



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 17, 2017 – 09:15 PM EDT

PDB ID : 5KXI
Title : X-ray structure of the human Alpha4Beta2 nicotinic receptor
Authors : Morales-Perez, C.L.; Noviello, C.M.; Hibbs, R.E.
Deposited on : unknown
Resolution : 3.94 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

<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	:	1.7.2 (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

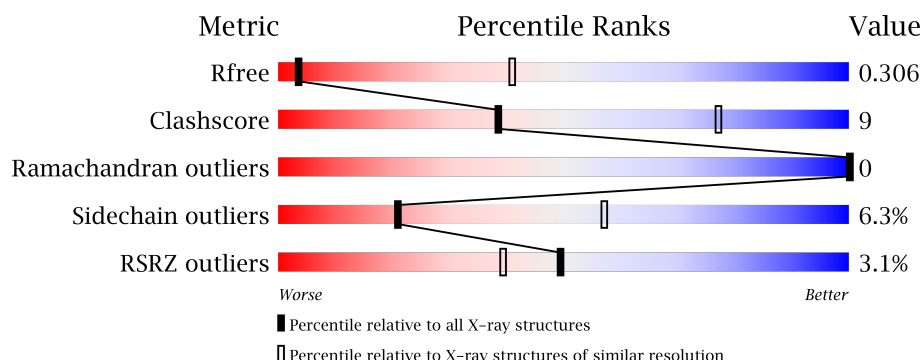
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.94 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	1021 (4.28-3.60)
Clashscore	112137	1117 (4.28-3.60)
Ramachandran outliers	110173	1076 (4.28-3.60)
Sidechain outliers	110143	1067 (4.28-3.60)
RSRZ outliers	101464	1034 (4.28-3.60)

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	386	<div> <div>3%</div> <div>71%</div> <div>22%</div> <div>6%</div> </div>
1	D	386	<div> <div>3%</div> <div>73%</div> <div>20%</div> <div>6%</div> </div>
2	B	403	<div> <div>3%</div> <div>63%</div> <div>24%</div> <div>11%</div> </div>
2	C	403	<div> <div>0%</div> <div>64%</div> <div>24%</div> <div>11%</div> </div>
2	E	403	<div> <div>3%</div> <div>64%</div> <div>24%</div> <div>11%</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
3	NAG	C	500	-	-	-	X
4	NCT	A	402	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14805 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 Neuronal acetylcholine receptor subunit alpha-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2983	1968	482	516	17			
1	D	363	Total	C	N	O	S	0	0	0
			2983	1968	482	516	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	-	linker	UNP P43681
A	340	THR	-	linker	UNP P43681
A	341	ASP	-	linker	UNP P43681
A	342	PHE	-	linker	UNP P43681
A	343	GLU	-	linker	UNP P43681
A	344	ARG	-	linker	UNP P43681
D	339	ASP	-	linker	UNP P43681
D	340	THR	-	linker	UNP P43681
D	341	ASP	-	linker	UNP P43681
D	342	PHE	-	linker	UNP P43681
D	343	GLU	-	linker	UNP P43681
D	344	ARG	-	linker	UNP P43681

- Molecule 2 is a protein called Neuronal acetylcholine receptor subunit beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	358	Total	C	N	O	S	0	0	0
			2913	1915	459	521	18			
2	C	358	Total	C	N	O	S	0	0	0
			2913	1915	459	521	18			
2	E	358	Total	C	N	O	S	0	0	0
			2913	1915	459	521	18			

There are 48 discrepancies between the modelled and reference sequences:

