



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:32 PM GMT

PDB ID : 1KSI
Title : CRYSTAL STRUCTURE OF A EUKARYOTIC (PEA SEEDLING)
COPPER-CONTAINING AMINE OXIDASE AT 2.2Å RESOLUTION
Authors : Wilce, M.C.J.; Kumar, V.; Freeman, H.C.; Guss, J.M.
Deposited on : 1996-07-20
Resolution : 2.20 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

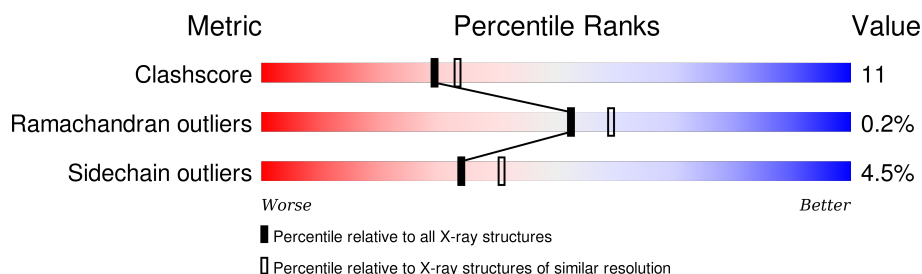
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	642	
1	B	642	

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
2	NAG	A	655	X	-	X	-
2	NAG	A	656	X	-	X	-
2	NAG	A	657	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	655	X	-	-	-
2	NAG	B	656	X	-	-	-
2	NAG	B	657	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10995 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.

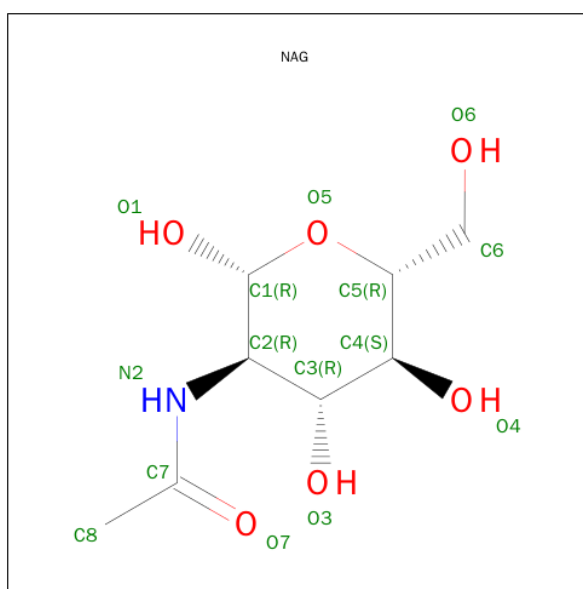
- Molecule 1 is a protein called COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	10	1	0
			5168	3319	877	961	11			
1	B	642	Total	C	N	O	S	12	1	0
			5168	3319	877	961	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	TPQ	TYR	MODIFIED RESIDUE	UNP Q43077
B	387	TPQ	TYR	MODIFIED RESIDUE	UNP Q43077

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cu	0	0
			1	1		
3	A	1	Total	Cu	0	0
			1	1		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is water.

