



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:21 PM GMT

PDB ID : 2C11  
Title : CRYSTAL STRUCTURE OF THE 2-HYDRAZINOPYRIDINE OF SEMIC  
ARBAZIDE-SENSITIVEAMINE OXIDASE  
Authors : Jakobsson, E.; Kleywegt, G.J.  
Deposited on : 2005-09-09  
Resolution : 2.90 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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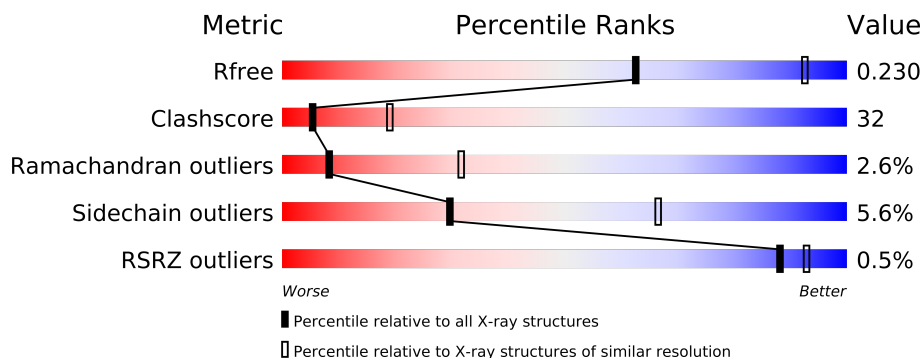
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	735	
1	B	735	
1	C	735	
1	D	735	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	D	1738	-	X
6	CU	A	1744	-	X
6	CU	B	1747	-	X
6	CU	B	1748	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21917 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MEMBRANE COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	1
			5340	3434	924	965	17			
1	B	672	Total	C	N	O	S	0	0	1
			5340	3434	924	965	17			
1	C	672	Total	C	N	O	S	0	0	1
			5340	3434	924	965	17			
1	D	672	Total	C	N	O	S	0	0	1
			5340	3434	924	965	17			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	A	2	Total	Ca	0	0
			2	2		
5	D	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Ca	0	0
			2	2		

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	8	Total	Cu	0	0
			8	8		
6	A	7	Total	Cu	0	0
			7	7		
6	D	7	Total	Cu	0	0
			7	7		
6	C	8	Total	Cu	0	0
			8	8		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Cl	0	0
			2	2		
7	D	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	3	Total	C	N	O	0	0
			39	22	2	15		
8	D	3	Total	C	N	O	0	0
			39	22	2	15		

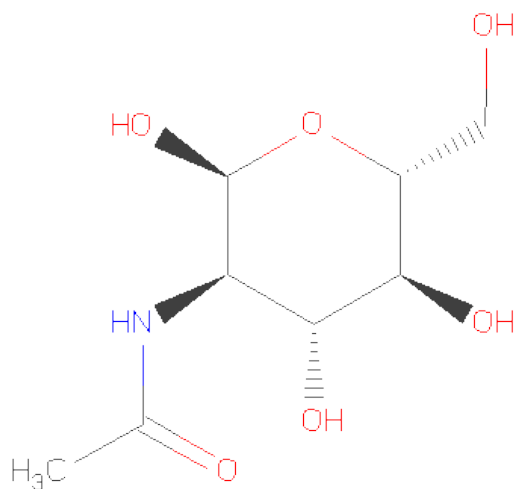
- Molecule 9 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	5	Total	C	N	O	0	0
			60	34	2	24		
9	D	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 11 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is water.

