



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:34 AM GMT

PDB ID : 2AYL  
Title : 2.0 Angstrom Crystal Structure of Manganese Protoporphyrin IX-reconstituted Ovine Prostaglandin H2 Synthase-1 Complexed With Flurbiprofen  
Authors : Gupta, K.; Selinsky, B.S.; Loll, P.J.  
Deposited on : 2005-09-07  
Resolution : 2.00 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](mailto: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.

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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 : 1.7 (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

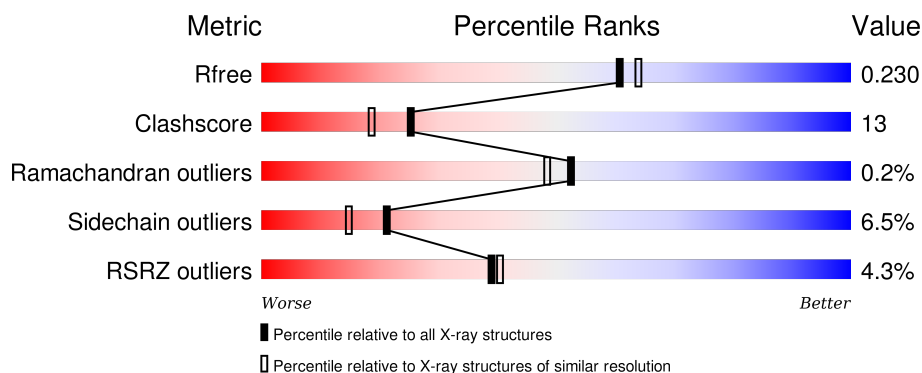
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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	553	<div> <div>5%</div> <div>79%</div> <div>18%</div> <div>•</div> </div>
1	B	553	<div> <div>4%</div> <div>77%</div> <div>20%</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
2	BOG	A	751	-	-	-	X
2	BOG	A	752	-	-	-	X
2	BOG	A	753	-	-	-	X
2	BOG	A	754	-	-	-	X
2	BOG	B	1751	-	-	-	X
2	BOG	B	1753	-	-	-	X
3	NAG	A	661	-	-	-	X
3	NAG	A	662	X	-	-	-
3	NAG	B	1661	-	-	-	X
3	NAG	B	1662	X	-	-	-
4	NAG	A	672	X	-	X	-
4	MAN	A	673	X	-	X	-
4	MAN	A	675	X	-	-	-
4	NAG	B	1672	X	-	-	-
4	MAN	B	1673	X	-	-	-
4	MAN	B	1674	X	-	-	-
4	MAN	B	1675	X	-	-	-
5	MAN	A	683	X	-	-	-
5	MAN	A	684	X	-	-	-
5	MAN	B	1684	X	-	-	-
8	GOL	A	758	-	X	-	X
8	GOL	A	759	-	X	-	X
8	GOL	A	760	-	X	-	-
8	GOL	B	1759	-	X	-	X
8	GOL	B	1760	-	X	-	-

## 2 Entry composition [i](#)

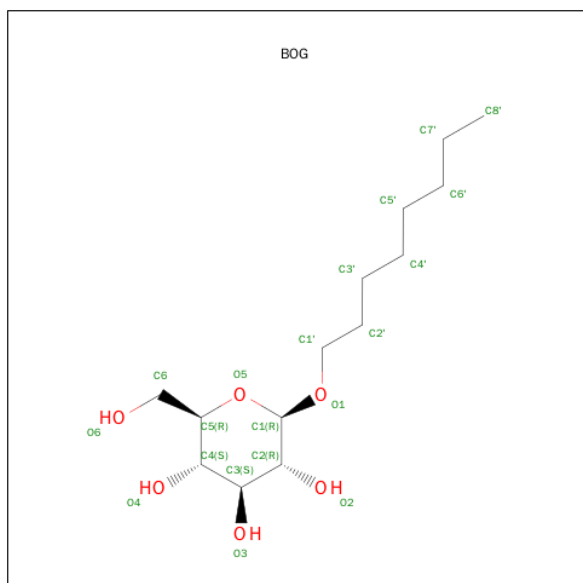
There are 9 unique types of molecules in this entry. The entry contains 10505 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Prostaglandin G/H synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	2	0
			4504	2918	762	795	29			
1	B	553	Total	C	N	O	S	0	2	0
			4504	2918	762	795	29			

