



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:17 PM GMT

PDB ID : 5CP7
Title : Crystal Structure of an Antigen-Binding Fragment of Monoclonal Antibody
against Sulfonamides
Authors : Wang, Z.; Shen, J.; Li, C.; Li, Y.; Wen, K.; Yu, X.; Zhang, X.
Deposited on : 2015-07-21
Resolution : 3.01 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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

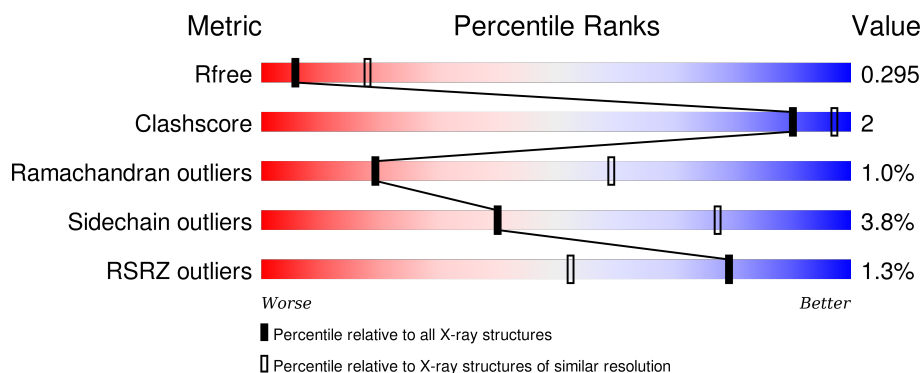
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

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	218	<div> <div></div> <div>91%8%</div> </div>
1	C	218	<div> <div></div> <div>89%11%</div> </div>
1	E	218	<div> <div>4%</div> <div>91%8%</div> </div>
1	G	218	<div> <div></div> <div>93%6%</div> </div>
2	B	214	<div> <div></div> <div>93%6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	214	<div><div>%</div><div><div></div><div>87%</div><div>8%5%</div></div></div>
2	F	214	<div><div>4%</div><div><div></div><div>88%</div><div>8%•</div></div></div>
2	H	214	<div><div>%</div><div><div></div><div>85%</div><div>13%••</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13178 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 Light Chain of Antigen-Binding Fragment of Monoclonal Antibody of 4C7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	1	0
			1700	1061	288	345	6			
1	C	218	Total	C	N	O	S	0	1	0
			1702	1062	288	346	6			
1	E	218	Total	C	N	O	S	0	0	0
			1686	1052	285	343	6			
1	G	218	Total	C	N	O	S	0	1	0
			1702	1062	289	345	6			

- Molecule 2 is a protein called Heavy Chain of Antigen-Binding Fragment of Monoclonal Antibody of 4C7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1628	1027	272	323	6			
2	D	204	Total	C	N	O	S	0	1	0
			1573	999	260	308	6			
2	F	207	Total	C	N	O	S	0	0	0
			1576	995	264	311	6			
2	H	212	Total	C	N	O	S	0	0	0
			1610	1017	268	319	6			

- Molecule 3 is water.

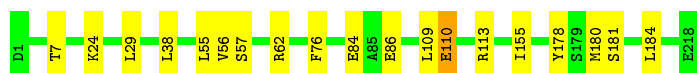
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	O	0	0
			1	1		

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.

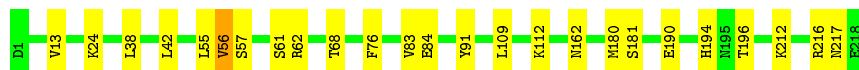
- Molecule 1: Light Chain of Antigen-Binding Fragment of Monoclonal Antibody of 4C7

Chain A: 



- Molecule 1: Light Chain of Antigen-Binding Fragment of Monoclonal Antibody of 4C7

Chain C: 



- Molecule 1: Light Chain of Antigen-Binding Fragment of Monoclonal Antibody of 4C7

Chain E: 



- Molecule 1: Light Chain of Antigen-Binding Fragment of Monoclonal Antibody of 4C7

Chain G: 




- Molecule 2: Heavy Chain of Antigen-Binding Fragment of Monoclonal Antibody of 4C7

Chain B: 

