



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 11:39 PM UTC

PDB ID : 5L5G / pdb_00005l5g
Title : Plexin A2 full extracellular region, domains 1 to 8 modeled, data to 10 angstrom
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 : 10.00 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

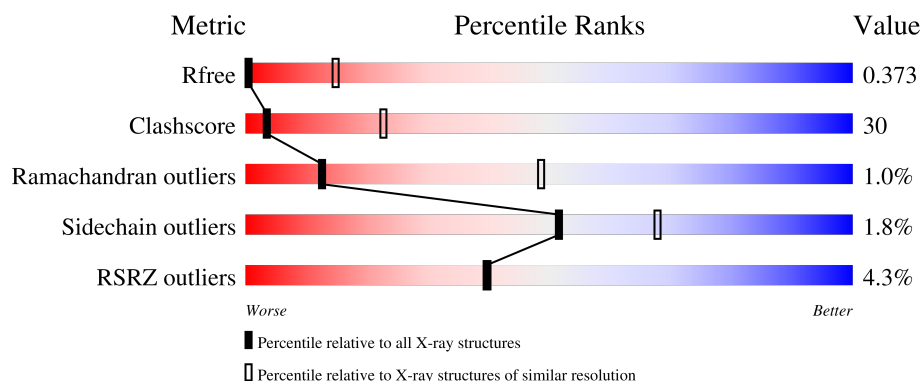
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 10.00 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	1002 (15.00-4.06)
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	1212	4% 50% 22% •• 25%
1	B	1212	2% 45% 20% • 33%
1	C	1212	4% 52% 26% • 18%
1	D	1212	3% 52% 27% •• 18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28787 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-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	906	Total	C	N	O	S	0	0	0
			7060	4461	1214	1333	52			
1	B	809	Total	C	N	O	S	0	0	0
			6337	4004	1092	1195	46			
1	C	993	Total	C	N	O	S	0	0	0
			7695	4856	1321	1462	56			
1	D	993	Total	C	N	O	S	0	0	0
			7695	4856	1321	1462	56			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLU	-	expression tag	UNP P70207
A	1232	GLY	-	expression tag	UNP P70207
A	1233	GLY	-	expression tag	UNP P70207
A	1234	SER	-	expression tag	UNP P70207
A	1235	ARG	-	expression tag	UNP P70207
A	1236	THR	-	expression tag	UNP P70207
A	1237	LYS	-	expression tag	UNP P70207
A	1238	HIS	-	expression tag	UNP P70207
A	1239	HIS	-	expression tag	UNP P70207
A	1240	HIS	-	expression tag	UNP P70207
A	1241	HIS	-	expression tag	UNP P70207
A	1242	HIS	-	expression tag	UNP P70207
A	1243	HIS	-	expression tag	UNP P70207
B	32	GLU	-	expression tag	UNP P70207
B	1232	GLY	-	expression tag	UNP P70207
B	1233	GLY	-	expression tag	UNP P70207
B	1234	SER	-	expression tag	UNP P70207
B	1235	ARG	-	expression tag	UNP P70207
B	1236	THR	-	expression tag	UNP P70207
B	1237	LYS	-	expression tag	UNP P70207
B	1238	HIS	-	expression tag	UNP P70207

