



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:27 pm BST

PDB ID : 3IG3
Title : Crystal structure of mouse Plexin A3 intracellular domain
Authors : He, H.; Zhang, X.
Deposited on : 2009-07-27
Resolution : 1.99 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

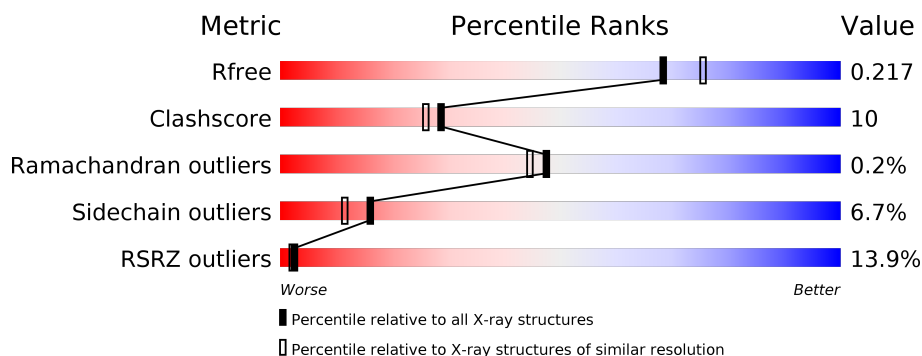
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	627	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4848 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 Plxna3 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	561	4479	2849	767	842	21	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1246	SER	-	EXPRESSION TAG	UNP A5D6Q5

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0

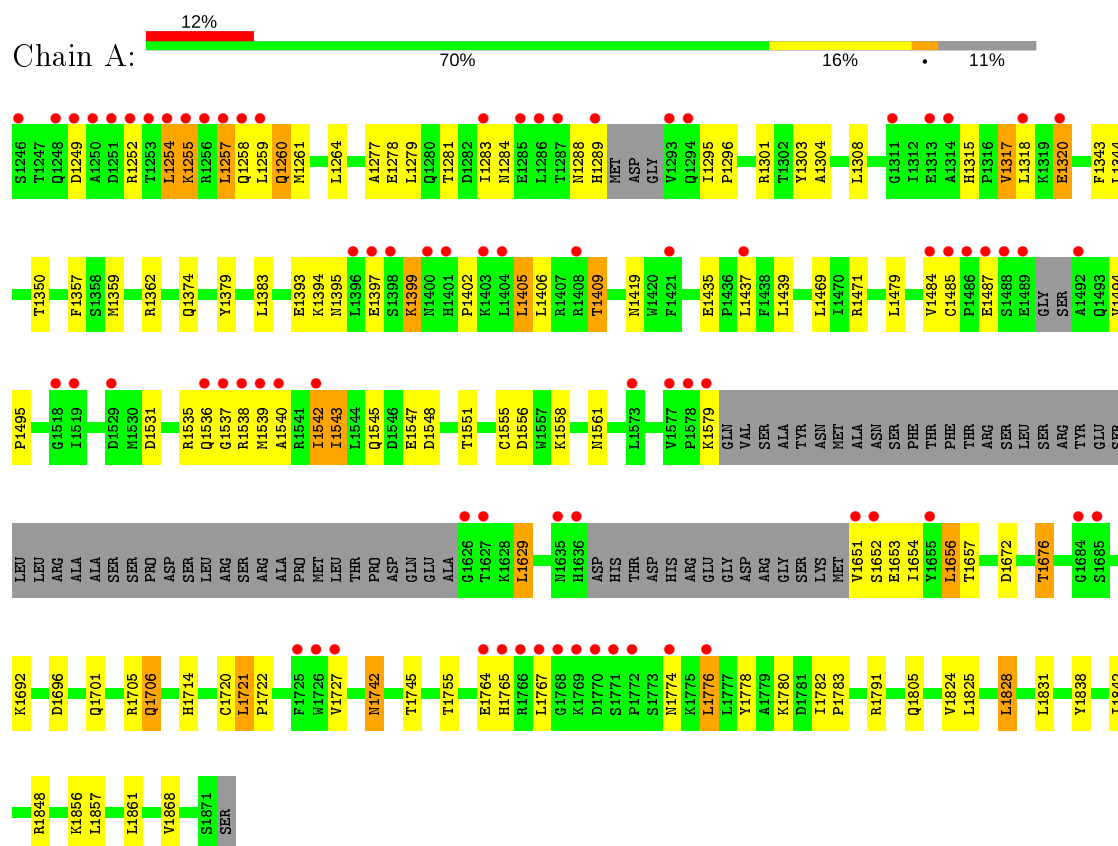
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	363	Total 363	O 363	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Plxna3 protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.79Å 47.20Å 101.18Å 90.00° 118.69° 90.00°	Depositor
Resolution (Å)	34.08 – 1.99 34.08 – 1.99	Depositor EDS
% Data completeness (in resolution range)	95.1 (34.08-1.99) 95.1 (34.08-1.99)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.188 , 0.223 0.184 , 0.217	Depositor DCC
R_{free} test set	2007 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4848	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.25	0/4562	0.42	0/6178

