



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2025 – 01:39 PM JST

PDB ID : 8ZU9
Title : The complex structure of MPXV M1R and neutralizing antibody A129
Authors : Ge, J.W.
Deposited on : 2024-06-08
Resolution : 2.17 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) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

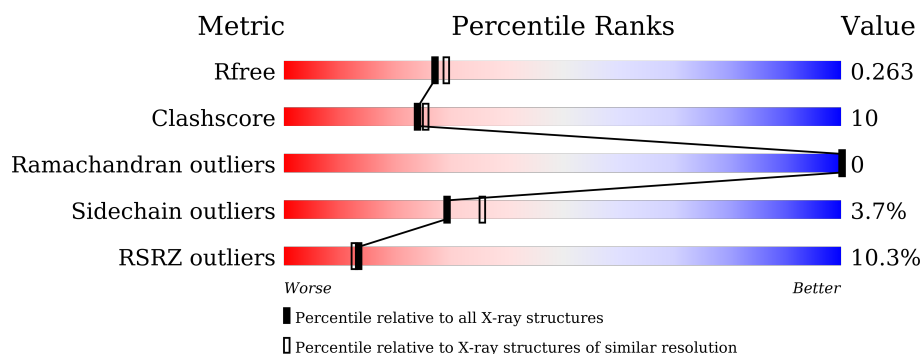
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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}	164625	8336 (2.20-2.16)
Clashscore	180529	9404 (2.20-2.16)
Ramachandran outliers	177936	9297 (2.20-2.16)
Sidechain outliers	177891	9297 (2.20-2.16)
RSRZ outliers	164620	8337 (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 $\leq 5\%$. 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	B	223	<div> <div>4%</div> <div>84%</div> <div>15%</div> </div>
2	A	214	<div> <div>%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
3	E	187	<div> <div>27%</div> <div>57%</div> <div>30%</div> <div>.</div> <div>11%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6094 atoms, of which 1451 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 A129 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	223	Total	C	N	O	S	0	0	0
			1671	1047	284	332	8			

- Molecule 2 is a protein called A129 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	214	Total	C	H	N	O	S	0	0
			3083	1023	1451	273	331	5		

- Molecule 3 is a protein called Entry-fusion complex associated protein OPG095.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	166	Total	C	N	O	S	0	0	0
			1229	753	208	258	10			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	146	MET	LEU	conflict	UNP M1LBP0
E	182	HIS	-	expression tag	UNP M1LBP0
E	183	HIS	-	expression tag	UNP M1LBP0
E	184	HIS	-	expression tag	UNP M1LBP0
E	185	HIS	-	expression tag	UNP M1LBP0
E	186	HIS	-	expression tag	UNP M1LBP0
E	187	HIS	-	expression tag	UNP M1LBP0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	44	Total	O	0	0
			44	44		

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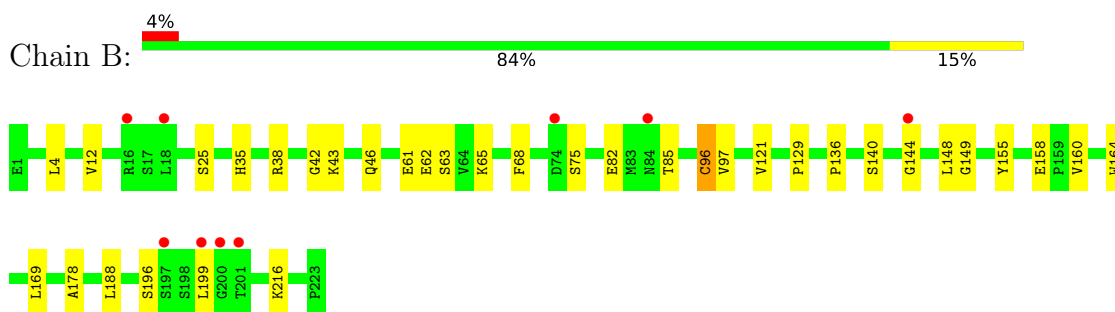
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total 51	O 51	0	0
4	E	16	Total 16	O 16	0	0

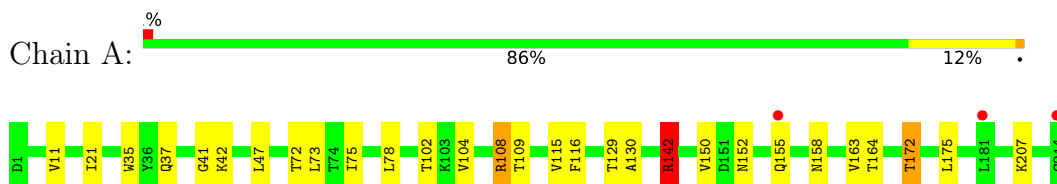
3 Residue-property plots

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.

