



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2016 – 11:03 AM EDT

PDB ID : 5L0E
Title : Crystal Structure of Autotaxin and Compound 1
Authors : Durbin, J.D.
Deposited on : 2016-07-27
Resolution : 3.06 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20027939

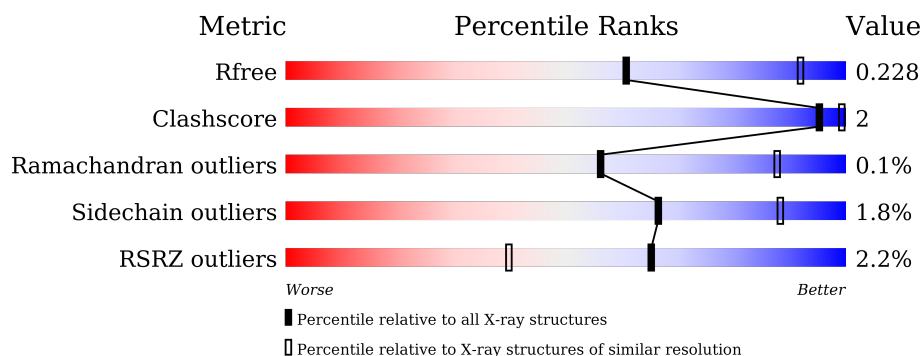
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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. 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	871	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>10%</div> </div> </div>
1	B	871	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>6%</div> <div>10%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	A	909	-	-	-	X
4	MAN	B	905	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12992 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.

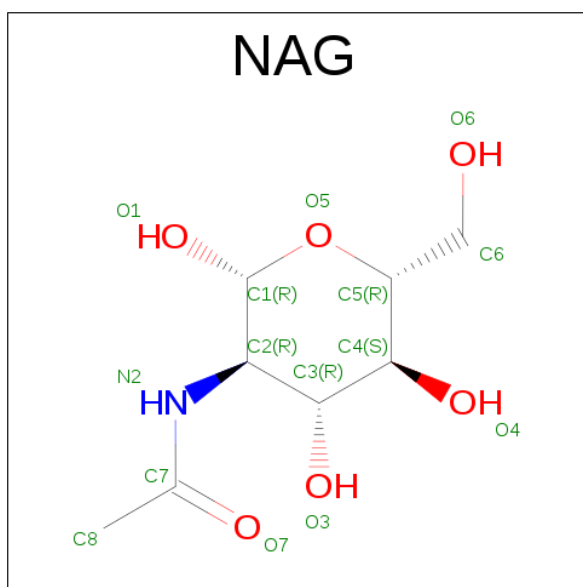
- Molecule 1 is a protein called Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	783	Total	C	N	O	S	0	0	0
			6319	4001	1088	1181	49			
1	B	782	Total	C	N	O	S	0	0	0
			6310	3995	1086	1180	49			

There are 22 discrepancies between the modelled and reference sequences:

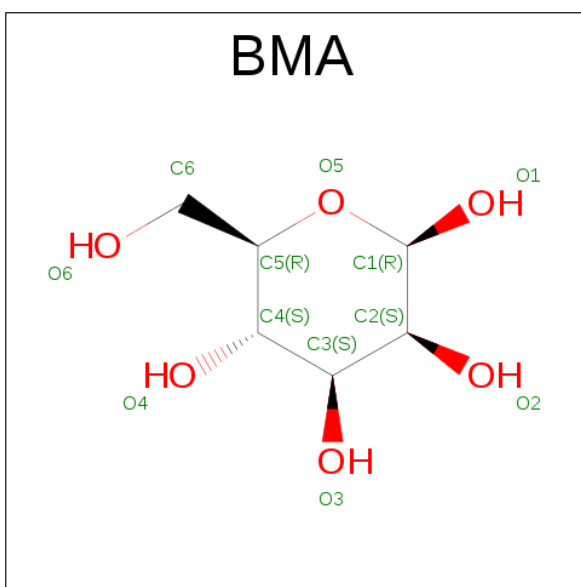
Chain	Residue	Modelled	Actual	Comment	Reference
A	591	THR	ARG	engineered mutation	UNP Q64610
A	592	GLU	LYS	engineered mutation	UNP Q64610
A	863	ALA	-	expression tag	UNP Q64610
A	864	ALA	-	expression tag	UNP Q64610
A	865	ALA	-	expression tag	UNP Q64610
A	866	HIS	-	expression tag	UNP Q64610
A	867	HIS	-	expression tag	UNP Q64610
A	868	HIS	-	expression tag	UNP Q64610
A	869	HIS	-	expression tag	UNP Q64610
A	870	HIS	-	expression tag	UNP Q64610
A	871	HIS	-	expression tag	UNP Q64610
B	591	THR	ARG	engineered mutation	UNP Q64610
B	592	GLU	LYS	engineered mutation	UNP Q64610
B	863	ALA	-	expression tag	UNP Q64610
B	864	ALA	-	expression tag	UNP Q64610
B	865	ALA	-	expression tag	UNP Q64610
B	866	HIS	-	expression tag	UNP Q64610
B	867	HIS	-	expression tag	UNP Q64610
B	868	HIS	-	expression tag	UNP Q64610
B	869	HIS	-	expression tag	UNP Q64610
B	870	HIS	-	expression tag	UNP Q64610
B	871	HIS	-	expression tag	UNP Q64610

