



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2017 – 08:53 AM EDT

PDB ID : 5J68  
Title : Structure of Astrotactin-2, a conserved vertebrate-specific and perforin-like membrane protein involved in neuronal development  
Authors : Ni, T.; Harlos, K.; Gilbert, R.J.C.  
Deposited on : unknown  
Resolution : 5.22 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

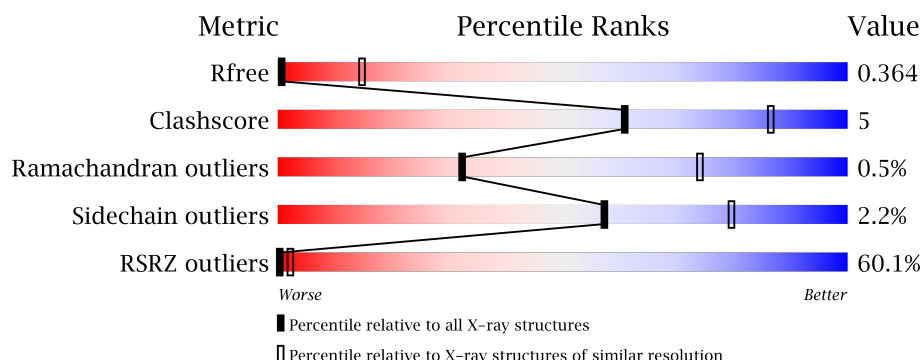
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 5.22 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))
$R_{free}$	100719	1019 (6.74-3.70)
Clashscore	112137	1003 (6.70-3.72)
Ramachandran outliers	110173	1051 (6.70-3.70)
Sidechain outliers	110143	1026 (6.70-3.70)
RSRZ outliers	101464	1028 (6.70-3.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	572	<div> <div>59%</div> <div>86%</div> <div>10%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4610 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 Astrotactin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	4456	2823	758	846	29	0	0	0

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	14	0
2	A	1	14	8	1	5	14	0
2	A	1	14	8	1	5	14	0

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	11	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



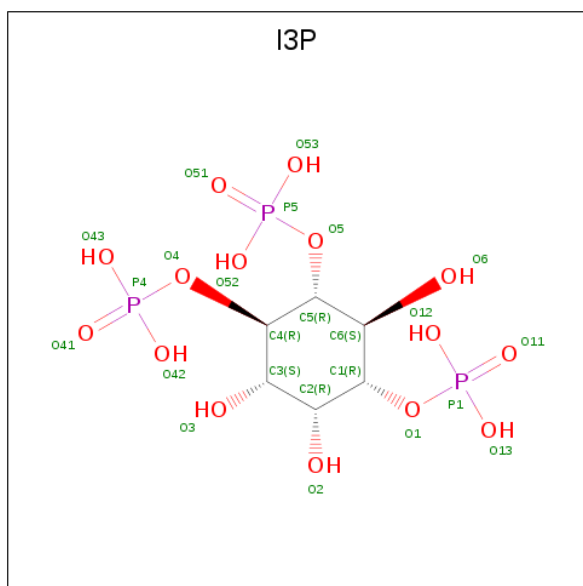
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	11	0
			11	6	5		
4	A	1	Total	C	O	11	0
			11	6	5		
4	A	1	Total	C	O	11	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	11	0
			11	6	5		
4	A	1	Total	C	O	11	0
			11	6	5		
4	A	1	Total	C	O	11	0
			11	6	5		
4	A	1	Total	C	O	11	0
			11	6	5		

- Molecule 5 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula:  $C_6H_{15}O_{15}P_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	24	0
			24	6	15	3		

### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: Astrotactin-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.90Å 103.90Å 304.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.80 – 5.22 85.80 – 5.22	Depositor EDS
% Data completeness (in resolution range)	99.9 (85.80-5.22) 100.0 (85.80-5.22)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 5.12Å)	Xtriage
Refinement program	PHENIX (dev_2283: ???)	Depositor
R, $R_{free}$	0.348 , 0.364 0.347 , 0.364	Depositor DCC
$R_{free}$ test set	358 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	330.4	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 458.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	4610	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	336.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, I3P, BMA, NAG

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	0.27	0/4552	0.49	1/6166 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1216	LEU	CA-CB-CG	-5.46	102.75	115.30

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	4456	0	4386	46	0
2	A	42	0	37	0	0
3	A	11	0	8	0	0
4	A	77	0	65	0	0
5	A	24	0	9	0	0
All	All	4610	0	4505	46	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 5.