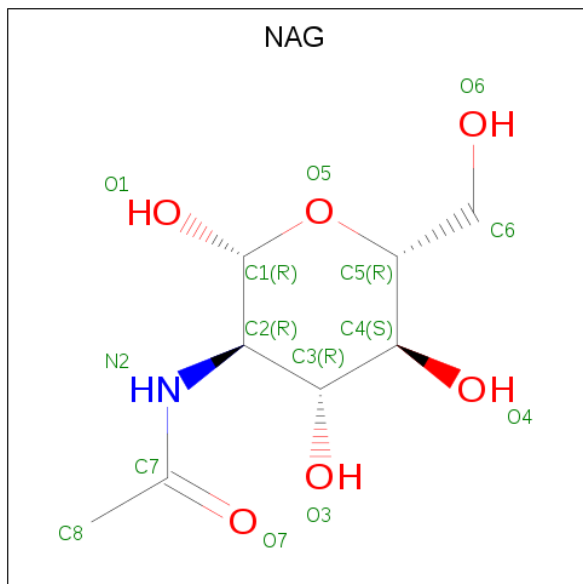
Chain	Residue	Modelled	Actual	Comment	Reference
B	331	ASP	-	linker	UNP P17787
B	332	ASP	-	linker	UNP P17787
B	333	ASP	-	linker	UNP P17787
B	334	GLN	-	linker	UNP P17787
B	335	GLU	-	linker	UNP P17787
B	336	ARG	-	linker	UNP P17787
B	394	SER	-	expression tag	UNP P17787
B	395	ALA	-	expression tag	UNP P17787
B	396	TRP	-	expression tag	UNP P17787
B	397	SER	-	expression tag	UNP P17787
B	398	HIS	-	expression tag	UNP P17787
B	399	PRO	-	expression tag	UNP P17787
B	400	GLN	-	expression tag	UNP P17787
B	401	PHE	-	expression tag	UNP P17787
B	402	GLU	-	expression tag	UNP P17787
B	403	LYS	-	expression tag	UNP P17787
C	331	ASP	-	linker	UNP P17787
C	332	ASP	-	linker	UNP P17787
C	333	ASP	-	linker	UNP P17787
C	334	GLN	-	linker	UNP P17787
C	335	GLU	-	linker	UNP P17787
C	336	ARG	-	linker	UNP P17787
C	394	SER	-	expression tag	UNP P17787
C	395	ALA	-	expression tag	UNP P17787
C	396	TRP	-	expression tag	UNP P17787
C	397	SER	-	expression tag	UNP P17787
C	398	HIS	-	expression tag	UNP P17787
C	399	PRO	-	expression tag	UNP P17787
C	400	GLN	-	expression tag	UNP P17787
C	401	PHE	-	expression tag	UNP P17787
C	402	GLU	-	expression tag	UNP P17787
C	403	LYS	-	expression tag	UNP P17787
E	331	ASP	-	linker	UNP P17787
E	332	ASP	-	linker	UNP P17787
E	333	ASP	-	linker	UNP P17787
E	334	GLN	-	linker	UNP P17787
E	335	GLU	-	linker	UNP P17787
E	336	ARG	-	linker	UNP P17787
E	394	SER	-	expression tag	UNP P17787
E	395	ALA	-	expression tag	UNP P17787
E	396	TRP	-	expression tag	UNP P17787
E	397	SER	-	expression tag	UNP P17787
E	398	HIS	-	expression tag	UNP P17787

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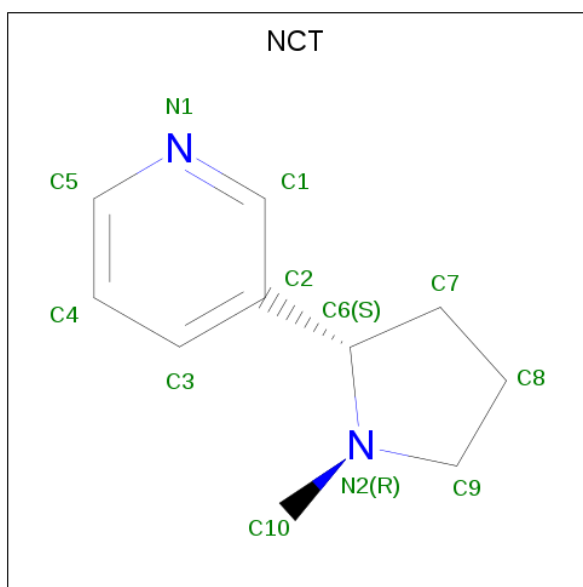
Chain	Residue	Modelled	Actual	Comment	Reference
E	399	PRO	-	expression tag	UNP P17787
E	400	GLN	-	expression tag	UNP P17787
E	401	PHE	-	expression tag	UNP P17787
E	402	GLU	-	expression tag	UNP P17787
E	403	LYS	-	expression tag	UNP P17787