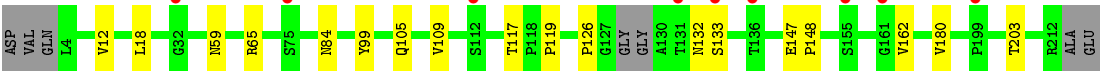
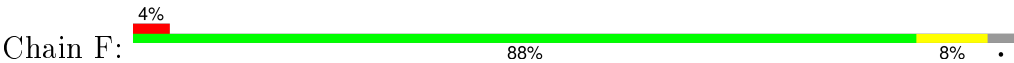


- Molecule 2: Heavy Chain of Antigen-Binding Fragment of Monoclonal Antibody of 4C7

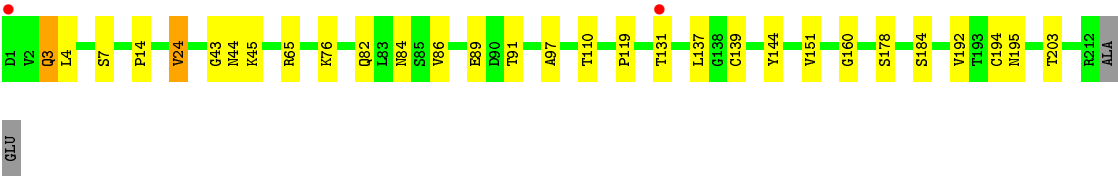
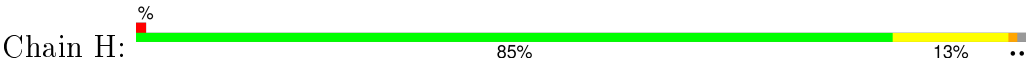
Chain D: 



● Molecule 2: Heavy Chain of Antigen-Binding Fragment of Monoclonal Antibody of 4C7



● Molecule 2: Heavy Chain of Antigen-Binding Fragment of Monoclonal Antibody of 4C7



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	176.10Å 96.51Å 138.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.01 29.86 – 3.01	Depositor EDS
% Data completeness (in resolution range)	94.6 (29.88-3.01) 94.7 (29.86-3.01)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 3.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.260 , 0.302 0.257 , 0.295	Depositor DCC
R_{free} test set	2275 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 23.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 44814 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	13178	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.30	0/1735	0.51	0/2356
1	C	0.30	0/1737	0.52	0/2357
1	E	0.29	0/1721	0.49	0/2338
1	G	0.29	0/1737	0.48	0/2357
2	B	0.29	0/1675	0.52	0/2297
2	D	0.29	0/1619	0.50	0/2220
2	F	0.30	0/1622	0.49	0/2224
2	H	0.31	0/1655	0.53	0/2270
All	All	0.30	0/13501	0.51	0/18419

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 [i](#)

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	1700	0	1655	8	0
1	C	1702	0	1659	8	0
1	E	1686	0	1634	9	0
1	G	1702	0	1661	6	0
2	B	1628	0	1566	8	0
2	D	1573	0	1515	7	0
2	F	1576	0	1506	4	0
2	H	1610	0	1549	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
All	All	13178	0	12745	59	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 2.