- Molecule 2 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- 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
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

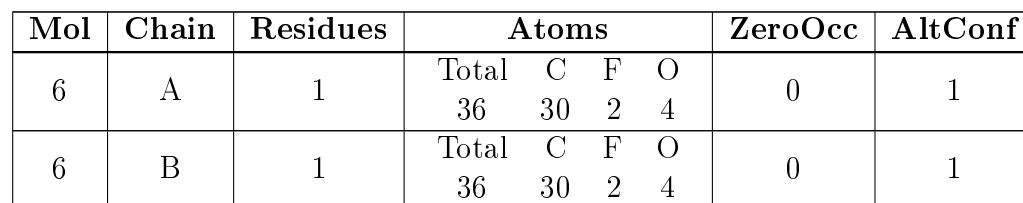
- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		
4	B	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total	C	N	O	0	0
			50	28	2	20		
5	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is FLURBIPROFEN (three-letter code: FLP) (formula: C<sub>15</sub>H<sub>13</sub>FO<sub>2</sub>).



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- The ORTEP diagram shows the Mn(II) complex structure. The central Mn(II) ion is coordinated by four nitrogen atoms (NA, NB, NC, ND) in a distorted tetrahedral geometry. The Mn-N bond lengths are approximately 2.15 Å (Mn-NA), 2.18 Å (Mn-NB), 2.12 Å (Mn-NC), and 2.15 Å (Mn-ND). The Mn(II) ion is also coordinated by two water molecules (O1A, O1D) and two hydroxide ions (O2A, O2D) in a bidentate fashion, forming a dimeric structure. The Mn-O bond lengths are approximately 2.05 Å (Mn-O1A), 2.08 Å (Mn-O1D), 2.02 Å (Mn-O2A), and 2.05 Å (Mn-O2D). The Mn(II) ion is also coordinated by two water molecules (O1A, O1D) and two hydroxide ions (O2A, O2D) in a bidentate fashion, forming a dimeric structure. The Mn-O bond lengths are approximately 2.05 Å (Mn-O1A), 2.08 Å (Mn-O1D), 2.02 Å (Mn-O2A), and 2.05 Å (Mn-O2D). The Mn(II) ion is also coordinated by two water molecules (O1A, O1D) and two hydroxide ions (O2A, O2D) in a bidentate fashion, forming a dimeric structure. The Mn-O bond lengths are approximately 2.05 Å (Mn-O1A), 2.08 Å (Mn-O1D), 2.02 Å (Mn-O2A), and 2.05 Å (Mn-O2D).

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

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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

