



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2017 – 11:37 PM EST

PDB ID : 4LP5
Title : Crystal structure of the full-length human RAGE extracellular domain (VC1C2 fragment)
Authors : Yatime, L.; Andersen, G.R.
Deposited on : unknown
Resolution : 3.80 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

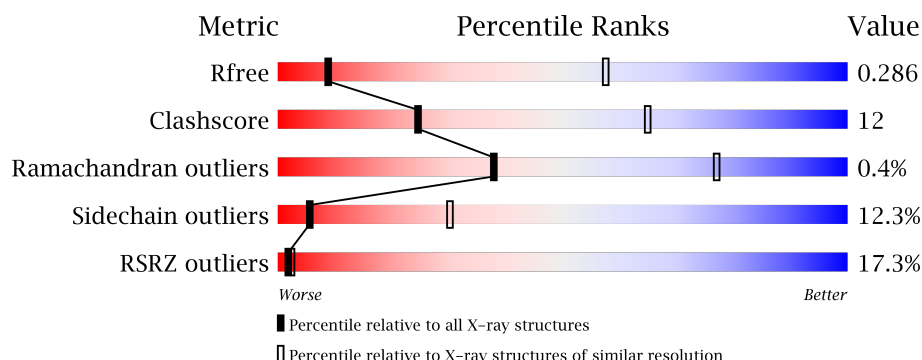
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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	304	
1	B	304	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3902 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 Advanced glycosylation end product-specific receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	211	Total	C	N	O	S	0	0	0
			1622	1022	300	294	6			
1	A	302	Total	C	N	O	S	0	0	0
			2280	1439	408	423	10			

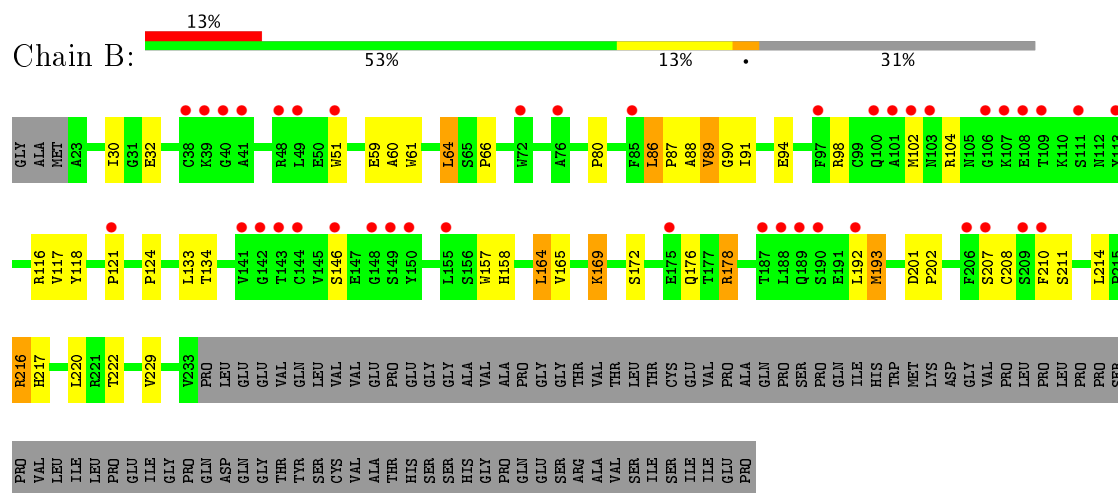
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	GLY	-	EXPRESSION TAG	UNP Q15109
B	21	ALA	-	EXPRESSION TAG	UNP Q15109
B	22	MET	-	EXPRESSION TAG	UNP Q15109
A	20	GLY	-	EXPRESSION TAG	UNP Q15109
A	21	ALA	-	EXPRESSION TAG	UNP Q15109
A	22	MET	-	EXPRESSION TAG	UNP Q15109