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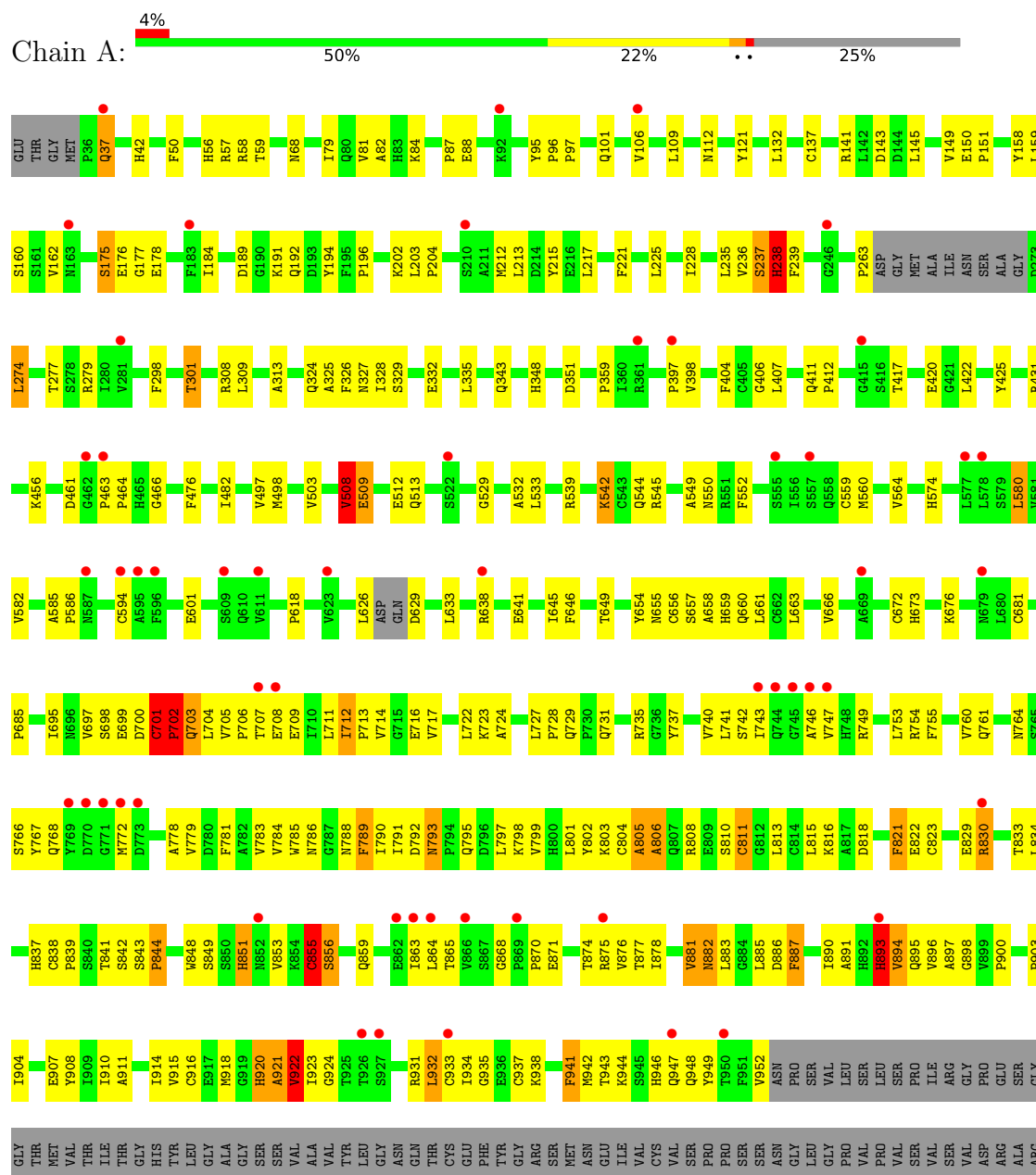
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1239	HIS	-	expression tag	UNP P70207
B	1240	HIS	-	expression tag	UNP P70207
B	1241	HIS	-	expression tag	UNP P70207
B	1242	HIS	-	expression tag	UNP P70207
B	1243	HIS	-	expression tag	UNP P70207
C	32	GLU	-	expression tag	UNP P70207
C	1232	GLY	-	expression tag	UNP P70207
C	1233	GLY	-	expression tag	UNP P70207
C	1234	SER	-	expression tag	UNP P70207
C	1235	ARG	-	expression tag	UNP P70207
C	1236	THR	-	expression tag	UNP P70207
C	1237	LYS	-	expression tag	UNP P70207
C	1238	HIS	-	expression tag	UNP P70207
C	1239	HIS	-	expression tag	UNP P70207
C	1240	HIS	-	expression tag	UNP P70207
C	1241	HIS	-	expression tag	UNP P70207
C	1242	HIS	-	expression tag	UNP P70207
C	1243	HIS	-	expression tag	UNP P70207
D	32	GLU	-	expression tag	UNP P70207
D	1232	GLY	-	expression tag	UNP P70207
D	1233	GLY	-	expression tag	UNP P70207
D	1234	SER	-	expression tag	UNP P70207
D	1235	ARG	-	expression tag	UNP P70207
D	1236	THR	-	expression tag	UNP P70207
D	1237	LYS	-	expression tag	UNP P70207
D	1238	HIS	-	expression tag	UNP P70207
D	1239	HIS	-	expression tag	UNP P70207
D	1240	HIS	-	expression tag	UNP P70207
D	1241	HIS	-	expression tag	UNP P70207
D	1242	HIS	-	expression tag	UNP P70207
D	1243	HIS	-	expression tag	UNP P70207