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



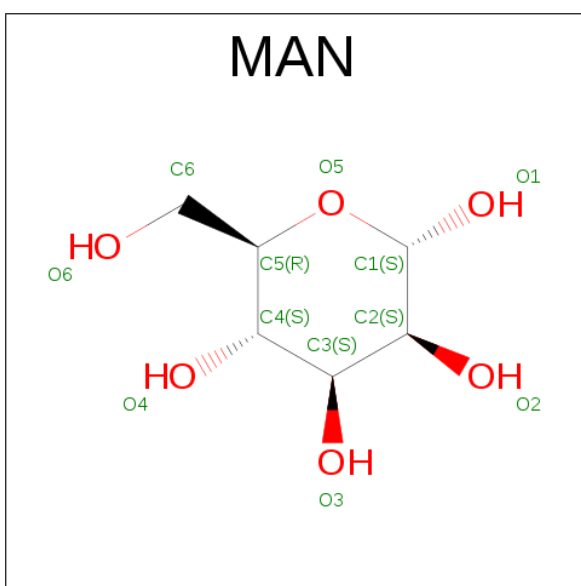
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



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

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



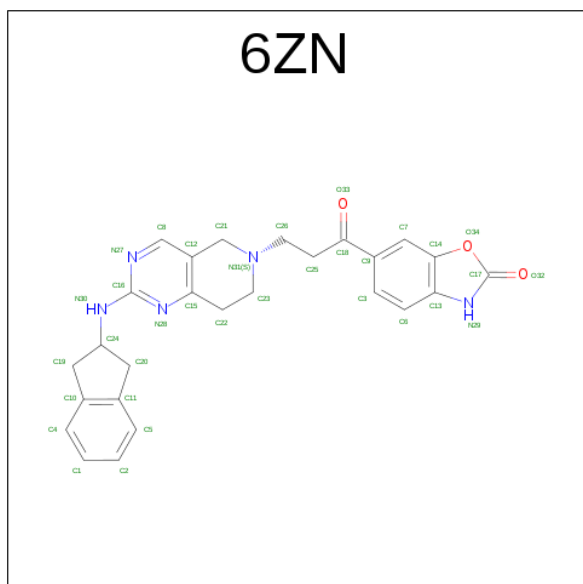
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

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

- Molecule 5 is 6-(3-{2-[(2,3-dihydro-1H-inden-2-yl)amino]-7,8-dihydropyrido[4,3-d]pyrimidin-6(5H)-yl}propanoyl)-1,3-benzoxazol-2(3H)-one (three-letter code: 6ZN) (formula: C₂₆H₂₅N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			34	26	5	3		
5	B	1	Total	C	N	O	0	0
			34	26	5	3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Cl 1	0	0
6	A	1	Total 1	Cl 1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	3	Total 3	Zn 3	0	0
7	A	3	Total 3	Zn 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	40	Total 40	O 40	0	0
8	B	42	Total 42	O 42	0	0

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

- [illegible]