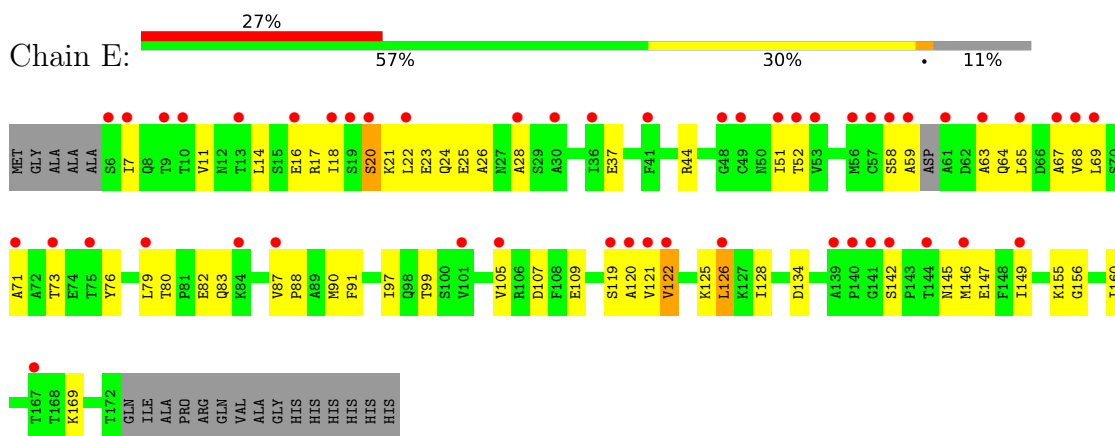
- Molecule 1: A129 heavy chain



- Molecule 2: A129 light chain



- Molecule 3: Entry-fusion complex associated protein OPG095



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.73Å 89.30Å 100.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.33 – 2.17 38.33 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.33-2.17) 99.9 (38.33-2.17)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.211 , 0.262 0.225 , 0.263	Depositor DCC
R_{free} test set	34340 reflections (5.51%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6094	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 4.38% 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 [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	B	0.52	0/1711	0.71	0/2329
2	A	0.61	0/1669	0.73	0/2267
3	E	0.52	0/1241	0.74	0/1688
All	All	0.55	0/4621	0.73	0/6284

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	108	ARG	Sidechain
2	A	142	ARG	Sidechain

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	B	1671	0	1617	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1632	1451	1584	18	0
3	E	1229	0	1184	50	0
4	A	51	0	0	0	0
4	B	44	0	0	2	0
4	E	16	0	0	0	0
All	All	4643	1451	4385	88	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 10.