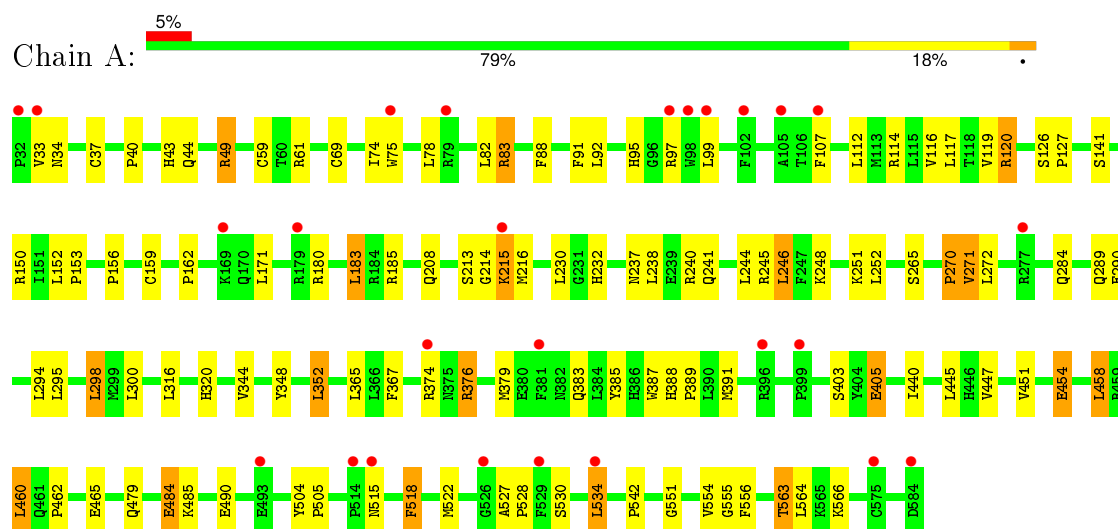
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	434	Total	O	0	0
			434	434		
9	B	457	Total	O	0	0
			457	457		

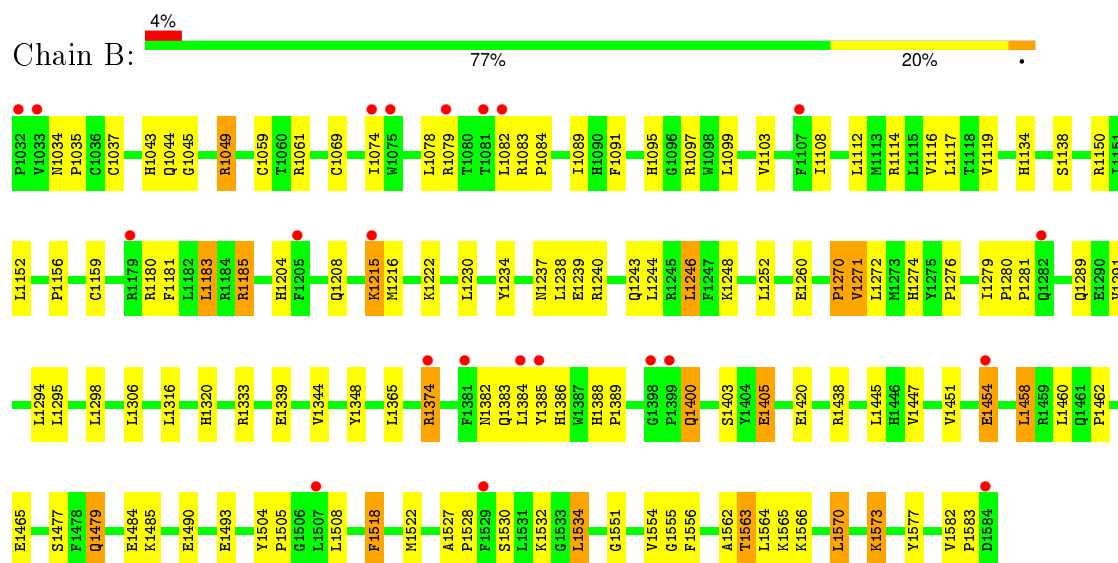
### 3 Residue-property plots [i](#)

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: Prostaglandin G/H synthase 1



#### • Molecule 1: Prostaglandin G/H synthase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.93Å 206.55Å 221.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.33 – 2.00 43.32 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.33-2.00) 99.4 (43.32-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.237 0.211 , 0.230	Depositor DCC
$R_{free}$ test set	11371 reflections (8.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 176618 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, FLP, MNH, BOG, 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	0.34	0/4643	0.60	0/6302
1	B	0.35	0/4643	0.60	0/6302
All	All	0.34	0/9286	0.60	0/12604

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
3	A	1	0
3	B	1	0
4	A	3	0
4	B	4	0
5	A	2	0
5	B	1	0
All	All	12	0

There are no bond length outliers.

