1:A:116:THR:HA	2.01	0.43
2:B:113:ARG:NH2	2:B:116:ALA:HB2	2.34	0.43
2:L:127:SER:O	2:L:131:THR:HG23	2.19	0.43
1:A:154:GLU:HB3	1:A:155:PRO:HA	2.01	0.42
2:B:125:PRO:HD3	2:B:137:VAL:HG22	2.01	0.42
1:H:4:LEU:HG	1:H:24:VAL:HG12	2.01	0.42
2:L:55:LEU:O	2:L:56:VAL:HB	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASN:N	1:A:139:ASN:ND2	2.66	0.42
1:H:24:VAL:HG21	1:H:29:ILE:HG23	2.01	0.42
1:A:33:TYR:O	1:A:54:TYR:HB3	2.19	0.42
1:H:24:VAL:HG23	1:H:77:ASN:ND2	2.34	0.42
1:H:219:ARG:NH2	2:L:125:PRO:O	2.51	0.42
2:L:136:SER:HA	2:L:184:LEU:O	2.20	0.42
2:L:63:VAL:HA	2:L:64:PRO:HD3	1.94	0.41
1:A:53:HIS:CE1	1:A:54:TYR:CE1	3.08	0.41
1:H:170:HIS:HE1	2:L:143:ASN:OD1	2.04	0.41
1:A:144:LEU:HG	1:A:216:ILE:HG21	2.03	0.41
1:H:100:THR:HG22	1:H:102:TYR:H	1.85	0.41
1:H:28:SER:C	1:H:30:THR:H	2.24	0.41
2:B:215:ASN:C	2:B:215:ASN:ND2	2.74	0.41
2:B:112:LYS:HD3	2:B:112:LYS:HA	1.89	0.41
1:H:179:ASP:O	1:H:180:LEU:HD12	2.21	0.40
1:H:88:ILE:HA	1:H:117:VAL:HB	2.02	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	212/241 (88%)	206 (97%)	6 (3%)	0	100	100
1	H	210/241 (87%)	200 (95%)	10 (5%)	0	100	100
2	B	215/239 (90%)	206 (96%)	9 (4%)	0	100	100
2	L	214/239 (90%)	209 (98%)	5 (2%)	0	100	100
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	P	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
All	All	863/976 (88%)	832 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	195/215 (91%)	188 (96%)	7 (4%)	40	70
1	H	193/215 (90%)	185 (96%)	8 (4%)	35	66
2	B	194/214 (91%)	180 (93%)	14 (7%)	17	39
2	L	193/214 (90%)	184 (95%)	9 (5%)	30	60
3	C	6/6 (100%)	5 (83%)	1 (17%)	2	6
3	P	6/6 (100%)	6 (100%)	0	100	100
All	All	787/870 (90%)	748 (95%)	39 (5%)	28	57

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	32	ASP
1	H	39	ARG
1	H	52	ILE
1	H	83	LEU
1	H	86	VAL
1	H	147	LEU
1	H	156	VAL
1	H	159	THR
2	L	2	VAL
2	L	95	GLN
2	L	110	GLU
2	L	152	LYS
2	L	177	THR
2	L	186	LEU
2	L	198	THR
2	L	205	THR
2	L	212	LYS
1	A	11	LEU
1	A	25	THR

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Mol	Chain	Res	Type
1	A	58	THR
1	A	123	THR
1	A	139	ASN
1	A	146	CYS
1	A	213	ASP
2	B	9	LEU
2	B	21	ILE
2	B	29	LEU
2	B	38	LEU
2	B	80	ILE
2	B	94	VAL
2	B	95	GLN
2	B	112	LYS
2	B	115	ASP
2	B	156	ASP
2	B	160	ARG
2	B	162	ASN
2	B	214	PHE
2	B	215	ASN
3	C	1	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	170	HIS
1	A	170	HIS
2	B	98	HIS
2	B	129	GLN
2	B	215	ASN

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 [i](#)

There are no carbohydrates 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	216/241 (89%)	-0.02	1 (0%) 90 92	36, 51, 75, 113	0
1	H	214/241 (88%)	-0.01	1 (0%) 90 92	36, 54, 79, 100	0
2	B	216/239 (90%)	0.14	11 (5%) 29 27	30, 53, 108, 134	0
2	L	216/239 (90%)	-0.10	1 (0%) 90 92	28, 49, 79, 88	0
3	C	8/8 (100%)	0.42	1 (12%) 4 3	37, 49, 71, 77	0
3	P	8/8 (100%)	-0.10	0 100 100	41, 47, 60, 65	0
All	All	878/976 (89%)	0.00	15 (1%) 70 72	28, 52, 86, 134	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1	CYS	4.1
2	B	157	GLY	3.4
2	B	192[A]	GLU	2.8
2	B	211	VAL	2.5
1	A	221	CYS	2.3
1	H	1	ASP	2.3
2	B	200	GLU	2.2
2	B	134	GLY	2.2
2	B	185	THR	2.2
2	B	155	ILE	2.2
2	L	202	THR	2.2
2	B	132	SER	2.0
2	B	153	TRP	2.0
2	B	159	GLU	2.0
2	B	186	LEU	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.