



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:50 AM 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 Full wwPDB X-ray Structure Validation 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.

---

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

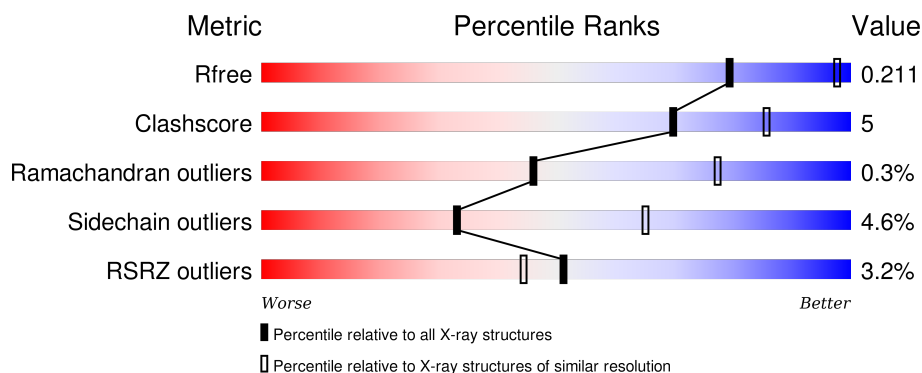
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (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  $\geq 3$ , 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>3%</div> <div>88%</div> <div>11%</div> </div>
2	B	553	<div> <div>3%</div> <div>89%</div> <div>10%</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:

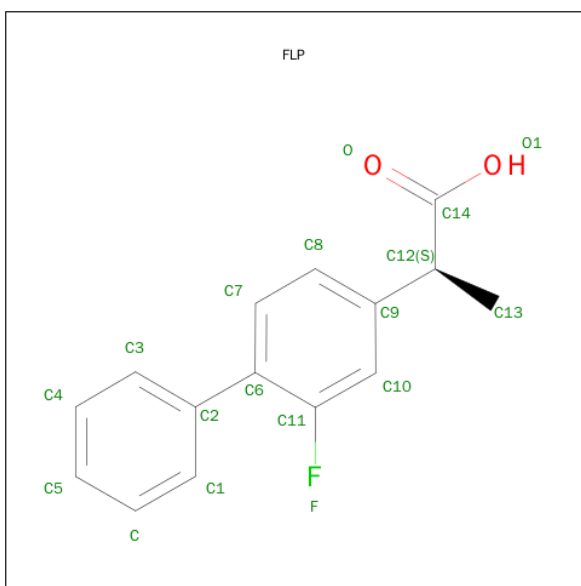
Chain	Residue	Modelled	Actual	Comment	Reference
B	92	LEU	MET	CONFLICT	UNP P05979
B	120	GLN	ARG	CONFLICT	UNP P05979

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- 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		

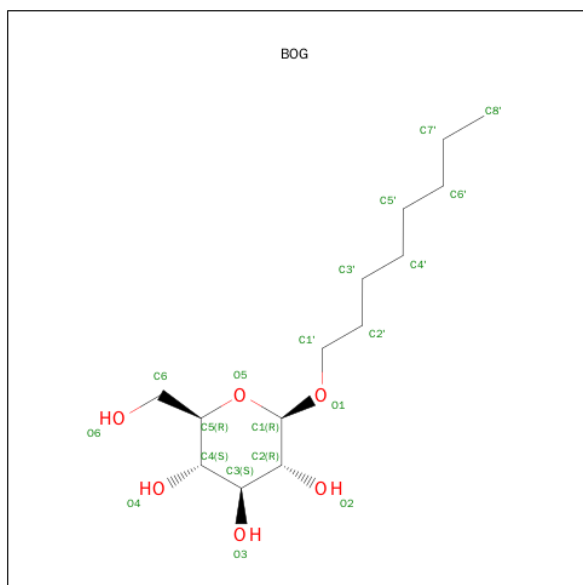
- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

