



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:54 AM UTC

PDB ID : 1ZKD / pdb_00001zkd
Title : X-Ray structure of the putative protein Q6N1P6 from Rhodopseudomonas palustris at the resolution 2.1 Å , Northeast Structural Genomics Consortium target RpR58
Authors : Kuzin, A.P.; Yong, W.; Vorobiev, S.M.; Acton, T.; Ma, L.; Xiao, R.; Montelione, G.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2005-05-02
Resolution : 2.10 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

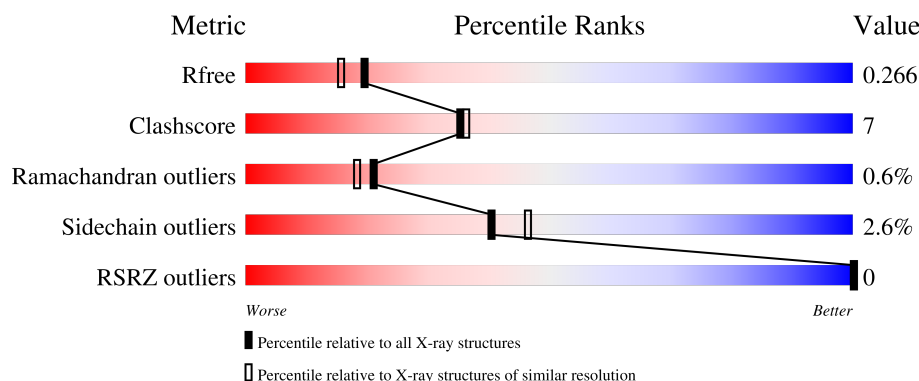
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	A	387	 76% 15% • 8%
1	B	387	 74% 17% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5740 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 DUF185.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	Se	0	0	0
			2740	1745	483	503	1	8			
1	B	356	Total	C	N	O	S	Se	0	0	0
			2729	1739	479	502	1	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MSE	MET	modified residue	UNP Q6N1P6
A	27	MSE	MET	modified residue	UNP Q6N1P6
A	60	MSE	MET	modified residue	UNP Q6N1P6
A	94	MSE	MET	modified residue	UNP Q6N1P6
A	95	MSE	MET	modified residue	UNP Q6N1P6
A	317	MSE	MET	modified residue	UNP Q6N1P6
A	343	MSE	MET	modified residue	UNP Q6N1P6
A	346	MSE	MET	modified residue	UNP Q6N1P6
A	380	LEU	-	cloning artifact	UNP Q6N1P6
A	381	GLU	-	cloning artifact	UNP Q6N1P6
A	382	HIS	-	cloning artifact	UNP Q6N1P6
A	383	HIS	-	cloning artifact	UNP Q6N1P6
A	384	HIS	-	cloning artifact	UNP Q6N1P6
A	385	HIS	-	cloning artifact	UNP Q6N1P6
A	386	HIS	-	cloning artifact	UNP Q6N1P6
A	387	HIS	-	cloning artifact	UNP Q6N1P6
B	21	MSE	MET	modified residue	UNP Q6N1P6
B	27	MSE	MET	modified residue	UNP Q6N1P6
B	60	MSE	MET	modified residue	UNP Q6N1P6
B	94	MSE	MET	modified residue	UNP Q6N1P6
B	95	MSE	MET	modified residue	UNP Q6N1P6
B	317	MSE	MET	modified residue	UNP Q6N1P6
B	343	MSE	MET	modified residue	UNP Q6N1P6
B	346	MSE	MET	modified residue	UNP Q6N1P6
B	380	LEU	-	cloning artifact	UNP Q6N1P6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	381	GLU	-	cloning artifact	UNP Q6N1P6
B	382	HIS	-	cloning artifact	UNP Q6N1P6
B	383	HIS	-	cloning artifact	UNP Q6N1P6
B	384	HIS	-	cloning artifact	UNP Q6N1P6
B	385	HIS	-	cloning artifact	UNP Q6N1P6
B	386	HIS	-	cloning artifact	UNP Q6N1P6
B	387	HIS	-	cloning artifact	UNP Q6N1P6

- Molecule 2 is water.