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is (S)-3-(1-METHYLPYRROLIDIN-2-YL)PYRIDINE (three-letter code: NCT) (formula: $C_{10}H_{14}N_2$).



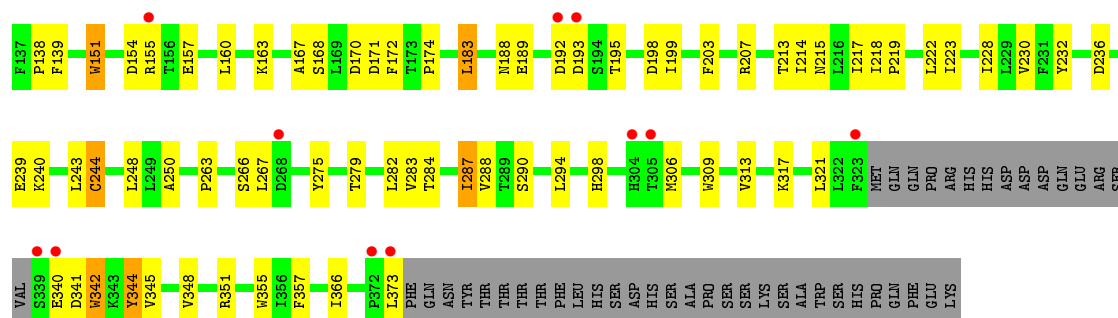
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			12	10	2		
4	D	1	Total	C	N	0	0
			12	10	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

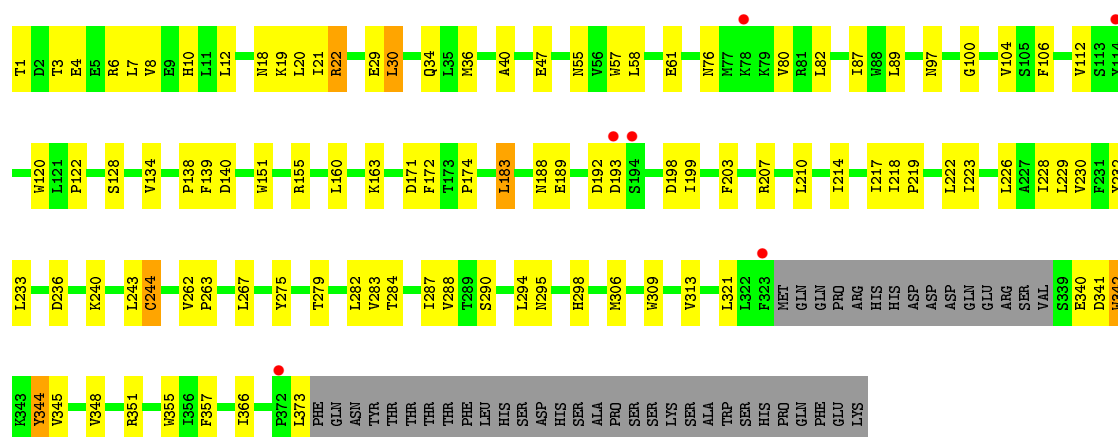
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