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4479	0	4457	87	0
2	A	6	0	8	0	0
3	A	363	0	0	5	0
All	All	4848	0	4465	87	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 10.

All (87) 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:1344:LEU:HD23	1:A:1383:LEU:HD13	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1284:ASN:O	1:A:1288:ASN:HB2	1.86	0.76
1:A:1672:ASP:O	1:A:1676:THR:HG23	1.88	0.74
1:A:1344:LEU:HD23	1:A:1383:LEU:CD1	2.20	0.71
1:A:1629:LEU:HD12	1:A:1629:LEU:H	1.60	0.67
1:A:1742:ASN:C	1:A:1742:ASN:HD22	1.98	0.67
1:A:1548:ASP:H	1:A:1551:THR:CG2	2.09	0.64
1:A:1742:ASN:ND2	1:A:1745:THR:H	1.94	0.64
1:A:1653:GLU:O	1:A:1657:THR:HG23	1.97	0.64
1:A:1705:ARG:C	1:A:1706:GLN:HG2	2.18	0.64
1:A:1805:GLN:NE2	3:A:142:HOH:O	2.32	0.62
1:A:1548:ASP:H	1:A:1551:THR:HG23	1.64	0.61
1:A:1838:TYR:O	1:A:1842:ILE:HG12	2.02	0.59
1:A:1548:ASP:O	1:A:1551:THR:HG23	2.03	0.59
1:A:1395:ASN:HD21	1:A:1409:THR:HG21	1.68	0.59
1:A:1320:GLU:H	1:A:1320:GLU:CD	2.07	0.58
1:A:1405:LEU:HD22	1:A:1406:LEU:HG	1.86	0.57
1:A:1277:ALA:O	1:A:1281:THR:HG23	2.04	0.57
1:A:1547:GLU:HA	1:A:1551:THR:HG21	1.87	0.57
1:A:1308:LEU:HD22	1:A:1419:ASN:ND2	2.20	0.56
1:A:1406:LEU:HD13	1:A:1720:CYS:SG	2.46	0.56
1:A:1379:TYR:CZ	1:A:1383:LEU:HD12	2.42	0.55
1:A:1542:ILE:O	1:A:1542:ILE:HG13	2.09	0.52
1:A:1547:GLU:HG3	1:A:1551:THR:HG21	1.91	0.52
1:A:1405:LEU:HD23	1:A:1406:LEU:H	1.74	0.51
1:A:1824:VAL:HG12	1:A:1828:LEU:HD22	1.91	0.51
1:A:1721:LEU:HB3	1:A:1722:PRO:CD	2.41	0.50
1:A:1357:PHE:CE2	1:A:1362:ARG:HG3	2.46	0.50
1:A:1782:ILE:HB	1:A:1783:PRO:HD3	1.93	0.50
1:A:1254:LEU:HD23	1:A:1257:LEU:HD22	1.93	0.49
1:A:1257:LEU:HD23	1:A:1258:GLN:N	2.27	0.49
1:A:1259:LEU:HD12	1:A:1260:GLN:N	2.28	0.49
1:A:1543:ILE:HD11	1:A:1545:GLN:HE21	1.77	0.49
1:A:1485:CYS:SG	1:A:1494:VAL:HG13	2.53	0.48
1:A:1304:ALA:O	1:A:1308:LEU:HG	2.14	0.48
1:A:1537:GLY:HA2	1:A:1540:ALA:H	1.79	0.48
1:A:1261:MET:CE	1:A:1656:LEU:HD11	2.44	0.48
1:A:1359:MET:HA	1:A:1362:ARG:HD3	1.95	0.48
1:A:1543:ILE:HD11	1:A:1545:GLN:NE2	2.28	0.48
1:A:1547:GLU:HA	1:A:1551:THR:CG2	2.43	0.48
1:A:1397:GLU:C	1:A:1399:LYS:N	2.67	0.47
1:A:1755:THR:HG23	1:A:1782:ILE:CD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1856:LYS:HG3	1:A:1856:LYS:O	2.12	0.47
