



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:14 PM GMT

PDB ID : 1WP1
Title : Crystal structure of the drug-discharge outer membrane protein, OprM
Authors : Akama, H.; Kanemaki, M.; Yoshimura, M.; Tsukihara, T.; Kashiwagi, T.;
Narita, S.; Nakagawa, A.; Nakae, T.
Deposited on : 2004-08-28
Resolution : 2.56 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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

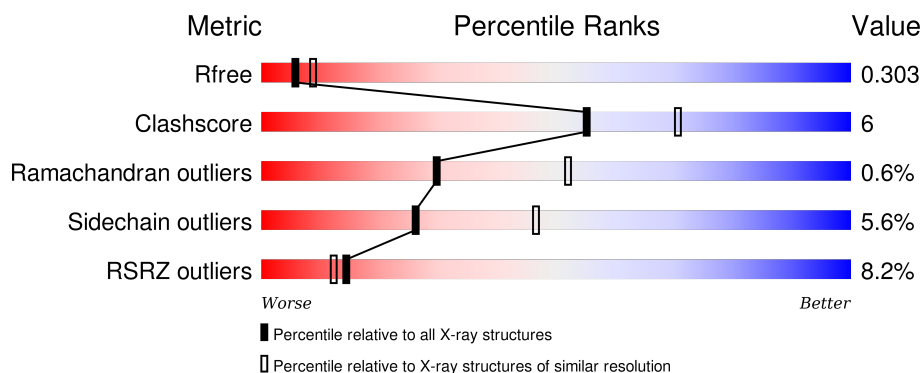
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

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	474	<div> <div>3%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
1	B	474	<div> <div>12%</div> <div>69%</div> <div>15%</div> <div>• 15%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6671 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 Outer membrane protein oprM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3494	2186	622	683	3			
1	B	405	Total	C	N	O	S	0	0	0
			3153	1983	559	609	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	HIS	-	EXPRESSION TAG	UNP Q51487
A	470	HIS	-	EXPRESSION TAG	UNP Q51487
A	471	HIS	-	EXPRESSION TAG	UNP Q51487
A	472	HIS	-	EXPRESSION TAG	UNP Q51487
A	473	HIS	-	EXPRESSION TAG	UNP Q51487
A	474	HIS	-	EXPRESSION TAG	UNP Q51487
B	469	HIS	-	EXPRESSION TAG	UNP Q51487
B	470	HIS	-	EXPRESSION TAG	UNP Q51487
B	471	HIS	-	EXPRESSION TAG	UNP Q51487
B	472	HIS	-	EXPRESSION TAG	UNP Q51487
B	473	HIS	-	EXPRESSION TAG	UNP Q51487
B	474	HIS	-	EXPRESSION TAG	UNP Q51487

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	O	0	0
			17	17		
2	B	7	Total	O	0	0
			7	7		

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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 81% 3% 14%
- Y358
E359
K391
D394
E395
R403
T406
D409
Q426
Q435
L436
K444
G447
G448
G449
V455
T456
GLN
GLN
GLN
THR
ALA
LYS
LYS
GLU
ASP
PRO
GLN
ALA
HIS
HIS
HIS
HIS
HIS
HIS
- C1
S2
L3
P10
E11
A12
P13
A16
P19
Y24
A35
I38
R41
D46
P47
Q48
L49
Q50
E58
R61
R64
E71
R74
D83
L84
F85
P86
R87
G94
T95
T105
A110
I111
G116
G120
T121
T122
A123
W124
Y125
L126
- T155
D171
Q174
V198
L204
T211
D230
S240
N245
L246
G251
Q254
V260
P265
L269
R272
P273
D274
L275
R293
I300
A304
N305
R311
F317
W324
L325
N331
I334
F335
T336
A337
G338
S339
L340
R341

- [illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	85.43Å 85.43Å 1044.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.63 – 2.56 36.37 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.63-2.56) 99.2 (36.37-2.56)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.252 , 0.308 0.249 , 0.303	Depositor DCC
R_{free} test set	2438 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	77.7	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 48264 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6671	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	0.64	0/3550	0.70	3/4829 (0.1%)
1	B	0.90	9/3202 (0.3%)	0.80	7/4353 (0.2%)
All	All	0.77	9/6752 (0.1%)	0.75	10/9182 (0.1%)

