



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 04:42 pm GMT

PDB ID : 3N8W
Title : Crystal Structure of R120Q/Native Cyclooxygenase-1 Heterodimer mutant in complex with Flurbiprofen
Authors : Sidhu, R.S.
Deposited on : 2010-05-28
Resolution : 2.75 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

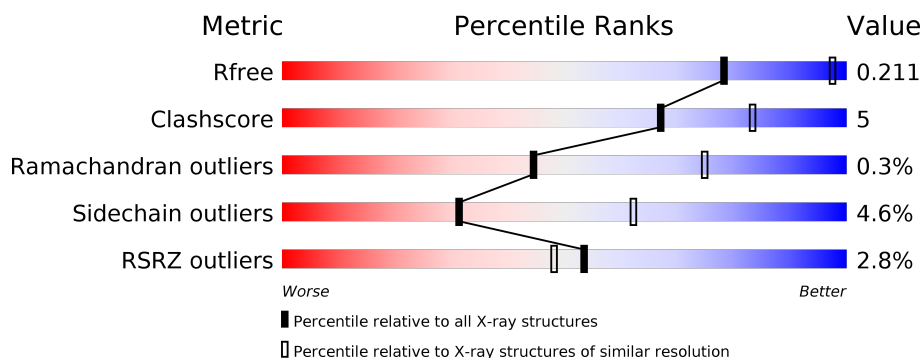
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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>3%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div></div> </div> </div>
2	B	553	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>10%</div> <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
4	FLP	A	701	X	-	-	-
5	NAG	A	661	X	-	-	-
5	NAG	B	1661	-	-	-	X
7	NDG	A	672	-	-	-	X
8	BOG	A	751	-	-	-	X
9	NDG	B	1681	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9505 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	0	0
			4437	2877	747	785	28			

There is a discrepancy between the modelled and reference sequences:

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

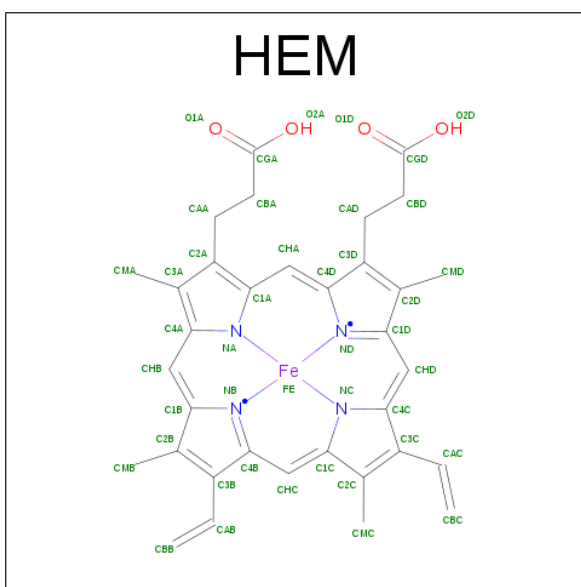
- Molecule 2 is a protein called Prostaglandin G/H synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	553	Total	C	N	O	S	0	8	0
			4472	2901	744	800	27			

There are 2 discrepancies between the modelled and reference sequences:

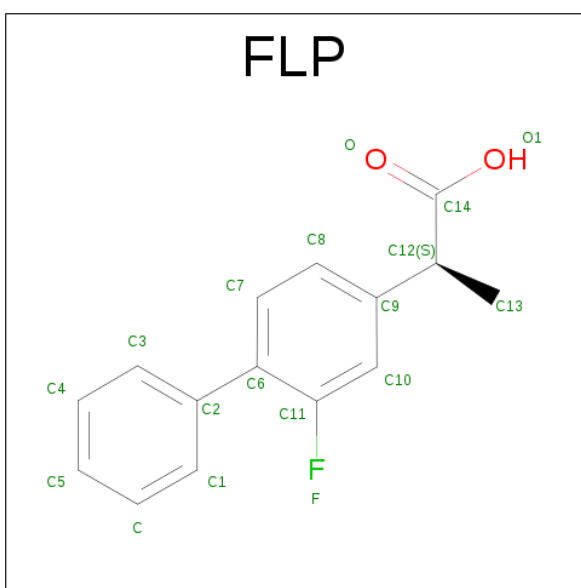
Chain	Residue	Modelled	Actual	Comment	Reference
B	92	LEU	MET	CONFLICT	UNP P05979
B	120	GLN	ARG	CONFLICT	UNP P05979