1:A:1249:ASP:HA	1:A:1252:ARG:NH1	2.30	0.47
1:A:1558:LYS:O	1:A:1629:LEU:HA	2.15	0.47
1:A:1651:VAL:HG22	1:A:1652:SER:N	2.31	0.46
1:A:1402:PRO:O	1:A:1405:LEU:HB2	2.16	0.46
1:A:1531:ASP:CG	1:A:1579:LYS:HG2	2.35	0.46
1:A:1485:CYS:C	1:A:1487:GLU:H	2.19	0.46
1:A:1714:HIS:HD2	3:A:143:HOH:O	1.99	0.46
1:A:1755:THR:HG23	1:A:1782:ILE:HD11	1.96	0.45
1:A:1538:ARG:HG2	1:A:1538:ARG:O	2.16	0.45
1:A:1537:GLY:CA	1:A:1539:MET:N	2.80	0.45
1:A:1701:GLN:NE2	1:A:1705:ARG:HH22	2.16	0.44
1:A:1778:TYR:O	1:A:1782:ILE:HG12	2.17	0.44
1:A:1350:THR:HG21	1:A:1842:ILE:HD13	1.99	0.44
1:A:1722:PRO:O	1:A:1727:VAL:HG23	2.18	0.44
1:A:1484:VAL:HG21	1:A:1535:ARG:NH1	2.33	0.44
1:A:1257:LEU:HD21	1:A:1767:LEU:CD2	2.48	0.43
1:A:1742:ASN:HD21	1:A:1745:THR:H	1.64	0.43
1:A:1767:LEU:HD11	1:A:1776:LEU:HD23	2.00	0.43
1:A:1343:PHE:HB2	1:A:1857:LEU:HD13	2.00	0.43
1:A:1393:GLU:OE2	1:A:1397:GLU:HG3	2.18	0.43
1:A:1264:LEU:CD1	1:A:1656:LEU:HD12	2.49	0.43
1:A:1435:GLU:O	1:A:1439:LEU:HG	2.18	0.43
1:A:1374:GLN:HB3	3:A:340:HOH:O	2.19	0.42
1:A:1394:LYS:HG2	3:A:328:HOH:O	2.19	0.42
1:A:1555:CYS:O	1:A:1556:ASP:HB2	2.19	0.42
1:A:1301:ARG:NH2	1:A:1318:LEU:HD22	2.33	0.42
1:A:1405:LEU:HD23	1:A:1406:LEU:N	2.34	0.42
1:A:1551:THR:HG22	1:A:1561:ASN:ND2	2.35	0.42
1:A:1288:ASN:O	1:A:1289:HIS:CB	2.67	0.42
1:A:1825:LEU:HA	1:A:1825:LEU:HD23	1.82	0.42
1:A:1848:ARG:HB2	1:A:1848:ARG:NH1	2.34	0.42
1:A:1494:VAL:HA	1:A:1495:PRO:HD3	1.85	0.42
1:A:1295:ILE:HA	1:A:1296:PRO:HD3	1.81	0.41
1:A:1742:ASN:C	1:A:1742:ASN:ND2	2.71	0.41
1:A:1255:LYS:HB3	1:A:1255:LYS:HE3	1.77	0.41
1:A:1692:LYS:HE3	1:A:1696:ASP:OD2	2.20	0.41
1:A:1536:GLN:HB3	1:A:1536:GLN:HE21	1.60	0.41
1:A:1629:LEU:N	1:A:1629:LEU:HD12	2.33	0.41
1:A:1780:LYS:HD2	3:A:214:HOH:O	2.21	0.41
1:A:1397:GLU:C	1:A:1399:LYS:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1264:LEU:HB3	1:A:1657:THR:HG22	2.02	0.40
1:A:1652:SER:OG	1:A:1654:ILE:HG22	2.20	0.40
1:A:1315:HIS:ND1	1:A:1317:VAL:HB	2.36	0.40
1:A:1264:LEU:HD22	1:A:1657:THR:HG22	2.04	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	551/627 (88%)	532 (97%)	18 (3%)	1 (0%)	47	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1721	LEU

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	493/565 (87%)	460 (93%)	33 (7%)	16	11

