



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:40 PM GMT

PDB ID : 1Q4G
Title : 2.0 Angstrom Crystal Structure of Ovine Prostaglandin H2 Synthase-1, in complex with alpha-methyl-4-biphenylacetic acid
Authors : Gupta, K.; Selinsky, B.S.; Kaub, C.J.; Katz, A.K.; Loll, P.J.
Deposited on : 2003-08-03
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
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

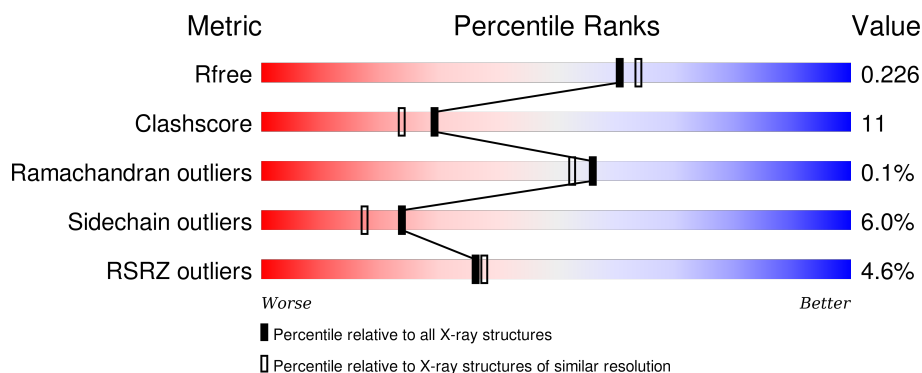
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 ≥ 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>6%</div> <div>78%</div> <div>19%</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	752	-	-	-	X
2	BOG	A	753	-	-	-	X
2	BOG	A	754	-	-	-	X
2	BOG	B	1751	-	-	-	X
2	BOG	B	1752	-	-	-	X
2	BOG	B	1753	-	-	-	X
3	NAG	A	661	-	-	-	X
3	NAG	B	1661	-	-	-	X
7	BFL	A	701	-	-	-	X
9	GOL	A	758	-	X	-	X
9	GOL	A	759	-	X	-	-
9	GOL	B	1758	-	X	-	X
9	GOL	B	1759	-	X	-	X
9	GOL	B	1760	-	X	-	-

2 Entry composition [i](#)

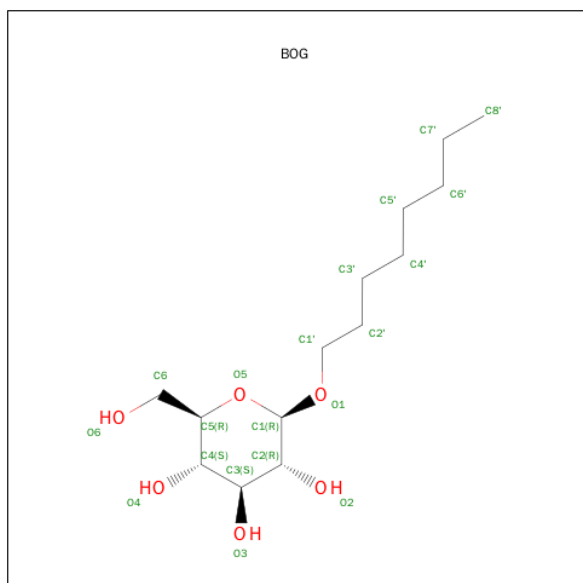
There are 10 unique types of molecules in this entry. The entry contains 10336 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: C₁₄H₂₈O₆).



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		
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 (4-MER).

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

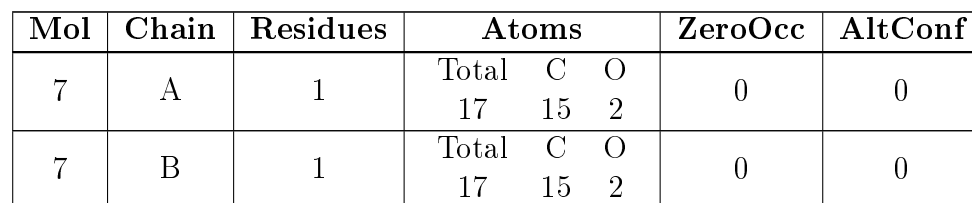
- Molecule 5 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 7 is 2-(1,1'-BIPHENYL-4-YL)PROPANOIC ACID (three-letter code: BFL) (formula: C₁₅H₁₄O₂).