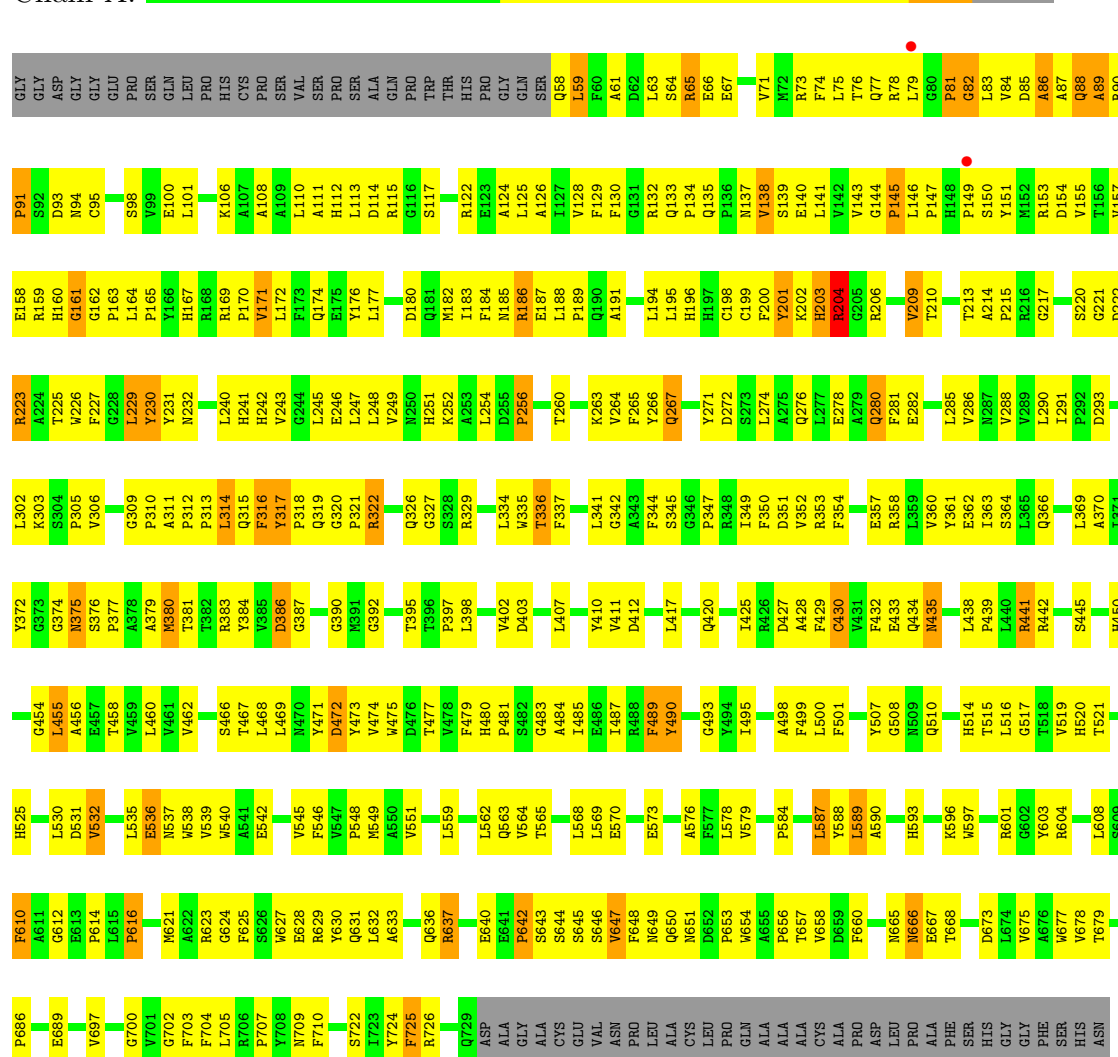
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	19	Total	O	0	0
			19	19		
12	B	20	Total	O	0	0
			20	20		
12	C	11	Total	O	0	0
			11	11		
12	D	9	Total	O	0	0
			9	9		

### 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 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 ( $RSRZ > 2$ ). 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.