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)
2:A:37:GLN:HB2	2:A:47:LEU:HD11	1.74	0.69
3:E:63:ALA:O	3:E:67:ALA:N	2.25	0.69
3:E:28:ALA:HB2	3:E:58:SER:HB3	1.74	0.68
1:B:61:GLU:OE1	1:B:63:SER:HB3	1.94	0.67
3:E:20:SER:O	3:E:23:GLU:HG2	1.97	0.64
3:E:73:THR:HG22	3:E:105:VAL:HG13	1.80	0.64
3:E:76:TYR:HA	3:E:79:LEU:HD12	1.80	0.63
3:E:22:LEU:O	3:E:26:ALA:HB3	1.99	0.62
3:E:82:GLU:OE1	3:E:82:GLU:N	2.28	0.62
2:A:115:VAL:O	2:A:207:LYS:HD2	2.00	0.62
3:E:155:LYS:H	3:E:155:LYS:HE2	1.66	0.61
1:B:85:THR:HG22	1:B:85:THR:O	2.01	0.61
2:A:41:GLY:O	2:A:42:LYS:HE2	2.02	0.59
3:E:87:VAL:N	3:E:88:PRO:HD2	2.17	0.59
2:A:21:ILE:HD12	2:A:102:THR:HG21	1.86	0.57
3:E:37:GLU:O	3:E:128:ILE:HA	2.05	0.57
3:E:87:VAL:CG1	3:E:91:PHE:HE1	2.19	0.56
1:B:38:ARG:HD2	1:B:46:GLN:OE1	2.06	0.56
2:A:155:GLN:HG3	2:A:158:ASN:HD21	1.70	0.55
2:A:155:GLN:CG	2:A:158:ASN:HD21	2.20	0.55
3:E:14:LEU:O	3:E:18:ILE:HG12	2.06	0.55
3:E:69:LEU:O	3:E:73:THR:HG23	2.07	0.55
3:E:155:LYS:H	3:E:155:LYS:CE	2.19	0.54
3:E:52:THR:O	3:E:147:GLU:HA	2.08	0.54
3:E:17:ARG:O	3:E:21:LYS:HG3	2.08	0.53
1:B:144:GLY:O	1:B:196:SER:CB	2.57	0.52
3:E:18:ILE:O	3:E:22:LEU:HG	2.11	0.51
2:A:163:VAL:HG22	2:A:175:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:156:GLY:O	3:E:160:ILE:HG12	2.10	0.51
2:A:108:ARG:HG2	2:A:109:THR:N	2.27	0.50
3:E:44:ARG:HB2	3:E:134:ASP:O	2.10	0.50
1:B:129:PRO:HB3	1:B:155:TYR:HB3	1.94	0.50
1:B:62:GLU:OE1	1:B:65:LYS:NZ	2.40	0.49
1:B:144:GLY:O	1:B:196:SER:N	2.34	0.49
2:A:73:LEU:C	2:A:73:LEU:HD23	2.34	0.48
1:B:149:GLY:HA2	1:B:164:TRP:CH2	2.47	0.48
3:E:80:THR:HG23	3:E:82:GLU:HG2	1.96	0.48
3:E:23:GLU:CG	3:E:24:GLN:N	2.77	0.48
1:B:25:SER:OG	4:B:301:HOH:O	2.20	0.48
3:E:18:ILE:HD13	3:E:71:ALA:HB3	1.96	0.48
1:B:4:LEU:HD23	1:B:96:CYS:SG	2.54	0.47
3:E:87:VAL:O	3:E:90:MET:HG2	2.13	0.47
3:E:99:THR:OG1	3:E:107:ASP:OD2	2.22	0.47
3:E:122:VAL:HB	3:E:155:LYS:HD2	1.96	0.47
3:E:169:LYS:HD3	3:E:169:LYS:HA	1.65	0.47
3:E:17:ARG:HH11	3:E:21:LYS:NZ	2.13	0.47
3:E:87:VAL:HG12	3:E:91:PHE:CE1	2.50	0.46
3:E:87:VAL:CG1	3:E:91:PHE:CE1	2.99	0.46
2:A:11:VAL:CG1	2:A:104:VAL:HG22	2.45	0.46
1:B:35:HIS:HB2	1:B:97:VAL:HG22	1.96	0.46
1:B:158:GLU:OE2	1:B:178:ALA:HB3	2.16	0.46
2:A:35:TRP:CE2	2:A:73:LEU:HB2	2.50	0.45
1:B:155:TYR:CE2	1:B:160:VAL:HG23	2.51	0.45
3:E:80:THR:HG22	3:E:83:GLN:CG	2.47	0.45
3:E:119:SER:O	3:E:120:ALA:C	2.55	0.45
3:E:16:GLU:O	3:E:20:SER:OG	2.34	0.45
1:B:42:GLY:C	1:B:43:LYS:HD2	2.37	0.45
3:E:155:LYS:N	3:E:155:LYS:HD3	2.33	0.44
3:E:80:THR:HG23	3:E:83:GLN:H	1.82	0.44
3:E:125:LYS:HB3	3:E:125:LYS:HE3	1.78	0.44
3:E:58:SER:OG	3:E:59:ALA:N	2.51	0.43
3:E:21:LYS:HA	3:E:24:GLN:HG2	2.00	0.43
2:A:129:THR:HG22	2:A:130:ALA:N	2.32	0.43
3:E:24:GLN:HG3	3:E:25:GLU:HG2	2.01	0.43
3:E:7:ILE:O	3:E:11:VAL:HG23	2.19	0.43
3:E:64:GLN:O	3:E:68:VAL:HG12	2.19	0.43
1:B:188:LEU:HD12	1:B:188:LEU:C	2.39	0.42
4:B:323:HOH:O	2:A:172:THR:HG23	2.19	0.42
2:A:150:VAL:HG21	2:A:155:GLN:HE21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:87:VAL:O	3:E:91:PHE:HD1	2.03	0.42
3:E:126:LEU:HD13	3:E:126:LEU:HA	1.72	0.42
3:E:155:LYS:H	3:E:155:LYS:CD	2.33	0.41
3:E:76:TYR:O	3:E:79:LEU:HB2	2.19	0.41
3:E:119:SER:O	3:E:121:VAL:N	2.53	0.41
3:E:97:ILE:HD13	3:E:97:ILE:HA	1.83	0.41
1:B:35:HIS:HB2	1:B:97:VAL:CG2	2.50	0.41
2:A:75:ILE:HG21	2:A:78:LEU:HD12	2.03	0.41
1:B:140:SER:HA	2:A:116:PHE:CD1	2.55	0.41
2:A:142:ARG:CZ	2:A:163:VAL:HG21	2.51	0.41
3:E:18:ILE:HD12	3:E:68:VAL:HG23	2.03	0.41
3:E:80:THR:HG22	3:E:83:GLN:HG3	2.02	0.41
1:B:68:PHE:HA	1:B:82:GLU:O	2.21	0.40
2:A:163:VAL:HG12	2:A:164:THR:O	2.21	0.40
1:B:136:PRO:HG3	1:B:148:LEU:HD13	2.03	0.40
1:B:12:VAL:CG1	1:B:121:VAL:HG22	2.52	0.40
3:E:87:VAL:N	3:E:88:PRO:CD	2.84	0.40
1:B:178:ALA:HA	1:B:188:LEU:HB3	2.02	0.40
3:E:24:GLN:HG3	3:E:25:GLU:CG	2.52	0.40

