



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 12:52 PM GMT

PDB ID : 3N8Y
Title : Structure of Aspirin Acetylated Cyclooxygenase-1 in Complex with Diclofenac
Authors : Sidhu, R.S.
Deposited on : 2010-05-28
Resolution : 2.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

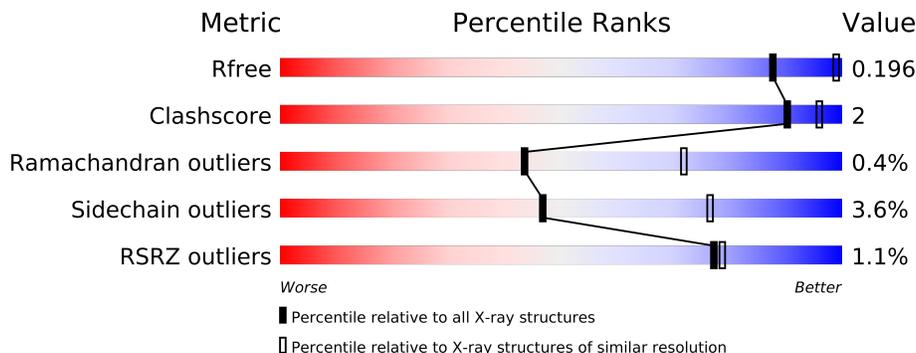
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	553	
2	B	553	

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 9465 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Prostaglandin G/H synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	553	4427	2870	742	787	28	0	5	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	LEU	MET	CONFLICT	UNP P05979

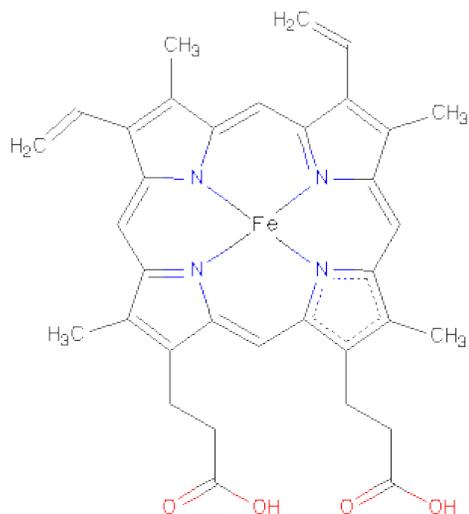
- Molecule 2 is a protein called Prostaglandin G/H synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	553	4443	2887	740	789	27	3	4	0

There are 2 discrepancies between the modelled and reference sequences:

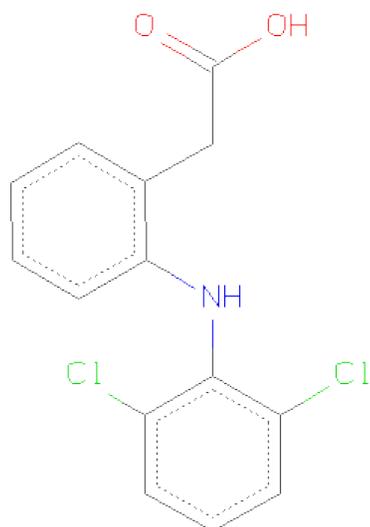
Chain	Residue	Modelled	Actual	Comment	Reference
B	92	LEU	MET	CONFLICT	UNP P05979
B	530	OAS	SER	MICROHETEROGENEITY	UNP P05979

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 4 is 2-[2,6-DICHLOROPHENYL)AMINO]BENZENEACETICACID (three-letter code: DIF) (formula: C₁₄H₁₁Cl₂NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
4	A	1	19	14	2	1	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
4	B	1	19	14	2	1	2	0	1

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

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	LEU	MET	CONFLICT	UNP P05979
B	92	LEU	MET	CONFLICT	UNP P05979
B	530	OAS	SER	MICROHETEROGENEITY	UNP P05979