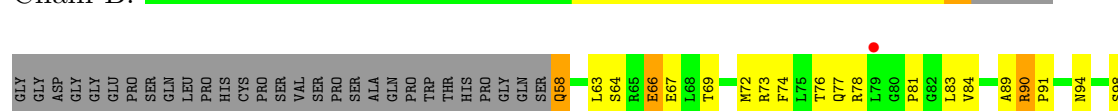
#### • Molecule 1: MEMBRANE COPPER AMINE OXIDASE

Chain A:



#### • Molecule 1: MEMBRANE COPPER AMINE OXIDASE

Chain B:









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.40Å 127.40Å 219.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 29.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-2.90) 90.7 (29.75-2.60)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.215 , 0.276 0.238 , 0.230	Depositor DCC
$R_{free}$ test set	4335 reflections (4.68%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.3	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 32.2	EDS
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 96971 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PAQ, BMA, NAG, CL, CA, NDG, FUL, CU, 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	0/5488	0.72	2/7481 (0.0%)
1	B	0.48	0/5488	0.72	1/7481 (0.0%)
1	C	0.49	0/5488	0.71	2/7481 (0.0%)
1	D	0.48	0/5488	0.72	1/7481 (0.0%)
All	All	0.49	0/21952	0.72	6/29924 (0.0%)

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	1	0
1	B	1	0
1	C	1	0
1	D	1	0
All	All	4	0

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	LEU	CA-CB-CG	7.19	131.83	115.30
1	D	373	GLY	N-CA-C	-6.13	97.78	113.10
1	B	373	GLY	N-CA-C	-5.95	98.23	113.10
1	C	204	ARG	N-CA-C	5.47	125.78	111.00
1	A	204	ARG	N-CA-C	5.24	125.15	111.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	471	PAQ	CG
1	B	471	PAQ	CG
1	C	471	PAQ	CG
1	D	471	PAQ	CG

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5340	0	5112	410	0
1	B	5340	0	5110	323	0
1	C	5340	0	5112	399	0
1	D	5340	0	5111	338	0
2	A	28	0	25	2	0
2	C	28	0	25	3	0
3	A	24	0	22	4	0
4	A	28	0	26	4	0
4	B	42	0	39	3	0
4	C	28	0	26	2	0
4	D	28	0	26	2	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	7	0	0	0	0
6	B	8	0	0	0	0
6	C	8	0	0	0	0
6	D	7	0	0	0	0
7	A	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	39	0	34	1	0
8	D	39	0	34	5	0
9	B	60	0	52	3	0
9	D	60	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	38	0	34	5	0
11	D	14	0	13	0	0
12	A	19	0	0	5	0
12	B	20	0	0	5	0
12	C	11	0	0	5	0
12	D	9	0	0	4	0
All	All	21917	0	20853	1388	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

The worst 5 of 1388 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:360:VAL:HG11	1:B:363:ILE:HG13	1.37	1.04
1:C:90:ARG:HG2	1:C:91:PRO:HD2	1.42	1.02
1:B:106:LYS:HB2	1:B:637:ARG:HH21	1.27	0.99
1:A:90:ARG:HG2	1:A:91:PRO:HD2	1.43	0.96
1:A:344:PHE:HA	1:A:390:GLY:HA2	1.45	0.95

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	669/735 (91%)	571 (85%)	72 (11%)	26 (4%)	5	18
1	B	669/735 (91%)	585 (87%)	76 (11%)	8 (1%)	19	57
1	C	669/735 (91%)	575 (86%)	69 (10%)	25 (4%)	5	20
1	D	669/735 (91%)	587 (88%)	71 (11%)	11 (2%)	14	47
All	All	2676/2940 (91%)	2318 (87%)	288 (11%)	70 (3%)	8	32

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	MET
1	A	637	ARG
1	B	267	GLN
1	B	386	ASP
1	B	596	LYS

