



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:32 AM UTC

PDB ID : 5L5K / pdb_00005l5k
Title : Plexin A4 full extracellular region, domains 1 to 10, data to 7.5 angstrom, spacegroup P4(1)
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 : 7.50 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

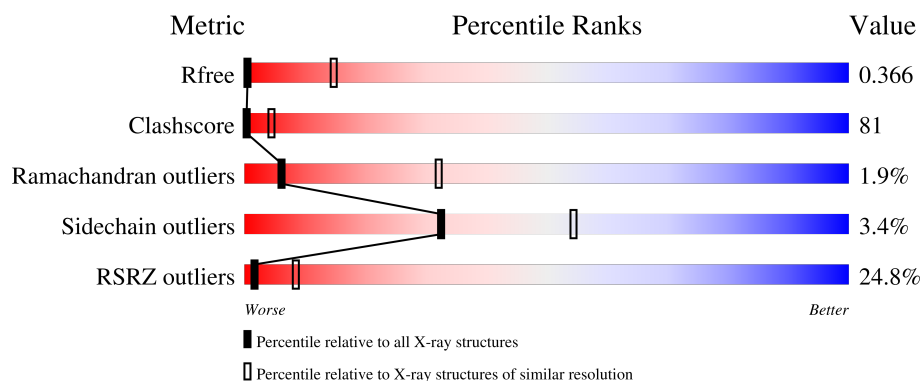
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.50 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	24% 30% 56% 10% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9134 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	1168	Total	C	N	O	S	0	0	0
			9134	5761	1572	1729	72			

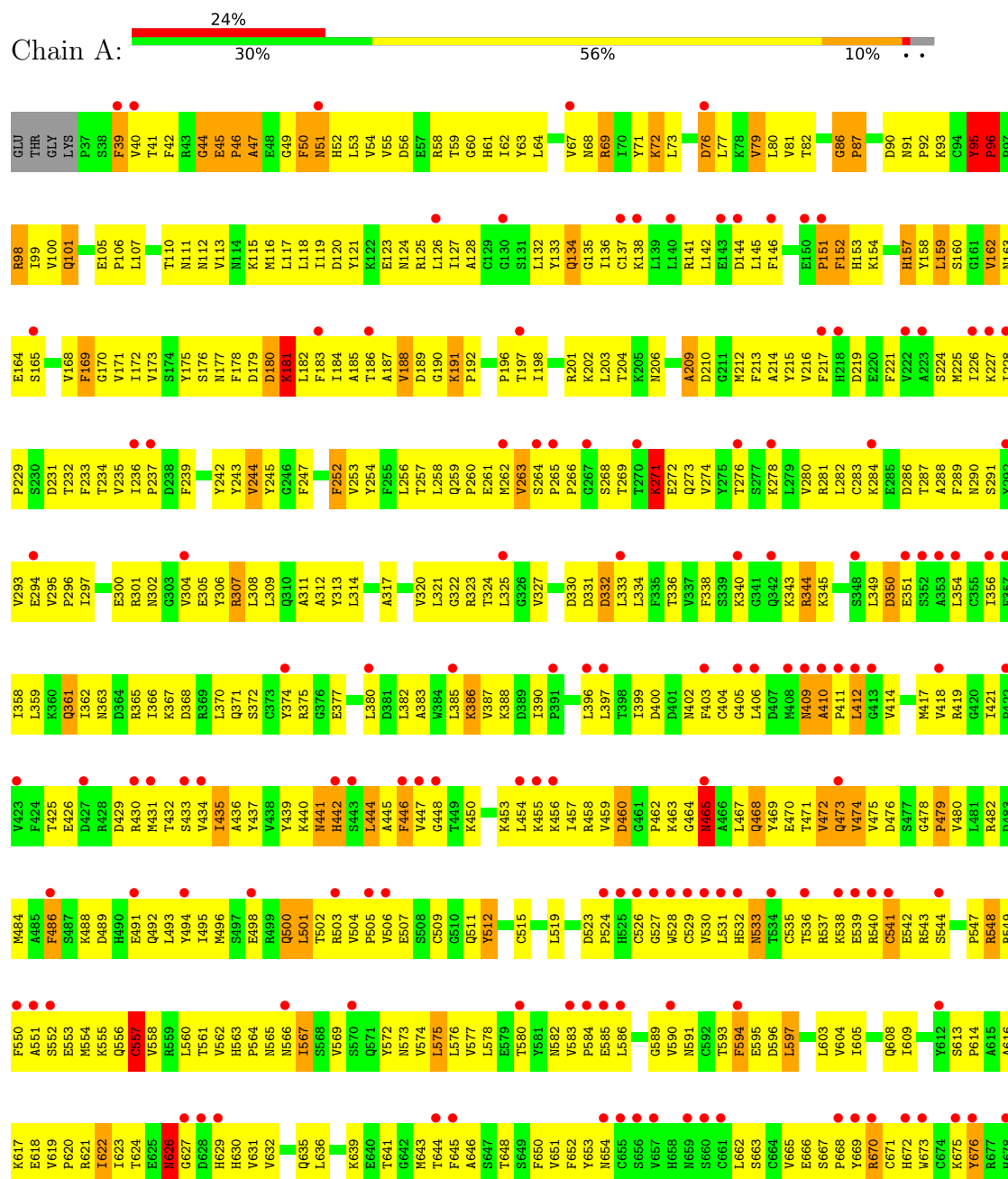
There are 13 discrepancies between the modelled and reference sequences:

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



S1194	V679	Q743	K815	N881	N941	I1003	H1063	M1131	S1194
D1195	C680	G744	A616	N882	A942	I1004	L1064	K1132	D1195
V1196	T681	T745	D817	L883	R943	C1005	D1065	M1133	V1196
Q1197	H682	E746	F820	G883	S944	N1006	L1066	T1134	Q1197
L1198	D683	Q747	F821	E884	S945	T1007	Q1067	T1135	L1198
L1199	P684	R748	C822	E885	Q946	T1008	Q1068	T1136	L1199
C1200	N685	R753	Q823	F886	L947	S1009	N1069	Y1137	C1200
E1201	T686	F754	W824	R887	Y948	S1010	N1070	P1071	E1201
S1202	G687	F754	Q825	R888	Y949	E1012	Q1071	Q1072	S1202
F1203	S688	W759	Q826	I889	F950	V1013	I1072	R1073	F1203
N1204	F689	Q760	S827	A890	T952	L1014	L1073	R1073	N1204
LEU	Q690	C761	P828	S891	L953	D1015	H1076	H1076	LEU
ILE	E691	Q762	Q829	H892	T954	M1016	H1081	A1144	ILE
GLY	V694	W763	Q830	V893	L955	K1017	H1082	A1145	GLY
ARG	K695	T764	Q831	K894	A956	V1018	I1082	SER	ARG
HIS	L696	S765	C931	V895	A957	V1019	N1083	PRO	HIS
K1210	P697	S766	T832	A896	D957	T1020	I1084	GLY	K1210
V1211	F698	S767	L833	G897	L958	V1021	C1085	ILE	V1211
M1212	D699	T773	Q834	V898	K959	Q1021	E1086	LEU	M1212
A1213	C700	W774	Q835	E899	P960	V1022	V1087	LEU	A1213
R1214	P701	C779	H836	P902	R962	D1023	L1088	GLU	R1214
V1215	Q702	W779	C837	L903	G963	A1025	N1089	LYS	V1215
G1216	L703	E778	P838	V904	P964	R1026	A1090	PRO	G1216
G1217	L704	S779	D905	D905	N965	I1027	A1090	GLY	G1217
M1218	R705	L780	G906	G906	S866	R1028	M1093	T1158	M1218
E1219	V706	T781	Y907	Y907	G967	Q1029	T1094	P1159	E1219
Y1220	D707	W782	S842	I908	G968	D1030	C1095	I1160	Y1220
S1221	W783	Q783	R843	R843	T969	L1031	Q1096	L1161	S1221
PRO	K708	W784	W844	P909	Q970	V1032	A1097	L1162	PRO
GLY	L709	W785	L845	A910	V971	F1033	P1098	K1163	GLY
MET	L710	W785	E846	E911	T972	Q1034	A1099	G1164	MET
VAL	W711	L711	L847	Q912	T973	Y1035	L1100	K1165	VAL
TYR	F712	G786	S848	Q913	R974	E1037	A1101	M1166	TYR
ILE	W713	H787	G849	V914	T974	V1036	G1103	L1167	ILE
ALA	E714	F788	C851	C915	G975	E1037	L1102	L1167	ALA
PRO	W715	W789	N851	E916	T976	D1038	P1104	I1168	PRO
GLY	L716	D791	S852	M917	N977	P1039	D1105	P1169	GLY
ARG	W717	W792	K853	G918	L978	T1040	H1106	P1170	ARG
THR	F718	F793	C884	E919	R979	I1041	H1107	V1171	THR
LYS	I719	A794	T855	A920	A980	V1042	Q1107	A1172	LYS
HIS	K722	W795	N856	K921	G981	R1043	S1108	N1175	HIS
HIS	A723	K797	P857	P922	S982	I1044	D1109	V1176	HIS
HIS	K724	W798	Q923	S923	N983	E1045	L1110	K1177	HIS
HIS	W725	W799	H824	Q924	V984	P1046	E1112	L1178	HIS
L726	L726	L800	T863	H925	V986	E1047	E1116	N1179	L726
P727	W726	Y801	P864	A926	N987	W1048	F1117	V1180	P727
Q728	Q728	X802	V865	G927	F988	S1049	G1118	T1181	Q728
P729	Q729	C803	T866	F928	G989	I1050	F1119	V1182	P729
Q730	Q730	G804	G867	V929	S990	S1052	I1120	L1183	Q730
		A805	P868	C932	Q991	G1053	L1121	V1184	
Q733	Q733	R806	R869	N1054	P992	T1054	D1122	G1185	Q733
R734	R734	E807	E870	V933	C993	T1055	N1123	E1186	R734
G735	G735	E808	G871	A934	L994	P1056	I1057	K1187	G735
Y736	Y736	S809	T873	C936	H995	A1058	V1124	P1188	Y736
		C810	T874	R837	R997	V1059	L1127	C1189	
I739	I739	G811	K874	P938	R998	W1060	L1128	T1190	I739
L740	L740	L812	V875	E939	R999	G1061	I1129	V1191	L740
N741	N741	C813	T876			T1062	L1130	T1192	N741
I742	I742	L814	I877	F940	Y1002			V1193	I742