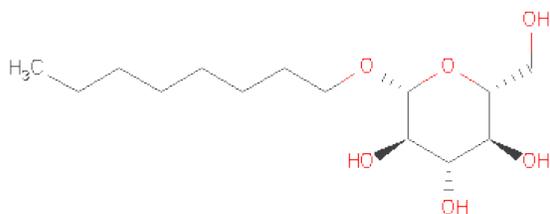
- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	LEU	MET	CONFLICT	UNP P05979

- Molecule 7 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



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

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	LEU	MET	CONFLICT	UNP P05979
B	530	OAS	SER	MICROHETEROGENEITY	UNP P05979

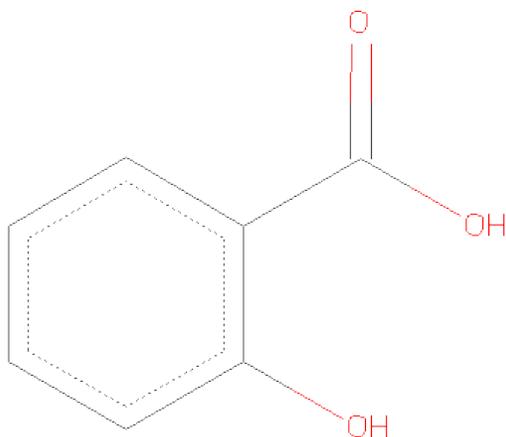
- Molecule 9 is a polymer of unknown type called SUGAR (4-MER).

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	LEU	MET	CONFLICT	UNP P05979
B	530	OAS	SER	MICROHETEROGENEITY	UNP P05979

- Molecule 10 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: C₇H₆O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 10 7 3	0	1

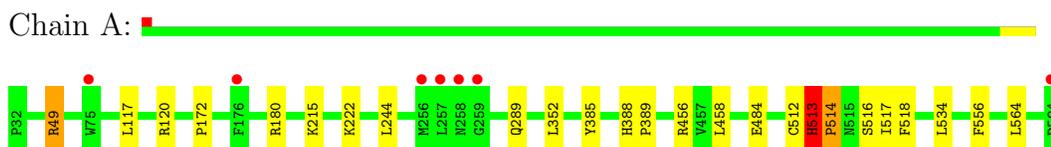
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	74	Total O 74 74	0	0
11	B	68	Total O 68 68	0	0

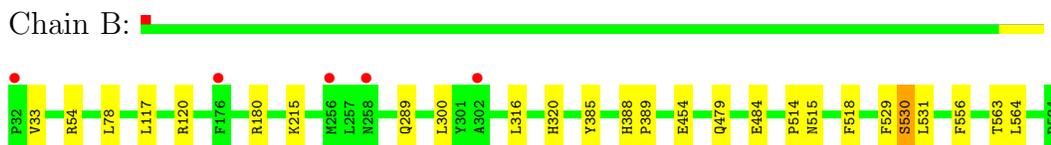
3 Residue-property plots

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 ($RSRZ > 2$). 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 2: Prostaglandin G/H synthase 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	182.33Å 182.33Å 103.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.84 – 2.60 29.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.84-2.60) 99.0 (29.84-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.184 , 0.200 0.185 , 0.196	Depositor DCC
R_{free} test set	1595 reflections (2.76%)	DCC
Wilson B-factor (Å ²)	48.7	Xtrriage
Anisotropy	0.303	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 11.9	EDS
Estimated twinning fraction	0.501 for H, K, L 0.499 for -H-K, K, -L 0.057 for h,-h-k,-l	Xtrriage
Reported twinning fraction	0.501 for H, K, L 0.499 for -H-K, K, -L	Depositor
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	0 of 59356 reflections	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9465	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: BMA, NAG, SAL, DIF, NDG, OAS, 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	0.32	0/4572	0.47	0/6228
2	B	0.33	0/4569	0.47	1/6218 (0.0%)
All	All	0.32	0/9141	0.47	1/12446 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	479	GLN	CG-CD-OE1	-5.19	111.22	121.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	529[B]	PHE	Mainchain
2	B	530[A]	OAS	Mainchain
2	B	530[B]	OAS	Mainchain