### 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	562/609 (92%)	523 (93%)	39 (7%)	22	54
1	B	562/609 (92%)	538 (96%)	24 (4%)	40	78
1	C	562/609 (92%)	527 (94%)	35 (6%)	26	61
1	D	562/609 (92%)	535 (95%)	27 (5%)	35	74
All	All	2248/2436 (92%)	2123 (94%)	125 (6%)	30	66

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	515	THR
1	C	203	HIS
1	D	513	GLU
1	B	528	VAL
1	C	88	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	510	GLN
1	C	219	GLN
1	D	420	GLN
1	B	560	GLN
1	C	160	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	PAQ	A	471	1	22,22,23	4.20	6 (27%)	26,29,31	2.26	7 (26%)
1	PAQ	B	471	1	22,22,23	4.17	7 (31%)	26,29,31	2.29	8 (30%)
1	PAQ	C	471	1	22,22,23	4.14	6 (27%)	26,29,31	2.29	7 (26%)
1	PAQ	D	471	1	22,22,23	3.99	6 (27%)	26,29,31	2.24	7 (26%)

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
1	PAQ	A	471	1	1/1/5/10	0/7/27/29	0/2/2/2
1	PAQ	B	471	1	1/1/5/10	0/7/27/29	0/2/2/2
1	PAQ	C	471	1	1/1/5/10	0/7/27/29	0/2/2/2
1	PAQ	D	471	1	1/1/5/10	0/7/27/29	0/2/2/2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	PAQ	O-C	18.07	1.23	1.11
1	B	471	PAQ	O-C	17.90	1.23	1.11
1	C	471	PAQ	O-C	17.68	1.23	1.11
1	D	471	PAQ	O-C	16.97	1.23	1.11
1	A	471	PAQ	CG-CD2	-4.85	1.39	1.50

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	471	PAQ	CD2-CG-CD1	5.59	119.02	104.68
1	B	471	PAQ	CD2-CG-CD1	5.59	119.01	104.68
1	A	471	PAQ	CD2-CG-CD1	5.55	118.92	104.68
1	C	471	PAQ	CD2-CG-CD1	5.53	118.86	104.68
1	C	471	PAQ	CD2-CE2-N1	-5.18	117.45	125.58

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	471	PAQ	CG
1	A	471	PAQ	CG
1	D	471	PAQ	CG
1	C	471	PAQ	CG