- Chain B:
-
- 2% 84% 6% 10%
- Met Ala Arg Gly Gln Cys Leu Gly Ser Phe Glu Val Ile Ser Leu Phe Thr Phe Ala Ile Ser Ser Val Asn Ile Cys Leu Gly Phe Thr Ala Arg Ile Lys Lys Arg Ala Glu Trp Asp Gly Gly Pro Pro Thr Val Leu Ser Asp Ser Ser Pro Trp
- Q134 E140 V161 R162 P163 I166 D171 K183 P199 P206 L216 P222 E225 M232 F241 R246 F249 T272 L297 P310 C350 V351 D363 E370 L389 S396 I397 S400 K401 P416 D417 L446 R449
- R450 V451 W452 D459 VAL TYR LYS LYS PRO PRO SER GLY LYS C468 P502 P504 P505 D570 LYS VAL GLU LYS PRO LYS ASN LYS LEU LEU GLU GLU LEU ASN LYS LYS ARG LEU HIS THR LYS G589 S590 T591 E592 L604 Y605 R606 Y609 D610 L611 P625 S659 Y669 P682

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.18Å 96.84Å 136.92Å 90.00° 112.82° 90.00°	Depositor
Resolution (Å)	19.98 – 3.06 19.98 – 3.06	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.98-3.06) 95.0 (19.98-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.04Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.183 , 0.211 0.197 , 0.228	Depositor DCC
R_{free} test set	983 reflections (2.47%)	DCC
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12992	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: ZN, BMA, NAG, CL, 6ZN, MAN

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	0.50	0/6497	0.68	0/8814
1	B	0.51	0/6488	0.69	0/8803
All	All	0.51	0/12985	0.68	0/17617

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	6319	0	6049	20	0
1	B	6310	0	6036	21	0
2	A	42	0	37	0	0
2	B	42	0	37	0	0
3	A	11	0	8	0	0
3	B	11	0	9	0	0
4	A	66	0	56	0	0
4	B	33	0	28	0	0
5	A	34	0	0	1	0
5	B	34	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	3	0	0	0	0
7	B	3	0	0	0	0
8	A	40	0	0	0	0
8	B	42	0	0	1	0
All	All	12992	0	12260	40	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 2.

All (40) 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:163:PRO:HB3	1:A:350:CYS:O	1.87	0.75
1:B:77:ASN:OD1	1:B:272:THR:HG21	1.99	0.62
1:A:243:LEU:HD22	5:A:911:6ZN:C7	2.31	0.61
1:A:171:ASP:O	1:A:310:PRO:HD2	2.03	0.58
1:B:171:ASP:O	1:B:310:PRO:HD2	2.05	0.56
1:A:71:PRO:HB3	1:B:549:ARG:HH22	1.72	0.54
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.44	0.53
1:B:222:PRO:HA	1:B:225:HIS:CE1	2.45	0.52
1:A:166:ILE:HD12	1:A:351:VAL:HG11	1.93	0.51
1:B:166:ILE:HD12	1:B:351:VAL:HG11	1.93	0.50
1:B:625:PHE:HD1	1:B:762:PRO:HG3	1.76	0.50
1:A:456:LYS:HG3	1:A:458:LEU:HB3	1.94	0.49
1:B:134:GLN:HB3	1:B:140:GLU:HG3	1.95	0.48
1:A:134:GLN:HB3	1:A:140:GLU:HG3	1.95	0.48
1:B:682:PRO:HB3	1:B:716:GLN:HB3	1.96	0.47
1:B:669:TYR:CE2	1:B:701:MET:CE	2.97	0.47
1:A:669:TYR:CE2	1:A:701:MET:CE	2.98	0.46
1:A:682:PRO:HB3	1:A:716:GLN:HB3	1.96	0.46
1:B:81:SER:HA	8:B:1038:HOH:O	2.15	0.46
1:B:449:ARG:O	1:B:450:ARG:HB2	2.17	0.45
1:B:604:LEU:HD11	1:B:836:ASP:HB2	1.98	0.45
1:A:199:PRO:HG2	1:A:502:PRO:HG3	1.98	0.44
1:A:604:LEU:HD11	1:A:836:ASP:HB2	1.98	0.44
1:B:246:ARG:HA	1:B:249:PHE:HD2	1.84	0.43
1:B:856:HIS:HD2	1:B:858:TYR:CZ	2.36	0.43
1:B:199:PRO:HG2	1:B:502:PRO:HG3	2.00	0.42
1:A:124:LEU:HD12	1:A:129:CYS:SG	2.60	0.42
1:B:550:PRO:HB2	1:B:611:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:HIS:HD2	1:A:858:TYR:CZ	2.38	0.42
1:B:206:PRO:HB3	1:B:389:LEU:HD22	2.02	0.41
1:A:188:ILE:HD11	1:A:331:ILE:HG22	2.02	0.41
1:B:163:PRO:HB3	1:B:350:CYS:O	2.20	0.41
1:A:550:PRO:HB3	1:A:609:TYR:CE2	2.55	0.41
1:B:232:MET:HB2	1:B:241:PHE:HB3	2.01	0.41
1:A:232:MET:HB2	1:A:241:PHE:HB3	2.01	0.41
1:B:550:PRO:HB3	1:B:609:TYR:CE2	2.56	0.41
1:B:669:TYR:CE2	1:B:701:MET:HE1	2.56	0.40
1:A:456:LYS:HE3	1:A:458:LEU:HD22	2.03	0.40
1:A:550:PRO:HB2	1:A:611:ILE:HG12	2.02	0.40
1:A:591:THR:HG21	1:A:613:TYR:HB3	2.04	0.40

