WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Mar 23, 2024 – 01:21 PM EDT

PDB ID : 1Z3G

Title : Crystal structure of complex between Pvs25 and Fab fragment of malaria transmission blocking antibody 2A8

Authors : Saxena, A.K.; Singh, K.; Su, H.P.; Klein, M.M.; Stowers, A.W.; Saul, A.J.; Long, C.A.; Garboczi, D.N.

Deposited on : 2005-03-12
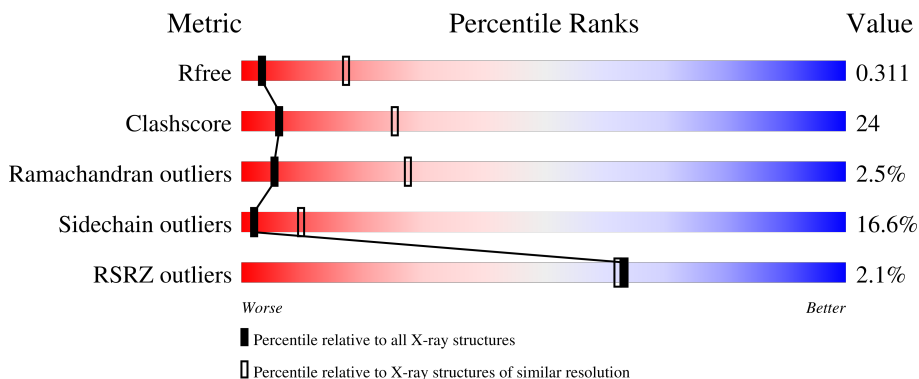
Resolution : 3.30 Å(reported)

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 3.30 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.
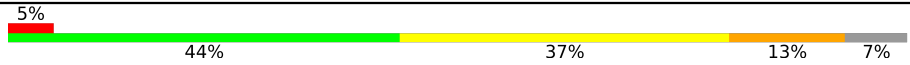
Metric	Percentile Ranks	Value
Rfree		0.311
Clashscore		24
Ramachandran outliers		2.5%
Sidechain outliers		16.6%
RSRZ outliers		2.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	L	213	70% 28% •
1	M	213	.% 72% 25% •
2	H	216	3% 47% 42% 9% ••
2	I	216	44% 44% 11% •
3	A	186	2% 44% 40% 8% • 7%

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Mol	Chain	Length	Quality of chain
3	B	186	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9120 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 2A8 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1634	1011	274	339	10			
1	M	213	Total	C	N	O	S	0	0	0
			1634	1011	274	339	10			

- Molecule 2 is a protein called 2A8 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1617	1027	267	315	8			
2	I	214	Total	C	N	O	S	0	0	0
			1617	1027	267	315	8			

- Molecule 3 is a protein called ookinete surface protein Pvs25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	173	Total	C	N	O	S	0	0	0
			1309	795	216	272	26			
3	B	173	Total	C	N	O	S	0	0	0
			1309	795	216	272	26			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLU	-	cloning artifact	UNP O96555
A	-3	ALA	-	cloning artifact	UNP O96555
A	-2	GLU	-	cloning artifact	UNP O96555
A	-1	ALA	-	cloning artifact	UNP O96555
A	0	SER	-	cloning artifact	UNP O96555
A	174	GLY	-	cloning artifact	UNP O96555
A	175	PRO	-	cloning artifact	UNP O96555
A	176	HIS	-	expression tag	UNP O96555