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



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

- Molecule 4 is FLURBIPROFEN (three-letter code: FLP) (formula: $C_{15}H_{13}FO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			18	15	1	2		

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

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

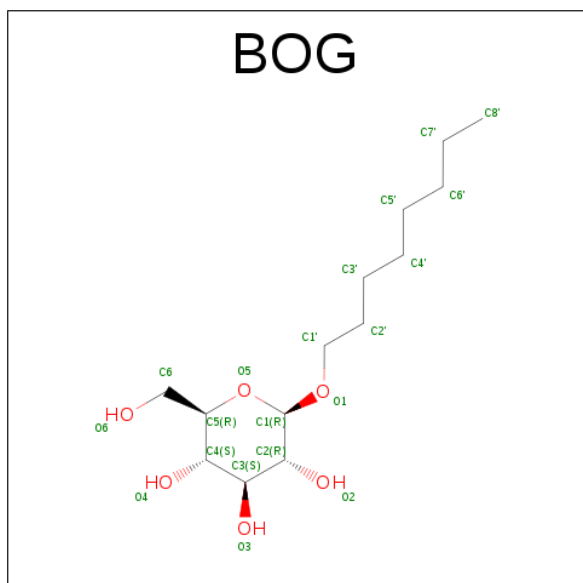
- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 8 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			20	14	6		
8	B	1	Total	C	O	0	0
			13	7	6		
8	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	3	Total	C	N	O	0	0
			39	22	2	15		

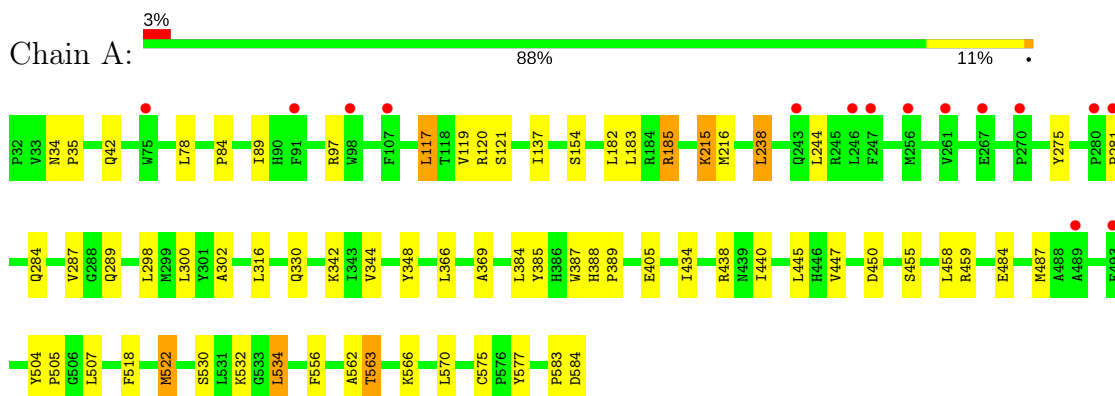
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	105	Total	O	0	0
			105	105		
11	B	108	Total	O	0	0
			108	108		