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

25 carbohydrates 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	1730	1,2	12,14,15	0.52	0	15,19,21	1.19	1 (6%)
2	NAG	A	1731	2	12,14,15	0.52	0	15,19,21	0.87	1 (6%)
3	NAG	A	1732	1,3	12,14,15	0.51	0	15,19,21	1.06	1 (6%)
3	FUL	A	1733	3	9,10,11	0.53	0	10,14,16	0.65	0
8	NAG	B	1730	1,8	12,14,15	0.70	0	15,19,21	0.83	1 (6%)
8	NAG	B	1731	8	12,14,15	0.93	0	15,19,21	0.88	1 (6%)
9	NDG	B	1732	1,9	12,14,15	0.62	0	15,19,21	1.48	3 (20%)
9	NAG	B	1733	9	12,14,15	0.64	0	15,19,21	0.76	0
9	FUL	B	1734	9	9,10,11	0.68	0	10,14,16	0.67	0
8	BMA	B	1737	8	10,11,12	0.54	0	11,15,17	0.48	0
9	BMA	B	1739	9	10,11,12	0.72	0	11,15,17	0.44	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	B	1740	9	10,11,12	0.49	0	11,15,17	0.32	0
2	NAG	C	1730	1,2	12,14,15	0.57	0	15,19,21	0.75	0
2	NAG	C	1731	2	12,14,15	0.50	0	15,19,21	0.91	1 (6%)
10	NAG	C	1732	1,10	12,14,15	0.53	0	15,19,21	1.05	2 (13%)
10	NAG	C	1733	10	12,14,15	0.45	0	15,19,21	0.68	0
10	FUL	C	1734	10	9,10,11	0.44	0	10,14,16	0.60	0
8	NAG	D	1730	1,8	12,14,15	0.56	0	15,19,21	0.64	0
8	NAG	D	1731	8	12,14,15	0.73	0	15,19,21	0.63	0
9	NDG	D	1732	1,9	12,14,15	0.66	0	15,19,21	1.08	1 (6%)
9	NAG	D	1733	9	12,14,15	0.63	0	15,19,21	0.74	0
9	FUL	D	1734	9	9,10,11	0.66	0	10,14,16	0.58	0
8	BMA	D	1737	8	10,11,12	0.52	0	11,15,17	0.42	0
9	BMA	D	1739	9	10,11,12	0.85	0	11,15,17	0.45	0
9	MAN	D	1740	9	10,11,12	0.65	0	11,15,17	0.33	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	1730	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1731	2	-	1/6/23/26	0/1/1/1
3	NAG	A	1732	1,3	-	0/6/23/26	0/1/1/1
3	FUL	A	1733	3	-	0/0/17/20	1/1/1/1
8	NAG	B	1730	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1731	8	-	0/6/23/26	0/1/1/1
9	NDG	B	1732	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	1733	9	-	0/6/23/26	0/1/1/1
9	FUL	B	1734	9	-	0/0/17/20	0/1/1/1
8	BMA	B	1737	8	-	0/2/19/22	0/1/1/1
9	BMA	B	1739	9	-	0/2/19/22	0/1/1/1
9	MAN	B	1740	9	-	0/2/19/22	0/1/1/1
2	NAG	C	1730	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1731	2	-	0/6/23/26	0/1/1/1
10	NAG	C	1732	1,10	-	0/6/23/26	0/1/1/1
10	NAG	C	1733	10	-	0/6/23/26	0/1/1/1
10	FUL	C	1734	10	-	0/0/17/20	0/1/1/1
8	NAG	D	1730	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	1731	8	-	0/6/23/26	0/1/1/1
9	NDG	D	1732	1,9	-	0/6/23/26	0/1/1/1
9	NAG	D	1733	9	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FUL	D	1734	9	-	0/0/17/20	0/1/1/1
8	BMA	D	1737	8	-	0/2/19/22	0/1/1/1
9	BMA	D	1739	9	-	0/2/19/22	0/1/1/1
9	MAN	D	1740	9	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1730	NAG	C3-C2-N2	-3.22	106.86	111.76
9	B	1732	NDG	C3-C4-C5	-3.20	104.49	110.20
9	B	1732	NDG	C4-C3-C2	-2.59	104.97	111.32
9	D	1732	NDG	C3-C4-C5	-2.57	105.61	110.20
8	B	1731	NAG	C2-N2-C7	-2.33	119.18	123.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1731	NAG	C1-C2-N2-C7
9	D	1733	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1733	FUL	C1-C2-C3-C4-C5-O5

## 5.6 Ligand geometry

Of 52 ligands modelled in this entry, 42 are monoatomic - leaving 10 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
4	NAG	A	1734	1	12,14,15	0.34	0	15,19,21	0.86	1 (6%)
4	NAG	A	1735	1	12,14,15	0.56	0	15,19,21	0.66	0
4	NAG	B	1735	1	12,14,15	0.70	0	15,19,21	0.77	0
4	NAG	B	1736	1	12,14,15	0.47	0	15,19,21	0.75	0
4	NAG	B	1738	1	12,14,15	0.53	0	15,19,21	0.73	0
4	NAG	C	1735	1	12,14,15	0.52	0	15,19,21	0.68	0
4	NAG	C	1736	1	12,14,15	0.47	0	15,19,21	0.90	1 (6%)
4	NAG	D	1735	1	12,14,15	0.63	0	15,19,21	0.69	0
11	NDG	D	1736	1	12,14,15	0.53	0	15,19,21	0.71	0
4	NAG	D	1738	1	12,14,15	0.59	0	15,19,21	0.92	1 (6%)

