



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:48 PM GMT

PDB ID : 1QPA
Title : LIGNIN PEROXIDASE ISOZYME LIP4.65 (PI 4.65)
Authors : Choinowski, T.H.; Piontek, K.
Deposited on : 1996-10-08
Resolution : 1.80 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) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

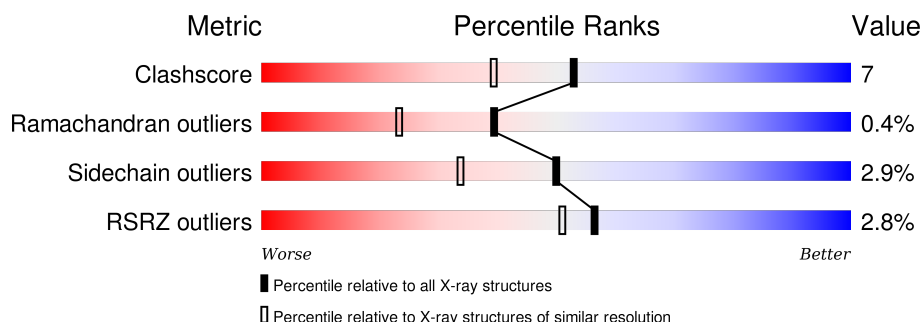
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	345	<div> <div>2%</div> <div>77%</div> <div>19%</div> <div>...</div> </div>
1	B	345	<div> <div>4%</div> <div>80%</div> <div>17%</div> <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
3	MAN	A	370	-	-	-	X
3	MAN	B	370	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FUC	B	365	X	-	X	-
5	MAN	B	386	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5821 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.

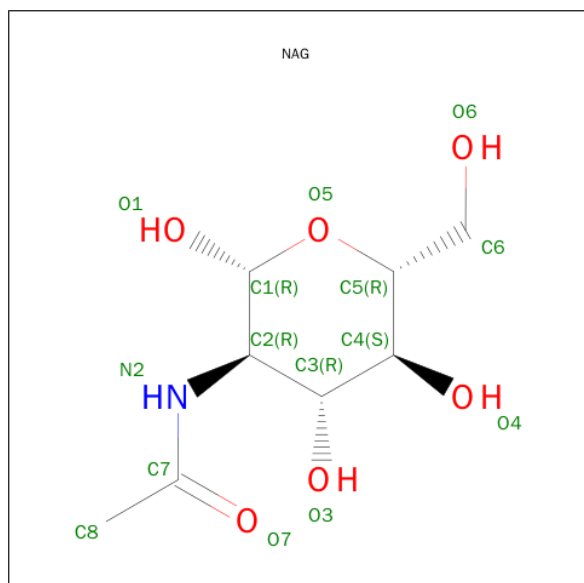
- Molecule 1 is a protein called LIGNIN PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2569	1630	432	492	15			
1	B	344	Total	C	N	O	S	0	0	0
			2569	1630	432	492	15			

There are 6 discrepancies between the modelled and reference sequences:

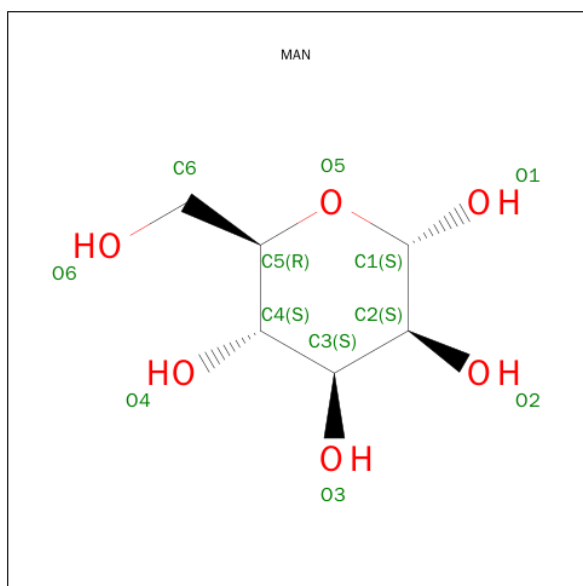
Chain	Residue	Modelled	Actual	Comment	Reference
A	105	PRO	ARG	CONFLICT	UNP P11542
A	171	HTR	TRP	MODIFIED RESIDUE	UNP P11542
A	283	ILE	THR	CONFLICT	UNP P11542
B	105	PRO	ARG	CONFLICT	UNP P11542
B	171	HTR	TRP	MODIFIED RESIDUE	UNP P11542
B	283	ILE	THR	CONFLICT	UNP P11542