All (46) 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:1200:VAL:HG22	1:A:1216:LEU:HD11	1.72	0.71
1:A:792:ILE:HG21	1:A:1021:LEU:HD12	1.78	0.66
1:A:1029:SER:HA	1:A:1137:THR:HB	1.78	0.66
1:A:1063:THR:OG1	1:A:1064:ASP:N	2.30	0.64
1:A:966:ILE:HD12	1:A:972:LYS:HA	1.80	0.64
1:A:1212:ALA:O	1:A:1216:LEU:HD22	1.99	0.62
1:A:1216:LEU:HD12	1:A:1219:LEU:HD12	1.82	0.61
1:A:1083:THR:HB	1:A:1084:SER:HA	1.84	0.60
1:A:1224:SER:HA	1:A:1227:SER:HB3	1.85	0.59
1:A:1200:VAL:HG13	1:A:1216:LEU:HD21	1.83	0.59
1:A:1217:ARG:HA	1:A:1220:GLU:HG3	1.83	0.59
1:A:1209:PRO:O	1:A:1213:HIS:ND1	2.25	0.58
1:A:1122:ASP:OD1	1:A:1126:ARG:N	2.38	0.55
1:A:753:ILE:HG22	1:A:754:LYS:HG3	1.89	0.55
1:A:963:TYR:HA	1:A:966:ILE:HG13	1.90	0.54
1:A:1029:SER:HB2	1:A:1110:PRO:HB3	1.90	0.54
1:A:1209:PRO:HA	1:A:1212:ALA:HB3	1.90	0.53
1:A:1224:SER:HA	1:A:1227:SER:CB	2.40	0.51
1:A:1204:GLU:HG3	1:A:1209:PRO:HG3	1.92	0.50
1:A:1222:VAL:HG12	1:A:1223:SER:O	2.13	0.48
1:A:793:ARG:HH21	1:A:1136:ARG:NH2	2.13	0.47
1:A:1021:LEU:HD23	1:A:1034:LEU:HD23	1.96	0.46
1:A:1210:ARG:HG3	1:A:1211:LYS:N	2.30	0.46
1:A:818:SER:HA	1:A:819:THR:HA	1.59	0.46
1:A:1236:GLN:O	1:A:1281:THR:N	2.45	0.45
1:A:1113:LEU:HD13	1:A:1136:ARG:HG2	2.00	0.44
1:A:1113:LEU:HD22	1:A:1136:ARG:NH2	2.32	0.44
1:A:1181:MET:O	1:A:1185:VAL:HG13	2.19	0.43
1:A:1030:THR:HG22	1:A:1110:PRO:HD3	1.99	0.43
1:A:1208:GLY:HA2	1:A:1209:PRO:HD3	1.59	0.43
1:A:725:GLU:OE1	1:A:725:GLU:N	2.49	0.43
1:A:992:ILE:HD13	1:A:997:ARG:HB2	2.00	0.43
1:A:1058:ASP:N	1:A:1058:ASP:OD1	2.52	0.43
1:A:1113:LEU:HD22	1:A:1136:ARG:HH21	1.84	0.42
1:A:1141:LEU:HD21	1:A:1278:ALA:HB1	2.00	0.42
1:A:923:GLU:OE1	1:A:925:ARG:NH2	2.53	0.42
1:A:919:ILE:O	1:A:919:ILE:HG22	2.20	0.42
1:A:1212:ALA:C	1:A:1216:LEU:HD22	2.40	0.41
1:A:793:ARG:HH21	1:A:1136:ARG:HH22	1.68	0.41
1:A:968:ASP:O	1:A:972:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:LEU:HA	1:A:1082:GLY:HA3	1.60	0.41
1:A:1215:ILE:HG22	1:A:1216:LEU:HD13	2.03	0.41
1:A:1244:TYR:CD1	1:A:1275:VAL:HG23	2.56	0.41
1:A:1225:HIS:N	1:A:1225:HIS:ND1	2.69	0.40
1:A:1109:GLU:HG2	1:A:1110:PRO:HD2	2.03	0.40
1:A:994:ASP:O	1:A:1046:LYS:HE2	2.21	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	553/572 (97%)	522 (94%)	28 (5%)	3 (0%)	32 74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1161	TYR
1	A	942	PRO
1	A	1287	GLY