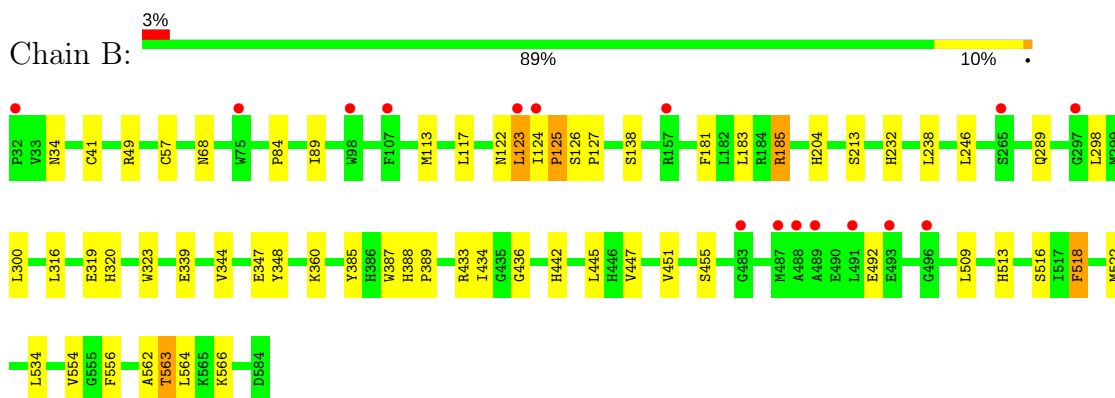
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 2: Prostaglandin G/H synthase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	182.48Å 182.48Å 103.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.91 – 2.75 46.91 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.91-2.75) 99.5 (46.91-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.178 , 0.201 0.191 , 0.211	Depositor DCC
R_{free} test set	1708 reflections (3.49%)	DCC
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.532 for H, K, L 0.468 for -H-K, K, -L	Depositor
Outliers	0 of 50719 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9505	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: BMA, NAG, FLP, NDG, 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	0/4576	0.51	0/6224
2	B	0.35	0/4612	0.51	0/6281
All	All	0.35	0/9188	0.51	0/12505

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
5	A	1	0
9	B	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	661	NAG	C1
9	B	1681	NDG	C1

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	4437	0	4280	36	0
2	B	4472	0	4299	47	0
3	A	43	0	30	1	0
3	B	43	0	30	1	0
4	A	18	0	12	0	0
5	A	28	0	25	0	0
5	B	28	0	25	0	0
6	A	39	0	34	0	0
7	A	61	0	52	0	0
8	A	20	0	28	1	0
8	B	25	0	22	0	0
9	B	39	0	33	0	0
10	B	39	0	34	1	0
11	A	105	0	0	5	0
11	B	108	0	0	5	0
All	All	9505	0	8904	82	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 5.

The worst 5 of 82 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)
2:B:124[B]:ILE:O	2:B:126[B]:SER:N	1.71	1.21
2:B:122[B]:ASN:O	2:B:124[B]:ILE:N	1.87	1.07
2:B:185:ARG:HG3	2:B:185:ARG:HH11	1.24	1.02
2:B:122[B]:ASN:C	2:B:124[B]:ILE:H	1.63	1.01
2:B:124[B]:ILE:C	2:B:126[B]:SER:H	1.65	0.99

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	551/553 (100%)	525 (95%)	26 (5%)	0	100	100
2	B	559/553 (101%)	528 (94%)	26 (5%)	5 (1%)	20	49
All	All	1110/1106 (100%)	1053 (95%)	52 (5%)	5 (0%)	44	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	123[A]	LEU
2	B	123[B]	LEU
2	B	125[A]	PRO
2	B	125[B]	PRO
2	B	204	HIS

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	475/488 (97%)	449 (94%)	26 (6%)	25	54
2	B	480/488 (98%)	462 (96%)	18 (4%)	38	70
All	All	955/976 (98%)	911 (95%)	44 (5%)	31	62

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	522	MET
1	A	575	CYS
2	B	534	LEU
1	A	534	LEU
1	A	563	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	GLN
2	B	581	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 ⓘ