There are no bond angle outliers.

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	662	NAG	C1
4	A	672	NAG	C1
4	A	673	MAN	C1
4	A	675	MAN	C1
5	A	683	MAN	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	4504	0	4407	103	0
1	B	4504	0	4405	114	0
2	A	80	0	112	7	0
2	B	60	0	84	5	0
3	A	28	0	25	1	0
3	B	28	0	25	1	0
4	A	61	0	52	13	0
4	B	61	0	52	8	0
5	A	50	0	43	3	0
5	B	50	0	43	2	0
6	A	36	0	24	0	0
6	B	36	0	24	0	0
7	A	43	0	30	3	0
7	B	43	0	30	0	0
8	A	18	0	12	2	0
8	B	12	0	8	0	0
9	A	434	0	0	8	0
9	B	457	0	0	13	0
All	All	10505	0	9376	236	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 13.

The worst 5 of 236 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:B:1215:LYS:H	1:B:1215:LYS:HD3	1.28	0.98
1:B:1215:LYS:NZ	1:B:1222:LYS:HD2	1.84	0.93
1:A:83:ARG:HH12	2:A:751:BOG:H3	1.32	0.93
1:A:127:PRO:HD3	1:A:374:ARG:HH22	1.37	0.89
1:A:352:LEU:HD21	1:A:518:PHE:CZ	2.08	0.87

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	553/553 (100%)	538 (97%)	14 (2%)	1 (0%)	52	48
1	B	553/553 (100%)	538 (97%)	14 (2%)	1 (0%)	52	48
All	All	1106/1106 (100%)	1076 (97%)	28 (2%)	2 (0%)	52	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	PRO
1	B	1270	PRO

### 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	490/488 (100%)	458 (94%)	32 (6%)	21	15
1	B	490/488 (100%)	459 (94%)	31 (6%)	22	16
All	All	980/976 (100%)	917 (94%)	63 (6%)	21	15

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	LEU
1	B	1180	ARG
1	B	1556	PHE
1	A	556	PHE

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Mol	Chain	Res	Type
1	A	564	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1056	GLN
1	B	1203	GLN
1	B	1442	HIS
1	B	1095	HIS
1	B	1204	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