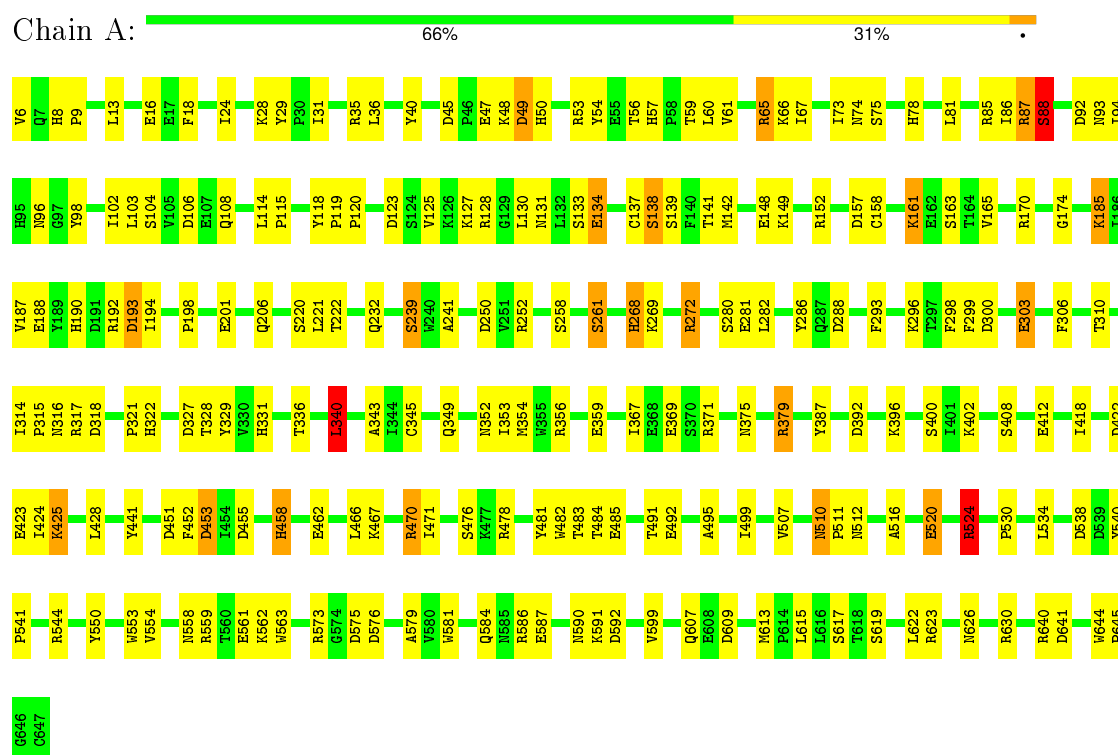
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	280	Total	O	0	0
			280	280		
5	B	291	Total	O	0	0
			291	291		

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.

Note EDS was not executed.

• Molecule 1: COPPER AMINE OXIDASE



D539	Y540	P541	Q542	I543	R544	V552	N558	R559	T560	E561	K562	D570	R573	G574	D575	W581	R586	V589	N590	H602	Q607	E608	M613	P614	L615	I616	S617	T618	S619	F620	E621	L622	R623	P624	E629	R630	K635	R640	D641	W644	P645	G646	C647
I418	K421	D422	E423	T424	K425	D427	Y441	H442	D443	Y446	D453	T454	D455	H458	T464	S465	R470	D473	R478	W482	K490	T491	D494	T497	T498	I499	G500	L501	A502	P503	A504	V507	K514	R524	P530	L534	L535	D538					

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.37Å 114.64Å 199.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	86.5 (7.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10995	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MN, TPQ, CU, 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	0.80	1/5297 (0.0%)	1.75	102/7211 (1.4%)
1	B	0.82	4/5297 (0.1%)	1.68	91/7211 (1.3%)
All	All	0.81	5/10594 (0.0%)	1.72	193/14422 (1.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	640	ARG	NE-CZ	10.87	1.47	1.33
1	B	148	GLU	CA-CB	7.35	1.70	1.53
1	B	640	ARG	CD-NE	6.34	1.57	1.46
1	B	148	GLU	CD-OE2	5.17	1.31	1.25
1	A	258	SER	CA-CB	5.14	1.60	1.52

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ARG	CD-NE-CZ	20.12	151.76	123.60
1	A	317	ARG	NE-CZ-NH1	19.41	130.01	120.30
1	A	478	ARG	NE-CZ-NH1	17.62	129.11	120.30
1	A	575	ASP	CB-CG-OD1	16.53	133.17	118.30
1	A	478	ARG	NE-CZ-NH2	-16.32	112.14	120.30

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	5168	0	5085	119	1
1	B	5168	0	5085	102	1
2	A	42	0	39	32	0
2	B	42	0	38	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	280	0	0	7	0
5	B	291	0	0	6	0
All	All	10995	0	10247	226	1

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 11.