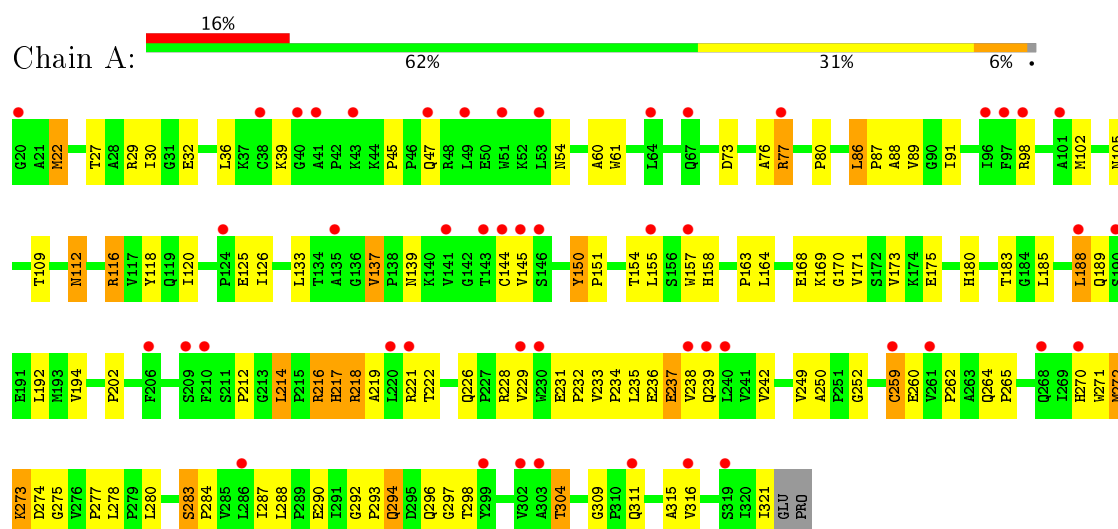
3 Residue-property plots [i](#)

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: Advanced glycosylation end product-specific receptor



• Molecule 1: Advanced glycosylation end product-specific receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	180.01Å 180.01Å 48.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.18 – 3.80 77.95 – 3.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (31.18-3.80) 96.3 (77.95-3.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 3.78Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.242 , 0.286 0.239 , 0.286	Depositor DCC
R_{free} test set	891 reflections (10.11%)	DCC
Wilson B-factor (Å ²)	136.1	Xtriage
Anisotropy	0.885	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 115.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3902	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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	A	0.29	0/2343	0.52	1/3202 (0.0%)
1	B	0.27	0/1665	0.51	0/2265
All	All	0.28	0/4008	0.51	1/5467 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	LEU	CA-CB-CG	5.52	127.99	115.30

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	2280	0	2291	75	0
1	B	1622	0	1638	23	0
All	All	3902	0	3929	96	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 12.