- 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		

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



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

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

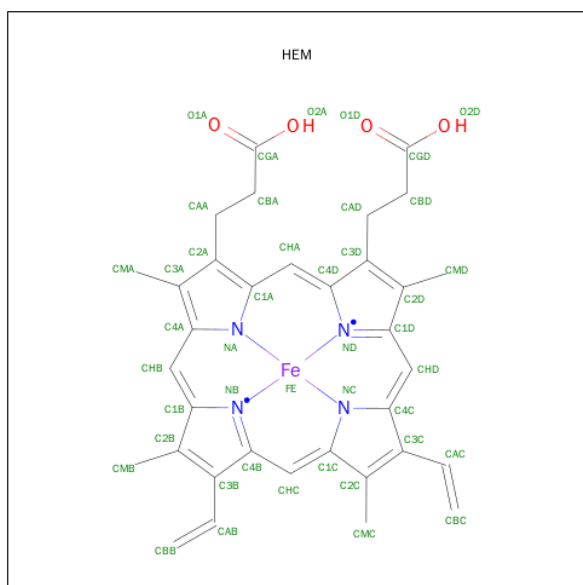
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	2	Total	C	O	0	0
			22	12	10		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
7	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

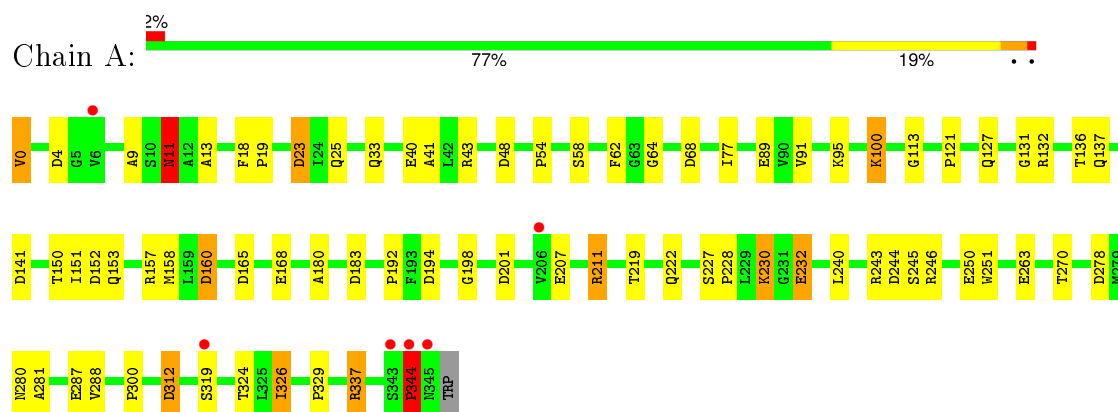
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	267	Total O 267 267	0	0
8	B	197	Total O 197 197	0	0

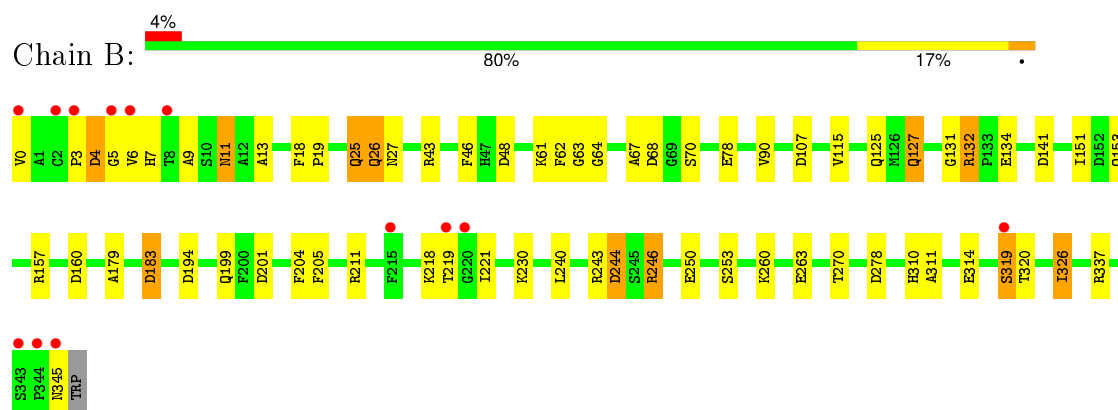
3 Residue-property plots

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: LIGNIN PEROXIDASE



• Molecule 1: LIGNIN PEROXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.79Å 94.02Å 81.26Å 90.00° 106.47° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 24.70 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.80) 96.1 (24.70-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 1.80Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	(Not available) , (Not available) 0.163 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 84.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 74081 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5821	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NAG, CA, HTR, FUC, HEM, 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	0.98	1/2625 (0.0%)	1.93	64/3581 (1.8%)
1	B	0.87	2/2625 (0.1%)	1.99	53/3581 (1.5%)
All	All	0.92	3/5250 (0.1%)	1.96	117/7162 (1.6%)