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
1	A	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	ARG	CZ-NH1	29.47	1.71	1.33
1	B	81	ARG	CZ-NH1	12.68	1.49	1.33
1	B	78	ARG	NE-CZ	10.33	1.46	1.33
1	B	141	GLU	CD-OE2	8.78	1.35	1.25
1	B	279	GLU	CD-OE2	7.88	1.34	1.25
1	B	141	GLU	CD-OE1	6.58	1.32	1.25
1	B	78	ARG	CZ-NH2	5.79	1.40	1.33
1	B	136	ARG	CZ-NH1	5.42	1.40	1.33
1	B	81	ARG	CZ-NH2	5.31	1.40	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ARG	NE-CZ-NH2	-21.36	109.62	120.30
1	B	81	ARG	NE-CZ-NH2	-16.23	112.19	120.30
1	B	81	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	B	78	ARG	CD-NE-CZ	-7.67	112.86	123.60
1	B	78	ARG	NE-CZ-NH1	5.66	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ARG	NH1-CZ-NH2	5.40	125.33	119.40
1	A	394	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	272	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	136	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	230	ASP	CB-CG-OD1	5.07	122.87	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	447	GLY	Peptide

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	3494	0	3473	43	0
1	B	3153	0	3138	40	0
2	A	17	0	0	2	0
2	B	7	0	0	0	0
All	All	6671	0	6611	83	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 6.