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- Chemical structure of HEM (heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme group.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	Fe	N	O	0	1
			86	68	2	8	8		



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	Fe	N	O	
			86	68	2	8	8	
							0	1

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

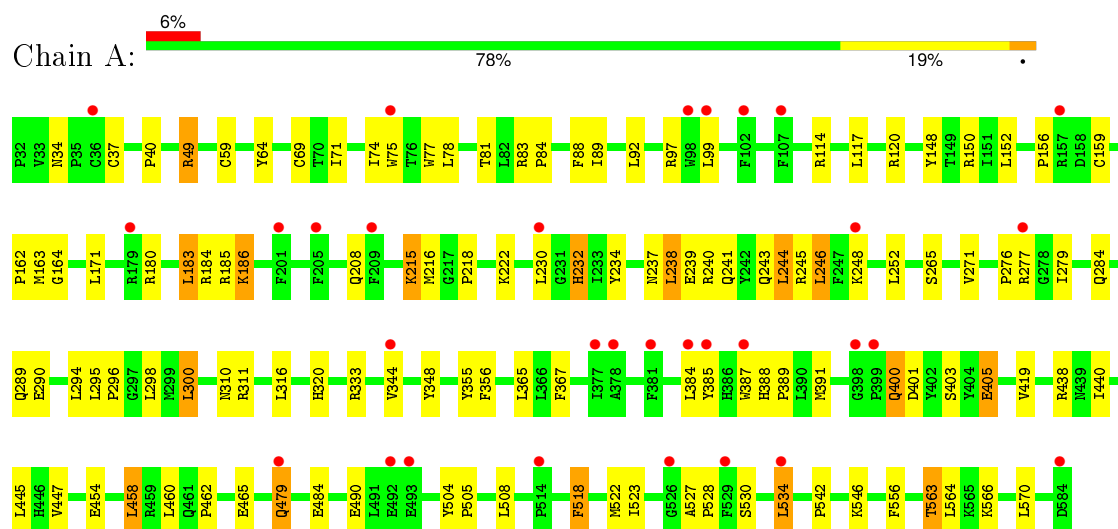
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	321	Total	O		
			321	321		
					0	0
10	B	333	Total	O		
			333	333		
					0	0

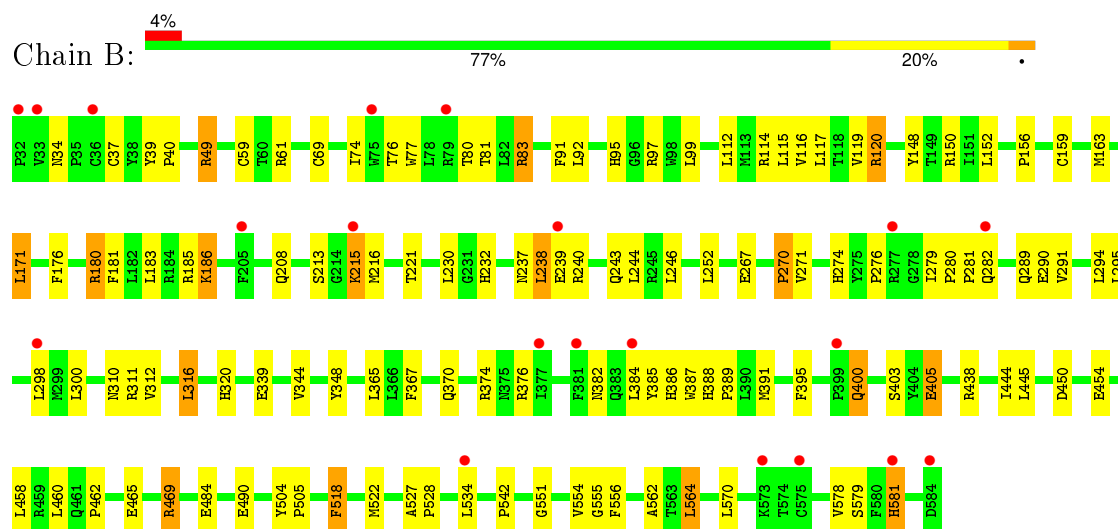
3 Residue-property plots [i](#)