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<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



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		

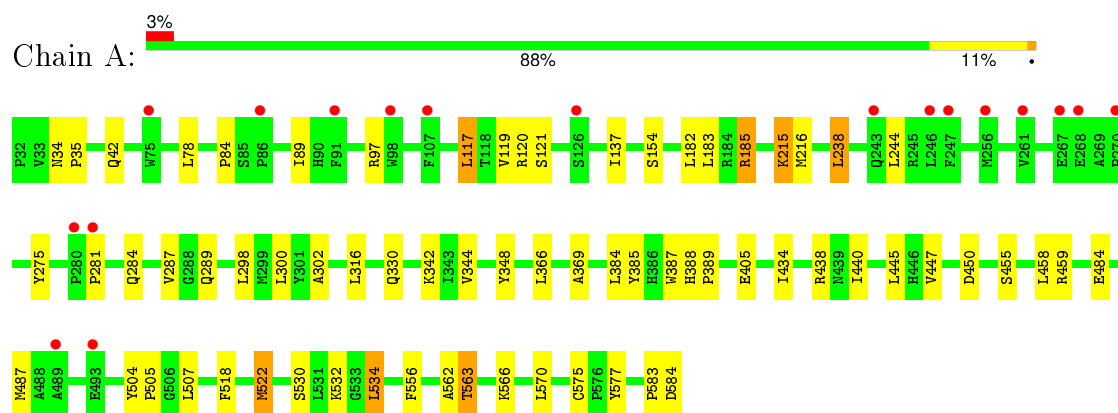
- Molecule 11 is water.

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

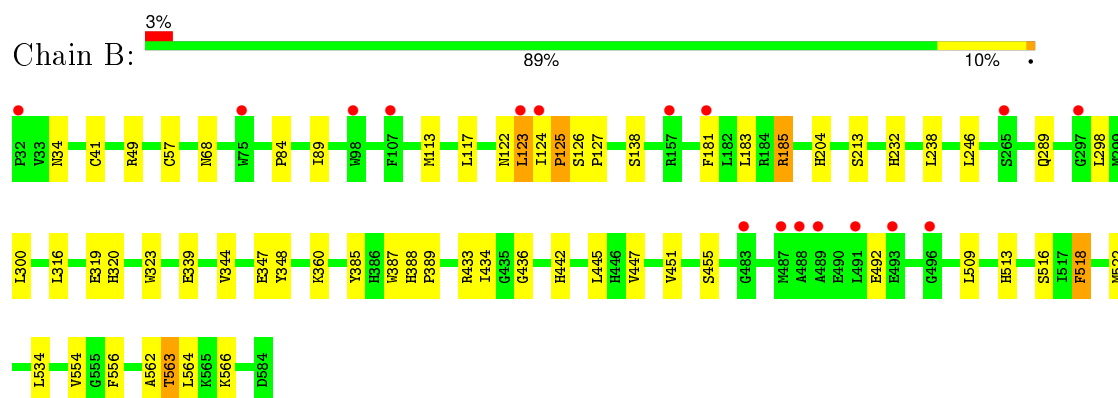
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 32.5	EDS
Estimated twinning fraction	0.532 for H, K, L 0.468 for -H-K, K, -L 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
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
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 <sup>2</sup> )	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.*

<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 [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.