All (83) 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:B:78:ARG:NH1	1:B:78:ARG:CZ	1.71	1.54
1:A:336:THR:HG21	1:A:339:SER:HB3	1.26	1.08
1:A:336:THR:CG2	1:A:339:SER:HB3	1.89	1.02
1:B:87:ARG:HB2	1:B:124:TRP:HB2	1.59	0.84
1:A:336:THR:HG21	1:A:339:SER:CB	2.11	0.79
1:A:336:THR:CG2	1:A:339:SER:CB	2.64	0.76
1:B:435:GLN:HG3	1:B:436:LEU:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:LEU:O	1:B:437:THR:HG23	1.86	0.75
1:A:403:ARG:NH1	1:A:409:ASP:OD2	2.21	0.73
1:B:39:GLY:HA2	1:B:451:ASN:O	1.90	0.71
1:A:272:ARG:HD3	1:A:274:ASP:OD1	1.91	0.71
1:A:251:GLY:H	1:A:254:GLN:HE21	1.38	0.70
1:B:289:ILE:HD11	1:B:351:LYS:HD2	1.72	0.70
1:B:67:ALA:HA	1:B:150:GLN:HE21	1.57	0.69
1:A:305:ASN:HB2	1:A:325:LEU:HB3	1.73	0.69
1:A:12:ALA:HB2	1:A:269:LEU:HD11	1.75	0.69
1:A:38:ILE:HD12	1:A:260:VAL:HG22	1.75	0.69
1:B:9:ARG:CD	1:B:279:GLU:OE2	2.42	0.68
1:B:345:ASP:O	1:B:349:ILE:HG12	1.94	0.68
1:B:365:ALA:O	1:B:369:VAL:HG23	1.93	0.68
1:B:9:ARG:HD2	1:B:279:GLU:OE2	1.95	0.67
1:B:282:LEU:HD11	1:B:355:VAL:HG23	1.75	0.67
1:A:121:THR:HG21	1:A:124:TRP:HB2	1.80	0.62
1:A:336:THR:HG22	1:A:339:SER:H	1.66	0.59
1:B:77:TYR:HA	1:B:139:ALA:HB1	1.85	0.59
1:A:331:ASN:C	1:A:331:ASN:OD1	2.43	0.57
1:B:7:TYR:OH	1:B:279:GLU:HG2	2.03	0.57
1:B:272:ARG:NH1	1:B:274:ASP:OD2	2.38	0.57
1:B:70:VAL:HG21	1:B:150:GLN:NE2	2.21	0.55
1:B:9:ARG:HD3	1:B:279:GLU:OE2	2.06	0.55
1:B:41:ARG:HG3	1:B:452:GLN:HG3	1.89	0.55
1:B:397:TYR:HA	1:B:417:ALA:HB1	1.89	0.54
1:A:35:ALA:HB2	1:A:260:VAL:HG13	1.90	0.54
1:A:16:ALA:O	1:A:265:PRO:HG2	2.09	0.52
1:B:67:ALA:HA	1:B:150:GLN:NE2	2.24	0.52
1:B:67:ALA:O	1:B:70:VAL:HB	2.11	0.51
1:B:399:LEU:O	1:B:403:ARG:HG3	2.11	0.50
1:B:403:ARG:NH1	1:B:409:ASP:OD2	2.45	0.50
1:A:41:ARG:HD2	1:A:50:GLN:OE1	2.11	0.50
1:A:174:GLN:HE22	1:A:426:GLN:HA	1.76	0.50
1:A:3:LEU:O	1:A:293:ARG:NH1	2.36	0.49
1:B:60:ASN:ND2	1:B:157:LEU:HD11	2.28	0.48
1:A:171:ASP:OD2	1:A:230:ASP:OD2	2.31	0.47
1:B:140:LEU:O	1:B:143:TYR:HB3	2.15	0.47
1:A:41:ARG:CD	1:A:50:GLN:OE1	2.64	0.46
1:B:298:PRO:HB3	1:B:331:ASN:H	1.79	0.46
1:B:349:ILE:HA	1:B:352:ASP:HB2	1.98	0.46
1:A:174:GLN:HE22	1:A:426:GLN:HG2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:GLN:HG3	1:A:436:LEU:N	2.30	0.46
1:A:46:ASP:OD1	1:A:48:GLN:N	2.46	0.46
1:A:46:ASP:C	1:A:46:ASP:OD1	2.54	0.45
1:A:391:LYS:O	1:A:395:GLU:HG2	2.17	0.45
1:A:120:GLY:HA3	1:A:304:ALA:O	2.17	0.45
1:A:71:GLU:OE1	1:A:74:ARG:NH1	2.44	0.44
1:B:84:LEU:O	1:B:124:TRP:HZ2	2.01	0.44
1:A:10:PRO:HD2	1:A:358:TYR:CE2	2.53	0.43
1:B:7:TYR:OH	1:B:279:GLU:CG	2.65	0.43
1:A:35:ALA:CB	1:A:260:VAL:HG13	2.48	0.43
1:A:245:ASN:HB3	2:A:477:HOH:O	2.17	0.43
1:A:300:ILE:H	1:A:300:ILE:HG13	1.59	0.43
1:A:336:THR:HG22	1:A:337:ALA:N	2.34	0.43
1:A:13:PRO:HG3	1:A:359:GLU:HG2	2.00	0.43
1:A:58:GLU:O	1:A:64:ARG:NH2	2.52	0.42
1:A:272:ARG:HB3	1:A:275:ILE:HD12	2.00	0.42
1:B:242:ILE:HA	1:B:243:PRO:HD3	1.88	0.42
1:B:8:GLN:HG3	1:B:8:GLN:H	1.65	0.42
1:A:155:THR:HG22	1:A:449:GLY:H	1.85	0.42
1:B:64:ARG:O	1:B:68:LEU:HG	2.20	0.42
1:A:46:ASP:HA	1:A:47:PRO:HD3	1.95	0.42
1:B:13:PRO:HB2	1:B:363:GLN:HE21	1.84	0.42
1:B:452:GLN:HG2	1:B:453:GLN:HG2	2.01	0.41
1:B:9:ARG:HA	1:B:10:PRO:HD3	1.93	0.41
1:B:383:LEU:CD1	1:B:435:GLN:HE21	2.33	0.41
1:A:19:PRO:HB2	1:A:24:TYR:CZ	2.55	0.41
1:B:271:ARG:O	1:B:273:PRO:HD3	2.20	0.41
1:A:121:THR:HG22	1:A:122:THR:N	2.35	0.41
1:B:148:GLN:NE2	1:B:273:PRO:HA	2.36	0.41
1:A:87:ARG:O	1:A:121:THR:HG23	2.19	0.41
1:A:272:ARG:HA	1:A:273:PRO:HD3	1.87	0.40
1:A:174:GLN:HA	1:A:174:GLN:HE21	1.86	0.40
1:B:48:GLN:HE21	1:B:165:TYR:HE1	1.69	0.40
1:B:18:TYR:CZ	1:B:369:VAL:HG11	2.57	0.40
1:A:331:ASN:HB2	2:A:479:HOH:O	2.21	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	454/474 (96%)	432 (95%)	20 (4%)	2 (0%)	39	62
1	B	397/474 (84%)	368 (93%)	26 (6%)	3 (1%)	24	43
All	All	851/948 (90%)	800 (94%)	46 (5%)	5 (1%)	30	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	PRO
1	B	296	PHE
1	B	82	ALA
1	A	94	GLY
1	A	116	GLY