### 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	501/513 (98%)	490 (98%)	11 (2%)	57 79

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	720	ASP
1	A	732	ASN
1	A	793	ARG
1	A	880	LEU
1	A	1064	ASP
1	A	1141	LEU
1	A	1210	ARG
1	A	1216	LEU
1	A	1220	GLU
1	A	1224	SER
1	A	1227	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	875	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 ⓘ

12 ligands are 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	NAG	A	1300	1,2	14,14,15	1.52	1 (7%)	15,19,21	2.59	1 (6%)
2	NAG	A	1301	3,2	14,14,15	0.41	0	15,19,21	0.50	0
3	BMA	A	1302	2,4	11,11,12	0.46	0	13,15,17	0.78	0
4	MAN	A	1303	3,4	11,11,12	1.01	1 (9%)	13,15,17	1.24	2 (15%)
4	MAN	A	1304	4	11,11,12	0.71	0	13,15,17	0.97	1 (7%)
4	MAN	A	1305	4	11,11,12	0.80	0	13,15,17	1.64	2 (15%)
4	MAN	A	1306	4	11,11,12	2.13	2 (18%)	13,15,17	1.80	3 (23%)
4	MAN	A	1307	4	11,11,12	1.69	4 (36%)	13,15,17	1.31	2 (15%)
4	MAN	A	1308	3,4	11,11,12	0.61	0	13,15,17	1.05	2 (15%)
4	MAN	A	1309	4	11,11,12	0.57	0	13,15,17	1.10	2 (15%)
2	NAG	A	1310	1	14,14,15	0.37	0	15,19,21	0.80	1 (6%)
5	I3P	A	1311	-	24,24,24	1.26	3 (12%)	36,39,39	0.64	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	NAG	A	1300	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1301	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1302	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1303	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1304	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1305	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1306	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1307	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1308	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1309	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
5	I3P	A	1311	-	-	0/15/39/39	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1303	MAN	O5-C1	-2.57	1.39	1.43
4	A	1307	MAN	O5-C1	-2.18	1.40	1.43
4	A	1306	MAN	C4-C3	2.01	1.57	1.52
4	A	1307	MAN	C4-C3	2.13	1.57	1.52
4	A	1307	MAN	O5-C5	2.81	1.49	1.43
5	A	1311	I3P	P5-O5	3.00	1.64	1.59
5	A	1311	I3P	P1-O1	3.10	1.65	1.59
5	A	1311	I3P	P4-O4	3.11	1.65	1.59
4	A	1307	MAN	C4-C5	3.13	1.59	1.53
2	A	1300	NAG	O5-C1	5.54	1.52	1.43
4	A	1306	MAN	C2-C3	6.17	1.60	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1307	MAN	C1-C2-C3	-2.75	106.16	109.65
4	A	1309	MAN	O2-C2-C3	-2.28	105.69	110.17
4	A	1303	MAN	O2-C2-C3	-2.26	105.74	110.17
4	A	1305	MAN	O2-C2-C3	-2.23	105.79	110.17
4	A	1307	MAN	O5-C1-C2	-2.11	107.49	110.79
4	A	1308	MAN	O2-C2-C3	-2.07	106.11	110.17
4	A	1303	MAN	C3-C4-C5	2.25	114.18	110.22
4	A	1304	MAN	C1-O5-C5	2.62	115.77	112.17
4	A	1308	MAN	C1-O5-C5	2.63	115.79	112.17
2	A	1310	NAG	C1-O5-C5	2.68	115.86	112.17
4	A	1309	MAN	C1-O5-C5	2.78	116.00	112.17
4	A	1306	MAN	C2-C3-C4	2.97	116.05	110.88
4	A	1306	MAN	O2-C2-C3	3.21	116.48	110.17
4	A	1306	MAN	O3-C3-C2	3.29	116.00	110.02
4	A	1305	MAN	C1-O5-C5	5.13	119.24	112.17
2	A	1300	NAG	C1-O5-C5	9.82	125.70	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	559/572 (97%)	3.51	336 (60%) 0 2	282, 335, 369, 393	0