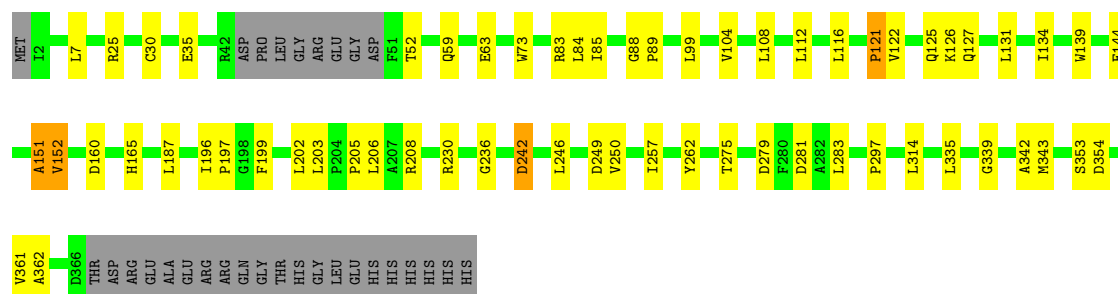
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total 132	O 132	0	0
2	B	139	Total 139	O 139	0	0

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.

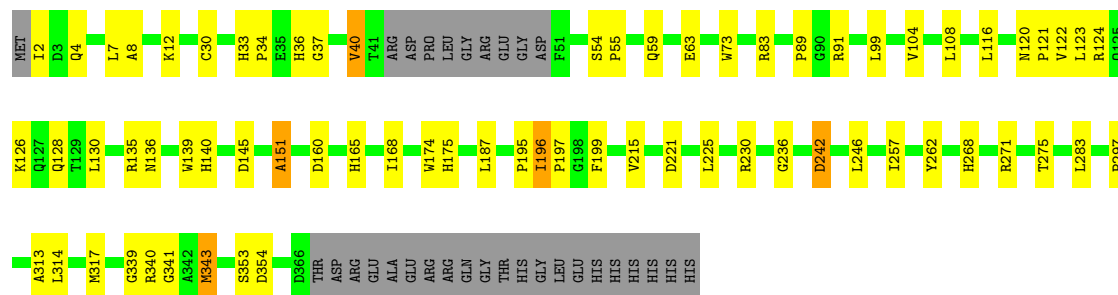
• Molecule 1: DUF185

Chain A: 



• Molecule 1: DUF185

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	79.80Å 79.80Å 247.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	22.19 – 2.10 22.19 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.4 (22.19-2.10) 95.9 (22.19-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	13.90 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.258 0.230 , 0.266	Depositor DCC
R_{free} test set	4876 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.472 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5740	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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	0.40	0/2795	0.89	5/3787 (0.1%)
1	B	0.41	0/2784	0.90	6/3773 (0.2%)
All	All	0.40	0/5579	0.89	11/7560 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	VAL	N-CA-C	-6.69	106.14	113.43
1	B	354	ASP	N-CA-C	-6.46	100.18	109.48
1	B	151	ALA	N-CA-C	6.30	117.79	108.60
1	A	354	ASP	N-CA-C	-6.09	100.71	109.48
1	A	353	SER	N-CA-C	5.97	117.66	109.18
1	B	353	SER	N-CA-C	5.56	117.08	109.18
1	A	151	ALA	N-CA-C	5.51	117.18	108.96
1	B	343	MSE	N-CA-C	5.43	119.60	112.92
1	B	196	ILE	N-CA-C	-5.37	104.01	108.63
1	A	281	ASP	N-CA-C	-5.28	105.44	111.14
1	A	85	ILE	N-CA-C	5.16	115.74	108.36

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	2740	0	2747	39	0
1	B	2729	0	2734	46	0
2	A	132	0	0	1	0
2	B	139	0	0	2	0
All	All	5740	0	5481	81	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 7.