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, α , β , γ	98.15Å 203.86Å 223.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.68 – 2.00 43.68 – 1.98	Depositor EDS
% Data completeness (in resolution range)	94.8 (43.68-2.00) 93.1 (43.68-1.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.231 0.211 , 0.226	Depositor DCC
R_{free} test set	10694 reflections (8.09%)	DCC
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 144143 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10336	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: GOL, BMA, NAG, NDG, BFL, HEM, 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	0.35	0/4643	0.59	1/6302 (0.0%)
1	B	0.37	0/4643	0.60	0/6302
All	All	0.36	0/9286	0.60	1/12604 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	TYR	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4504	0	4403	101	0
1	B	4504	0	4403	100	0
2	A	80	0	112	2	0
2	B	80	0	112	6	0
3	A	28	0	25	3	0
3	B	28	0	25	1	0
4	A	50	0	43	5	0
4	B	50	0	43	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	61	0	52	6	0
6	B	61	0	52	8	0
7	A	17	0	13	1	0
7	B	17	0	13	0	0
8	A	86	0	60	4	0
8	B	86	0	60	4	0
9	A	12	0	8	1	0
9	B	18	0	12	1	0
10	A	321	0	0	6	0
10	B	333	0	0	5	0
All	All	10336	0	9436	215	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 11.

The worst 5 of 215 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:185:ARG:HH21	1:A:438:ARG:NH1	1.56	1.02
1:A:59:CYS:SG	1:A:69[B]:CYS:HB2	2.01	1.01
1:A:59:CYS:SG	1:A:69[B]:CYS:CB	2.53	0.96
1:B:215:LYS:H	1:B:215:LYS:HE2	1.32	0.93
1:A:215:LYS:H	1:A:215:LYS:HE2	1.35	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/553 (100%)	537 (97%)	16 (3%)	0	100	100
1	B	553/553 (100%)	535 (97%)	17 (3%)	1 (0%)	52	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1106/1106 (100%)	1072 (97%)	33 (3%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	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%)	462 (94%)	28 (6%)	25	19
1	B	490/488 (100%)	459 (94%)	31 (6%)	22	16
All	All	980/976 (100%)	921 (94%)	59 (6%)	24	17

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	563	THR
1	B	171	LEU
1	B	518	PHE
1	A	564	LEU
1	B	83	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	GLN
1	B	56	GLN
1	B	443	HIS
1	A	443	HIS
1	B	42	GLN