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4427	0	0	6	0
2	B	4443	0	2	7	0
3	A	43	0	0	0	0
3	B	43	0	0	0	0
4	A	19	0	0	0	0
4	B	19	0	10	11	0
5	A	50	0	0	0	0
5	B	50	0	0	0	0
6	A	61	0	0	0	0
7	A	40	0	28	0	0
7	B	40	0	56	0	0
8	B	28	0	0	0	0
9	B	50	0	0	0	0
10	B	10	0	4	0	0
11	A	74	0	0	0	0
11	B	68	0	0	0	0
All	All	9465	0	100	20	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

The worst 5 of 20 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:530[B]:OAS:OG	4:B:585[B]:DIF:O2	1.64	1.15
4:B:585[B]:DIF:O2	4:B:585[B]:DIF:N1	2.01	0.94
2:B:530[B]:OAS:OG	4:B:585[B]:DIF:C14	2.30	0.80
1:A:513[A]:HIS:CB	1:A:514[A]:PRO:CD	2.62	0.77
4:B:585[B]:DIF:C9	4:B:585[B]:DIF:CL2	2.70	0.77

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	556/553 (100%)	534 (96%)	16 (3%)	6 (1%)	21	42
2	B	553/553 (100%)	533 (96%)	19 (3%)	1 (0%)	56	82
All	All	1109/1106 (100%)	1067 (96%)	35 (3%)	7 (1%)	43	63

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	513[A]	HIS
1	A	513[B]	HIS
2	B	33	VAL
1	A	514[A]	PRO
1	A	514[B]	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	471/488 (96%)	452 (96%)	19 (4%)	42	73
2	B	471/487 (97%)	455 (97%)	16 (3%)	49	78
All	All	942/975 (97%)	907 (96%)	35 (4%)	47	75

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	518	PHE
2	B	54	ARG
2	B	556	PHE
1	A	534	LEU

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Mol	Chain	Res	Type
1	A	556	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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
2	OAS	B	530[A]	2	8,8,9	6.11	4 (50%)	7,9,11	2.83	2 (28%)
2	OAS	B	530[B]	2	5,5,9	7.30	1 (20%)	3,5,11	8.46	2 (66%)

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	OAS	B	530[A]	2	-	0/5/7/9	0/0/0/0
2	OAS	B	530[B]	2	-	0/2/4/9	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	530[B]	OAS	O-C	16.19	1.22	1.11
2	B	530[A]	OAS	O-C	16.07	1.22	1.11
2	B	530[A]	OAS	C2A-C1A	-4.52	1.32	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	530[A]	OAS	OAC-C1A	3.33	1.33	1.20
2	B	530[A]	OAS	OG-C1A	2.38	1.46	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	530[B]	OAS	OG-CB-CA	14.00	119.83	113.63
2	B	530[A]	OAS	C-CA-N	-5.31	108.53	113.83
2	B	530[A]	OAS	OG-CB-CA	4.58	119.96	108.80
2	B	530[B]	OAS	C-CA-N	-4.33	109.50	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates i