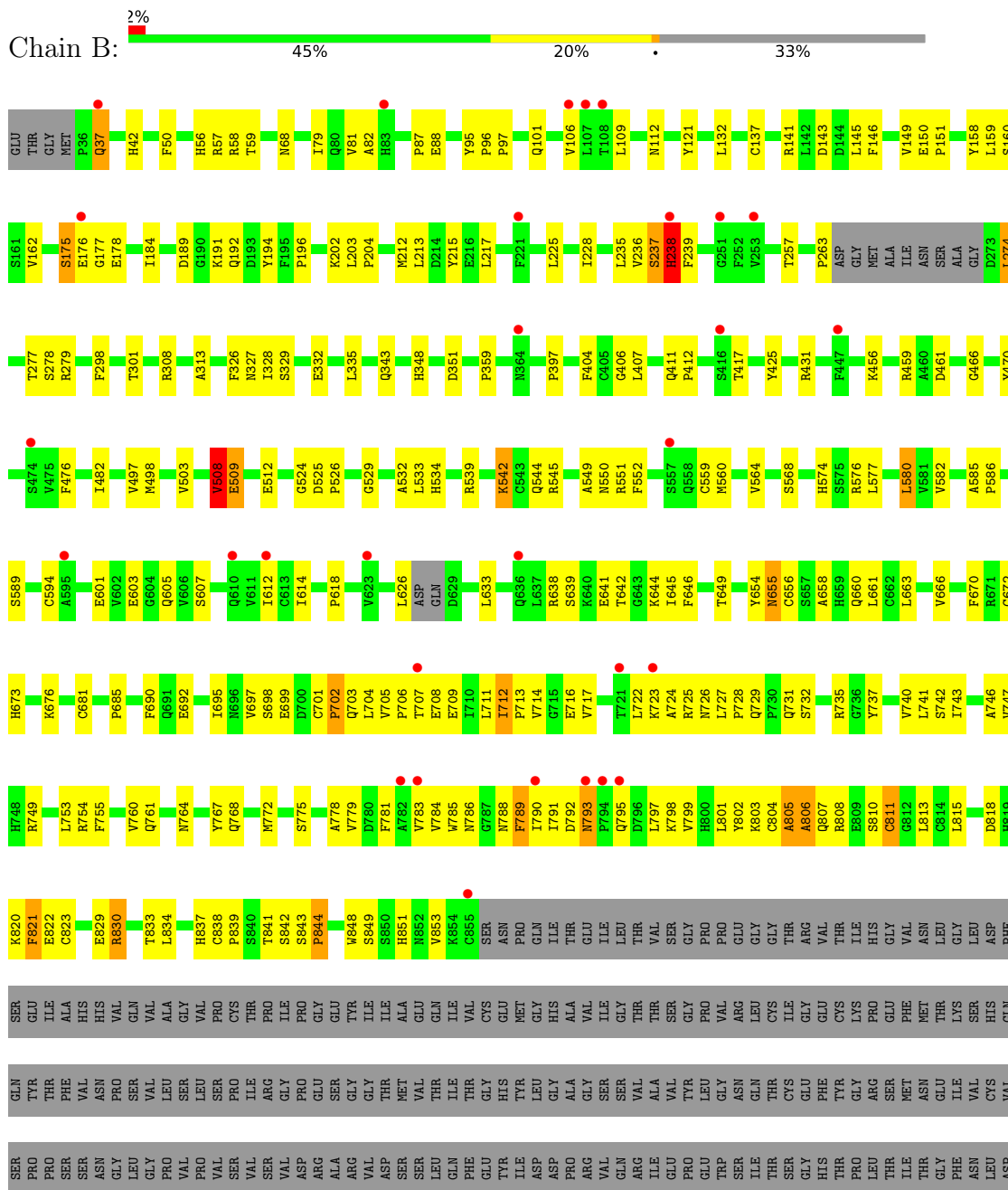
3 Residue-property plots

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.