22 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	$\# Z  > 2$
3	NAG	A	661	1,3	14,14,15	0.60	0	15,19,21	0.78	1 (6%)
3	NAG	A	662	3	14,14,15	0.58	0	15,19,21	0.83	1 (6%)
4	NAG	A	671	1,4	14,14,15	0.67	0	15,19,21	0.94	1 (6%)
4	NAG	A	672	4	14,14,15	0.76	0	15,19,21	1.89	3 (20%)
4	MAN	A	673	4	11,11,12	0.77	0	14,15,17	1.71	2 (14%)
4	MAN	A	674	4	11,11,12	0.60	0	14,15,17	1.23	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	A	675	4	11,11,12	0.57	0	14,15,17	0.82	1 (7%)
5	NAG	A	681	1,5	14,14,15	0.49	0	15,19,21	0.80	1 (6%)
5	NAG	A	682	5	14,14,15	0.63	0	15,19,21	0.78	1 (6%)
5	MAN	A	683	5	11,11,12	0.68	0	14,15,17	1.06	2 (14%)
5	MAN	A	684	5	11,11,12	0.58	0	14,15,17	0.95	1 (7%)
3	NAG	B	1661	1,3	14,14,15	0.85	0	15,19,21	0.96	1 (6%)
3	NAG	B	1662	3	14,14,15	0.65	0	15,19,21	0.92	1 (6%)
4	NAG	B	1671	1,4	14,14,15	0.66	0	15,19,21	0.86	1 (6%)
4	NAG	B	1672	4	14,14,15	0.72	1 (7%)	15,19,21	1.62	2 (13%)
4	MAN	B	1673	4	11,11,12	0.48	0	14,15,17	0.68	0
4	MAN	B	1674	4	11,11,12	0.62	0	14,15,17	1.24	1 (7%)
4	MAN	B	1675	4	11,11,12	0.64	0	14,15,17	0.94	1 (7%)
5	NAG	B	1681	1,5	14,14,15	0.45	0	15,19,21	0.67	1 (6%)
5	NAG	B	1682	5	14,14,15	0.51	0	15,19,21	0.90	1 (6%)
5	MAN	B	1683	5	11,11,12	0.48	0	14,15,17	0.78	0
5	MAN	B	1684	5	11,11,12	0.51	0	14,15,17	0.94	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
3	NAG	A	661	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	662	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	671	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	672	4	1/1/5/7	0/6/23/26	0/1/1/1
4	MAN	A	673	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	674	4	-	0/2/19/22	1/1/1/1
4	MAN	A	675	4	1/1/4/5	0/2/19/22	1/1/1/1
5	NAG	A	681	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	682	5	-	0/6/23/26	0/1/1/1
5	MAN	A	683	5	1/1/4/5	0/2/19/22	1/1/1/1
5	MAN	A	684	5	1/1/4/5	0/2/19/22	1/1/1/1
3	NAG	B	1661	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1662	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	1671	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1672	4	1/1/5/7	0/6/23/26	0/1/1/1
4	MAN	B	1673	4	1/1/4/5	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	B	1674	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	1675	4	1/1/4/5	0/2/19/22	1/1/1/1
5	NAG	B	1681	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1682	5	-	0/6/23/26	0/1/1/1
5	MAN	B	1683	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1684	5	1/1/4/5	0/2/19/22	1/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1672	NAG	C1-C2	2.06	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	672	NAG	C4-C3-C2	-4.14	104.80	111.23
4	B	1672	NAG	C4-C3-C2	-3.39	105.96	111.23
4	A	673	MAN	C2-C3-C4	-2.63	106.57	111.04
4	A	672	NAG	C3-C4-C5	-2.63	105.61	110.20
3	B	1661	NAG	C2-N2-C7	-2.50	119.83	123.04

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1673	MAN	C1
3	A	662	NAG	C1
3	B	1662	NAG	C1
4	B	1672	NAG	C1
5	A	684	MAN	C1

There are no torsion outliers.

5 of 6 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	674	MAN	C1-C2-C3-C4-C5-O5
4	B	1675	MAN	C1-C2-C3-C4-C5-O5
4	A	675	MAN	C1-C2-C3-C4-C5-O5
5	A	684	MAN	C1-C2-C3-C4-C5-O5
5	A	683	MAN	C1-C2-C3-C4-C5-O5

15 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	661	NAG	1	0
4	A	672	NAG	8	0
4	A	673	MAN	6	0
4	A	674	MAN	3	0
4	A	675	MAN	4	0
5	A	682	NAG	3	0
5	A	683	MAN	3	0
3	B	1661	NAG	1	0
3	B	1662	NAG	1	0
4	B	1672	NAG	4	0
4	B	1673	MAN	1	0
4	B	1674	MAN	3	0
4	B	1675	MAN	3	0
5	B	1682	NAG	1	0
5	B	1683	MAN	2	0