All (96) 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:22:MET:O	1:A:112:ASN:ND2	1.89	1.04
1:A:273:LYS:HB3	1:A:278:LEU:HD21	1.58	0.86
1:A:54:ASN:ND2	1:A:60:ALA:O	2.10	0.84
1:A:60:ALA:O	1:A:61:TRP:CD1	2.30	0.84
1:A:218:ARG:HD3	1:A:219:ALA:H	1.48	0.78
1:A:273:LYS:HE2	1:A:274:ASP:H	1.52	0.75
1:A:292:GLY:HA3	1:A:294:GLN:HE21	1.52	0.73
1:B:88:ALA:HB2	1:A:80:PRO:HG3	1.72	0.72
1:A:218:ARG:HD2	1:A:221:ARG:HH22	1.56	0.70
1:A:171:VAL:HG22	1:A:194:VAL:HG12	1.73	0.70
1:B:80:PRO:HG2	1:A:88:ALA:HB2	1.73	0.70
1:B:157:TRP:HB2	1:B:164:LEU:HD11	1.78	0.65
1:A:242:VAL:HG21	1:A:316:VAL:HG21	1.78	0.65
1:A:169:LYS:H	1:A:170:GLY:HA2	1.60	0.65
1:A:273:LYS:HG3	1:A:274:ASP:N	2.12	0.64
1:A:272:MET:HB2	1:A:277:PRO:HA	1.80	0.64
1:A:60:ALA:C	1:A:61:TRP:CD1	2.72	0.63
1:B:51:TRP:HB2	1:B:64:LEU:HD21	1.84	0.60
1:A:76:ALA:HB2	1:A:86:LEU:HD23	1.84	0.60
1:A:118:TYR:CZ	1:A:216:ARG:HD3	2.37	0.59
1:A:293:PRO:HA	1:A:296:GLN:HG3	1.85	0.58
1:B:30:ILE:HG23	1:B:90:GLY:HA2	1.84	0.58
1:A:259:CYS:HB2	1:A:271:TRP:CH2	2.39	0.57
1:A:126:ILE:HG13	1:A:222:THR:HG21	1.86	0.56
1:A:169:LYS:N	1:A:170:GLY:HA2	2.19	0.56
1:B:216:ARG:NH1	1:B:217:HIS:HB2	2.21	0.56
1:A:271:TRP:NE1	1:A:283:SER:O	2.39	0.55
1:A:29:ARG:HB2	1:A:118:TYR:CZ	2.41	0.55
1:A:137:VAL:O	1:A:139:ASN:ND2	2.41	0.54
1:A:158:HIS:HA	1:A:163:PRO:HA	1.89	0.54
1:A:155:LEU:HG	1:A:188:LEU:HD12	1.88	0.54
1:A:45:PRO:HA	1:A:47:GLN:HG3	1.89	0.54
1:A:60:ALA:C	1:A:61:TRP:HD1	2.09	0.54
1:A:273:LYS:H	1:A:278:LEU:HG	1.73	0.53
1:A:239:GLN:HB2	1:A:260:GLU:HB2	1.90	0.53
1:A:250:ALA:HA	1:A:321:ILE:HG12	1.91	0.53
1:A:218:ARG:HD2	1:A:221:ARG:NH2	2.24	0.53
1:A:202:PRO:HA	1:A:229:VAL:HB	1.91	0.53
1:A:32:GLU:O	1:A:89:VAL:HG12	2.09	0.53
1:A:264:GLN:HE21	1:A:265:PRO:HD2	1.74	0.52
1:B:121:PRO:HG3	1:B:210:PHE:CE2	2.45	0.52
1:B:124:PRO:HG3	1:B:220:LEU:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LYS:HB2	1:A:171:VAL:N	2.25	0.51
1:A:180:HIS:HB3	1:A:183:THR:O	2.12	0.50
1:A:273:LYS:CE	1:A:274:ASP:H	2.21	0.50
1:A:29:ARG:HH12	1:A:120:ILE:HD13	1.76	0.50
1:B:214:LEU:HB2	1:B:216:ARG:NE	2.28	0.49
1:A:91:ILE:HG23	1:A:150:TYR:HE2	1.77	0.49
1:A:218:ARG:HD3	1:A:219:ALA:N	2.23	0.49
1:A:54:ASN:HB2	1:A:61:TRP:CE2	2.47	0.49
1:A:171:VAL:HG13	1:A:192:LEU:HD11	1.95	0.48
1:A:30:ILE:HG13	1:A:118:TYR:O	2.14	0.48
1:A:118:TYR:CE2	1:A:216:ARG:HD3	2.49	0.47