All (81) 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:120:ASN:HD22	1:B:123:LEU:HB2	1.47	0.79
1:A:205:PRO:HA	1:A:208:ARG:HH11	1.52	0.71
1:B:4:GLN:NE2	1:B:268:HIS:H	1.88	0.71
1:B:160:ASP:HB3	1:B:242:ASP:OD1	1.91	0.69
1:B:313:ALA:O	1:B:317:MSE:HG2	1.95	0.67
1:A:160:ASP:HB3	1:A:242:ASP:OD1	1.97	0.65
1:A:89:PRO:HG2	1:A:116:LEU:HB3	1.80	0.63
1:A:246:LEU:HD22	1:A:297:PRO:HG2	1.81	0.63
1:B:196:ILE:HB	1:B:199:PHE:HB2	1.81	0.62
1:A:84:LEU:HA	1:A:152:VAL:HG23	1.83	0.61
1:B:124:ARG:O	1:B:128:GLN:HG3	2.00	0.61
1:B:83:ARG:HB2	1:B:151:ALA:HB2	1.82	0.60
1:B:165:HIS:HD2	2:B:426:HOH:O	1.84	0.60
1:B:59:GLN:O	1:B:63:GLU:HG3	2.01	0.60
1:B:246:LEU:HD22	1:B:297:PRO:HG2	1.83	0.59
1:A:199:PHE:O	1:A:202:LEU:HG	2.03	0.58
1:A:59:GLN:O	1:A:63:GLU:HG3	2.04	0.58
1:B:116:LEU:HD12	1:B:139:TRP:CZ3	2.40	0.57
1:B:8:ALA:O	1:B:12:LYS:HG2	2.06	0.56
1:A:196:ILE:HB	1:A:199:PHE:HB2	1.87	0.56
1:B:175:HIS:CE1	1:B:195:PRO:HG3	2.41	0.55
1:A:279:ASP:O	1:A:283:LEU:HD13	2.06	0.54
1:A:52:THR:HG21	1:B:340:ARG:NH1	2.22	0.54
1:A:52:THR:HG21	1:B:340:ARG:HH12	1.72	0.53
1:B:4:GLN:HE22	1:B:268:HIS:H	1.58	0.52
1:A:116:LEU:HD12	1:A:139:TRP:CZ3	2.45	0.51
1:A:165:HIS:HD2	2:A:422:HOH:O	1.93	0.51
1:B:33:HIS:HD2	1:B:36:HIS:H	1.60	0.50
1:B:126:LYS:NZ	1:B:130:LEU:HD12	2.27	0.50
1:A:342:ALA:O	1:A:343:MSE:HE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:HD11	1:A:275:THR:HG21	1.93	0.49
1:A:126:LYS:HD3	1:A:126:LYS:C	2.38	0.48
1:A:131:LEU:O	1:A:134:ILE:HG22	2.12	0.48
1:B:120:ASN:HD21	1:B:122:VAL:HG12	1.78	0.48
1:A:83:ARG:HB2	1:A:151:ALA:HB2	1.94	0.48
1:B:126:LYS:HZ3	1:B:130:LEU:HD12	1.79	0.48
1:B:168:ILE:HD12	1:B:215:VAL:HG22	1.96	0.48
1:B:140:HIS:HB3	1:B:145:ASP:HB2	1.96	0.47
1:A:73:TRP:CD2	1:A:108:LEU:HD13	2.50	0.47
1:B:34:PRO:O	1:B:40:VAL:HG11	2.15	0.47
1:B:73:TRP:CD2	1:B:108:LEU:HD13	2.49	0.47
1:A:121:PRO:HG2	1:A:122:VAL:H	1.81	0.46
1:B:174:TRP:O	1:B:196:ILE:HG12	2.15	0.46
1:B:165:HIS:HE1	2:B:480:HOH:O	1.97	0.46
1:B:168:ILE:CD1	1:B:215:VAL:HG22	2.47	0.45
1:B:130:LEU:O	1:B:130:LEU:HD23	2.16	0.45
1:A:127:GLN:HB3	1:A:139:TRP:CZ3	2.52	0.44
1:A:151:ALA:O	1:A:236:GLY:HA3	2.18	0.44
1:A:205:PRO:CA	1:A:208:ARG:HH11	2.27	0.44
1:B:221:ASP:O	1:B:225:LEU:HG	2.18	0.44
1:A:127:GLN:HB3	1:A:139:TRP:CH2	2.52	0.44
1:B:257:ILE:HD11	1:B:275:THR:HG21	2.00	0.44
1:B:151:ALA:O	1:B:236:GLY:HA3	2.18	0.44
1:A:88:GLY:N	1:A:89:PRO:HD3	2.33	0.44