## 5.6 Ligand geometry

18 ligands 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	$\# Z  > 2$
6	FLP	A	1701[A]	-	16,19,19	2.35	8 (50%)	21,26,26	1.08	1 (4%)
6	FLP	A	1701[B]	-	16,19,19	2.28	7 (43%)	21,26,26	1.01	1 (4%)
7	MNH	A	601	-	30,50,50	1.65	5 (16%)	28,82,82	6.58	21 (75%)
2	BOG	A	751	-	20,20,20	1.67	6 (30%)	25,25,25	0.91	1 (4%)
2	BOG	A	752	-	20,20,20	1.74	5 (25%)	25,25,25	0.94	2 (8%)
2	BOG	A	753	-	20,20,20	1.66	5 (25%)	25,25,25	0.93	2 (8%)
2	BOG	A	754	-	20,20,20	1.66	5 (25%)	25,25,25	0.96	2 (8%)
8	GOL	A	758	-	5,5,5	4.72	5 (100%)	5,5,5	5.62	3 (60%)
8	GOL	A	759	-	5,5,5	4.80	5 (100%)	5,5,5	5.63	3 (60%)
8	GOL	A	760	-	5,5,5	4.80	5 (100%)	5,5,5	5.73	3 (60%)
7	MNH	B	1601	-	30,50,50	1.66	5 (16%)	28,82,82	6.22	18 (64%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BOG	B	1750	-	20,20,20	1.67	5 (25%)	25,25,25	0.97	2 (8%)
2	BOG	B	1751	-	20,20,20	1.67	6 (30%)	25,25,25	0.94	2 (8%)
2	BOG	B	1753	-	20,20,20	1.65	5 (25%)	25,25,25	0.95	2 (8%)
8	GOL	B	1759	-	5,5,5	4.80	5 (100%)	5,5,5	5.71	3 (60%)
8	GOL	B	1760	-	5,5,5	4.79	5 (100%)	5,5,5	5.62	3 (60%)
6	FLP	B	2701[A]	-	16,19,19	2.37	8 (50%)	21,26,26	1.13	1 (4%)
6	FLP	B	2701[B]	-	16,19,19	2.31	7 (43%)	21,26,26	1.04	1 (4%)

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
6	FLP	A	1701[A]	-	-	0/8/12/12	0/2/2/2
6	FLP	A	1701[B]	-	-	0/8/12/12	0/2/2/2
7	MNH	A	601	-	-	0/8/94/94	0/0/8/8
2	BOG	A	751	-	-	0/11/31/31	0/1/1/1
2	BOG	A	752	-	-	0/11/31/31	0/1/1/1
2	BOG	A	753	-	-	0/11/31/31	0/1/1/1
2	BOG	A	754	-	-	0/11/31/31	0/1/1/1
8	GOL	A	758	-	-	0/4/4/4	0/0/0/0
8	GOL	A	759	-	-	0/4/4/4	0/0/0/0
8	GOL	A	760	-	-	0/4/4/4	0/0/0/0
7	MNH	B	1601	-	-	0/8/94/94	0/0/8/8
2	BOG	B	1750	-	-	0/11/31/31	0/1/1/1
2	BOG	B	1751	-	-	0/11/31/31	0/1/1/1
2	BOG	B	1753	-	-	0/11/31/31	0/1/1/1
8	GOL	B	1759	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1760	-	-	0/4/4/4	0/0/0/0
6	FLP	B	2701[A]	-	-	0/8/12/12	0/2/2/2
6	FLP	B	2701[B]	-	-	0/8/12/12	0/2/2/2

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	759	GOL	C3-C2	-8.19	1.21	1.52
8	B	1759	GOL	C3-C2	-8.12	1.21	1.52
8	B	1760	GOL	C3-C2	-8.10	1.21	1.52
8	A	760	GOL	C3-C2	-8.08	1.21	1.52
8	A	758	GOL	C3-C2	-7.83	1.22	1.52

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	B	1601	MNH	CAA-C2A-C1A	-9.59	116.60	127.01
7	A	601	MNH	CAA-C2A-C1A	-7.51	118.85	127.01
7	B	1601	MNH	C1D-C2D-C3D	-4.07	102.04	106.91
6	B	2701[A]	FLP	C14-C12-C9	-3.51	105.43	112.32
6	B	2701[B]	FLP	C14-C12-C9	-3.27	105.90	112.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	MNH	3	0
2	A	751	BOG	6	0
2	A	754	BOG	1	0
8	A	759	GOL	2	0
2	B	1751	BOG	4	0
2	B	1753	BOG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 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	553/553 (100%)	0.15	26 (4%) 35 37	20, 30, 43, 53	0
1	B	553/553 (100%)	0.14	22 (3%) 42 44	20, 29, 42, 55	0
All	All	1106/1106 (100%)	0.14	48 (4%) 39 40	20, 29, 42, 55	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	TRP	6.0
1	B	1584	ASP	5.8
1	A	107	PHE	5.7
1	A	584	ASP	5.6
1	B	1075	TRP	5.3