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	990	ASP	17.4
1	A	989	GLY	16.3
1	A	998	CYS	15.8
1	A	974	ALA	14.8
1	A	1012	SER	14.2
1	A	887	THR	13.6
1	A	885	GLU	13.6
1	A	837	SER	13.4
1	A	839	ARG	13.4
1	A	810	SER	13.2
1	A	999	ASP	13.2
1	A	1011	CYS	13.0
1	A	834	THR	12.9
1	A	1287	GLY	12.4
1	A	997	ARG	12.1
1	A	1088	ALA	11.7
1	A	886	THR	11.5
1	A	971	THR	11.3
1	A	1286	LYS	11.1
1	A	996	CYS	11.0
1	A	975	PHE	10.8
1	A	1044	GLY	10.8
1	A	1009	PRO	10.8
1	A	1280	ASN	10.7
1	A	835	LYS	10.6
1	A	836	GLU	10.5
1	A	838	SER	10.4

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Mol	Chain	Res	Type	RSRZ
1	A	849	TYR	10.3
1	A	1090	ARG	10.3
1	A	1282	TYR	10.0
1	A	1045	THR	9.9
1	A	1279	ARG	9.7
1	A	1288	ARG	9.7
1	A	931	ARG	9.6
1	A	991	VAL	9.6
1	A	988	LYS	9.5
1	A	1142	VAL	9.4
1	A	833	LEU	9.3
1	A	942	PRO	9.3
1	A	884	LYS	9.2
1	A	850	GLY	9.2
1	A	1257	MET	9.1
1	A	973	GLU	9.1
1	A	1010	ASN	9.1
1	A	978	ALA	9.1
1	A	729	GLY	9.0
1	A	841	GLU	8.8
1	A	972	LYS	8.8
1	A	918	LEU	8.6
1	A	842	LEU	8.6
1	A	1261	SER	8.5
1	A	1124	ARG	8.5
1	A	943	GLY	8.4
1	A	984	TRP	8.2
1	A	977	SER	8.2
1	A	941	ARG	8.2
1	A	1089	GLY	8.1
1	A	970	GLY	8.0
1	A	881	GLN	7.9
1	A	1043	ILE	7.8
1	A	1285	SER	7.8
1	A	965	LEU	7.7
1	A	944	LYS	7.7
1	A	826	PHE	7.6
1	A	966	ILE	7.5
1	A	830	LEU	7.5
1	A	976	LYS	7.4
1	A	916	ASP	7.4
1	A	1001	SER	7.4

