



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5L5M / pdb_00005l5m
Title : Plexin A4 full extracellular region, domains 1 to 7 modeled, data to 8 angstrom, spacegroup P4(3)2(1)2
Authors : Janssen, B.J.C.; Kong, Y.; Malinauskas, T.; Vangoor, V.R.; Coles, C.H.; Kaufmann, R.; Ni, T.; Gilbert, R.J.C.; Padilla-Parra, S.; Pasterkamp, R.J.; Jones, E.Y.
Deposited on : 2016-05-28
Resolution : 8.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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)
Validation Pipeline (wwPDB-VP)	:	2.49

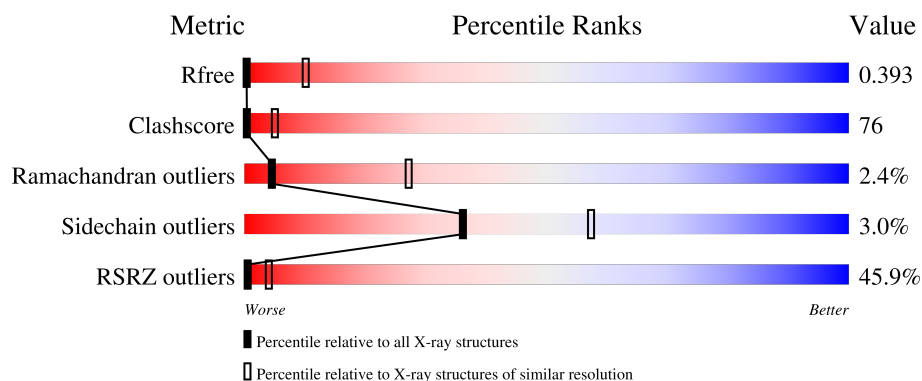
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.00 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	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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	1207	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7189 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 Plexin-A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	915	Total	C	N	O	S	0	0	0
			7189	4533	1239	1357	60			

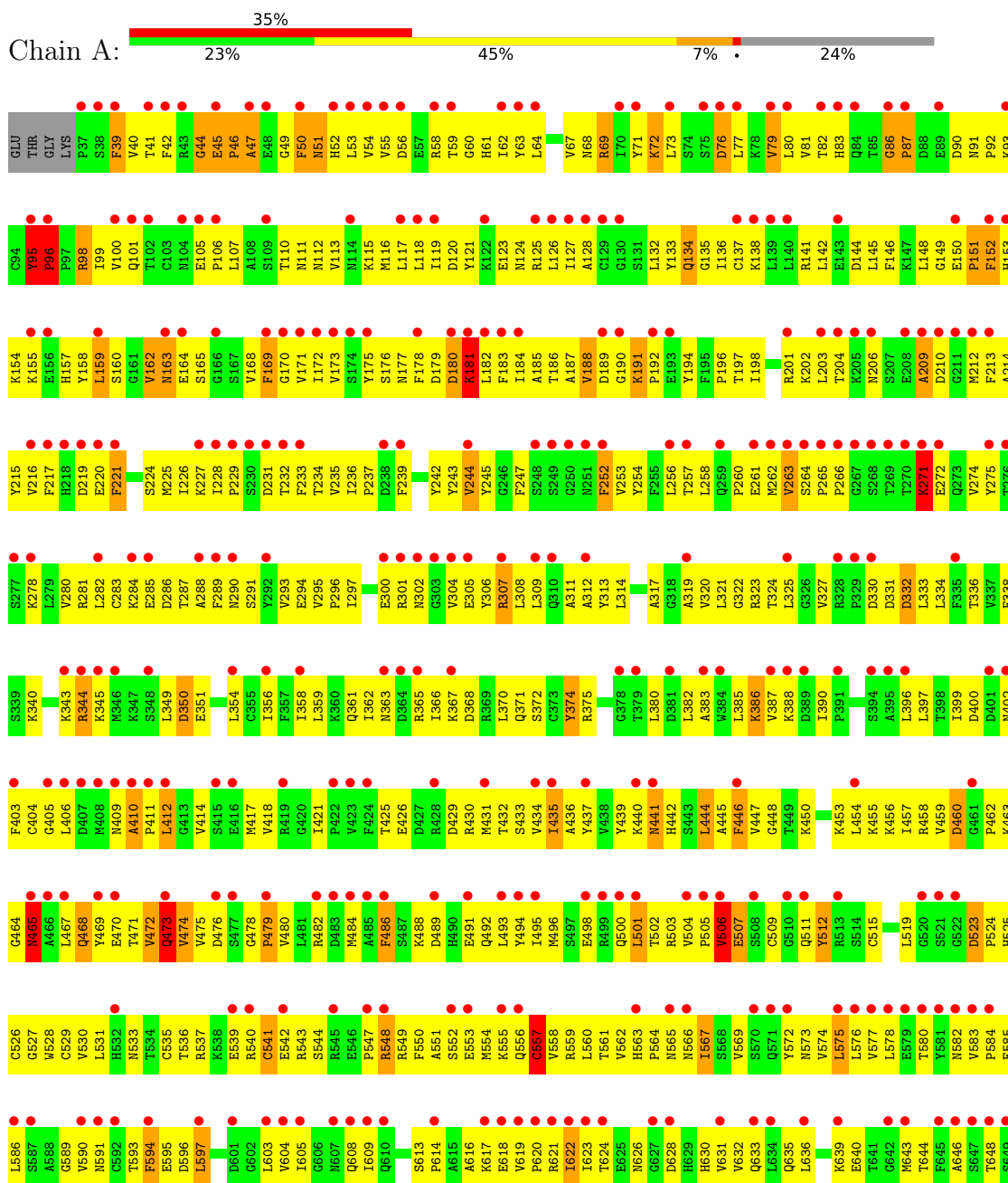
There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLU	-	expression tag	UNP Q80UG2
A	34	THR	-	expression tag	UNP Q80UG2
A	35	GLY	-	expression tag	UNP Q80UG2
A	1230	GLY	-	expression tag	UNP Q80UG2
A	1231	ARG	-	expression tag	UNP Q80UG2
A	1232	THR	-	expression tag	UNP Q80UG2
A	1233	LYS	-	expression tag	UNP Q80UG2
A	1234	HIS	-	expression tag	UNP Q80UG2
A	1235	HIS	-	expression tag	UNP Q80UG2
A	1236	HIS	-	expression tag	UNP Q80UG2
A	1237	HIS	-	expression tag	UNP Q80UG2
A	1238	HIS	-	expression tag	UNP Q80UG2
A	1239	HIS	-	expression tag	UNP Q80UG2