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	0.66	0	15,19,21	0.73	0
3	NDG	A	662	3	14,14,15	0.57	0	15,19,21	0.95	1 (6%)
5	NAG	A	671	1,5	14,14,15	0.72	0	15,19,21	1.12	1 (6%)
5	NDG	A	672	5	14,14,15	0.88	1 (7%)	15,19,21	1.77	3 (20%)
5	BMA	A	673	5	11,11,12	0.80	0	14,15,17	1.80	3 (21%)
5	MAN	A	674	5	11,11,12	0.65	0	14,15,17	0.84	1 (7%)
5	MAN	A	675	5	11,11,12	0.53	0	14,15,17	0.76	1 (7%)
4	NAG	A	681	1,4	14,14,15	0.48	0	15,19,21	0.77	1 (6%)
4	NAG	A	682	4	14,14,15	0.64	0	15,19,21	0.79	1 (6%)
4	BMA	A	683	4	11,11,12	0.71	0	14,15,17	1.15	2 (14%)
4	BMA	A	684	4	11,11,12	0.57	0	14,15,17	0.97	1 (7%)
3	NAG	B	1661	1,3	14,14,15	0.63	0	15,19,21	0.99	1 (6%)
3	NDG	B	1662	3	14,14,15	0.62	0	15,19,21	0.85	1 (6%)
6	NAG	B	1671	1,6	14,14,15	0.69	0	15,19,21	0.95	1 (6%)
6	NDG	B	1672	6	14,14,15	0.74	1 (7%)	15,19,21	1.48	2 (13%)
6	BMA	B	1673	6	11,11,12	0.52	0	14,15,17	0.69	0
6	BMA	B	1674	6	11,11,12	0.63	0	14,15,17	1.12	1 (7%)
6	BMA	B	1675	6	11,11,12	0.64	0	14,15,17	0.90	1 (7%)
4	NAG	B	1681	1,4	14,14,15	0.54	0	15,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1682	4	14,14,15	0.61	0	15,19,21	0.84	1 (6%)
4	BMA	B	1683	4	11,11,12	0.64	0	14,15,17	1.15	1 (7%)
4	BMA	B	1684	4	11,11,12	0.57	0	14,15,17	0.96	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	NDG	A	662	3	-	0/6/23/26	0/1/1/1
5	NAG	A	671	1,5	-	0/6/23/26	0/1/1/1
5	NDG	A	672	5	-	0/6/23/26	0/1/1/1
5	BMA	A	673	5	-	0/2/19/22	0/1/1/1
5	MAN	A	674	5	-	0/2/19/22	0/1/1/1
5	MAN	A	675	5	-	0/2/19/22	1/1/1/1
4	NAG	A	681	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	682	4	-	0/6/23/26	0/1/1/1
4	BMA	A	683	4	-	0/2/19/22	1/1/1/1
4	BMA	A	684	4	-	0/2/19/22	1/1/1/1
3	NAG	B	1661	1,3	-	0/6/23/26	0/1/1/1
3	NDG	B	1662	3	-	0/6/23/26	0/1/1/1
6	NAG	B	1671	1,6	-	0/6/23/26	0/1/1/1
6	NDG	B	1672	6	-	0/6/23/26	0/1/1/1
6	BMA	B	1673	6	-	0/2/19/22	0/1/1/1
6	BMA	B	1674	6	-	0/2/19/22	0/1/1/1
6	BMA	B	1675	6	-	0/2/19/22	1/1/1/1
4	NAG	B	1681	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1682	4	-	0/6/23/26	0/1/1/1
4	BMA	B	1683	4	-	0/2/19/22	1/1/1/1
4	BMA	B	1684	4	-	0/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1672	NDG	C1-C2	2.20	1.55	1.52
5	A	672	NDG	C1-C2	2.30	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	672	NDG	C4-C3-C2	-3.37	106.00	111.23
6	B	1672	NDG	C4-C3-C2	-2.80	106.87	111.23
3	B	1661	NAG	C2-N2-C7	-2.66	119.63	123.04
5	A	672	NDG	C3-C4-C5	-2.57	105.71	110.20
3	A	662	NDG	C2-N2-C7	-2.54	119.78	123.04

There are no chirality outliers.

There are no torsion outliers.

5 of 6 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1675	BMA	C1-C2-C3-C4-C5-O5
5	A	675	MAN	C1-C2-C3-C4-C5-O5
4	A	684	BMA	C1-C2-C3-C4-C5-O5
4	B	1684	BMA	C1-C2-C3-C4-C5-O5
4	A	683	BMA	C1-C2-C3-C4-C5-O5

14 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	661	NAG	2	0
3	A	662	NDG	2	0
5	A	671	NAG	1	0
5	A	672	NDG	5	0
5	A	673	BMA	3	0
4	A	682	NAG	3	0
4	A	683	BMA	5	0
4	A	684	BMA	1	0
3	B	1661	NAG	1	0
6	B	1672	NDG	4	0
6	B	1674	BMA	3	0
6	B	1675	BMA	3	0
4	B	1682	NAG	2	0
4	B	1683	BMA	4	0