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	B	221/223 (99%)	212 (96%)	9 (4%)	0	100	100
2	A	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
3	E	162/187 (87%)	151 (93%)	11 (7%)	0	100	100
All	All	595/624 (95%)	567 (95%)	28 (5%)	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	B	188/188 (100%)	183 (97%)	5 (3%)	40	49
2	A	186/186 (100%)	182 (98%)	4 (2%)	47	58
3	E	137/155 (88%)	127 (93%)	10 (7%)	11	11
All	All	511/529 (97%)	492 (96%)	19 (4%)	29	35

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	75	SER
1	B	96	CYS
1	B	169	LEU
1	B	199	LEU
1	B	216	LYS
2	A	72	THR
2	A	142	ARG
2	A	152	ASN
2	A	172	THR
3	E	20	SER
3	E	51	ILE
3	E	65	LEU
3	E	109	GLU
3	E	122	VAL
3	E	126	LEU
3	E	142	SER
3	E	145	ASN
3	E	146	MET
3	E	149	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides 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	B	223/223 (100%)	0.52	9 (4%) 43 42	32, 43, 56, 75	0
2	A	214/214 (100%)	0.15	3 (1%) 73 72	34, 46, 59, 99	0
3	E	166/187 (88%)	1.54	50 (30%) 1 1	40, 69, 91, 99	0
All	All	603/624 (96%)	0.67	62 (10%) 13 12	32, 46, 82, 99	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	7	ILE	4.7
3	E	41	PHE	4.2
3	E	18	ILE	4.0
3	E	19	SER	3.9
3	E	6	SER	3.6
3	E	146	MET	3.4
1	B	16	ARG	3.4
3	E	120	ALA	3.3
3	E	79	LEU	3.3
3	E	68	VAL	3.3
3	E	140	PRO	3.2
1	B	201	THR	3.1
3	E	56	MET	3.1
3	E	36	ILE	3.1
3	E	142	SER	3.0
1	B	199	LEU	2.9
3	E	139	ALA	2.9
2	A	214	CYS	2.9
3	E	73	THR	2.9
3	E	16	GLU	2.8
3	E	22	LEU	2.8
3	E	59	ALA	2.8
3	E	71	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	48	GLY	2.7
3	E	121	VAL	2.7
3	E	144	THR	2.7
3	E	30	ALA	2.6
3	E	101	VAL	2.6
3	E	126	LEU	2.6
3	E	149	ILE	2.5
3	E	119	SER	2.5
2	A	181	LEU	2.5
1	B	74	ASP	2.5
3	E	105	VAL	2.5
1	B	18	LEU	2.4
3	E	63	ALA	2.4
1	B	197	SER	2.4
3	E	58	SER	2.4
3	E	51	ILE	2.4
3	E	61	ALA	2.4
2	A	155	GLN	2.4
3	E	9	THR	2.3
3	E	69	LEU	2.3
3	E	49	CYS	2.3
3	E	52	THR	2.3
3	E	122	VAL	2.2
3	E	84	LYS	2.2
1	B	84	ASN	2.2
1	B	144	GLY	2.2
3	E	75	THR	2.1
3	E	53	VAL	2.1
3	E	10	THR	2.1
3	E	167	THR	2.1
3	E	67	ALA	2.1
1	B	200	GLY	2.1
3	E	87	VAL	2.1
3	E	65	LEU	2.1
3	E	20	SER	2.1
3	E	28	ALA	2.1
3	E	141	GLY	2.0
3	E	13	THR	2.0
3	E	57	CYS	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 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.