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
4	B	1	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ASN	CG-OD1	5.69	1.36	1.24
1	B	153	GLN	CD-OE1	5.51	1.36	1.24
1	B	26	GLN	CD-OE1	5.25	1.35	1.24

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	ARG	NE-CZ-NH1	41.65	141.12	120.30
1	B	337	ARG	CD-NE-CZ	23.20	156.09	123.60
1	A	160	ASP	CB-CG-OD2	19.84	136.16	118.30
1	B	246	ARG	NE-CZ-NH2	-18.94	110.83	120.30
1	A	246	ARG	NE-CZ-NH2	18.63	129.62	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	365	FUC	C1

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	2569	0	2448	27	0
1	B	2569	0	2447	33	0
2	A	14	0	13	0	0
3	A	22	0	20	0	0
3	B	33	0	30	5	0
4	B	38	0	34	7	0
5	B	22	0	19	4	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	43	0	30	4	0
7	B	43	0	30	4	0
8	A	267	0	0	3	0
8	B	197	0	0	1	0
All	All	5821	0	5071	69	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 7.

The worst 5 of 69 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:11:ASN:HD22	1:A:13:ALA:H	0.99	0.93
1:B:260:LYS:HE3	4:B:365:FUC:H2	1.54	0.90
1:B:4:ASP:HB3	1:B:6:VAL:H	1.36	0.89
1:B:211:ARG:HB2	1:B:211:ARG:NH1	1.95	0.82
1:B:4:ASP:OD2	1:B:7:HIS:ND1	2.12	0.81

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	341/345 (99%)	332 (97%)	7 (2%)	2 (1%)	30	14
1	B	341/345 (99%)	326 (96%)	14 (4%)	1 (0%)	46	29
All	All	682/690 (99%)	658 (96%)	21 (3%)	3 (0%)	39	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	PRO
1	A	131	GLY
1	B	131	GLY

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	274/275 (100%)	266 (97%)	8 (3%)	50	34
1	B	274/275 (100%)	266 (97%)	8 (3%)	50	34
All	All	548/550 (100%)	532 (97%)	16 (3%)	50	34

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	PRO
1	B	11	ASN
1	B	230	LYS

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Mol	Chain	Res	Type
1	A	337	ARG
1	B	319	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	11	ASN
1	B	25	GLN
1	B	127	GLN
1	A	127	GLN
1	B	119	ASN

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	HTR	A	171	1	15,16,17	1.46	1 (6%)	12,22,24	2.11	5 (41%)
1	HTR	B	171	1	15,16,17	1.17	1 (6%)	12,22,24	1.81	4 (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	HTR	A	171	1	-	0/4/10/12	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HTR	B	171	1	-	0/4/10/12	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	HTR	OH-CB	2.18	1.47	1.42
1	A	171	HTR	CG-CD2	4.00	1.45	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	HTR	O-C-CA	-3.22	116.93	125.44
1	A	171	HTR	CH2-CZ2-CE2	-3.09	115.11	120.06
1	B	171	HTR	O-C-CA	-2.67	118.39	125.44
1	B	171	HTR	CH2-CZ2-CE2	-2.19	116.56	120.06
1	B	171	HTR	OH-CB-CG	2.26	114.50	110.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

5 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
4	NAG	B	360	1,4	14,14,15	1.34	2 (14%)	15,19,21	3.64	6 (40%)
4	NAG	B	361	4	14,14,15	1.18	1 (7%)	15,19,21	3.01	9 (60%)
4	FUC	B	365	4	10,10,11	1.16	0	14,14,16	2.57	4 (28%)
5	MAN	B	385	1,5	11,11,12	0.70	0	14,15,17	2.48	6 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	B	386	5	11,11,12	0.83	1 (9%)	14,15,17	1.92	4 (28%)

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	B	360	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	361	4	-	0/6/23/26	0/1/1/1
4	FUC	B	365	4	1/1/4/5	0/0/17/20	0/1/1/1
5	MAN	B	385	1,5	-	0/2/19/22	0/1/1/1
5	MAN	B	386	5	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	360	NAG	O7-C7	-3.03	1.16	1.23
4	B	361	NAG	O7-C7	-2.79	1.16	1.23
4	B	360	NAG	O6-C6	-2.38	1.32	1.42
5	B	386	MAN	C1-C2	2.16	1.57	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	360	NAG	C4-C3-C2	-6.56	101.04	111.23
4	B	361	NAG	C1-O5-C5	-6.07	104.55	112.25
4	B	365	FUC	C1-O5-C5	-4.95	104.73	112.38
5	B	385	MAN	O4-C4-C3	-3.87	101.61	110.34
4	B	361	NAG	C4-C3-C2	-3.77	105.37	111.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	365	FUC	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	365	FUC	7	0
5	B	386	MAN	4	0