All (59) 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:A:55:LEU:O	1:A:57:SER:N	2.23	0.70
1:C:55:LEU:O	1:C:57:SER:N	2.25	0.69
1:G:55:LEU:O	1:G:57:SER:N	2.28	0.66
2:H:14:PRO:O	2:H:86:VAL:O	2.14	0.66
1:E:55:LEU:O	1:E:57:SER:N	2.30	0.64
1:C:91:TYR:CE1	1:C:109:LEU:HD12	2.33	0.64
2:F:18:LEU:HD11	2:F:109:VAL:HG11	1.85	0.58
2:H:91:THR:HG23	2:H:110:THR:HA	1.88	0.54
1:G:41:LEU:HD23	1:G:51:ARG:HA	1.88	0.54
2:H:3:GLN:C	2:H:4:LEU:HD23	2.29	0.53
2:B:41:PHE:O	2:B:43:GLY:O	2.26	0.53
2:H:82:GLN:NE2	2:H:84:ASN:OD1	2.41	0.52
2:D:30:THR:HG21	2:D:74:THR:HG23	1.92	0.52
2:B:91:THR:HG23	2:B:110:THR:HA	1.93	0.51
2:F:147:GLU:HB3	2:F:148:PRO:HA	1.93	0.50
2:D:4:LEU:HD22	2:D:24:VAL:HG12	1.94	0.49
1:E:66:ARG:NH2	1:E:87:ASP:OD2	2.43	0.49
2:D:91:THR:HG23	2:D:110:THR:HA	1.95	0.48
2:F:162:VAL:O	2:F:162:VAL:HG13	2.13	0.48
1:C:42:LEU:HD13	1:C:91:TYR:CE1	2.49	0.47
1:A:84:GLU:HG2	2:B:31:SER:CB	2.46	0.46
2:D:32:GLY:O	2:D:54:TYR:CD1	2.69	0.46
1:G:38:LEU:HD22	1:G:76:PHE:CG	2.51	0.46
1:C:38:LEU:HD13	1:C:76:PHE:CD1	2.51	0.46
1:E:42:LEU:HB2	1:E:52:LEU:HD11	1.97	0.46
1:E:94:TRP:CD1	1:E:94:TRP:C	2.89	0.46
1:G:29:LEU:HD12	1:G:76:PHE:CE1	2.51	0.45
1:C:83:VAL:HG23	1:C:83:VAL:O	2.15	0.45
2:B:3:GLN:C	2:B:4:LEU:HD12	2.37	0.45
1:A:84:GLU:HG2	2:B:31:SER:HB3	1.98	0.45
1:E:187:THR:HB	1:E:190:GLU:HB2	1.99	0.45
2:B:176:LEU:C	2:B:176:LEU:HD12	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:151:VAL:HG11	2:H:178:SER:HB3	2.00	0.44
2:H:4:LEU:HD22	2:H:24:VAL:HB	2.00	0.43
1:E:50:LYS:NZ	1:E:60:ASP:OD2	2.51	0.43
1:C:194:HIS:O	1:C:216:ARG:NH1	2.52	0.42
1:A:38:LEU:HD22	1:A:76:PHE:CG	2.54	0.42
2:B:14:PRO:O	2:B:86:VAL:O	2.37	0.42
2:H:43:GLY:O	2:H:44:ASN:HB2	2.20	0.42
2:B:52:ILE:O	2:B:52:ILE:HG23	2.19	0.42
1:G:2:VAL:HG21	1:G:98:HIS:HB2	2.02	0.42
2:F:119:PRO:HD2	2:F:203:THR:HG21	2.00	0.42
2:H:151:VAL:HG11	2:H:178:SER:CB	2.49	0.42
1:E:42:LEU:HD13	1:E:91:TYR:CZ	2.55	0.41
2:H:137:LEU:HD12	2:H:192:VAL:HG11	2.02	0.41
1:A:155:ILE:HD11	1:A:184:LEU:HD21	2.01	0.41
1:A:38:LEU:HD22	1:A:76:PHE:CD2	2.54	0.41
1:E:62:ARG:HG3	1:E:62:ARG:O	2.19	0.41
1:A:110:GLU:HG3	1:A:178:TYR:OH	2.21	0.41
2:H:119:PRO:HB3	2:H:144:TYR:HB3	2.03	0.41
1:G:94:TRP:CH2	1:G:96:GLY:HA3	2.55	0.41
2:D:176:LEU:HD12	2:D:176:LEU:C	2.41	0.41
1:C:56:VAL:HG23	1:C:57:SER:N	2.36	0.40
2:D:211:PRO:O	2:D:212:ARG:HB3	2.21	0.40
2:H:4:LEU:HD12	2:H:97:ALA:HA	2.03	0.40
2:D:4:LEU:HD12	2:D:97:ALA:HA	2.04	0.40
1:C:13:VAL:HG21	1:C:83:VAL:HG11	2.01	0.40
1:A:29:LEU:HD12	1:A:76:PHE:CE1	2.56	0.40
1:E:55:LEU:O	1:E:56:VAL:C	2.59	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	217/218 (100%)	209 (96%)	7 (3%)	1 (0%)	34	75
1	C	217/218 (100%)	208 (96%)	8 (4%)	1 (0%)	34	75
1	E	216/218 (99%)	197 (91%)	15 (7%)	4 (2%)	10	41
1	G	217/218 (100%)	204 (94%)	11 (5%)	2 (1%)	21	62
2	B	212/214 (99%)	195 (92%)	16 (8%)	1 (0%)	34	75
2	D	201/214 (94%)	184 (92%)	15 (8%)	2 (1%)	19	59
2	F	203/214 (95%)	178 (88%)	21 (10%)	4 (2%)	9	39
2	H	210/214 (98%)	189 (90%)	19 (9%)	2 (1%)	19	59
All	All	1693/1728 (98%)	1564 (92%)	112 (7%)	17 (1%)	19	59