1:A:232:PRO:O	1:A:234:PRO:HD3	2.14	0.47
1:A:273:LYS:CG	1:A:274:ASP:N	2.77	0.47
1:A:39:LYS:O	1:A:109:THR:OG1	2.19	0.47
1:A:144:CYS:HB2	1:A:157:TRP:CZ2	2.50	0.47
1:A:292:GLY:HA3	1:A:294:GLN:NE2	2.24	0.47
1:A:73:ASP:HA	1:A:77:ARG:HG2	1.97	0.47
1:A:212:PRO:HB3	1:A:217:HIS:HE2	1.80	0.47
1:B:169:LYS:HD3	1:B:169:LYS:H	1.79	0.46
1:B:86:LEU:HA	1:B:87:PRO:HD3	1.75	0.46
1:A:273:LYS:HE3	1:A:297:GLY:HA3	1.98	0.46
1:A:27:THR:HA	1:A:116:ARG:O	2.16	0.46
1:A:237:GLU:HG3	1:A:238:VAL:N	2.30	0.45
1:A:155:LEU:HA	1:A:155:LEU:HD23	1.85	0.45
1:A:271:TRP:HZ2	1:A:284:PRO:C	2.19	0.45
1:B:172:SER:HB3	1:B:193:MET:HB2	1.97	0.44
1:A:98:ARG:HG2	1:A:112:ASN:HB3	1.99	0.44
1:B:202:PRO:HA	1:B:229:VAL:HB	2.00	0.44
1:A:235:LEU:HD23	1:A:235:LEU:H	1.82	0.44
1:B:116:ARG:HD3	1:B:116:ARG:HA	1.74	0.43
1:A:236:GLU:HB3	1:A:262:PRO:HG2	2.00	0.43
1:B:61:TRP:HH2	1:B:98:ARG:HH11	1.65	0.43
1:B:158:HIS:N	1:B:207:SER:O	2.50	0.43
1:B:32:GLU:O	1:B:89:VAL:HG12	2.19	0.43
1:A:168:GLU:O	1:A:169:LYS:NZ	2.44	0.43
1:B:94:GLU:HG3	1:B:117:VAL:HG22	2.00	0.42
1:A:273:LYS:HE3	1:A:298:THR:N	2.34	0.42
1:B:208:CYS:HB3	1:B:222:THR:HG21	2.01	0.42
1:B:176:GLN:HE21	1:B:178:ARG:HD3	1.84	0.42
1:A:252:GLY:HA2	1:A:290:GLU:HA	2.01	0.42
1:A:304:THR:HA	1:A:309:GLY:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASP:HA	1:A:275:GLY:HA2	1.72	0.42
1:A:249:VAL:HG12	1:A:250:ALA:O	2.20	0.41
1:B:192:LEU:O	1:B:193:MET:HG2	2.19	0.41
1:A:273:LYS:NZ	1:A:274:ASP:O	2.40	0.41
1:A:91:ILE:HG12	1:A:150:TYR:CE2	2.55	0.41
1:A:145:VAL:HG22	1:A:189:GLN:HG3	2.03	0.41
1:A:216:ARG:HE	1:A:216:ARG:C	2.23	0.41
1:A:86:LEU:HA	1:A:87:PRO:HD3	1.94	0.41
1:B:59:GLU:HA	1:B:60:ALA:HA	1.60	0.41
1:A:150:TYR:HD1	1:A:151:PRO:HA	1.86	0.41
1:A:29:ARG:NH1	1:A:120:ILE:HD13	2.35	0.41
1:A:173:VAL:HG12	1:A:175:GLU:HG3	2.03	0.41
1:B:91:ILE:HA	1:B:117:VAL:HG21	2.02	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	A	300/304 (99%)	268 (89%)	31 (10%)	1 (0%)	44	81
1	B	209/304 (69%)	187 (90%)	21 (10%)	1 (0%)	32	73
All	All	509/608 (84%)	455 (89%)	52 (10%)	2 (0%)	38	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	ALA
1	B	66	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	253/255 (99%)	217 (86%)	36 (14%)	4	26
1	B	177/255 (69%)	160 (90%)	17 (10%)	10	41
All	All	430/510 (84%)	377 (88%)	53 (12%)	5	30