All (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
2:B:41:CYS:HB2	11:B:640:HOH:O	1.63	0.98
2:B:126[B]:SER:HA	2:B:127[B]:PRO:C	1.91	0.90
2:B:124[B]:ILE:C	2:B:126[B]:SER:N	2.25	0.83
1:A:563:THR:HG22	1:A:566:LYS:H	1.43	0.82
2:B:125[B]:PRO:O	2:B:127[B]:PRO:O	1.99	0.79
2:B:124[B]:ILE:HG22	2:B:124[B]:ILE:O	1.84	0.77
1:A:369:ALA:HB3	11:A:628:HOH:O	1.87	0.74
2:B:122[B]:ASN:OD1	2:B:123[B]:LEU:N	2.22	0.70
2:B:122[B]:ASN:CG	2:B:123[B]:LEU:H	1.97	0.69
2:B:122[B]:ASN:C	2:B:124[B]:ILE:N	2.34	0.68
2:B:185:ARG:NH1	2:B:185:ARG:HG3	2.03	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:CYS:SG	11:B:640:HOH:O	2.54	0.66
2:B:122[B]:ASN:CG	2:B:123[B]:LEU:N	2.50	0.65
2:B:124[B]:ILE:O	2:B:125[B]:PRO:C	2.33	0.65
2:B:563:THR:HG22	2:B:566:LYS:H	1.62	0.65
1:A:459:ARG:HD3	11:A:24:HOH:O	2.01	0.59
1:A:344:VAL:HA	1:A:348:TYR:HB3	1.88	0.56
1:A:342:LYS:HG2	1:A:562:ALA:HB3	1.87	0.55
1:A:185:ARG:HH21	1:A:438:ARG:HG2	1.73	0.54
2:B:113:MET:O	2:B:117:LEU:HD13	2.08	0.54
1:A:119:VAL:HG12	8:A:751:BOG:H62	1.90	0.53
1:A:387:TRP:HB2	3:A:801:HEM:HAC	1.91	0.53
2:B:344:VAL:HA	2:B:348:TYR:HB3	1.90	0.52
1:A:121:SER:HB2	1:A:532:LYS:HD3	1.91	0.52
2:B:433:ARG:HH11	2:B:436:GLY:HA3	1.75	0.51
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.92	0.51
2:B:126[A]:SER:HA	2:B:127[A]:PRO:C	2.31	0.51
1:A:287:VAL:HG11	1:A:302:ALA:HB1	1.92	0.51
1:A:388:HIS:N	1:A:389:PRO:CD	2.75	0.50
1:A:275:TYR:CE2	1:A:284:GLN:HB2	2.47	0.50
2:B:41:CYS:SG	2:B:68:ASN:HA	2.53	0.49
2:B:387:TRP:HB2	3:B:601:HEM:HAC	1.94	0.49
1:A:507:LEU:HB3	1:A:522:MET:CE	2.43	0.48
2:B:344:VAL:O	2:B:348:TYR:HB3	2.14	0.48
2:B:447:VAL:O	2:B:451:VAL:HG23	2.13	0.48
2:B:124[B]:ILE:HG22	2:B:126[B]:SER:N	2.28	0.48
1:A:281:PRO:HA	1:A:284:GLN:HG2	1.96	0.48
2:B:124[B]:ILE:HG22	2:B:126[B]:SER:H	1.78	0.48
2:B:339:GLU:HG2	2:B:562:ALA:HB2	1.96	0.47
1:A:216:MET:HE1	11:A:614:HOH:O	2.13	0.47
1:A:532:LYS:HE3	11:A:615:HOH:O	2.15	0.47
2:B:319:GLU:OE2	2:B:554:VAL:HG21	2.14	0.47
1:A:487:MET:HB3	1:A:487:MET:HE2	1.78	0.47
2:B:34:ASN:HA	2:B:49:ARG:HH21	1.80	0.47
2:B:124[B]:ILE:O	2:B:126[B]:SER:O	2.34	0.46
2:B:183:LEU:HD13	2:B:445:LEU:HD22	1.98	0.46
1:A:389:PRO:HB2	1:A:434:ILE:HA	1.97	0.46
1:A:182:LEU:HB3	1:A:440:ILE:HD12	1.98	0.45
2:B:122[B]:ASN:OD1	2:B:123[B]:LEU:HD23	2.15	0.45
1:A:183:LEU:HD13	1:A:445:LEU:HD22	1.97	0.45
1:A:97:ARG:HB3	1:A:97:ARG:NH1	2.32	0.44
1:A:507:LEU:HD22	1:A:522:MET:HE2	2.00	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD13	10:B:1672:NDG:H6C2	2.00	0.43
2:B:84:PRO:HG2	2:B:89:ILE:HD11	2.00	0.43
2:B:181:PHE:HB3	2:B:509:LEU:HD21	2.00	0.43
2:B:388:HIS:N	2:B:389:PRO:CD	2.82	0.43
2:B:320:HIS:HB3	2:B:323:TRP:CG	2.53	0.43
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.54	0.43
2:B:518:PHE:CD1	2:B:522:MET:HG2	2.54	0.42
1:A:344:VAL:O	1:A:348:TYR:HB3	2.18	0.42
2:B:126[B]:SER:CA	2:B:127[B]:PRO:C	2.72	0.42
2:B:185:ARG:CG	2:B:185:ARG:NH1	2.72	0.42
1:A:330:GLN:HB3	2:B:138:SER:HB2	2.00	0.42
1:A:84:PRO:HG2	1:A:89:ILE:HD11	2.01	0.42
2:B:389:PRO:HB2	2:B:434:ILE:HA	2.01	0.42
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.56	0.41
2:B:124[B]:ILE:HG22	2:B:126[B]:SER:O	2.20	0.41
2:B:513:HIS:HB2	2:B:516:SER:OG	2.21	0.41
2:B:442:HIS:CD2	11:B:671:HOH:O	2.72	0.41
1:A:530:SER:O	1:A:534:LEU:HD22	2.20	0.41
1:A:34:ASN:HA	1:A:35:PRO:HD2	1.95	0.41
2:B:455:SER:C	11:B:623:HOH:O	2.59	0.41
1:A:117:LEU:HB3	1:A:366:LEU:HD21	2.03	0.41
1:A:215:LYS:H	1:A:215:LYS:HD3	1.86	0.41
1:A:137:ILE:HD12	11:B:635:HOH:O	2.21	0.41
1:A:154:SER:HB2	1:A:459:ARG:HB2	2.03	0.40
1:A:120:ARG:HG2	11:A:663:HOH:O	2.21	0.40