### 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](#)

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	B	1661	14/15	0.84	0.23	6.12	48,51,53,57	0
3	NAG	A	661	14/15	0.81	0.17	3.60	47,51,54,59	0
4	NAG	A	671	14/15	0.93	0.10	0.42	28,29,33,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	1671	14/15	0.94	0.10	-0.44	25,26,30,35	0
5	NAG	A	681	14/15	0.90	0.10	-0.51	40,42,45,50	0
5	NAG	B	1681	14/15	0.94	0.07	-0.95	33,35,38,41	0
4	NAG	B	1672	14/15	0.78	0.23	-	42,45,48,54	0
4	MAN	A	674	11/12	0.47	0.51	-	75,77,78,79	0
5	MAN	A	684	11/12	0.38	0.52	-	80,81,81,81	0
4	MAN	B	1674	11/12	0.32	0.57	-	73,75,77,79	0
5	NAG	B	1682	14/15	0.88	0.15	-	44,46,51,57	0
4	MAN	A	675	11/12	0.78	0.44	-	79,79,79,80	0
3	NAG	A	662	14/15	0.51	0.59	-	63,65,66,67	0
4	MAN	A	673	11/12	0.59	0.44	-	62,66,70,73	0
3	NAG	B	1662	14/15	0.75	0.41	-	59,61,62,62	0
5	MAN	B	1684	11/12	0.53	0.57	-	75,77,77,78	0
4	MAN	B	1675	11/12	0.51	0.47	-	80,80,81,81	0
4	NAG	A	672	14/15	0.67	0.25	-	45,48,52,57	0
5	MAN	B	1683	11/12	0.63	0.39	-	62,66,69,73	0
4	MAN	B	1673	11/12	0.70	0.40	-	59,62,66,70	0
5	MAN	A	683	11/12	0.69	0.57	-	69,72,75,78	0
5	NAG	A	682	14/15	0.75	0.22	-	53,56,60,65	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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BOG	B	1753	20/20	0.44	0.49	11.46	90,94,95,95	0
2	BOG	A	752	20/20	0.04	0.52	10.50	94,101,102,102	0
8	GOL	B	1759	6/6	0.80	0.21	9.80	36,39,41,46	0
8	GOL	A	758	6/6	0.78	0.28	5.60	38,44,45,45	0
2	BOG	A	754	20/20	0.32	0.54	4.78	96,99,99,100	0
8	GOL	A	759	6/6	0.80	0.22	4.55	43,45,47,47	0
2	BOG	B	1751	20/20	0.57	0.32	4.06	77,80,81,81	0
2	BOG	A	751	20/20	0.73	0.26	2.59	69,70,71,71	0
2	BOG	A	753	20/20	0.70	0.25	2.15	63,67,68,69	0
7	MNH	A	601	43/43	0.88	0.17	1.14	32,37,42,44	0
7	MNH	B	1601	43/43	0.90	0.16	0.56	32,36,42,44	0
6	FLP	B	2701[A]	18/18	0.89	0.18	0.32	25,26,27,27	18

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	FLP	B	2701[B]	18/18	0.89	0.18	0.32	37,38,38,38	18
6	FLP	A	1701[B]	18/18	0.88	0.17	0.04	35,36,37,37	18
6	FLP	A	1701[A]	18/18	0.88	0.17	0.04	29,29,30,31	18
2	BOG	B	1750	20/20	0.72	0.40	-	84,84,89,89	0
8	GOL	B	1760	6/6	0.55	0.36	-	66,67,67,68	0
8	GOL	A	760	6/6	0.76	0.21	-	61,62,62,63	0

## 6.5 Other polymers

There are no such residues in this entry.