There are no symmetry-related clashes.

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	777/871 (89%)	745 (96%)	31 (4%)	1 (0%)	56	88
1	B	776/871 (89%)	743 (96%)	33 (4%)	0	100	100
All	All	1553/1742 (89%)	1488 (96%)	64 (4%)	1 (0%)	56	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	SER

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	710/786 (90%)	699 (98%)	11 (2%)	72	90
1	B	709/786 (90%)	695 (98%)	14 (2%)	63	87
All	All	1419/1572 (90%)	1394 (98%)	25 (2%)	66	88

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	LEU
1	A	162	ARG
1	A	216	LEU
1	A	246	ARG
1	A	446	LEU
1	A	452	HIS
1	A	606	ARG
1	A	659	SER
1	A	750	ASP
1	A	760	SER
1	A	810	ASP
1	B	124	LEU
1	B	161	VAL
1	B	162	ARG
1	B	183	LYS
1	B	216	LEU
1	B	246	ARG
1	B	363	ASP
1	B	370	GLU
1	B	446	LEU
1	B	452	HIS
1	B	570	ASP
1	B	606	ARG
1	B	659	SER
1	B	750	ASP

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	118	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 8 are monoatomic - leaving 19 for Mogul analysis.

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	901	1,2	14,14,15	0.35	0	15,19,21	0.63	0
2	NAG	A	902	3,2	14,14,15	0.31	0	15,19,21	0.65	0
3	BMA	A	903	2,4	11,11,12	0.75	0	15,15,17	1.24	1 (6%)
4	MAN	A	904	3,4	11,11,12	0.47	0	15,15,17	0.92	2 (13%)
4	MAN	A	905	4	11,11,12	0.44	0	15,15,17	0.87	1 (6%)
4	MAN	A	906	4	11,11,12	0.40	0	15,15,17	0.77	1 (6%)
4	MAN	A	907	3	11,11,12	0.37	0	15,15,17	0.68	1 (6%)
4	MAN	A	908	4	11,11,12	0.35	0	15,15,17	0.85	1 (6%)
4	MAN	A	909	4	11,11,12	0.34	0	15,15,17	0.64	0
2	NAG	A	910	1	14,14,15	0.31	0	15,19,21	0.54	0
5	6ZN	A	911	7	35,39,39	1.53	4 (11%)	42,56,56	2.13	16 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	901	1,2	14,14,15	0.38	0	15,19,21	0.66	0
2	NAG	B	902	3,2	14,14,15	0.28	0	15,19,21	0.67	0
3	BMA	B	903	2,4	11,11,12	0.78	0	15,15,17	1.17	0
4	MAN	B	904	3,4	11,11,12	0.43	0	15,15,17	0.95	1 (6%)
4	MAN	B	905	4	11,11,12	0.43	0	15,15,17	0.85	1 (6%)
4	MAN	B	906	4	11,11,12	0.38	0	15,15,17	0.81	1 (6%)
2	NAG	B	907	1	14,14,15	0.28	0	15,19,21	0.51	0
5	6ZN	B	908	7	35,39,39	1.40	3 (8%)	42,56,56	2.30	10 (23%)