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	64	LEU
1	B	86	LEU
1	B	89	VAL
1	B	102	MET
1	B	104	ARG
1	B	118	TYR
1	B	133	LEU
1	B	134	THR
1	B	146	SER
1	B	164	LEU
1	B	165	VAL
1	B	169	LYS
1	B	178	ARG
1	B	193	MET
1	B	201	ASP
1	B	211	SER
1	B	216	ARG
1	A	22	MET
1	A	36	LEU
1	A	77	ARG
1	A	86	LEU
1	A	102	MET
1	A	105	ASN
1	A	112	ASN
1	A	116	ARG
1	A	125	GLU
1	A	133	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	137	VAL
1	A	150	TYR
1	A	154	THR
1	A	164	LEU
1	A	185	LEU
1	A	188	LEU
1	A	214	LEU
1	A	216	ARG
1	A	217	HIS
1	A	218	ARG
1	A	226	GLN
1	A	228	ARG
1	A	231	GLU
1	A	233	VAL
1	A	237	GLU
1	A	259	CYS
1	A	270	HIS
1	A	272	MET
1	A	273	LYS
1	A	280	LEU
1	A	283	SER
1	A	287	ILE
1	A	288	LEU
1	A	294	GLN
1	A	304	THR
1	A	311	GLN

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

Mol	Chain	Res	Type
1	B	167	ASN
1	B	176	GLN
1	B	226	GLN
1	A	176	GLN
1	A	264	GLN
1	A	294	GLN
1	A	296	GLN

5.3.3 RNA ⓘ

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	302/304 (99%)	0.84	48 (15%) 2 3	78, 121, 189, 278	0
1	B	211/304 (69%)	0.93	41 (19%) 1 2	106, 139, 198, 270	0
All	All	513/608 (84%)	0.88	89 (17%) 2 2	78, 130, 196, 278	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	THR	6.1
1	B	190	SER	5.7
1	B	189	GLN	5.3
1	A	146	SER	5.0
1	B	206	PHE	4.8
1	A	145	VAL	4.6
1	B	141	VAL	4.6
1	A	43	LYS	4.5
1	B	143	THR	4.5
1	A	206	PHE	4.3
1	B	49	LEU	4.3
1	B	188	LEU	4.2
1	A	220	LEU	4.0
1	A	143	THR	3.8
1	B	107	LYS	3.5
1	A	240	LEU	3.5
1	B	209	SER	3.4
1	B	142	GLY	3.4
1	B	192	LEU	3.4
1	B	41	ALA	3.3
1	A	49	LEU	3.2
1	B	103	ASN	3.2
1	A	20	GLY	3.2
1	B	108	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	47	GLN	3.2
1	A	64	LEU	3.1
1	A	230	TRP	3.1
1	B	100	GLN	3.1
1	A	311	GLN	3.1
1	A	40	GLY	3.0
1	A	51	TRP	3.0
1	A	299	TYR	3.0
1	A	239	GLN	3.0
1	A	238	VAL	2.9
1	A	188	LEU	2.9
1	B	187	THR	2.8
1	A	157	TRP	2.8
1	B	207	SER	2.8
1	A	303	ALA	2.8
1	A	270	HIS	2.8
1	A	77	ARG	2.7
1	B	101	ALA	2.7
1	A	97	PHE	2.7
1	A	190	SER	2.7
1	B	210	PHE	2.7
1	B	144	CYS	2.6
1	B	146	SER	2.6
1	A	53	LEU	2.6
1	B	148	GLY	2.6
1	A	124	PRO	2.5
1	A	101	ALA	2.5
1	B	175	GLU	2.5
1	A	96	ILE	2.5
1	A	261	VAL	2.4
1	A	41	ALA	2.4
1	A	221	ARG	2.4
1	B	38	CYS	2.4
1	A	209	SER	2.4
1	B	85	PHE	2.4
1	B	97	PHE	2.4
1	B	155	LEU	2.4
1	A	286	LEU	2.4
1	A	210	PHE	2.3
1	B	39	LYS	2.3
1	B	40	GLY	2.3
1	B	113	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	121	PRO	2.3
1	A	268	GLN	2.3
1	B	102	MET	2.3
1	A	302	VAL	2.3
1	A	67	GLN	2.3
1	B	111	SER	2.2
1	B	51	TRP	2.2
1	A	259	CYS	2.2
1	B	106	GLY	2.2
1	A	155	LEU	2.2
1	B	76	ALA	2.2
1	A	38	CYS	2.2
1	A	141	VAL	2.1
1	B	150	TYR	2.1
1	A	229	VAL	2.1
1	A	144	CYS	2.1
1	B	72	TRP	2.1
1	A	98	ARG	2.0
1	B	149	SER	2.0
1	A	319	SER	2.0
1	A	316	VAL	2.0
1	B	48	ARG	2.0
1	A	135	ALA	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.