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1254	LEU
1	A	1255	LYS
1	A	1257	LEU
1	A	1260	GLN
1	A	1278	GLU
1	A	1279	LEU
1	A	1283	ILE
1	A	1303	TYR
1	A	1317	VAL
1	A	1320	GLU
1	A	1399	LYS
1	A	1405	LEU
1	A	1409	THR
1	A	1437	LEU
1	A	1469	LEU
1	A	1471	ARG
1	A	1479	LEU
1	A	1542	ILE
1	A	1543	ILE
1	A	1629	LEU
1	A	1656	LEU
1	A	1676	THR
1	A	1706	GLN
1	A	1742	ASN
1	A	1764	GLU
1	A	1765	HIS
1	A	1774	ASN
1	A	1776	LEU
1	A	1791	ARG
1	A	1828	LEU
1	A	1831	LEU
1	A	1861	LEU
1	A	1868	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1260	GLN
1	A	1284	ASN
1	A	1326	ASN
1	A	1395	ASN
1	A	1419	ASN
1	A	1482	HIS

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Mol	Chain	Res	Type
1	A	1493	GLN
1	A	1536	GLN
1	A	1545	GLN
1	A	1565	HIS
1	A	1667	GLN
1	A	1701	GLN
1	A	1714	HIS
1	A	1742	ASN
1	A	1784	ASN
1	A	1805	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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	366	-	5,5,5	0.35	0	5,5,5	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	366	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	366	GOL	C1-C2-C3-O3
2	A	366	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	561/627 (89%)	0.71	78 (13%) 2 2	23, 40, 81, 110	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1651	VAL	6.8
1	A	1765	HIS	6.8
1	A	1636	HIS	6.7
1	A	1767	LEU	6.7
1	A	1259	LEU	6.0
1	A	1492	ALA	6.0
1	A	1539	MET	6.0
1	A	1684	GLY	5.8
1	A	1488	SER	5.8
1	A	1537	GLY	5.7
1	A	1769	LYS	5.6
1	A	1635	ASN	4.9
1	A	1538	ARG	4.8
1	A	1768	GLY	4.7
1	A	1770	ASP	4.5
1	A	1578	PRO	4.4
1	A	1254	LEU	4.4
1	A	1489	GLU	4.4
1	A	1685	SER	4.3
1	A	1256	ARG	4.3
1	A	1486	PRO	4.3
1	A	1314	ALA	4.2
1	A	1255	LYS	4.2
1	A	1540	ALA	4.0
1	A	1253	THR	4.0
1	A	1766	ARG	4.0
1	A	1485	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1487	GLU	3.9
1	A	1772	PRO	3.9
1	A	1397	GLU	3.9
1	A	1286	LEU	3.8
1	A	1246	SER	3.7
1	A	1626	GLY	3.6
1	A	1252	ARG	3.6
1	A	1249	ASP	3.5
1	A	1764	GLU	3.4
1	A	1257	LEU	3.3
1	A	1404	LEU	3.3
1	A	1287	THR	3.3
1	A	1573	LEU	3.1
1	A	1727	VAL	3.1
1	A	1771	SER	3.0
1	A	1289	HIS	3.0
1	A	1579	LYS	3.0
1	A	1251	ASP	2.9
1	A	1401	HIS	2.9
1	A	1250	ALA	2.9
1	A	1293	VAL	2.8
1	A	1258	GLN	2.8
1	A	1294	GLN	2.8
1	A	1627	THR	2.8
1	A	1774	ASN	2.8
1	A	1577	VAL	2.7
1	A	1396	LEU	2.6
1	A	1400	ASN	2.6
1	A	1726	TRP	2.5
1	A	1311	GLY	2.5
1	A	1519	ILE	2.4
1	A	1398	SER	2.4
1	A	1776	LEU	2.4
1	A	1518	GLY	2.4
1	A	1313	GLU	2.4
1	A	1542	ILE	2.4
1	A	1725	PHE	2.3
1	A	1484	VAL	2.3
1	A	1437	LEU	2.3
1	A	1655	TYR	2.3
1	A	1403	LYS	2.3
1	A	1320	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1285	GLU	2.3
1	A	1536	GLN	2.3
1	A	1529	ASP	2.2
1	A	1408	ARG	2.2
1	A	1421	PHE	2.2
1	A	1248	GLN	2.2
1	A	1283	ILE	2.1
1	A	1318	LEU	2.1
1	A	1652	SER	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	A	366	6/6	0.92	0.14	41,49,54,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.