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
7	HEM	A	350	1,8	30,50,50	3.14	9 (30%)	24,82,82	3.25	12 (50%)
2	NAG	A	360	1	14,14,15	0.98	1 (7%)	15,19,21	2.00	4 (26%)
3	MAN	A	370	1	11,11,12	1.17	1 (9%)	14,15,17	2.42	7 (50%)
3	MAN	A	375	1	11,11,12	1.10	2 (18%)	14,15,17	2.36	6 (42%)
7	HEM	B	350	1,8	30,50,50	2.51	9 (30%)	24,82,82	3.05	13 (54%)
3	MAN	B	370	1	11,11,12	1.16	1 (9%)	14,15,17	1.72	2 (14%)
3	MAN	B	375	1	11,11,12	1.08	1 (9%)	14,15,17	2.52	6 (42%)
3	MAN	B	380	1	11,11,12	0.88	0	14,15,17	1.45	1 (7%)

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
7	HEM	A	350	1,8	-	0/10/54/54	0/0/8/8
2	NAG	A	360	1	-	0/6/23/26	0/1/1/1
3	MAN	A	370	1	-	0/2/19/22	0/1/1/1
3	MAN	A	375	1	-	0/2/19/22	0/1/1/1
7	HEM	B	350	1,8	-	0/10/54/54	0/0/8/8
3	MAN	B	370	1	-	0/2/19/22	0/1/1/1
3	MAN	B	375	1	-	0/2/19/22	0/1/1/1
3	MAN	B	380	1	-	0/2/19/22	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	350	HEM	C3B-C4B	-9.36	1.43	1.51
7	B	350	HEM	C3B-C4B	-7.19	1.45	1.51
7	B	350	HEM	C2D-C3D	-7.04	1.33	1.54
7	A	350	HEM	C2D-C3D	-6.53	1.34	1.54
7	A	350	HEM	C2C-C1C	-6.04	1.41	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	375	MAN	O3-C3-C2	-5.45	100.15	110.00
7	A	350	HEM	C3B-CAB-CBB	-4.79	117.11	124.46
7	B	350	HEM	C1D-CHD-C4C	-4.78	117.83	125.82
7	B	350	HEM	C3B-CAB-CBB	-4.21	118.00	124.46
7	B	350	HEM	CMA-C3A-C4A	-3.50	122.57	128.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	350	HEM	4	0
7	B	350	HEM	4	0
3	B	380	MAN	5	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 [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	343/345 (99%)	-0.35	6 (1%) 73 69	10, 18, 33, 91	0
1	B	343/345 (99%)	-0.06	13 (3%) 44 38	12, 22, 45, 97	0
All	All	686/690 (99%)	-0.21	19 (2%) 56 51	10, 20, 38, 97	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	ASN	9.4
1	A	344	PRO	9.3
1	B	345	ASN	8.1
1	B	343	SER	6.4
1	A	343	SER	5.6

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	HTR	B	171	15/16	0.95	0.07	-	14,15,17,17	0
1	HTR	A	171	15/16	0.98	0.04	-	14,16,16,16	0

6.3 Carbohydrates [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
5	MAN	B	386	11/12	0.69	0.51	31.85	68,71,72,72	0
5	MAN	B	385	11/12	0.86	0.26	1.69	52,58,62,65	0
4	NAG	B	360	14/15	0.67	0.26	-	54,60,72,74	0
4	FUC	B	365	10/11	0.34	0.63	-	73,75,75,76	0
4	NAG	B	361	14/15	0.56	0.51	-	77,81,84,85	0

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
3	MAN	A	370	11/12	0.90	0.21	3.05	34,37,39,42	0
3	MAN	B	370	11/12	0.82	0.21	3.04	39,43,45,46	0
3	MAN	B	375	11/12	0.88	0.14	1.14	34,35,38,41	0
3	MAN	A	375	11/12	0.89	0.11	0.70	30,32,34,37	0
6	CA	A	352	1/1	0.99	0.07	0.70	14,14,14,14	0
2	NAG	A	360	14/15	0.85	0.19	0.45	36,42,47,47	0
7	HEM	B	350	43/43	0.98	0.09	-0.17	12,16,18,21	0
7	HEM	A	350	43/43	0.98	0.08	-0.21	9,11,14,15	0
6	CA	A	351	1/1	1.00	0.07	-0.92	13,13,13,13	0
6	CA	B	351	1/1	1.00	0.06	-1.31	13,13,13,13	0
6	CA	B	352	1/1	0.99	0.05	-1.68	18,18,18,18	0
3	MAN	B	380	11/12	0.78	0.17	-	55,58,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.