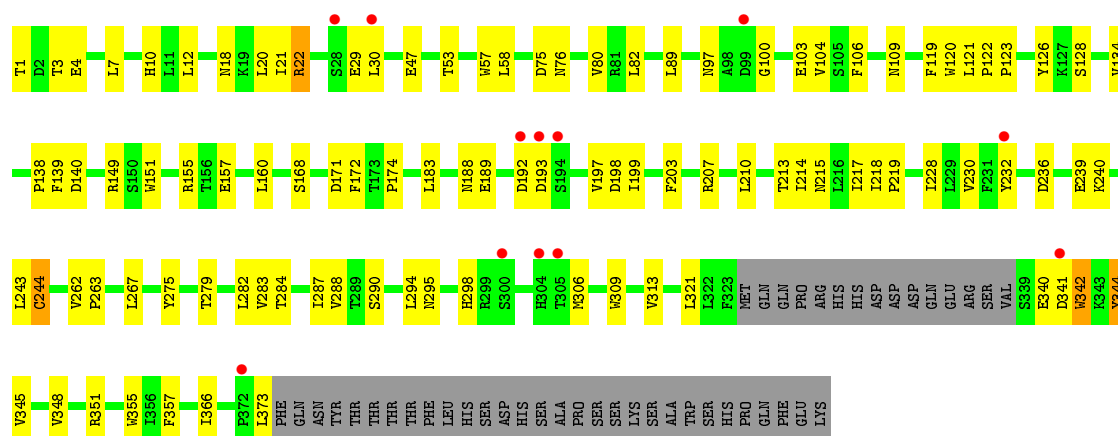
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	1	Total	O	0	0
			1	1		
6	C	1	Total	O	0	0
			1	1		
6	D	1	Total	O	0	0
			1	1		
6	E	1	Total	O	0	0
			1	1		



• Molecule 2: Neuronal acetylcholine receptor subunit beta-2



• Molecule 2: Neuronal acetylcholine receptor subunit beta-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.10Å 132.63Å 202.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.94 25.00 – 3.94	Depositor EDS
% Data completeness (in resolution range)	86.8 (25.00-3.94) 86.8 (25.00-3.94)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 3.97Å)	Xtriage
Refinement program	PHENIX (1.10_2155)	Depositor
R, R_{free}	0.285 , 0.307 0.280 , 0.306	Depositor DCC
R_{free} test set	1330 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	159.8	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14805	wwPDB-VP
Average B, all atoms (Å ²)	170.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, NCT, 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	0.26	0/3068	0.46	1/4191 (0.0%)
1	D	0.25	0/3068	0.45	1/4191 (0.0%)
2	B	0.26	0/2993	0.47	0/4089
2	C	0.26	0/2993	0.47	0/4089
2	E	0.26	0/2993	0.47	0/4089
All	All	0.26	0/15115	0.46	2/20649 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	378	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	378	LEU	CA-CB-CG	5.42	127.76	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	2983	0	3015	60	0
1	D	2983	0	3015	59	0
2	B	2913	0	2936	59	0
2	C	2913	0	2936	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2913	0	2936	53	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
3	E	14	0	13	0	0
4	A	12	0	14	2	0
4	D	12	0	14	4	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
All	All	14805	0	14931	255	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 9.

The worst 5 of 255 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)
2:B:97:ASN:HB3	2:B:100:GLY:HA3	1.52	0.91
2:C:97:ASN:HB3	2:C:100:GLY:HA3	1.53	0.90
2:E:97:ASN:HB3	2:E:100:GLY:HA3	1.53	0.88
1:A:325:ILE:HG21	1:A:360:ILE:HD11	1.58	0.83
1:D:325:ILE:HG21	1:D:360:ILE:HD11	1.62	0.79

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	359/386 (93%)	338 (94%)	21 (6%)	0	100	100
1	D	359/386 (93%)	338 (94%)	21 (6%)	0	100	100
2	B	354/403 (88%)	332 (94%)	22 (6%)	0	100	100
2	C	354/403 (88%)	330 (93%)	24 (7%)	0	100	100
2	E	354/403 (88%)	332 (94%)	22 (6%)	0	100	100
All	All	1780/1981 (90%)	1670 (94%)	110 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	338/359 (94%)	326 (96%)	12 (4%)	40	72
1	D	338/359 (94%)	327 (97%)	11 (3%)	43	73
2	B	335/379 (88%)	307 (92%)	28 (8%)	13	47
2	C	335/379 (88%)	308 (92%)	27 (8%)	14	48
2	E	335/379 (88%)	307 (92%)	28 (8%)	13	47
All	All	1681/1855 (91%)	1575 (94%)	106 (6%)	21	57