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: Plexin-A4



PRO	ASN	PHE	ASN	ASP	GLY	L903	S842	T781	V715	F650
ASN	ILE	GLU	ILE	ARG	PRO	V904	R843	V782	V716	V651
LEU	CYS	ALA	CYS	ALA	MET	D905	W844	W783	F717	F652
ILE	GLU	PHE	GLU	ARG	SER	G906	L845	W784	F718	Y653
GLY	SER	SER	VAL	ILE	GLY	Y907	E846	W785	I719	N654
ARG	LEU	PRO	LEU	ARG	GLY	I908	L847	G786	T720	G655
HIS	ASN	SER	ASN	GLN	THR	P909	S848	W787	L721	S656
LYS	ALA	GLY	ALA	ASP	GLN	A910	G849	F788	K722	V657
VAL	THR	ILE	THR	LEU	VAL	E911	A850	N789	A723	H658
MET	LEU	GLU	THR	VAL	THR	Q912	N851	I790	K724	N659
ALA	MET	GLU	ILE	PHE	ILE	I913	S852	D791	N725	
ARG	THR	LEU	THR	GLN	THR	V914	K853	N792	L726	L662
VAL	CYS	LYS	GLY	TYR	GLY	C915	C854	P793	P727	S663
GLY	GLN	PRO	THR	VAL	THR	E916	T855	A794	Q728	G664
GLY	ALA	GLY	ASN	GLU	ASN	M917	N856	Q795	Q728	V665
MET	PRO	THR	LEU	ASP	LEU	G918	P857	N796	Q730	E666
GLU	ALA	GLU	PRO	PRO	ASN	E919	R858	K797	S731	S667
TYR	ILE	LEU	LEU	THR	ALA	A920	E861	W798	G732	P668
SER	ALA	ILE	GLY	ILE	GLY	K921	L862	Y799	Q733	Y669
PRO	LEU	LEU	SER	VAL	SER	P922	I863	L900	W734	R670
GLY	GLY	LYS	GLY	ARG	ASN	S923	T864	Y801	G735	C671
MET	PRO	GLY	ILE	ILE	VAL	Q924	V865	K802	H672	W673
VAL	VAL	LYS	ASP	GLU	VAL	H925	T866	C803	G674	G674
TYR	ASN	ASN	HIS	PRO	VAL	A926	G867	G804	K675	K675
ILE	LEU	LEU	GLN	GLU	MET	G927	P868	A805	Y676	
ALA	ILE	ILE	SER	TRP	PHE	F928	R869	K806		
PRO	ASP	PRO	ASP	SER	GLY	V929	R869	R807		
GLY	LEU	VAL	LEU	ILE	SER	E930	E870	E808	V679	
ARG	THR	VAL	THR	VAL	GLN	I931	G871	S809	C680	
THR	ALA	ALA	GLU	SER	PRO	C932	G872	C810	T681	
LYS	GLY	GLY	ARG	GLY	CYS	V933	T873	G811	H682	
HIS	ASN	GLY	PRO	ASN	LEU	A934	K874	L812	D683	
HIS	ASN	VAL	GLU	THR	PHE	V935	W875	C813	T686	
HIS	LYS	VAL	GLU	PRO	HIS	C936	T876	L814		
HIS	LEU	LEU	GLY	ILE	ARG	R937	I877	K815		
HIS	ASN	ASN	GLY	VAL	ALA	P938	R878	A816	F689	
HIS	TYR	THR	ILE	TRP	VAL	F940	G879	D817	G690	
	THR	THR	LEU	GLY	SER	M941	E880		E691	
	VAL	VAL	ASP	THR	SER	A942	N881	F820	V694	
	LEU	LEU	ASN	THR	TYR	R943	L882	E821	K695	
	VAL	VAL	ASN	ILE	ILE	S944	G883	C922	L696	
	GLY	GLY	GLN	LEU	VAL	Q945	L884	G823	P697	
	GLU	GLU	SER	ASP	CYS	F886	E885	W824	E698	
	LYS	LYS	LEU	ILE	ASN	L947	R887	C825	D699	
	PRO	PRO	LEU	GLN	THR	Y948	D888	Q826	C700	
	CYS	THR	ILE	ASN	SER	Y949	I889	S827	P701	
	THR	THR	THR	PRO	SER	F950	A890	P828	Q702	
	VAL	VAL	ASN	GLN	GLU	M951	S891	Q830	L703	
	THR	THR	LYS	ILE	VAL	THR	H892	C831	L704	
	VAL	VAL	THR	ARG	VAL	LEU	V893	T832	R785	
	SER	SER	ASN	ALA	LEU	THR	K894	L833	V706	
	ASP	ASP	PHE	LYS	ASP	LEU	V895	R834	D707	
	VAL	VAL	THR	HIS	THR	ALA	Q835	I773	K708	
	GLN	GLN	TYR	GLY	LYS	ASP	G897	W774	I709	
	LEU	LEU	VAL	GLY	VAL	LEU	V898	C837	L710	
	LEU	LEU	PRO	LYS	THR	LYS	E899	P838	W775	
	CYS	CYS	ASN	GLU	VAL	PRO	C900	A839	V778	
	GLU	GLU	PRO	HIS	GLN	ASN	S901	H840	E779	
	SER	SER	SER	ILE	VAL	ARG	P902	E841	L780	