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	551/553 (100%)	525 (95%)	26 (5%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	559/553 (101%)	528 (94%)	26 (5%)	5 (1%)	21	52
All	All	1110/1106 (100%)	1053 (95%)	52 (5%)	5 (0%)	46	67

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%)	27	56
2	B	480/488 (98%)	462 (96%)	18 (4%)	40	73
All	All	955/976 (98%)	911 (95%)	44 (5%)	33	65

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	78	LEU
1	A	117	LEU
1	A	185	ARG
1	A	215	LYS
1	A	238	LEU
1	A	244	LEU
1	A	289	GLN
1	A	298	LEU
1	A	300	LEU
1	A	316	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	384	LEU
1	A	385	TYR
1	A	405	GLU
1	A	450	ASP
1	A	455	SER
1	A	458	LEU
1	A	484	GLU
1	A	518	PHE
1	A	522	MET
1	A	534	LEU
1	A	556	PHE
1	A	563	THR
1	A	570	LEU
1	A	575	CYS
1	A	584	ASP
2	B	185	ARG
2	B	213	SER
2	B	232	HIS
2	B	238	LEU
2	B	246	LEU
2	B	289	GLN
2	B	298	LEU
2	B	300	LEU
2	B	316	LEU
2	B	347	GLU
2	B	360	LYS
2	B	385	TYR
2	B	492	GLU
2	B	518	PHE
2	B	534	LEU
2	B	556	PHE
2	B	563	THR
2	B	564	LEU