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	128	SER
2	C	298	HIS
2	E	295	ASN
2	C	151	TRP
2	C	236	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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$
3	NAG	A	401	1	14,14,15	1.87	6 (42%)	15,19,21	1.26	2 (13%)
4	NCT	A	402	-	13,13,13	1.03	0	17,17,17	1.34	2 (11%)
3	NAG	B	500	2	14,14,15	1.82	6 (42%)	15,19,21	2.62	3 (20%)
3	NAG	C	500	2	14,14,15	1.74	5 (35%)	15,19,21	2.41	2 (13%)
3	NAG	D	401	1	14,14,15	1.85	6 (42%)	15,19,21	1.57	3 (20%)
4	NCT	D	402	-	13,13,13	0.95	0	17,17,17	1.35	2 (11%)
3	NAG	E	500	2	14,14,15	1.79	5 (35%)	15,19,21	2.56	3 (20%)

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
3	NAG	A	401	1	-	0/6/23/26	0/1/1/1
4	NCT	A	402	-	-	0/4/14/14	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	500	2	-	0/6/23/26	0/1/1/1
3	NAG	C	500	2	-	0/6/23/26	0/1/1/1
3	NAG	D	401	1	-	0/6/23/26	0/1/1/1
4	NCT	D	402	-	-	0/4/14/14	0/2/2/2
3	NAG	E	500	2	-	0/6/23/26	0/1/1/1

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	NAG	O5-C1	-3.23	1.38	1.43
3	A	401	NAG	O5-C1	-3.20	1.38	1.43
3	B	500	NAG	O5-C1	-2.96	1.38	1.43
3	E	500	NAG	O5-C1	-2.82	1.39	1.43
3	D	401	NAG	O5-C5	-2.75	1.37	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	NCT	C10-N2-C6	-3.81	100.46	112.77
4	A	402	NCT	C10-N2-C6	-3.72	100.74	112.77
3	D	401	NAG	C3-C4-C5	-2.11	106.50	110.22
3	A	401	NAG	C3-C4-C5	-2.10	106.52	110.22
3	E	500	NAG	C6-C5-C4	-2.05	108.21	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	NCT	2	0
4	D	402	NCT	4	0

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 [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	363/386 (94%)	-0.08	12 (3%) 47 37	123, 157, 261, 293	0
1	D	363/386 (94%)	-0.15	12 (3%) 47 37	138, 168, 234, 263	0
2	B	358/403 (88%)	-0.19	13 (3%) 43 34	122, 150, 231, 260	0
2	C	358/403 (88%)	-0.16	6 (1%) 70 61	124, 152, 251, 274	0
2	E	358/403 (88%)	-0.06	12 (3%) 46 36	130, 165, 251, 285	0
All	All	1800/1981 (90%)	-0.13	55 (3%) 49 39	122, 160, 245, 293	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	381	TRP	8.4
1	A	381	TRP	6.3
2	E	192	ASP	5.4
1	D	200	CYS	5.1
2	E	193	ASP	4.8

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	NCT	A	402	12/12	0.84	0.72	2.80	144,144,144,144	0
3	NAG	C	500	14/15	0.83	0.47	1.57	136,136,136,136	0
4	NCT	D	402	12/12	0.72	0.38	-0.17	158,158,158,158	0
3	NAG	E	500	14/15	0.83	0.19	-0.47	159,159,159,159	0
3	NAG	B	500	14/15	0.92	0.13	-0.96	137,137,137,137	0
3	NAG	A	401	14/15	0.87	0.18	-	137,137,137,137	0
5	NA	A	403	1/1	0.92	0.38	-	84,84,84,84	0
3	NAG	D	401	14/15	0.88	0.32	-	153,153,153,153	0

6.5 Other polymers

There are no such residues in this entry.