The worst 5 of 226 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:558:ASN:HD21	2:A:657:NAG:C1	1.07	1.58
1:B:558:ASN:HD21	2:B:657:NAG:C1	1.27	1.45
1:A:558:ASN:HD21	2:A:657:NAG:C2	1.34	1.41
1:A:558:ASN:ND2	2:A:657:NAG:H2	1.40	1.36
1:B:558:ASN:HD21	2:B:657:NAG:C2	1.47	1.25

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:HIS:NE2	1:B:640:ARG:NH1[4_455]	1.95	0.25

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	640/642 (100%)	612 (96%)	28 (4%)	0	100	100
1	B	640/642 (100%)	605 (94%)	33 (5%)	2 (0%)	46	50
All	All	1280/1284 (100%)	1217 (95%)	61 (5%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	473	ASP
1	B	502	ALA

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	576/575 (100%)	552 (96%)	24 (4%)	36	44
1	B	576/575 (100%)	548 (95%)	28 (5%)	31	36
All	All	1152/1150 (100%)	1100 (96%)	52 (4%)	34	41

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	613	MET
1	B	87	ARG
1	B	524	ARG
1	B	47	GLU
1	B	56	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	549	ASN

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Mol	Chain	Res	Type
1	A	558	ASN
1	B	360	ASN
1	A	542	GLN
1	B	542	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	TPQ	A	387	1	13,14,15	2.47	5 (38%)	15,19,21	2.78	8 (53%)
1	TPQ	B	387	1	13,14,15	2.57	5 (38%)	15,19,21	2.55	5 (33%)

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	TPQ	A	387	1	-	0/4/22/24	0/1/1/1
1	TPQ	B	387	1	-	0/4/22/24	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	387	TPQ	C1-C2	-6.09	1.41	1.49
1	A	387	TPQ	C1-C2	-5.36	1.42	1.49
1	B	387	TPQ	C6-C1	2.35	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	TPQ	C6-C1	2.35	1.40	1.34
1	B	387	TPQ	C3-C4	2.61	1.39	1.35

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	TPQ	C1-C6-C5	-7.20	118.58	122.97
1	A	387	TPQ	C1-C6-C5	-6.36	119.09	122.97
1	A	387	TPQ	O-C-CA	-4.08	114.87	125.49
1	B	387	TPQ	O-C-CA	-3.67	115.92	125.49
1	A	387	TPQ	C4-C3-C2	-2.44	117.66	120.77

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
1	A	387	TPQ	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	655	1,2	14,14,15	1.30	1 (7%)	15,19,21	2.15	4 (26%)
2	NAG	A	656	2	14,14,15	1.30	1 (7%)	15,19,21	2.16	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	657	1	14,14,15	1.30	1 (7%)	15,19,21	2.15	4 (26%)
2	NAG	B	655	1,2	14,14,15	1.53	3 (21%)	15,19,21	1.45	2 (13%)
2	NAG	B	656	2	14,14,15	1.17	2 (14%)	15,19,21	1.04	1 (6%)
2	NAG	B	657	1	14,14,15	1.29	1 (7%)	15,19,21	2.15	4 (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
2	NAG	A	655	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	656	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	657	1	-	0/6/23/26	0/1/1/1
2	NAG	B	655	1,2	2/2/5/7	0/6/23/26	0/1/1/1
2	NAG	B	656	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	657	1	-	0/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	656	NAG	O7-C7	-3.17	1.15	1.23
2	A	657	NAG	O7-C7	-3.17	1.15	1.23
2	A	655	NAG	O7-C7	-3.17	1.15	1.23
2	B	657	NAG	O7-C7	-3.17	1.15	1.23
2	B	656	NAG	O5-C1	-2.04	1.40	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	656	NAG	C4-C3-C2	-3.99	105.02	111.23
2	B	657	NAG	C4-C3-C2	-3.98	105.04	111.23
2	A	655	NAG	C4-C3-C2	-3.98	105.05	111.23
2	A	657	NAG	C4-C3-C2	-3.97	105.06	111.23
2	A	657	NAG	C3-C4-C5	-3.71	103.74	110.20

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	655	NAG	C1
2	B	655	NAG	C2

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Mol	Chain	Res	Type	Atom
2	B	656	NAG	C1
2	A	656	NAG	C1
2	A	655	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	655	NAG	19	0
2	A	656	NAG	19	0
2	A	657	NAG	13	0
2	B	655	NAG	2	0
2	B	657	NAG	10	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.