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	0.41	0	15,19,21	1.32	1 (6%)
5	NDG	A	662	5	14,14,15	0.53	0	15,19,21	1.43	3 (20%)
7	NAG	A	671	1,7	14,14,15	0.58	0	15,19,21	1.41	2 (13%)
7	NDG	A	672	7	14,14,15	0.62	0	15,19,21	2.01	2 (13%)
7	BMA	A	673	7	11,11,12	0.58	0	14,15,17	0.97	1 (7%)
7	MAN	A	674	7	11,11,12	0.52	0	14,15,17	1.64	2 (14%)
7	MAN	A	675	7	11,11,12	0.59	0	14,15,17	1.48	2 (14%)
6	NAG	A	681	1,6	14,14,15	1.82	1 (7%)	15,19,21	2.13	4 (26%)
6	NAG	A	682	6	14,14,15	0.38	0	15,19,21	1.32	2 (13%)
6	BMA	A	683	6	11,11,12	0.56	0	14,15,17	1.60	2 (14%)
5	NAG	B	1661	2,5	14,14,15	0.44	0	15,19,21	0.62	0
5	NDG	B	1662	5	14,14,15	0.46	0	15,19,21	1.10	1 (6%)
10	NAG	B	1671	10,2	14,14,15	0.47	0	15,19,21	1.30	1 (6%)
10	NDG	B	1672	10	14,14,15	0.63	0	15,19,21	1.93	5 (33%)
10	BMA	B	1673	10	11,11,12	0.57	0	14,15,17	1.03	1 (7%)
9	NDG	B	1681	9,2	14,14,15	0.71	0	15,19,21	1.75	4 (26%)
9	NAG	B	1682	9	14,14,15	0.47	0	15,19,21	1.05	1 (6%)
9	MAN	B	1683	9	11,11,12	0.54	0	14,15,17	1.19	2 (14%)



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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	681	NAG	O5-C1	-6.54	1.32	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	681	NAG	C1-O5-C5	-6.28	104.28	112.25
6	A	682	NAG	C4-C3-C2	-2.61	107.18	111.23
9	B	1681	NDG	C3-C2-N2	-2.20	105.30	110.56
6	A	681	NAG	C4-C3-C2	-2.02	108.09	111.23
9	B	1683	MAN	C1-C2-C3	2.17	112.11	109.54
5	A	662	NDG	C1-O-C5	2.20	115.05	112.25
7	A	671	NAG	O4-C4-C3	2.29	115.50	110.34
10	B	1672	NDG	C3-C4-C5	2.34	114.27	110.20
9	B	1682	NAG	C1-O5-C5	2.35	115.23	112.25
10	B	1673	BMA	C3-C4-C5	2.41	114.39	110.20
7	A	672	NDG	C2-N2-C7	2.41	126.14	123.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	1672	NDG	C2-N2-C7	2.45	126.19	123.04
6	A	681	NAG	C3-C4-C5	2.53	114.61	110.20
10	B	1672	NDG	O-C5-C6	2.61	112.99	107.35
5	A	662	NDG	C4-C3-C2	2.72	115.46	111.23
7	A	673	BMA	C1-O5-C5	2.73	115.71	112.25
9	B	1681	NDG	C2-N2-C7	2.75	126.58	123.04
7	A	674	MAN	C3-C4-C5	2.86	115.18	110.20
6	A	683	BMA	C1-C2-C3	2.88	112.95	109.54
6	A	681	NAG	C3-C2-N2	2.98	117.71	110.56
5	B	1662	NDG	C1-O-C5	3.02	116.09	112.25
6	A	682	NAG	C1-O5-C5	3.03	116.09	112.25
9	B	1681	NDG	C3-C4-C5	3.04	115.50	110.20
7	A	675	MAN	C3-C4-C5	3.18	115.74	110.20
9	B	1683	MAN	C1-O5-C5	3.45	116.63	112.25
5	A	662	NDG	C3-C4-C5	3.53	116.36	110.20
7	A	675	MAN	C1-O5-C5	3.57	116.78	112.25
10	B	1672	NDG	C4-C3-C2	3.77	117.08	111.23
7	A	671	NAG	C1-O5-C5	3.94	117.25	112.25
5	A	661	NAG	C1-O5-C5	3.99	117.31	112.25
10	B	1672	NDG	C1-O-C5	4.12	117.48	112.25
9	B	1681	NDG	C4-C3-C2	4.28	117.89	111.23
10	B	1671	NAG	C1-O5-C5	4.66	118.16	112.25
6	A	683	BMA	C1-O5-C5	4.68	118.19	112.25
7	A	674	MAN	C1-O5-C5	4.96	118.55	112.25
7	A	672	NDG	C1-O-C5	6.84	120.92	112.25