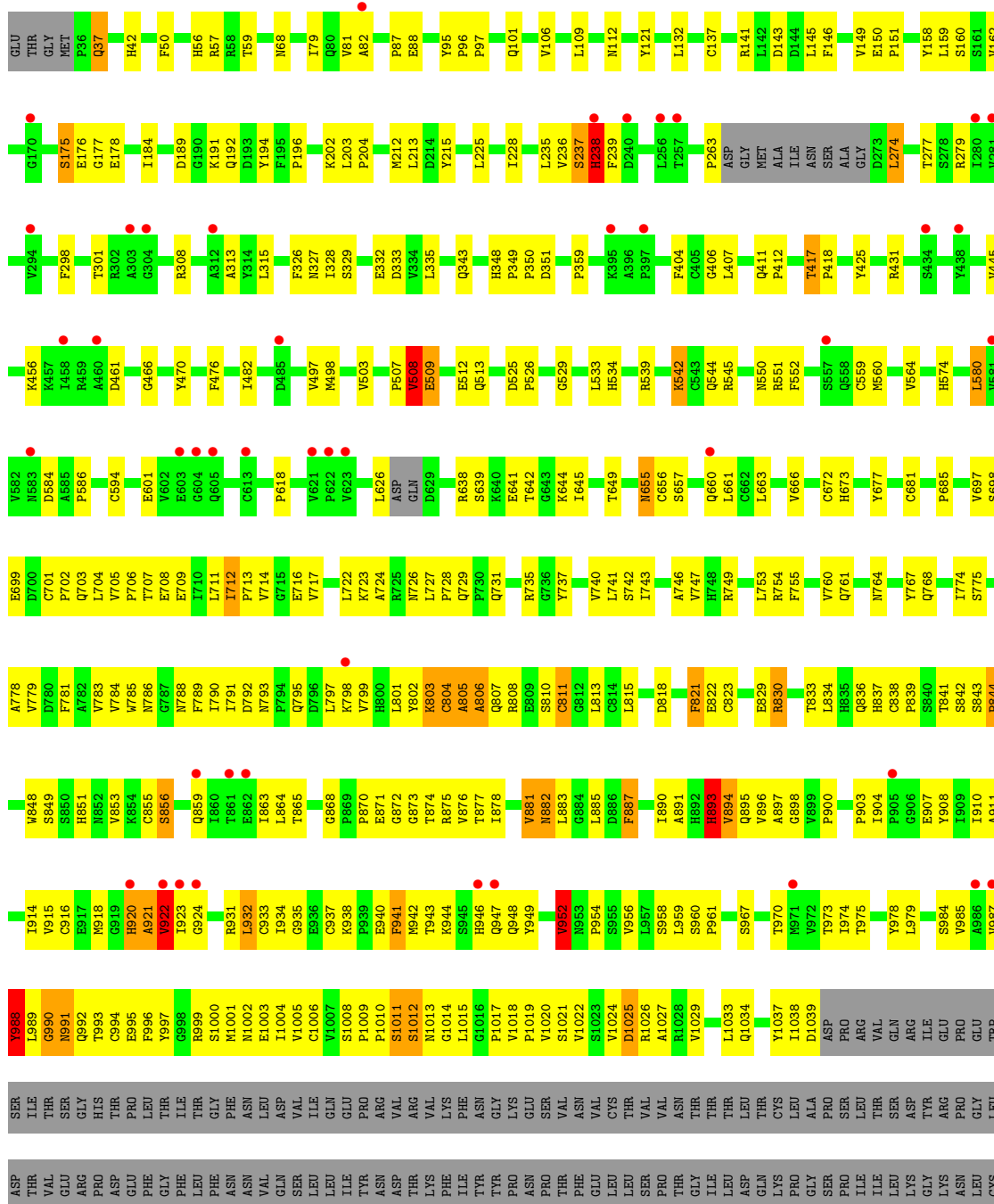
• Molecule 1: Plexin-A2



- Molecule 1: Plexin-A2



- Molecule 1: Plexin-A2



Chain D:

Category	Value	Color
ASP	3%	Red
THR	52%	Green
THR	27%	Yellow
THR	18%	Grey

ASP
GLY
GLY
SER
ARG
THR
LYS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	238.40Å 238.40Å 642.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.05 – 10.00 63.05 – 10.00	Depositor EDS
% Data completeness (in resolution range)	92.5 (63.05-10.00) 92.6 (63.05-10.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.335 , 0.370 0.334 , 0.373	Depositor DCC
R_{free} test set	529 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , 73.4	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	28787	wwPDB-VP
Average B, all atoms (Å ²)	236.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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

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	1.01	12/7230 (0.2%)	1.16	43/9821 (0.4%)
1	B	1.02	9/6488 (0.1%)	1.32	25/8804 (0.3%)
1	C	0.90	15/7878 (0.2%)	1.24	50/10705 (0.5%)
1	D	0.97	15/7879 (0.2%)	1.33	60/10708 (0.6%)
All	All	0.97	51/29475 (0.2%)	1.26	178/40038 (0.4%)