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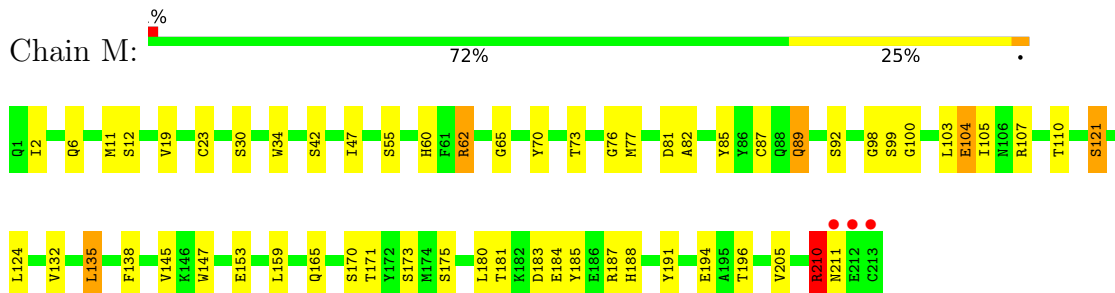| Chain	Residue	Modelled	Actual	Comment	Reference
A	177	HIS	-	expression tag	UNP O96555
A	178	HIS	-	expression tag	UNP O96555
A	179	HIS	-	expression tag	UNP O96555
A	180	HIS	-	expression tag	UNP O96555
A	181	HIS	-	expression tag	UNP O96555
B	-4	GLU	-	cloning artifact	UNP O96555
B	-3	ALA	-	cloning artifact	UNP O96555
B	-2	GLU	-	cloning artifact	UNP O96555
B	-1	ALA	-	cloning artifact	UNP O96555
B	0	SER	-	cloning artifact	UNP O96555
B	174	GLY	-	cloning artifact	UNP O96555
B	175	PRO	-	cloning artifact	UNP O96555
B	176	HIS	-	expression tag	UNP O96555
B	177	HIS	-	expression tag	UNP O96555
B	178	HIS	-	expression tag	UNP O96555
B	179	HIS	-	expression tag	UNP O96555
B	180	HIS	-	expression tag	UNP O96555
B	181	HIS	-	expression tag	UNP O96555

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.
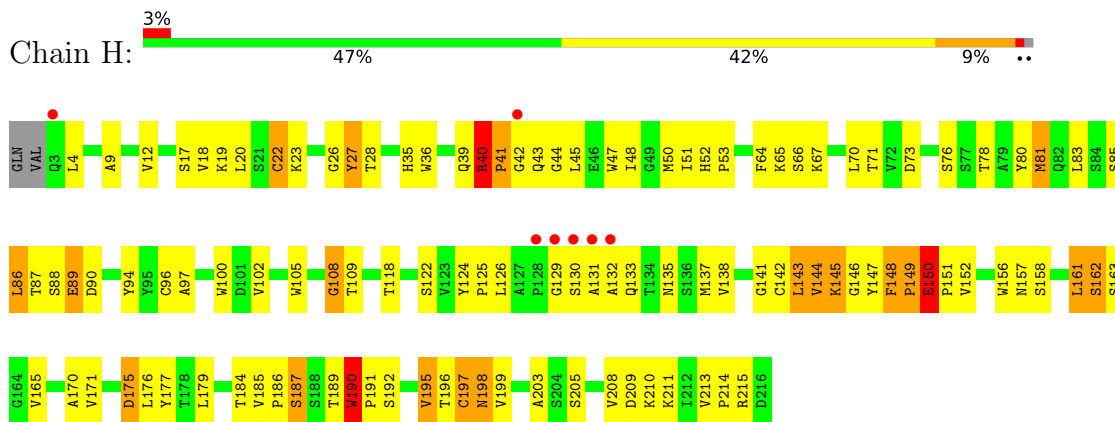
• Molecule 1: 2A8 Fab Light Chain
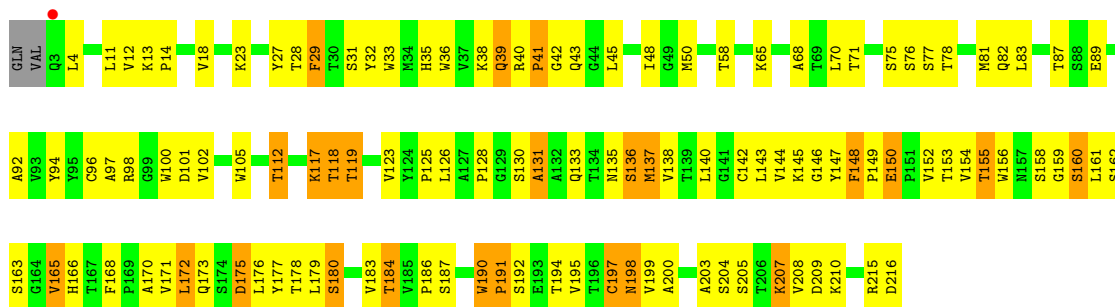
Chain L:

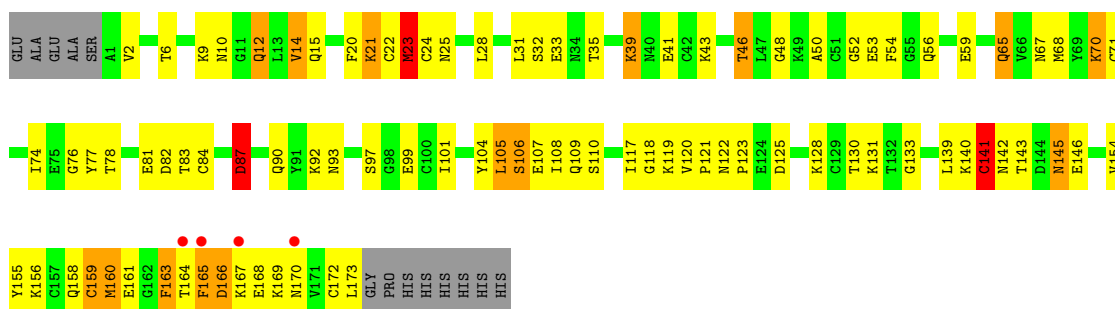• Molecule 1: 2A8 Fab Light Chain

Chain M:

• Molecule 2: 2A8 Fab Heavy Chain

Chain H:
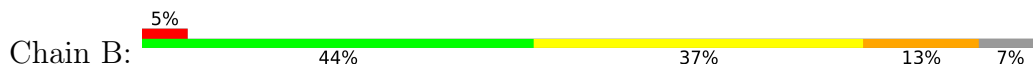

• Molecule 2: 2A8 Fab Heavy Chain

Chain I:

GLN VAL Q3 L4 L11 V12 K13 P14 V18 K23 Y27 T28 F29 T30 S31 Y32 W33 M34 H35 W36 V37 K38 Q39 R40 P41 G42 Q43 G44 L45 I48 G49 M50 T58 K65 A68 T69 L70 T71 S75 S76 S77 T78 M81 Q82 L83 T87 S88 E89

A92 V93 Y94 Y95 C96 A97 R98 G99 W100 D101 V102 W105 T112 K117 T118 T119 V123 Y124 P125 L126 A127 P128 G129 S130 A131 A132 Q133 T134 N135 S136 M137 V138 T139 L140 G141 C142 L143 V144 K145 G146 Y147 F148 P149 E150 P151 V152 T153 V154 T155 W156 N157 S158 G159 S160 L161 S162

S163 G164 V165 H166 T167 F168 P169 A170 V171 L172 Q173 S174 D175 L176 Y177 T178 L179 S180 V183 T184 V185 P186 S187 W190 P191 S192 E193 T194 V195 C197 N198 V199 A200 A203 S204 S205 T206 K207 V208 D209 K210 R215 D216

• Molecule 3: ookinete surface protein Pvs25

Chain A:

GLU ALA GLU ALA SER A1 V2 T6 K9 N10 G11 Q12 L13 V14 Q15 F20 K21 C22 M23 C24 N25 L28 L31 S32 E33 N34 T35 K39 N40 E41 C42 K43 T46 L47 G48 K49 A50 C51 G52 E53 F54 G55 Q56 E59 Q65 V66 N67 M68 Y69 K70 C71

I74 E75 G76 Y77 T78 E81 D82 T83 C84 D87 Q90 Y91 K92 N93 S97 G98 E99 C100 I101 Y104 L105 S106 E107 I108 Q109 S110 I117 G118 K119 V120 P121 N122 P123 E124 D125 K128 C129 T130 K131 T132 G133 L139 K140 C141 N142 T143 D144 N145 E146 V154

Y155 K156 C157 Q158 C159 M160 E161 G162 F163 T164 F165 D166 K167 E168 K169 N170 V171 C172 L173 GLY PRO HIS HIS HIS HIS HIS HIS

• Molecule 3: ookinete surface protein Pvs25

Chain B:

GLU ALA GLU ALA SER A1 V2 T3 V4 D5 T6 I7 C8 K9 N10 G11 Q12 L13 V14 Q15 M16 S17 N18 H19 F20 K21 C22 M23 E26 G27 L31 S32 E33 N34 T35 E41 C42 K43 K44 E45 T46 L47 A50 C51 Q56 C57 N60 P61 Q65 V66 N67 M68 Y69

K70 Y77 V85 L86 D87 V88 C89 Q90 Y91 K92 N93 C94 S97 G98 E99 C100 I101 V102 E103 Y104 L105 S106 E107 I108 Q109 S110 A111 G112 C113 S114 C115 A116 I117 G118 K119 V120 P121 N122 D125 E126 K127 K128 C129 T130 K131 T135 Q138 C141 D144 N145 E146