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	271.48Å 271.48Å 251.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.13 – 8.00 72.13 – 8.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (72.13-8.00) 99.1 (72.13-8.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 8.39Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.373 , 0.395 0.380 , 0.393	Depositor DCC
R_{free} test set	496 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	530.0	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 274.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	7189	wwPDB-VP
Average B, all atoms (Å ²)	250.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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	1.36	10/7346 (0.1%)	2.05	132/9949 (1.3%)

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	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	557	CYS	C-N	29.07	1.73	1.33
1	A	700	CYS	C-N	-10.61	1.09	1.33
1	A	49	GLY	C-N	9.87	1.45	1.33
1	A	180	ASP	C-N	7.53	1.44	1.33
1	A	506	VAL	C-N	-7.38	1.23	1.33

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	854	CYS	O-C-N	-59.41	78.66	122.03
1	A	506	VAL	O-C-N	-45.32	65.92	122.57
1	A	557	CYS	CA-C-N	-44.76	41.40	121.97
1	A	557	CYS	C-N-CA	-44.76	41.40	121.97
1	A	747	GLN	CG-CD-OE1	-38.43	43.94	120.80

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	506	VAL	Mainchain
1	A	700	CYS	Mainchain
1	A	802	LYS	Mainchain,Peptide
1	A	854	CYS	Mainchain
1	A	95	TYR	Peptide

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	7189	0	7046	1088	16
All	All	7189	0	7046	1088	16

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 76.

The worst 5 of 1088 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:439:TYR:CD1	1:A:537:ARG:NH1	1.70	1.55
1:A:439:TYR:CE1	1:A:537:ARG:NH1	1.71	1.54
1:A:548:ARG:CG	1:A:584:PRO:HA	1.31	1.52
1:A:556:GLN:HA	1:A:582:ASN:CB	1.40	1.51
1:A:548:ARG:HG3	1:A:584:PRO:CA	1.45	1.40

The worst 5 of 16 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:PHE:O	1:A:234:THR:OG1[8_665]	1.24	0.96
1:A:285:GLU:OE2	1:A:834:ARG:NH1[6_565]	1.32	0.88
1:A:146:PHE:CD1	1:A:730:GLN:OE1[4_455]	1.46	0.74
1:A:146:PHE:CE1	1:A:730:GLN:CD[4_455]	1.54	0.66
1:A:83:HIS:CE1	1:A:731:SER:OG[4_455]	1.63	0.57

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	911/1207 (76%)	843 (92%)	46 (5%)	22 (2%)	4 27

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PRO
1	A	181	LYS
1	A	191	LYS
1	A	410	ALA
1	A	465	ASN

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	812/1067 (76%)	788 (97%)	24 (3%)	36 57

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	575	LEU
1	A	722	LYS
1	A	670	ARG
1	A	743	GLN
1	A	435	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	582	ASN
1	A	836	HIS
1	A	672	HIS
1	A	946	GLN
1	A	789	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	653:TYR	C	654:ASN	N	2.02

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	557:CYS	C	558:VAL	N	1.73
1	A	700:CYS	C	701:PRO	N	1.09

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	915/1207 (75%)	2.25	420 (45%) 0 4	145, 231, 394, 394	0

The worst 5 of 420 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	PRO	12.8
1	A	269	THR	11.5
1	A	266	PRO	11.2
1	A	270	THR	10.5
1	A	566	ASN	10.5

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.