19 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
6	NAG	A	671	1,6	12,14,15	0.68	0	15,19,21	0.66	0
6	NDG	A	672	6	12,14,15	0.50	0	15,19,21	1.93	3 (20%)
6	BMA	A	673	6	10,11,12	0.66	0	11,15,17	1.12	1 (9%)
6	MAN	A	674	6	10,11,12	0.71	0	11,15,17	1.42	1 (9%)
6	MAN	A	675	6	10,11,12	0.69	0	11,15,17	1.18	1 (9%)
5	NAG	A	681	1,5	12,14,15	0.61	0	15,19,21	0.51	0
5	NAG	A	682	5	12,14,15	0.58	0	15,19,21	0.89	0
5	BMA	A	683	5	10,11,12	0.63	0	11,15,17	1.37	2 (18%)
5	BMA	A	684	5	10,11,12	0.61	0	11,15,17	1.34	2 (18%)
8	NAG	B	1661	8,2	12,14,15	0.60	0	15,19,21	0.98	1 (6%)
8	NDG	B	1662	8	12,14,15	0.57	0	15,19,21	0.92	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	B	1671	9,2	12,14,15	0.66	0	15,19,21	0.86	1 (6%)
9	NDG	B	1672	9	12,14,15	0.70	0	15,19,21	1.09	1 (6%)
9	BMA	B	1673	9	10,11,12	0.74	0	11,15,17	0.87	0
9	BMA	B	1674	9	10,11,12	0.60	0	11,15,17	1.54	2 (18%)
5	NAG	B	1681	2,5	12,14,15	0.66	0	15,19,21	0.74	0
5	NAG	B	1682	5	12,14,15	0.56	0	15,19,21	0.97	1 (6%)
5	BMA	B	1683	5	10,11,12	0.71	0	11,15,17	0.63	0
5	BMA	B	1684	5	10,11,12	0.73	0	11,15,17	1.07	1 (9%)

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	NAG	A	671	1,6	-	0/6/23/26	0/1/1/1
6	NDG	A	672	6	-	0/6/23/26	1/1/1/1
6	BMA	A	673	6	-	0/2/19/22	0/1/1/1
6	MAN	A	674	6	-	0/2/19/22	0/1/1/1
6	MAN	A	675	6	-	0/2/19/22	0/1/1/1
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	BMA	A	683	5	-	0/2/19/22	0/1/1/1
5	BMA	A	684	5	-	0/2/19/22	0/1/1/1
8	NAG	B	1661	8,2	-	0/6/23/26	0/1/1/1
8	NDG	B	1662	8	-	0/6/23/26	0/1/1/1
9	NAG	B	1671	9,2	-	0/6/23/26	0/1/1/1
9	NDG	B	1672	9	-	0/6/23/26	0/1/1/1
9	BMA	B	1673	9	-	0/2/19/22	0/1/1/1
9	BMA	B	1674	9	-	0/2/19/22	0/1/1/1
5	NAG	B	1681	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1682	5	-	0/6/23/26	0/1/1/1
5	BMA	B	1683	5	-	0/2/19/22	0/1/1/1
5	BMA	B	1684	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	672	NDG	O-C5-C6	5.30	112.54	106.98
9	B	1674	BMA	O5-C5-C6	4.30	111.49	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	674	MAN	O5-C5-C6	3.97	111.15	106.98
5	A	683	BMA	O5-C5-C6	3.78	110.95	106.98
5	A	684	BMA	O5-C5-C6	3.74	110.91	106.98

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	672	NDG	C1-C2-C3-C4-C5-O

5.6 Ligand geometry (i)

9 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
3	HEM	A	601	1,11	49,50,50	2.41	16 (32%)	46,82,82	2.07	8 (17%)
4	DIF	A	701	-	20,20,20	0.97	2 (10%)	27,27,27	1.10	3 (11%)
7	BOG	A	751	-	20,20,20	0.51	0	25,25,25	1.04	2 (8%)
7	BOG	A	754	-	20,20,20	0.52	0	25,25,25	0.61	0
7	BOG	B	1750	-	20,20,20	0.51	0	25,25,25	0.60	0
7	BOG	B	1751	-	20,20,20	0.43	0	25,25,25	0.68	0
4	DIF	B	585[B]	-	20,20,20	1.03	2 (10%)	27,27,27	1.11	2 (7%)
3	HEM	B	601	2	49,50,50	2.36	15 (30%)	46,82,82	1.99	8 (17%)
10	SAL	B	900[A]	-	10,10,10	0.89	0	13,13,13	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	601	1,11	-	0/14/114/114	0/0/8/8
4	DIF	A	701	-	-	0/8/8/8	0/2/2/2
7	BOG	A	751	-	-	0/11/31/31	0/1/1/1
7	BOG	A	754	-	-	0/11/31/31	0/1/1/1
7	BOG	B	1750	-	-	0/11/31/31	0/1/1/1
7	BOG	B	1751	-	-	0/11/31/31	0/1/1/1
4	DIF	B	585[B]	-	-	0/8/8/8	0/2/2/2
3	HEM	B	601	2	-	0/14/114/114	0/0/8/8
10	SAL	B	900[A]	-	-	0/4/4/4	0/1/1/1