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	C	56	VAL
1	E	56	VAL
1	E	101	GLN
1	G	56	VAL
2	B	65	ARG
2	D	14	PRO
2	D	171	SER
2	F	132	ASN
2	F	133	SER
2	H	160	GLY
2	F	180	VAL
1	G	143	ASN
2	H	131	THR
2	F	126	PRO
1	E	73	GLY
1	E	100	PRO

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	195/195 (100%)	186 (95%)	9 (5%)	33	72
1	C	196/195 (100%)	182 (93%)	14 (7%)	18	53
1	E	193/195 (99%)	189 (98%)	4 (2%)	61	89
1	G	196/195 (100%)	193 (98%)	3 (2%)	72	92
2	B	186/186 (100%)	180 (97%)	6 (3%)	46	81
2	D	181/186 (97%)	177 (98%)	4 (2%)	60	88
2	F	180/186 (97%)	173 (96%)	7 (4%)	39	77
2	H	185/186 (100%)	173 (94%)	12 (6%)	21	56
All	All	1512/1524 (99%)	1453 (96%)	59 (4%)	40	77

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	24	LYS
1	A	62	ARG
1	A	86	GLU
1	A	109	LEU
1	A	110	GLU
1	A	113	ARG
1	A	180	MET
1	A	181	SER
2	B	5	ARG
2	B	31	SER
2	B	65	ARG
2	B	67	ARG
2	B	88	THR
2	B	110	THR
1	C	24	LYS
1	C	61	SER
1	C	62	ARG
1	C	68	THR
1	C	84	GLU
1	C	112	LYS
1	C	162	ASN
1	C	180	MET
1	C	181	SER
1	C	190[A]	GLU
1	C	190[B]	GLU
1	C	196	THR

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Mol	Chain	Res	Type
1	C	212	LYS
1	C	217	ASN
2	D	5	ARG
2	D	6	GLU
2	D	68	ILE
2	D	77	ASN
1	E	75	ASP
1	E	94	TRP
1	E	113	ARG
1	E	161	GLN
2	F	12	VAL
2	F	59	ASN
2	F	65	ARG
2	F	84	ASN
2	F	99	TYR
2	F	105	GLN
2	F	117	THR
1	G	38	LEU
1	G	79	LYS
1	G	148	ASP
2	H	3	GLN
2	H	7	SER
2	H	24	VAL
2	H	45	LYS
2	H	65	ARG
2	H	76	LYS
2	H	89	GLU
2	H	139	CYS
2	H	184	SER
2	H	194	CYS
2	H	195	ASN
2	H	203	THR

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	43	GLN
2	B	105	GLN
2	B	198	HIS
2	D	16	GLN
1	E	47	GLN
1	E	101	GLN

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Mol	Chain	Res	Type
1	E	161	GLN
2	F	59	ASN
2	F	82	GLN
2	F	84	ASN
2	H	16	GLN
2	H	40	GLN
2	H	82	GLN
2	H	84	ASN
2	H	105	GLN

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 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	218/218 (100%)	-0.47	0 100 100	12, 17, 22, 31	0
1	C	218/218 (100%)	-0.45	0 100 100	13, 18, 23, 26	0
1	E	218/218 (100%)	0.23	8 (3%) 45 19	16, 45, 68, 72	0
1	G	218/218 (100%)	0.12	1 (0%) 91 76	23, 47, 59, 69	0
2	B	214/214 (100%)	-0.24	0 100 100	14, 23, 41, 58	0
2	D	204/214 (95%)	0.12	3 (1%) 76 48	9, 32, 71, 84	0
2	F	207/214 (96%)	0.56	9 (4%) 39 16	31, 52, 77, 80	0
2	H	212/214 (99%)	-0.36	2 (0%) 85 63	6, 16, 36, 55	0
All	All	1709/1728 (98%)	-0.07	23 (1%) 79 52	6, 26, 67, 84	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	131	THR	4.0
2	D	191	THR	3.7
1	E	217	ASN	3.5
1	E	85	ALA	3.5
2	F	155	SER	3.2
2	F	112	SER	3.1
2	F	199	PRO	3.0
1	E	199	CYS	2.9
2	H	1	ASP	2.8
1	E	209	PRO	2.8
2	F	32	GLY	2.6
2	F	161	GLY	2.4
1	E	207	THR	2.2
2	F	136	THR	2.2
2	D	159	SER	2.1
1	G	207	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	133	SER	2.1
2	D	183	PRO	2.1
1	E	208	SER	2.1
2	F	75	SER	2.1
1	E	148	ASP	2.0
2	H	131	THR	2.0
1	E	202	THR	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.