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	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	902	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	903	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	904	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	905	4	-	0/2/19/22	0/1/1/1
4	MAN	A	906	4	-	0/2/19/22	0/1/1/1
4	MAN	A	907	3	-	0/2/19/22	0/1/1/1
4	MAN	A	908	4	-	0/2/19/22	0/1/1/1
4	MAN	A	909	4	-	0/2/19/22	0/1/1/1
2	NAG	A	910	1	-	0/6/23/26	0/1/1/1
5	6ZN	A	911	7	-	0/13/30/30	0/5/6/6
2	NAG	B	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	902	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	903	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	904	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	905	4	-	0/2/19/22	0/1/1/1
4	MAN	B	906	4	-	0/2/19/22	0/1/1/1
2	NAG	B	907	1	-	0/6/23/26	0/1/1/1
5	6ZN	B	908	7	-	0/13/30/30	0/5/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	911	6ZN	C20-C11	-2.23	1.47	1.50
5	A	911	6ZN	C6-C13	-2.08	1.38	1.41
5	B	908	6ZN	C6-C13	-2.07	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	911	6ZN	O32-C17	2.78	1.22	1.19
5	B	908	6ZN	O32-C17	2.79	1.22	1.19
5	B	908	6ZN	C16-N30	5.99	1.41	1.34
5	A	911	6ZN	C16-N30	6.69	1.42	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	908	6ZN	C16-N30-C24	-8.13	114.46	123.51
5	A	911	6ZN	C16-N30-C24	-6.34	116.45	123.51
5	A	911	6ZN	C26-C25-C18	-4.39	108.01	112.79
5	B	908	6ZN	C11-C20-C24	-4.35	98.98	103.00
5	B	908	6ZN	N30-C16-N27	-4.34	110.89	116.97
5	B	908	6ZN	C10-C19-C24	-4.14	99.18	103.00
5	B	908	6ZN	C26-C25-C18	-3.49	108.99	112.79
5	A	911	6ZN	C3-C6-C13	-3.41	117.09	120.86
5	A	911	6ZN	C10-C19-C24	-3.13	100.11	103.00
5	A	911	6ZN	N27-C16-N28	-3.06	123.40	126.66
5	A	911	6ZN	C20-C24-N30	-2.85	106.19	111.63
5	B	908	6ZN	C3-C6-C13	-2.74	117.83	120.86
5	B	908	6ZN	C19-C24-N30	-2.72	106.44	111.63
5	B	908	6ZN	C7-C14-C13	-2.68	118.47	121.15
5	A	911	6ZN	C25-C18-C9	-2.60	115.29	119.23
3	A	903	BMA	C1-C2-C3	-2.53	106.49	109.55
5	A	911	6ZN	C1-C4-C10	-2.42	117.17	120.90
5	A	911	6ZN	C2-C5-C11	-2.28	117.40	120.90
5	A	911	6ZN	N30-C16-N27	-2.23	113.84	116.97
5	A	911	6ZN	C7-C14-C13	-2.16	118.99	121.15
5	B	908	6ZN	C1-C4-C10	-2.06	117.73	120.90
4	A	904	MAN	C1-C2-C3	2.06	112.05	109.55
4	A	907	MAN	C1-C2-C3	2.18	112.19	109.55
5	A	911	6ZN	C19-C10-C11	2.19	112.28	110.65
5	A	911	6ZN	C3-C9-C7	2.22	122.19	119.26
4	A	906	MAN	C1-O5-C5	2.31	115.54	112.14
5	A	911	6ZN	C5-C11-C10	2.44	122.80	120.01
5	A	911	6ZN	O33-C18-C25	2.48	124.89	120.26
4	B	906	MAN	C1-O5-C5	2.53	115.86	112.14
4	A	904	MAN	C1-O5-C5	2.55	115.89	112.14
4	B	905	MAN	C1-O5-C5	2.62	115.99	112.14
4	A	905	MAN	C1-O5-C5	2.64	116.02	112.14
4	B	904	MAN	C1-O5-C5	2.69	116.09	112.14
4	A	908	MAN	C1-O5-C5	2.78	116.23	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	911	6ZN	N30-C16-N28	4.01	122.71	116.97
5	B	908	6ZN	N30-C16-N28	5.28	124.52	116.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	911	6ZN	1	0