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
4	NAG	A	1734	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1735	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1735	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1736	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1738	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1735	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1736	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1735	1	-	0/6/23/26	0/1/1/1
11	NDG	D	1736	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1738	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1736	NAG	C3-C2-N2	-2.26	108.33	111.76
4	A	1734	NAG	C3-C2-N2	-2.18	108.43	111.76
4	D	1738	NAG	C3-C2-N2	-2.13	108.52	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	672/735 (91%)	-0.17	2 (0%) 91 95	43, 64, 79, 87	0
1	B	672/735 (91%)	-0.19	3 (0%) 90 94	41, 60, 75, 81	0
1	C	672/735 (91%)	-0.22	2 (0%) 91 95	43, 64, 79, 88	0
1	D	672/735 (91%)	-0.30	2 (0%) 91 95	41, 60, 75, 81	0
All	All	2688/2940 (91%)	-0.22	9 (0%) 88 95	41, 62, 77, 88	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	161	GLY	4.0
1	B	79	LEU	3.6
1	D	203	HIS	2.7
1	D	286	VAL	2.4
1	A	149	PRO	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	PAQ	B	471	21/22	0.35	3.97	55,59,61,61	0
1	PAQ	D	471	21/22	0.28	3.41	54,59,60,61	0
1	PAQ	A	471	21/22	0.28	2.60	56,59,60,63	0
1	PAQ	C	471	21/22	0.24	1.87	56,59,61,61	0

### 6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	FUL	B	1734	10/11	0.21	7.56	91,93,94,95	0
3	NAG	A	1732	14/15	0.18	3.92	80,81,83,85	0
9	FUL	D	1734	10/11	0.25	1.69	84,85,86,86	0
2	NAG	A	1730	14/15	0.18	0.07	75,77,80,84	0
9	NDG	B	1732	14/15	0.15	0.04	82,86,91,93	0
8	NAG	B	1730	14/15	0.18	-0.10	72,75,77,80	0
8	NAG	D	1731	14/15	0.17	-0.13	83,85,87,89	0
10	FUL	C	1734	10/11	0.16	-0.17	82,83,84,84	0
9	MAN	B	1740	11/12	0.20	-0.39	96,98,99,99	0
10	NAG	C	1732	14/15	0.15	-0.46	80,83,86,89	0
9	NDG	D	1732	14/15	0.13	-0.55	76,79,84,88	0
2	NAG	A	1731	14/15	0.15	-0.69	88,91,92,92	0
8	NAG	D	1730	14/15	0.16	-0.79	75,76,78,81	0
9	MAN	D	1740	11/12	0.16	-1.09	96,98,98,98	0
3	FUL	A	1733	10/11	0.12	-1.24	78,79,80,80	0
8	NAG	B	1731	14/15	0.13	-1.79	85,86,89,92	0
2	NAG	C	1730	14/15	0.12	-1.97	74,75,77,80	0
2	NAG	C	1731	14/15	0.15	-3.94	82,84,85,85	0
9	BMA	D	1739	11/12	0.11	-6.00	97,98,98,98	0
10	NAG	C	1733	14/15	0.20	-	91,92,93,93	0
9	NAG	B	1733	14/15	0.11	-	95,97,98,98	0
9	BMA	B	1739	11/12	0.10	-	97,97,98,98	0
9	NAG	D	1733	14/15	0.23	-	92,95,96,97	0
8	BMA	D	1737	11/12	0.15	-	89,90,91,91	0
8	BMA	B	1737	11/12	0.11	-	94,94,95,95	0