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	HEM	C3D-C2D	6.08	1.54	1.43
3	B	601	HEM	C3D-C2D	5.90	1.54	1.43
3	A	601	HEM	C3C-C2C	-5.34	1.34	1.43
3	B	601	HEM	C3B-C2B	-5.32	1.34	1.43
3	A	601	HEM	C3B-C2B	-5.30	1.34	1.43

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	HEM	C3B-C4B-NB	-8.76	107.73	114.00
3	B	601	HEM	C3B-C4B-NB	-8.54	107.89	114.00
3	A	601	HEM	C4D-ND-C1D	6.66	111.98	105.16
3	B	601	HEM	C4D-ND-C1D	6.43	111.74	105.16
3	A	601	HEM	C2D-C1D-ND	-3.86	108.37	112.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.42	7 (1%) 74 75	34, 47, 61, 68	1 (0%)
2	B	553/553 (100%)	-0.46	5 (0%) 81 82	34, 48, 61, 69	1 (0%)
All	All	1106/1106 (100%)	-0.44	12 (1%) 77 79	34, 47, 61, 69	2 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	176	PHE	3.0
1	A	258	ASN	2.9
1	A	584	ASP	2.8
2	B	302	ALA	2.5
2	B	256	MET	2.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	OAS	B	530[B]	6/10	0.13	-0.81	35,36,36,36	6
2	OAS	B	530[A]	9/10	0.13	-0.95	37,37,39,39	9

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	BMA	A	684	11/12	0.37	28.18	88,97,116,117	0
9	NDG	B	1672	14/15	0.27	10.03	65,66,68,68	0
6	MAN	A	675	11/12	0.22	8.60	69,71,72,73	0
9	NAG	B	1671	14/15	0.16	1.39	61,64,67,69	0
5	NAG	B	1682	14/15	0.21	1.29	84,85,86,87	0
8	NDG	B	1662	14/15	0.24	0.79	60,66,72,79	0
6	NDG	A	672	14/15	0.18	0.61	63,64,65,65	0
8	NAG	B	1661	14/15	0.21	0.54	58,59,66,73	0
5	NAG	B	1681	14/15	0.13	0.13	85,86,87,87	0
6	NAG	A	671	14/15	0.12	-0.67	58,60,60,62	0
5	NAG	A	682	14/15	0.09	-1.32	57,59,63,64	0
5	NAG	A	681	14/15	0.08	-1.38	56,58,61,62	0
6	BMA	A	673	11/12	0.24	-	65,66,67,68	0
5	BMA	B	1684	11/12	0.45	-	91,93,96,97	0
6	MAN	A	674	11/12	0.23	-	68,69,71,71	0
5	BMA	B	1683	11/12	0.21	-	85,86,89,90	0
9	BMA	B	1673	11/12	0.45	-	71,75,81,83	0
9	BMA	B	1674	11/12	0.40	-	84,89,98,99	0
5	BMA	A	683	11/12	0.23	-	67,76,86,87	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	BOG	A	754	20/20	0.18	1.66	46,46,46,46	0
7	BOG	A	751	20/20	0.16	1.38	39,47,64,69	0
4	DIF	B	585[B]	19/19	0.19	1.17	22,23,23,23	19
7	BOG	B	1750	20/20	0.16	0.61	42,43,44,44	0
3	HEM	A	601	43/43	0.16	0.30	40,45,49,51	0
7	BOG	B	1751	20/20	0.12	0.16	35,37,38,38	0
3	HEM	B	601	43/43	0.15	0.11	41,45,50,51	0
10	SAL	B	900[A]	10/10	0.12	-1.08	34,34,35,35	10

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	DIF	A	701	19/19	0.11	-1.28	46,47,48,50	0

6.5 Other polymers

There are no such residues in this entry.