18 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	$\# Z > 2$
5	NAG	A	661	1,5	14,14,15	0.42	0	15,19,21	1.26	1 (6%)
5	NDG	A	662	5	14,14,15	0.55	0	15,19,21	1.72	4 (26%)
7	NAG	A	671	1,7	14,14,15	0.59	0	15,19,21	1.39	2 (13%)
7	NDG	A	672	7	14,14,15	0.63	1 (7%)	15,19,21	2.02	3 (20%)
7	BMA	A	673	7	11,11,12	0.59	0	13,15,17	0.98	1 (7%)
7	MAN	A	674	7	11,11,12	0.53	0	13,15,17	1.54	2 (15%)
7	MAN	A	675	7	11,11,12	0.61	0	13,15,17	1.43	2 (15%)
6	NAG	A	681	1,6	14,14,15	1.86	1 (7%)	15,19,21	2.34	3 (20%)
6	NAG	A	682	6	14,14,15	0.39	0	15,19,21	1.40	2 (13%)
6	BMA	A	683	6	11,11,12	0.57	0	13,15,17	1.51	2 (15%)
5	NAG	B	1661	2,5	14,14,15	0.45	0	15,19,21	0.85	1 (6%)
5	NDG	B	1662	5	14,14,15	0.47	0	15,19,21	1.03	1 (6%)
10	NAG	B	1671	10,2	14,14,15	0.49	0	15,19,21	1.23	1 (6%)
10	NDG	B	1672	10	14,14,15	0.64	0	15,19,21	1.83	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BMA	B	1673	10	11,11,12	0.58	0	13,15,17	1.02	1 (7%)
9	NDG	B	1681	9,2	14,14,15	0.72	0	15,19,21	1.84	4 (26%)
9	NAG	B	1682	9	14,14,15	0.48	0	15,19,21	0.98	1 (6%)
9	MAN	B	1683	9	11,11,12	0.55	0	13,15,17	1.14	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
5	NAG	A	661	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NDG	A	662	5	-	0/6/23/26	0/1/1/1
7	NAG	A	671	1,7	-	0/6/23/26	0/1/1/1
7	NDG	A	672	7	-	0/6/23/26	0/1/1/1
7	BMA	A	673	7	-	0/2/19/22	0/1/1/1
7	MAN	A	674	7	-	0/2/19/22	0/1/1/1
7	MAN	A	675	7	-	0/2/19/22	0/1/1/1
6	NAG	A	681	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	682	6	-	0/6/23/26	0/1/1/1
6	BMA	A	683	6	-	0/2/19/22	0/1/1/1
5	NAG	B	1661	2,5	-	0/6/23/26	0/1/1/1
5	NDG	B	1662	5	-	0/6/23/26	0/1/1/1
10	NAG	B	1671	10,2	-	0/6/23/26	0/1/1/1
10	NDG	B	1672	10	-	0/6/23/26	0/1/1/1
10	BMA	B	1673	10	-	0/2/19/22	0/1/1/1
9	NDG	B	1681	9,2	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	B	1682	9	-	0/6/23/26	0/1/1/1
9	MAN	B	1683	9	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	681	NAG	O5-C1	-6.68	1.32	1.43
7	A	672	NDG	C1-C2	2.02	1.55	1.52

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	681	NAG	C1-O5-C5	-5.72	104.28	112.17
6	A	681	NAG	O5-C1-C2	-5.71	103.53	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	662	NDG	O-C1-C2	-3.54	106.55	111.47
6	A	682	NAG	C4-C3-C2	-2.62	107.18	111.02
9	B	1681	NDG	O-C1-C2	-2.46	108.05	111.47

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	661	NAG	C1
9	B	1681	NDG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1672	NDG	1	0

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	FLP	A	701	-	16,19,19	1.53	1 (6%)	22,26,26	1.29	3 (13%)
8	BOG	A	751	-	20,20,20	0.77	0	25,25,25	1.89	4 (16%)
3	HEM	A	801	11,1	28,50,50	2.28	7 (25%)	17,82,82	1.25	1 (5%)
8	BOG	B	1750	-	13,13,20	0.87	0	18,18,25	1.74	3 (16%)
8	BOG	B	1751	-	12,12,20	1.13	1 (8%)	17,17,25	1.81	4 (23%)
3	HEM	B	601	11,2	28,50,50	2.24	7 (25%)	17,82,82	1.36	2 (11%)