1:A:249:ASP:CG	1:A:250:VAL:H	2.26	0.43
1:A:339:GLY:HA3	1:B:262:TYR:CD2	2.53	0.43
1:B:91:ARG:HH21	1:B:126:LYS:HE3	1.82	0.43
1:B:341:GLY:O	1:B:343:MSE:HE2	2.18	0.43
1:B:120:ASN:ND2	1:B:123:LEU:HB2	2.25	0.43
1:B:7:LEU:HD21	1:B:30:CYS:HA	2.01	0.43
1:A:25:ARG:HH11	1:A:25:ARG:HG2	1.84	0.43
1:B:120:ASN:HD22	1:B:123:LEU:CB	2.26	0.43
1:A:121:PRO:O	1:A:125:GLN:HG3	2.19	0.43
1:B:135:ARG:HG2	1:B:136:ASN:H	1.84	0.43
1:A:108:LEU:O	1:A:112:LEU:HG	2.19	0.42
1:B:89:PRO:HG3	1:B:116:LEU:HB3	2.00	0.42
1:B:54:SER:N	1:B:55:PRO:HD2	2.35	0.42
1:A:262:TYR:CD2	1:B:339:GLY:HA3	2.55	0.42
1:A:7:LEU:CD2	1:A:30:CYS:HA	2.50	0.42
1:A:206:LEU:C	1:A:206:LEU:HD23	2.45	0.42
1:A:104:VAL:O	1:A:104:VAL:HG12	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:O	1:A:208:ARG:NH1	2.53	0.41
1:A:206:LEU:HD23	1:A:206:LEU:O	2.21	0.41
1:B:126:LYS:O	1:B:126:LYS:HD3	2.21	0.41
1:A:361:VAL:O	1:A:362:ALA:HB3	2.21	0.41
1:B:33:HIS:HB3	1:B:37:GLY:N	2.36	0.41
1:B:268:HIS:CD2	1:B:271:ARG:HH11	2.39	0.41
1:B:104:VAL:O	1:B:104:VAL:HG12	2.20	0.41
1:A:257:ILE:HD11	1:A:275:THR:CG2	2.51	0.40
1:B:2:ILE:HG12	1:B:2:ILE:O	2.21	0.40
1:A:7:LEU:HD21	1:A:30:CYS:HA	2.04	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	353/387 (91%)	346 (98%)	5 (1%)	2 (1%)	21	18
1	B	352/387 (91%)	346 (98%)	4 (1%)	2 (1%)	21	18
All	All	705/774 (91%)	692 (98%)	9 (1%)	4 (1%)	21	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	PRO
1	B	197	PRO
1	A	121	PRO
1	B	121	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	284/301 (94%)	275 (97%)	9 (3%)	34	38
1	B	283/301 (94%)	277 (98%)	6 (2%)	47	54
All	All	567/602 (94%)	552 (97%)	15 (3%)	40	46

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	99	LEU
1	A	144	GLU
1	A	152	VAL
1	A	187	LEU
1	A	230	ARG
1	A	242	ASP
1	A	314	LEU
1	A	335	LEU
1	B	99	LEU
1	B	187	LEU
1	B	230	ARG
1	B	242	ASP
1	B	283	LEU
1	B	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	128	GLN
1	A	165	HIS
1	A	267	GLN
1	B	4	GLN
1	B	33	HIS
1	B	120	ASN

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Mol	Chain	Res	Type
1	B	165	HIS
1	B	175	HIS
1	B	268	HIS

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	349/387 (90%)	-1.07	0 100 100	10, 25, 53, 65	0
1	B	348/387 (89%)	-1.08	0 100 100	11, 25, 53, 63	0
All	All	697/774 (90%)	-1.07	0 100 100	10, 25, 53, 65	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.