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Mol	Chain	Res	Type	RSRZ
1	A	1235	ILE	7.3
1	A	883	GLN	7.3
1	A	919	ILE	7.3
1	A	741	GLN	7.2
1	A	730	TYR	7.2
1	A	938	LEU	7.2
1	A	939	CYS	7.0
1	A	1013	PRO	7.0
1	A	861	SER	6.9
1	A	963	TYR	6.9
1	A	851	SER	6.9
1	A	995	TRP	6.8
1	A	1196	PHE	6.7
1	A	1144	ASP	6.7
1	A	1260	TYR	6.7
1	A	1126	ARG	6.7
1	A	1258	VAL	6.7
1	A	1000	LEU	6.5
1	A	1213	HIS	6.4
1	A	912	MET	6.4
1	A	731	ASN	6.4
1	A	831	LYS	6.3
1	A	1139	CYS	6.1
1	A	832	ILE	6.1
1	A	719	ASN	6.1
1	A	809	ARG	6.1
1	A	1002	ALA	6.1
1	A	992	ILE	6.0
1	A	932	CYS	6.0
1	A	964	THR	6.0
1	A	980	MET	6.0
1	A	968	ASP	6.0
1	A	1229	LEU	6.0
1	A	915	ASP	6.0
1	A	825	GLY	5.9
1	A	745	MET	5.8
1	A	897	SER	5.9
1	A	732	ASN	5.8
1	A	845	PHE	5.8
1	A	979	LEU	5.8
1	A	1140	PRO	5.8
1	A	1014	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	774	CYS	5.7
1	A	843	LEU	5.7
1	A	913	LEU	5.7
1	A	797	ALA	5.7
1	A	1143	ASP	5.7
1	A	1234	TYR	5.7
1	A	811	ASN	5.7
1	A	1238	ARG	5.7
1	A	846	ILE	5.7
1	A	1008	LEU	5.6
1	A	1222	VAL	5.6
1	A	981	SER	5.6
1	A	1245	LEU	5.6
1	A	922	VAL	5.6
1	A	1236	GLN	5.6
1	A	1233	ALA	5.6
1	A	829	VAL	5.5
1	A	900	PHE	5.5
1	A	994	ASP	5.5
1	A	739	GLN	5.4
1	A	1141	LEU	5.4
1	A	969	ASN	5.3
1	A	982	SER	5.3
1	A	1125	GLY	5.3
1	A	1278	ALA	5.2
1	A	1198	ASP	5.2
1	A	1193	TYR	5.2
1	A	1246	PHE	5.2
1	A	1154	ILE	5.2
1	A	1003	PHE	5.1
1	A	920	SER	5.1
1	A	933	PRO	5.1
1	A	869	PHE	5.1
1	A	806	TRP	5.1
1	A	921	GLY	5.1
1	A	804	GLN	5.1
1	A	1180	SER	5.1
1	A	985	CYS	5.0
1	A	940	ARG	5.0
1	A	917	GLN	5.0
1	A	742	VAL	4.9
1	A	1158	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	1195	LYS	4.9
1	A	848	HIS	4.9
1	A	870	PRO	4.8
1	A	1212	ALA	4.8
1	A	1179	ALA	4.8
1	A	1232	SER	4.8
1	A	1225	HIS	4.8
1	A	1184	ARG	4.8
1	A	1244	TYR	4.8
1	A	1237	SER	4.8
1	A	776	GLY	4.8
1	A	911	GLN	4.7
1	A	827	THR	4.7
1	A	796	GLU	4.7
1	A	1247	CYS	4.7
1	A	728	HIS	4.7
1	A	1206	GLU	4.6
1	A	738	ASN	4.6
1	A	847	GLN	4.6
1	A	987	GLY	4.6
1	A	1167	GLN	4.6
1	A	1281	THR	4.5
1	A	1189	TYR	4.5
1	A	1026	GLU	4.5
1	A	808	VAL	4.5
1	A	882	TYR	4.5
1	A	983	TYR	4.5
1	A	946	GLN	4.5
1	A	962	LEU	4.5
1	A	1174	LEU	4.4
1	A	937	HIS	4.4
1	A	993	ASP	4.4
1	A	898	MET	4.4
1	A	1209	PRO	4.4
1	A	1097	GLU	4.4
1	A	854	ILE	4.3
1	A	775	ARG	4.2
1	A	1256	GLY	4.2
1	A	1050	TYR	4.2
1	A	737	VAL	4.2
1	A	1220	GLU	4.2
1	A	1197	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	967	GLN	4.2
1	A	1087	ALA	4.2
1	A	1192	HIS	4.1
1	A	901	ILE	4.1
1	A	878	LEU	4.1
1	A	800	TYR	4.1
1	A	863	LEU	4.0
1	A	1042	ALA	4.0
1	A	1122	ASP	4.0
1	A	1284	GLU	4.0
1	A	879	TRP	4.0
1	A	949	PRO	4.0
1	A	945	GLU	4.0
1	A	1259	TRP	3.9
1	A	1040	GLN	3.9
1	A	1007	GLY	3.9
1	A	986	SER	3.9
1	A	1046	LYS	3.9
1	A	1063	THR	3.9
1	A	928	GLU	3.9
1	A	718	PHE	3.8
1	A	914	SER	3.8
1	A	1202	ARG	3.7
1	A	903	TYR	3.7
1	A	1219	LEU	3.7
1	A	740	GLY	3.7
1	A	1216	LEU	3.7