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	220.59Å 220.59Å 65.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.15 – 7.50 55.15 – 7.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (55.15-7.50) 98.4 (55.15-7.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 7.40Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.353 , 0.371 0.352 , 0.366	Depositor DCC
R_{free} test set	197 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	344.7	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 616.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	9134	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 5.45% 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	1.51	42/9324 (0.5%)	1.77	156/12638 (1.2%)

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	4

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	700	CYS	C-N	44.45	1.72	1.33
1	A	854	CYS	C-N	-34.83	0.85	1.33
1	A	557	CYS	C-N	-14.01	1.15	1.33
1	A	49	GLY	C-N	9.89	1.45	1.33
1	A	180	ASP	C-N	7.55	1.44	1.33

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	747	GLN	CG-CD-NE2	-48.30	43.95	116.40
1	A	557	CYS	CA-C-N	-37.03	74.63	123.14
1	A	557	CYS	C-N-CA	-37.03	74.63	123.14
1	A	747	GLN	OE1-CD-NE2	15.07	137.67	122.60
1	A	747	GLN	CG-CD-OE1	-13.54	93.71	120.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	557	CYS	Mainchain
1	A	854	CYS	Mainchain
1	A	863	ILE	Peptide
1	A	95	TYR	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	9134	0	8998	1462	10
All	All	9134	0	8998	1462	10

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 81.

The worst 5 of 1462 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:440:LYS:CD	1:A:538:LYS:HD2	1.28	1.55
1:A:700:CYS:C	1:A:701:PRO:N	1.72	1.47
1:A:854:CYS:C	1:A:855:THR:CA	1.93	1.42
1:A:440:LYS:HD3	1:A:538:LYS:CD	1.51	1.41
1:A:530:VAL:HG11	1:A:584:PRO:CD	1.50	1.38

The worst 5 of 10 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:146:PHE:CE1	1:A:730:GLN:NE2[4_555]	0.96	1.24
1:A:269:THR:CG2	1:A:377:GLU:OE1[2_455]	1.33	0.87
1:A:268:SER:OG	1:A:375:ARG:NH1[2_455]	1.48	0.72
1:A:146:PHE:CD1	1:A:730:GLN:OE1[4_555]	1.76	0.44
1:A:269:THR:CG2	1:A:377:GLU:CD[2_455]	1.90	0.30

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	1150/1207 (95%)	1071 (93%)	57 (5%)	22 (2%)	6	32

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	1035/1067 (97%)	1000 (97%)	35 (3%)	32	54

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1016	MET
1	A	1017	LYS
1	A	1107	GLN
1	A	548	ARG
1	A	529	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	134	GLN
1	A	490	HIS
1	A	1125	GLN

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	9

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1139:PRO	C	1140:ASN	N	4.11
1	A	506:VAL	C	507:GLU	N	2.75

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	951:MET	C	952:THR	N	2.26
1	A	802:LYS	C	803:CYS	N	2.24
1	A	1036:VAL	C	1037:GLU	N	2.02

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	1168/1207 (96%)	1.44	290 (24%) 2 8	185, 272, 310, 310	0

The worst 5 of 290 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	584	PRO	18.0
1	A	531	LEU	12.9
1	A	676	TYR	11.0
1	A	678	HIS	10.3
1	A	727	PRO	10.2

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.