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	FLP	A	701	-	1/1/2/2	0/8/12/12	0/2/2/2
8	BOG	A	751	-	-	0/11/31/31	0/1/1/1
3	HEM	A	801	11,1	-	0/6/54/54	0/0/8/8
8	BOG	B	1750	-	-	0/4/24/31	0/1/1/1
8	BOG	B	1751	-	-	0/2/22/31	0/1/1/1
3	HEM	B	601	11,2	-	0/6/54/54	0/0/8/8

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	FLP	C6-C2	-5.54	1.40	1.49
3	A	801	HEM	C3C-C2C	-4.79	1.34	1.40
3	B	601	HEM	C3C-C2C	-4.44	1.34	1.40
3	B	601	HEM	C3B-C2B	-4.35	1.34	1.40
3	A	801	HEM	C3B-C2B	-4.19	1.34	1.40

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	751	BOG	C1'-O1-C1	-5.56	104.32	113.87
8	B	1751	BOG	O5-C1-C2	-5.25	101.32	110.04
8	A	751	BOG	O5-C1-C2	-4.81	101.03	110.30
8	B	1750	BOG	O5-C1-C2	-4.23	102.14	110.30
8	B	1750	BOG	C1'-O1-C1	-3.84	107.29	113.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	701	FLP	C12

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	751	BOG	1	0
3	A	801	HEM	1	0
3	B	601	HEM	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%)	0.07	15 (2%) 55 49	43, 56, 71, 79	0
2	B	553/553 (100%)	0.01	16 (2%) 52 46	44, 58, 74, 81	0
All	All	1106/1106 (100%)	0.04	31 (2%) 53 48	43, 56, 72, 81	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	PRO	4.2
2	B	123[A]	LEU	4.1
2	B	124[A]	ILE	3.3
2	B	488	ALA	3.2
1	A	107	PHE	3.2

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
5	NAG	B	1661	14/15	0.92	0.29	2.81	59,65,67,71	0
7	NDG	A	672	14/15	0.88	0.34	2.31	64,67,69,73	0
9	NDG	B	1681	14/15	0.90	0.27	0.91	56,59,63,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	A	681	14/15	0.93	0.19	0.26	56,60,62,66	0
7	NAG	A	671	14/15	0.94	0.14	-0.90	46,49,53,58	0
10	NAG	B	1671	14/15	0.95	0.13	-1.39	45,48,51,56	0
6	BMA	A	683	11/12	0.90	0.33	-	77,78,79,79	0
5	NDG	B	1662	14/15	0.84	0.28	-	74,76,77,77	0
7	MAN	A	675	11/12	0.85	0.36	-	95,95,96,96	0
5	NDG	A	662	14/15	0.86	0.32	-	75,77,79,79	0
5	NAG	A	661	14/15	0.92	0.20	-	60,66,68,72	0
9	MAN	B	1683	11/12	0.84	0.31	-	79,80,80,80	0
9	NAG	B	1682	14/15	0.91	0.28	-	71,73,75,77	0
6	NAG	A	682	14/15	0.93	0.17	-	69,71,73,75	0
7	MAN	A	674	11/12	0.65	0.33	-	89,91,92,94	0
10	NDG	B	1672	14/15	0.84	0.33	-	61,64,65,68	0
7	BMA	A	673	11/12	0.91	0.38	-	77,80,84,87	0
10	BMA	B	1673	11/12	0.86	0.39	-	69,70,70,70	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(\AA^2)	Q<0.9
8	BOG	A	751	20/20	0.88	0.29	2.25	78,82,82,83	0
3	HEM	A	801	43/43	0.96	0.18	0.42	52,56,62,66	0
3	HEM	B	601	43/43	0.96	0.19	0.41	54,58,64,66	0
8	BOG	B	1751	12/20	0.91	0.19	-0.07	87,88,88,89	0
4	FLP	A	701	18/18	0.97	0.18	-0.15	53,55,57,58	0
8	BOG	B	1750	13/20	0.90	0.27	-	94,94,94,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.