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	783/871 (89%)	-0.29	21 (2%) 58 32	15, 47, 85, 105	0
1	B	782/871 (89%)	-0.28	14 (1%) 71 47	18, 46, 81, 113	0
All	All	1565/1742 (89%)	-0.28	35 (2%) 65 40	15, 46, 83, 113	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	589	GLY	5.7
1	B	52	THR	4.7
1	B	396	SER	4.2
1	A	54	THR	4.2
1	B	590	SER	4.0
1	A	400	SER	3.8
1	A	52	THR	3.4
1	B	417	ASP	3.3
1	A	416	PRO	3.3
1	B	400	SER	2.9
1	B	459	ASP	2.9
1	A	71	PRO	2.8
1	A	459	ASP	2.8
1	A	417	ASP	2.8
1	B	71	PRO	2.8
1	A	566	CYS	2.7
1	A	458	LEU	2.7
1	B	401	LYS	2.7
1	A	591	THR	2.6
1	B	591	THR	2.6
1	A	468	CYS	2.6
1	A	396	SER	2.5
1	B	416	PRO	2.5
1	A	401	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	567	THR	2.4
1	A	590	SER	2.4
1	A	67	GLU	2.4
1	A	549	ARG	2.3
1	A	56	GLY	2.3
1	A	569	ASP	2.2
1	B	297	ASN	2.2
1	B	592	GLU	2.2
1	A	53	ASN	2.2
1	B	397	ILE	2.1
1	A	246	ARG	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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	MAN	B	905	11/12	0.84	0.33	4.20	96,99,100,101	0
4	MAN	A	909	11/12	0.86	0.31	2.50	95,97,100,101	0
2	NAG	A	910	14/15	0.83	0.30	1.64	65,71,75,76	0
2	NAG	B	907	14/15	0.82	0.34	1.13	82,86,90,90	0
4	MAN	A	905	11/12	0.84	0.24	1.10	68,73,75,76	0
2	NAG	A	901	14/15	0.96	0.18	0.36	39,46,53,54	0
5	6ZN	A	911	34/34	0.95	0.17	0.22	27,47,61,61	0
5	6ZN	B	908	34/34	0.97	0.14	-0.52	29,36,56,59	0
2	NAG	B	901	14/15	0.97	0.14	-0.53	32,37,44,53	0
6	CL	B	912	1/1	0.98	0.15	-0.78	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	CL	A	912	1/1	0.94	0.10	-2.05	51,51,51,51	0
7	ZN	A	914	1/1	0.99	0.09	-2.18	30,30,30,30	0
7	ZN	B	910	1/1	0.97	0.07	-3.48	89,89,89,89	0
7	ZN	B	911	1/1	0.98	0.07	-3.54	74,74,74,74	0
7	ZN	A	915	1/1	0.99	0.03	-3.66	72,72,72,72	0
7	ZN	A	913	1/1	0.98	0.04	-6.68	61,61,61,61	1
7	ZN	B	909	1/1	1.00	0.07	-6.84	35,35,35,35	0
4	MAN	A	904	11/12	0.92	0.17	-	68,71,76,81	0
4	MAN	A	908	11/12	0.85	0.32	-	88,95,98,98	0
4	MAN	B	904	11/12	0.90	0.27	-	81,86,89,93	0
4	MAN	A	907	11/12	0.85	0.41	-	82,83,84,85	0
3	BMA	B	903	11/12	0.83	0.35	-	86,89,90,91	0
2	NAG	A	902	14/15	0.94	0.25	-	60,64,70,74	0
4	MAN	A	906	11/12	0.92	0.15	-	61,65,67,67	0
4	MAN	B	906	11/12	0.87	0.33	-	88,91,92,94	0
3	BMA	A	903	11/12	0.91	0.32	-	75,77,78,80	0
2	NAG	B	902	14/15	0.88	0.25	-	55,64,73,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.