5.6 Ligand geometry

19 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
7	BFL	A	701	-	15,18,18	2.07	7 (46%)	20,24,24	1.31	2 (10%)
2	BOG	A	751	-	20,20,20	1.63	6 (30%)	25,25,25	0.93	1 (4%)
2	BOG	A	752	-	20,20,20	1.74	5 (25%)	25,25,25	0.93	2 (8%)
2	BOG	A	753	-	20,20,20	1.63	5 (25%)	25,25,25	0.91	2 (8%)
2	BOG	A	754	-	20,20,20	1.65	5 (25%)	25,25,25	0.97	2 (8%)
9	GOL	A	758	-	5,5,5	4.81	5 (100%)	5,5,5	5.61	3 (60%)
9	GOL	A	759	-	5,5,5	4.76	5 (100%)	5,5,5	5.70	3 (60%)
8	HEM	A	801[A]	1	30,50,50	2.61	9 (30%)	24,82,82	7.05	17 (70%)
8	HEM	A	801[B]	1	30,50,50	2.56	9 (30%)	24,82,82	7.21	19 (79%)
8	HEM	B	1601[A]	1	30,50,50	2.77	10 (33%)	24,82,82	6.60	17 (70%)
8	HEM	B	1601[B]	1	30,50,50	2.69	10 (33%)	24,82,82	6.49	16 (66%)
7	BFL	B	1701	-	15,18,18	2.06	7 (46%)	20,24,24	1.25	2 (10%)
2	BOG	B	1750	-	20,20,20	1.67	5 (25%)	25,25,25	0.98	2 (8%)
2	BOG	B	1751	-	20,20,20	1.62	5 (25%)	25,25,25	0.85	1 (4%)
2	BOG	B	1752	-	20,20,20	1.66	5 (25%)	25,25,25	0.99	2 (8%)
2	BOG	B	1753	-	20,20,20	1.65	5 (25%)	25,25,25	0.97	2 (8%)
9	GOL	B	1758	-	5,5,5	4.88	5 (100%)	5,5,5	5.63	3 (60%)
9	GOL	B	1759	-	5,5,5	4.84	5 (100%)	5,5,5	5.65	3 (60%)
9	GOL	B	1760	-	5,5,5	4.77	5 (100%)	5,5,5	5.73	3 (60%)

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	BFL	A	701	-	-	0/8/12/12	0/2/2/2
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
9	GOL	A	758	-	-	0/4/4/4	0/0/0/0
9	GOL	A	759	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEM	A	801[A]	1	-	0/10/54/54	0/0/8/8
8	HEM	A	801[B]	1	-	0/10/54/54	0/0/8/8
8	HEM	B	1601[A]	1	-	0/10/54/54	0/0/8/8
8	HEM	B	1601[B]	1	-	0/10/54/54	0/0/8/8
7	BFL	B	1701	-	-	0/8/12/12	0/2/2/2
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	1752	-	-	0/11/31/31	0/1/1/1
2	BOG	B	1753	-	-	0/11/31/31	0/1/1/1
9	GOL	B	1758	-	-	0/4/4/4	0/0/0/0
9	GOL	B	1759	-	-	0/4/4/4	0/0/0/0
9	GOL	B	1760	-	-	0/4/4/4	0/0/0/0

The worst 5 of 118 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1758	GOL	C3-C2	-8.47	1.19	1.52
9	B	1759	GOL	C3-C2	-8.30	1.20	1.52
9	A	758	GOL	C3-C2	-8.11	1.21	1.52
9	B	1760	GOL	C3-C2	-8.04	1.21	1.52
9	A	759	GOL	C3-C2	-8.03	1.21	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	801[B]	HEM	CHD-C1D-ND	-6.96	107.76	124.52
8	A	801[A]	HEM	CAA-C2A-C1A	-6.44	120.01	127.01
8	A	801[A]	HEM	CHD-C1D-ND	-6.16	109.69	124.52
8	B	1601[B]	HEM	CHC-C4B-NB	-6.05	109.95	124.52
8	B	1601[A]	HEM	CHC-C4B-NB	-5.95	110.20	124.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	701	BFL	1	0
2	A	753	BOG	1	0
2	A	754	BOG	1	0
9	A	758	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	801[A]	HEM	2	0
8	A	801[B]	HEM	2	0
8	B	1601[A]	HEM	1	0
8	B	1601[B]	HEM	3	0
2	B	1751	BOG	4	0
2	B	1752	BOG	1	0
2	B	1753	BOG	1	0
9	B	1759	GOL	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, 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	553/553 (100%)	0.25	31 (5%) 28 29	30, 41, 55, 65	0
1	B	553/553 (100%)	0.17	20 (3%) 46 48	29, 41, 54, 66	0
All	All	1106/1106 (100%)	0.21	51 (4%) 36 38	29, 41, 55, 66	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	584	ASP	6.4
1	A	98	TRP	6.3
1	A	107	PHE	5.7
1	B	33	VAL	5.2
1	B	75	TRP	4.9