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	2
1	B	0	1
1	C	0	4
1	D	0	4
All	All	0	11

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	702	PRO	C-N	49.52	1.94	1.33
1	A	702	PRO	C-N	39.90	1.89	1.33
1	A	508	VAL	C-N	-38.57	0.78	1.33
1	D	655	ASN	C-N	-28.75	0.96	1.34
1	B	655	ASN	C-N	28.02	1.71	1.34

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	702	PRO	O-C-N	-65.13	51.99	122.98
1	B	508	VAL	O-C-N	-42.43	69.54	122.57
1	C	803	LYS	O-C-N	-36.79	72.31	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	559	CYS	O-C-N	-36.52	74.01	122.59
1	D	508	VAL	O-C-N	21.65	144.24	121.94

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	701	CYS	Mainchain
1	A	855	CYS	Mainchain
1	B	508	VAL	Mainchain
1	C	508	VAL	Mainchain
1	C	803	LYS	Mainchain

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	7060	0	6854	441	9
1	B	6337	0	6141	356	8
1	C	7695	0	7466	469	5
1	D	7695	0	7468	499	4
All	All	28787	0	27929	1690	13

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 30.

The worst 5 of 1690 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:463:PRO:HG2	1:B:612:ILE:CG2	1.25	1.55
1:A:407:LEU:CD2	1:C:944:LYS:HD2	1.03	1.48
1:D:533:LEU:CD1	1:D:642:THR:HG23	1.41	1.48
1:B:655:ASN:C	1:B:656:CYS:N	1.71	1.46
1:A:407:LEU:CD2	1:C:944:LYS:CD	1.93	1.43

The worst 5 of 13 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:839:PRO:CB	1:B:768:GLN:OE1[5_665]	1.27	0.93
1:B:397:PRO:CG	1:D:947:GLN:OE1[2_564]	1.51	0.69
1:A:731:GLN:OE1	1:C:146:PHE:CD1[3_455]	1.56	0.64
1:B:407:LEU:CD2	1:D:944:LYS:CD[2_564]	1.79	0.41
1:A:731:GLN:NE2	1:C:146:PHE:CE1[3_455]	1.87	0.33

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	896/1212 (74%)	861 (96%)	26 (3%)	9 (1%)	12	49
1	B	797/1212 (66%)	771 (97%)	19 (2%)	7 (1%)	14	51
1	C	981/1212 (81%)	937 (96%)	35 (4%)	9 (1%)	14	51
1	D	983/1212 (81%)	942 (96%)	31 (3%)	10 (1%)	12	49
All	All	3657/4848 (75%)	3511 (96%)	111 (3%)	35 (1%)	12	49

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	702	PRO
1	A	851	HIS
1	B	508	VAL
1	B	509	GLU
1	B	851	HIS

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	796/1064 (75%)	781 (98%)	15 (2%)	50	67
1	B	714/1064 (67%)	701 (98%)	13 (2%)	51	68
1	C	870/1064 (82%)	855 (98%)	15 (2%)	53	69
1	D	870/1064 (82%)	855 (98%)	15 (2%)	53	69
All	All	3250/4256 (76%)	3192 (98%)	58 (2%)	51	68

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	106	VAL
1	D	811	CYS
1	C	509	GLU
1	D	626	LEU
1	D	508	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1034	GLN
1	D	807	GLN
1	D	403	ASN
1	D	550	ASN
1	D	837	HIS

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 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	C	6
1	B	6
1	A	6
1	D	5

The worst 5 of 23 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	855:CYS	C	856:SER	N	5.61
1	C	702:PRO	C	703:GLN	N	3.75
1	D	702:PRO	C	703:GLN	N	3.35
1	C	559:CYS	C	560:MET	N	2.82
1	C	855:CYS	C	856:SER	N	2.48

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	906/1212 (74%)	0.07	54 (5%) 27 32	153, 176, 433, 433	0
1	B	809/1212 (66%)	-0.06	30 (3%) 45 43	147, 209, 350, 350	0
1	C	993/1212 (81%)	-0.17	44 (4%) 39 39	200, 270, 340, 340	0
1	D	993/1212 (81%)	-0.20	31 (3%) 51 46	184, 270, 345, 345	0
All	All	3701/4848 (76%)	-0.09	159 (4%) 40 40	147, 228, 345, 433	0

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	770	ASP	6.3
1	A	771	GLY	6.3
1	D	485	ASP	6.3
1	C	294	VAL	5.7
1	A	769	TYR	5.6

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.