V147 C148 K149 N150 V154 Y155 K156 C157 Q158 C159 M160 E161 G162 F163 T164 F165 D166 K167 E168 K169 N170 V171 C172 L173 GLY PRO HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.26Å　61.65Å　142.65Å 90.00°　101.68°　90.00°	Depositor
Resolution (Å)	49.15 – 3.30 49.16 – 3.28	Depositor EDS
% Data completeness (in resolution range)	94.8 (49.15-3.30) 94.9 (49.16-3.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.28	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.272　,　0.327 0.258　,　0.311	Depositor DCC
R_{free} test set	1095 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 11.4	EDS
L-test for twinning [2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	9120	wwPDB-VP
Average B, all atoms (Å^2)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	L	0.52	0/1673	0.68	1/2274 (0.0%)
1	M	0.57	0/1673	0.73	1/2274 (0.0%)
2	H	0.65	1/1664 (0.1%)	0.87	3/2278 (0.1%)
2	I	0.67	0/1664	0.83	0/2278
3	A	0.91	0/1323	1.06	3/1776 (0.2%)
3	B	0.77	0/1323	0.96	2/1776 (0.1%)
All	All	0.68	1/9320 (0.0%)	0.85	10/12656 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	190	TRP	NE1-CE2	-5.15	1.30	1.37

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	215	ARG	NE-CZ-NH2	8.46	124.53	120.30
2	H	40	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	L	210	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	M	210	ARG	NE-CZ-NH2	6.63	123.61	120.30
3	A	87	ASP	CB-CG-OD2	6.10	123.79	118.30

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	L	1634	0	1549	50	0
1	M	1634	0	1549	34	0
2	H	1617	0	1578	116	0
2	I	1617	0	1578	105	0
3	A	1309	0	1242	79	0
3	B	1309	0	1242	72	0
All	All	9120	0	8738	433	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 24.

The worst 5 of 433 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)
3:B:120:VAL:CG1	3:B:121:PRO:HD2	1.38	1.48
3:A:125:ASP:OD1	3:A:130:THR:HG21	1.35	1.21
2:I:190:TRP:HB3	2:I:191:PRO:CD	1.75	1.14
3:B:120:VAL:CG1	3:B:121:PRO:CD	2.24	1.13
2:H:148:PHE:HB3	2:H:149:PRO:HD3	1.24	1.12

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	L	211/213 (99%)	197 (93%)	14 (7%)	0	100	100
1	M	211/213 (99%)	197 (93%)	12 (6%)	2 (1%)	17	48
2	H	212/216 (98%)	177 (84%)	22 (10%)	13 (6%)	1	10
2	I	212/216 (98%)	184 (87%)	20 (9%)	8 (4%)	3	19
3	A	171/186 (92%)	143 (84%)	24 (14%)	4 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	171/186 (92%)	136 (80%)	32 (19%)	3 (2%)	8	35
All	All	1188/1230 (97%)	1034 (87%)	124 (10%)	30 (2%)	5	27

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	41	PRO
2	I	190	TRP
3	B	128	LYS
2	H	44	GLY
2	H	108	GLY

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	L	188/188 (100%)	175 (93%)	13 (7%)	15	44
1	M	188/188 (100%)	175 (93%)	13 (7%)	15	44
2	H	183/185 (99%)	152 (83%)	31 (17%)	2	9
2	I	183/185 (99%)	144 (79%)	39 (21%)	1	4
3	A	153/163 (94%)	120 (78%)	33 (22%)	1	4
3	B	153/163 (94%)	108 (71%)	45 (29%)	0	1
All	All	1048/1072 (98%)	874 (83%)	174 (17%)	2	10

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	105	LEU
3	B	44	LYS
3	A	141	CYS
3	B	5	ASP
3	B	92	LYS

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

Mol	Chain	Res	Type
3	B	142	ASN
3	B	145	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 ⓘ

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, 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(Å²)	Q<0.9
1	L	213/213 (100%)	-0.27	1 (0%)	91	91	2, 2, 2, 2	0
1	M	213/213 (100%)	-0.10	3 (1%)	75	75	2, 2, 2, 2	0
2	H	214/216 (99%)	-0.27	7 (3%)	46	44	2, 2, 2, 2	0
2	I	214/216 (99%)	-0.26	1 (0%)	91	91	2, 2, 2, 2	0
3	A	173/186 (93%)	-0.03	4 (2%)	60	59	2, 2, 2, 2	0
3	B	173/186 (93%)	0.36	9 (5%)	27	25	2, 2, 2, 2	0
All	All	1200/1230 (97%)	-0.11	25 (2%)	63	62	2, 2, 2, 2	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	213	CYS	6.5
3	B	170	ASN	6.0
2	H	131	ALA	4.3
2	H	3	GLN	4.0
3	A	170	ASN	3.7

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 monosaccharides 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.