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, 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	NAG	A	661	14/15	0.83	0.20	2.49	57,61,63,68	0
3	NAG	B	1661	14/15	0.84	0.17	2.47	59,62,64,66	0
5	NAG	A	671	14/15	0.95	0.10	-0.16	37,38,42,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	B	1671	14/15	0.95	0.10	-0.33	36,37,41,47	0
4	NAG	A	681	14/15	0.93	0.10	-0.45	50,53,56,60	0
4	NAG	B	1681	14/15	0.97	0.07	-0.88	43,45,49,50	0
4	NAG	B	1682	14/15	0.92	0.13	-	54,55,59,64	0
4	BMA	A	684	11/12	0.54	0.59	-	89,90,91,91	0
6	NDG	B	1672	14/15	0.84	0.23	-	53,56,60,65	0
3	NDG	A	662	14/15	0.55	0.51	-	72,74,75,75	0
4	NAG	A	682	14/15	0.84	0.19	-	63,66,69,74	0
6	BMA	B	1674	11/12	0.41	0.55	-	84,86,88,90	0
5	BMA	A	673	11/12	0.81	0.34	-	71,74,79,83	0
4	BMA	B	1684	11/12	0.67	0.48	-	81,82,82,83	0
6	BMA	B	1675	11/12	0.71	0.45	-	90,91,92,92	0
5	MAN	A	675	11/12	0.75	0.40	-	92,93,93,94	0
4	BMA	A	683	11/12	0.68	0.51	-	78,81,85,88	0
6	BMA	B	1673	11/12	0.78	0.32	-	70,73,78,81	0
4	BMA	B	1683	11/12	0.81	0.34	-	69,71,76,79	0
3	NDG	B	1662	14/15	0.83	0.35	-	68,70,71,71	0
5	MAN	A	674	11/12	0.79	0.47	-	86,88,90,91	0
5	NDG	A	672	14/15	0.85	0.21	-	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, 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
9	GOL	B	1758	6/6	0.60	0.39	10.69	79,82,82,83	0
2	BOG	A	752	20/20	0.09	0.54	10.18	96,104,105,105	0
2	BOG	B	1753	20/20	0.34	0.48	9.61	101,103,104,104	0
2	BOG	A	754	20/20	0.47	0.68	6.37	103,105,106,106	0
9	GOL	A	758	6/6	0.73	0.24	4.48	57,60,61,61	0
2	BOG	B	1752	20/20	0.31	0.47	4.40	112,113,113,113	0
9	GOL	B	1759	6/6	0.77	0.17	4.28	50,53,56,59	0
2	BOG	A	753	20/20	0.72	0.25	3.00	73,80,82,82	0
7	BFL	A	701	17/17	0.66	0.29	2.32	51,53,57,58	0
2	BOG	B	1751	20/20	0.83	0.20	2.15	76,78,78,78	0
7	BFL	B	1701	17/17	0.78	0.27	1.86	52,53,57,57	0
2	BOG	A	751	20/20	0.90	0.18	0.97	70,71,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	HEM	B	1601[B]	43/43	0.95	0.15	0.26	40,42,47,49	43
8	HEM	B	1601[A]	43/43	0.95	0.15	0.14	40,41,47,49	43
8	HEM	A	801[B]	43/43	0.94	0.15	0.01	39,41,46,48	43
8	HEM	A	801[A]	43/43	0.94	0.15	-0.01	41,42,48,50	43
9	GOL	B	1760	6/6	0.51	0.40	-	78,79,79,79	0
9	GOL	A	759	6/6	0.83	0.32	-	77,77,77,77	0
2	BOG	B	1750	20/20	0.76	0.42	-	91,91,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.