5.3.2 Protein sidechains [i](#)

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	359/375 (96%)	344 (96%)	15 (4%)	36	61
1	B	324/375 (86%)	301 (93%)	23 (7%)	18	34
All	All	683/750 (91%)	645 (94%)	38 (6%)	26	46

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG

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Mol	Chain	Res	Type
1	A	83	ASP
1	A	84	LEU
1	A	95	THR
1	A	126	LEU
1	A	198	VAL
1	A	204	LEU
1	A	211	THR
1	A	240	SER
1	A	260	VAL
1	A	272	ARG
1	A	334	ILE
1	A	406	THR
1	A	435	GLN
1	A	444	LYS
1	B	3	LEU
1	B	8	GLN
1	B	33	VAL
1	B	61	ARG
1	B	74	ARG
1	B	81	ARG
1	B	125	GLU
1	B	127	ASP
1	B	134	SER
1	B	136	ARG
1	B	152	SER
1	B	169	LYS
1	B	174	GLN
1	B	211	THR
1	B	260	VAL
1	B	270	GLN
1	B	272	ARG
1	B	293	ARG
1	B	345	ASP
1	B	409	ASP
1	B	435	GLN
1	B	456	THR
1	B	457	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN

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Mol	Chain	Res	Type
1	A	26	GLN
1	A	174	GLN
1	A	186	GLN
1	A	254	GLN
1	A	281	GLN
1	A	357	GLN
1	A	427	GLN
1	A	441	ASN
1	A	453	GLN
1	B	8	GLN
1	B	48	GLN
1	B	148	GLN
1	B	150	GLN
1	B	154	GLN
1	B	174	GLN
1	B	229	GLN
1	B	286	ASN
1	B	354	ASN
1	B	363	GLN
1	B	435	GLN

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 carbohydrates 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(Å ²)	Q<0.9
1	A	456/474 (96%)	0.22	12 (2%) 59 58	54, 70, 95, 99	0
1	B	405/474 (85%)	0.88	59 (14%) 3 2	66, 88, 133, 167	0
All	All	861/948 (90%)	0.53	71 (8%) 14 12	54, 78, 116, 167	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	TRP	8.7
1	B	344	LEU	8.4
1	B	85	PHE	7.1
1	B	90	VAL	6.9
1	B	323	SER	6.5
1	B	341	ARG	5.9
1	B	334	ILE	5.3
1	A	110	ALA	5.0
1	B	325	LEU	5.0
1	A	456	THR	4.9
1	B	86	PRO	4.9
1	B	4	ILE	4.8
1	B	122	THR	4.8
1	A	455	VAL	4.5
1	B	140	LEU	4.5
1	B	404	TYR	4.4
1	B	290	GLY	4.4
1	B	340	LEU	4.3
1	B	296	PHE	4.3
1	B	287	ALA	4.0
1	B	91	ASP	3.9
1	B	335	PHE	3.9
1	B	73	PHE	3.9
1	B	84	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	411	TYR	3.7
1	B	89	GLY	3.6
1	B	348	LYS	3.6
1	B	456	THR	3.5
1	B	68	LEU	3.5
1	B	7	TYR	3.4
1	B	291	ALA	3.3
1	B	77	TYR	3.2
1	B	128	LEU	3.1
1	B	88	ILE	3.1
1	A	105	THR	3.0
1	B	328	PRO	3.0
1	B	3	LEU	2.9
1	B	405	ARG	2.9
1	B	332	LEU	2.9
1	B	191	LEU	2.8
1	B	139	ALA	2.8
1	B	82	ALA	2.7
1	B	302	LEU	2.7
1	B	1	CYS	2.7
1	B	2	SER	2.6
1	B	330	ILE	2.6
1	B	351	LYS	2.5
1	B	284	ALA	2.5
1	A	311	ARG	2.5
1	B	449	GLY	2.5
1	A	86	PRO	2.4
1	B	326	PHE	2.4
1	A	246	LEU	2.4
1	B	414	LEU	2.4
1	B	293	ARG	2.4
1	A	85	PHE	2.4
1	B	294	ALA	2.4
1	B	126	LEU	2.3
1	A	341	ARG	2.3
1	B	333	PRO	2.3
1	B	189	PHE	2.3
1	B	40	TRP	2.1
1	B	353	ILE	2.1
1	B	269	LEU	2.1
1	A	317	PHE	2.1
1	B	457	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	198	VAL	2.1
1	A	111	ILE	2.0
1	B	283	MET	2.0
1	A	324	TRP	2.0
1	B	412	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.