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CU	A	1744	1/1	0.24	5.45	74,74,74,74	0
6	CU	B	1748	1/1	0.19	2.68	66,66,66,66	0
4	NAG	D	1738	14/15	0.18	2.37	81,83,85,85	0
6	CU	B	1747	1/1	0.15	2.33	81,81,81,81	0
4	NAG	A	1735	14/15	0.16	1.74	84,86,88,89	0
6	CU	B	1750	1/1	0.20	0.87	63,63,63,63	0
6	CU	A	1737	1/1	0.20	0.72	49,49,49,49	0
6	CU	B	1742	1/1	0.20	0.64	55,55,55,55	0
4	NAG	C	1736	14/15	0.14	0.50	82,85,88,88	0
5	CA	B	1743	1/1	0.18	0.35	47,47,47,47	0
4	NAG	B	1735	14/15	0.19	0.31	69,70,73,73	0
6	CU	A	1743	1/1	0.18	0.14	84,84,84,84	0
4	NAG	B	1738	14/15	0.14	0.14	81,83,84,85	0
6	CU	D	1749	1/1	0.17	0.02	67,67,67,67	0
6	CU	A	1745	1/1	0.14	-0.18	80,80,80,80	0
6	CU	C	1738	1/1	0.15	-0.28	49,49,49,49	0
6	CU	D	1742	1/1	0.15	-0.33	52,52,52,52	0
6	CU	B	1745	1/1	0.14	-0.54	75,75,75,75	0
4	NAG	C	1735	14/15	0.17	-0.59	70,72,73,74	0
11	NDG	D	1736	14/15	0.13	-0.65	83,84,86,86	0
6	CU	D	1748	1/1	0.13	-0.69	74,74,74,74	0
4	NAG	D	1735	14/15	0.14	-0.76	71,74,76,77	0
5	CA	A	1736	1/1	0.15	-0.84	52,52,52,52	0
4	NAG	A	1734	14/15	0.14	-0.90	71,73,74,74	0
5	CA	C	1739	1/1	0.12	-0.93	50,50,50,50	0
5	CA	D	1743	1/1	0.13	-0.99	46,46,46,46	0
4	NAG	B	1736	14/15	0.10	-1.01	84,86,88,88	0
6	CU	A	1742	1/1	0.13	-1.12	77,77,77,77	0
6	CU	C	1744	1/1	0.13	-1.15	90,90,90,90	0
6	CU	A	1741	1/1	0.10	-1.19	83,83,83,83	0
5	CA	B	1741	1/1	0.13	-1.20	46,46,46,46	0
6	CU	C	1747	1/1	0.10	-1.21	84,84,84,84	0
6	CU	C	1745	1/1	0.13	-1.30	77,77,77,77	0
6	CU	C	1743	1/1	0.13	-1.31	73,73,73,73	0
5	CA	A	1738	1/1	0.11	-1.32	49,49,49,49	0
6	CU	D	1746	1/1	0.11	-1.34	78,78,78,78	0
5	CA	C	1737	1/1	0.11	-1.34	50,50,50,50	0
7	CL	A	1746	1/1	0.10	-1.41	47,47,47,47	0
6	CU	C	1741	1/1	0.12	-1.53	79,79,79,79	0
7	CL	D	1744	1/1	0.09	-1.63	45,45,45,45	0
6	CU	B	1749	1/1	0.10	-1.64	69,69,69,69	0
5	CA	D	1741	1/1	0.11	-1.65	47,47,47,47	0
6	CU	D	1745	1/1	0.12	-1.67	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CL	A	1739	1/1	0.07	-2.10	47,47,47,47	0
6	CU	C	1742	1/1	0.08	-2.16	84,84,84,84	0
7	CL	C	1740	1/1	0.10	-2.35	49,49,49,49	0
6	CU	D	1750	1/1	0.10	-2.82	67,67,67,67	0
6	CU	B	1746	1/1	0.10	-3.76	71,71,71,71	0
6	CU	D	1747	1/1	0.06	-212.84	82,82,82,82	0
6	CU	A	1740	1/1	0.18	-	81,81,81,81	0
6	CU	C	1746	1/1	0.09	-	67,67,67,67	0
6	CU	B	1744	1/1	0.20	-	76,76,76,76	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.