1	A	1099	SER	3.7
1	A	733	ARG	3.6
1	A	874	VAL	3.6
1	A	1048	SER	3.6
1	A	1039	VAL	3.6
1	A	867	ILE	3.6
1	A	1118	LEU	3.6
1	A	1264	LYS	3.6
1	A	1136	ARG	3.6
1	A	1120	ALA	3.6
1	A	828	ASN	3.6
1	A	862	GLU	3.6
1	A	936	CYS	3.5
1	A	1230	LEU	3.5
1	A	1188	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1255	ALA	3.5
1	A	1263	LEU	3.5
1	A	1155	TYR	3.4
1	A	875	GLN	3.4
1	A	904	LEU	3.4
1	A	760	ALA	3.4
1	A	1091	SER	3.4
1	A	813	TYR	3.4
1	A	852	HIS	3.3
1	A	1101	TYR	3.3
1	A	1185	VAL	3.3
1	A	853	TYR	3.2
1	A	1183	PHE	3.2
1	A	1199	PHE	3.2
1	A	880	LEU	3.2
1	A	812	LEU	3.2
1	A	772	GLU	3.2
1	A	1157	LEU	3.2
1	A	1271	GLU	3.2
1	A	1151	ALA	3.1
1	A	840	GLU	3.1
1	A	1277	MET	3.1
1	A	1171	TYR	3.1
1	A	844	SER	3.1
1	A	858	LEU	3.0
1	A	1207	LEU	3.0
1	A	1065	LEU	3.0
1	A	1181	MET	3.0
1	A	1272	GLU	3.0
1	A	1194	GLU	3.0
1	A	725	GLU	3.0
1	A	1240	GLU	3.0
1	A	1038	ASP	2.9
1	A	1170	ALA	2.9
1	A	1273	LYS	2.9
1	A	1017	PRO	2.9
1	A	924	ILE	2.8
1	A	802	MET	2.8
1	A	1147	ALA	2.8
1	A	877	GLN	2.8
1	A	1190	ASN	2.8
1	A	743	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1191	SER	2.8
1	A	727	LEU	2.8
1	A	1123	THR	2.8
1	A	1073	PHE	2.7
1	A	909	THR	2.7
1	A	1226	CYS	2.7
1	A	1064	ASP	2.7
1	A	1253	ARG	2.7
1	A	954	LEU	2.7
1	A	865	CYS	2.6
1	A	1070	PHE	2.6
1	A	801	PRO	2.6
1	A	756	PHE	2.6
1	A	1148	GLU	2.6
1	A	1205	ASP	2.6
1	A	1127	HIS	2.5
1	A	1266	THR	2.5
1	A	908	LEU	2.5
1	A	1201	TRP	2.5
1	A	824	ALA	2.5
1	A	1182	LEU	2.4
1	A	857	ALA	2.4
1	A	794	TYR	2.4
1	A	1041	PRO	2.4
1	A	1254	PRO	2.4
1	A	1268	ILE	2.4
1	A	798	MET	2.3
1	A	1116	PHE	2.3
1	A	1049	ASP	2.3
1	A	1215	ILE	2.3
1	A	929	LYS	2.3
1	A	1265	ASP	2.3
1	A	783	PRO	2.2
1	A	1231	ARG	2.2
1	A	871	SER	2.2
1	A	763	LEU	2.2
1	A	1015	LEU	2.2
1	A	1218	ARG	2.2
1	A	1019	LEU	2.2
1	A	1051	ILE	2.1
1	A	1047	VAL	2.1
1	A	1150	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1078	LEU	2.1
1	A	951	PRO	2.1
1	A	950	THR	2.1
1	A	1004	ASP	2.1
1	A	1128	SER	2.1
1	A	1204	GLU	2.1
1	A	778	LEU	2.1
1	A	1036	TRP	2.1
1	A	1175	MET	2.1
1	A	744	GLN	2.1
1	A	1092	HIS	2.1
1	A	899	PRO	2.0
1	A	795	ASP	2.0
1	A	961	PRO	2.0
1	A	1283	GLY	2.0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MAN	A	1305	11/12	-	-	-	347,352,358,360	11
2	NAG	A	1301	14/15	-	-	-	330,333,339,341	14
2	NAG	A	1310	14/15	-	-	-	357,362,367,371	14
4	MAN	A	1306	11/12	-	-	-	340,343,354,363	11
4	MAN	A	1308	11/12	-	-	-	338,347,351,352	11
4	MAN	A	1303	11/12	-	-	-	341,345,354,359	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	1300	14/15	-	-	-	330,333,334,335	14
4	MAN	A	1307	11/12	-	-	-	349,353,357,360	11
3	BMA	A	1302	11/12	-	-	-	336,340,348,349	11
4	MAN	A	1309	11/12	-	-	-	338,347,352,354	11
4	MAN	A	1304	11/12	-	-	-	350,353,354,355	11
5	I3P	A	1311	24/24	-	-	-	332,350,361,362	24

## 6.5 Other polymers [i](#)

There are no such residues in this entry.