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

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	1.59	1 (6%)	21,26,26	1.38	3 (14%)
8	BOG	A	751	-	20,20,20	0.75	0	25,25,25	1.84	4 (16%)
3	HEM	A	801	11,1	30,50,50	2.20	10 (33%)	24,82,82	2.22	7 (29%)
8	BOG	B	1750	-	13,13,20	0.85	0	18,18,25	1.65	3 (16%)
8	BOG	B	1751	-	12,12,20	1.12	1 (8%)	17,17,25	1.84	4 (23%)
3	HEM	B	601	11,2	30,50,50	2.21	10 (33%)	24,82,82	2.29	10 (41%)

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	-	0/10/54/54	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	-	0/10/54/54	0/0/8/8

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HEM	C3B-C4B	-6.92	1.45	1.51
3	B	601	HEM	C3B-C4B	-6.78	1.45	1.51
4	A	701	FLP	C6-C2	-5.81	1.40	1.49
3	A	801	HEM	C3D-C4D	-5.25	1.44	1.51
3	B	601	HEM	C3D-C4D	-5.21	1.44	1.51
3	A	801	HEM	C2C-C1C	-3.77	1.45	1.52
3	B	601	HEM	C2C-C1C	-3.70	1.45	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1751	BOG	O5-C1	-2.13	1.39	1.43
3	B	601	HEM	C2D-C1D	-2.06	1.45	1.51
3	A	801	HEM	C2D-C1D	-2.03	1.45	1.51
3	A	801	HEM	C3C-CAC	2.11	1.55	1.51
3	B	601	HEM	C3B-CAB	2.17	1.55	1.51
3	A	801	HEM	CAA-C2A	2.19	1.55	1.52
3	B	601	HEM	CAA-C2A	2.25	1.55	1.52
3	B	601	HEM	C1C-NC	2.26	1.38	1.36
3	B	601	HEM	FE-NC	2.27	2.04	1.95
3	A	801	HEM	FE-NC	2.28	2.04	1.95
3	A	801	HEM	C3B-CAB	2.29	1.55	1.51
3	A	801	HEM	C4C-NC	2.34	1.38	1.36
3	B	601	HEM	C4C-NC	2.50	1.39	1.36
3	A	801	HEM	FE-ND	2.98	2.13	1.97
3	B	601	HEM	FE-ND	3.15	2.14	1.97

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	751	BOG	C1'-O1-C1	-5.51	104.32	113.94
8	B	1751	BOG	O5-C1-C2	-5.31	101.32	109.80
8	A	751	BOG	O5-C1-C2	-4.51	101.03	110.28
8	B	1750	BOG	O5-C1-C2	-3.96	102.14	110.28
8	B	1750	BOG	C1'-O1-C1	-3.67	107.29	113.29
8	B	1751	BOG	C1-C2-C3	-3.28	105.55	110.43
4	A	701	FLP	C10-C11-C6	-3.28	120.11	124.24
8	A	751	BOG	C1-C2-C3	-2.72	104.61	109.97
8	B	1750	BOG	C4-C3-C2	-2.69	105.77	110.79
8	A	751	BOG	C4-C3-C2	-2.65	105.84	110.79
4	A	701	FLP	C14-C12-C9	-2.65	107.12	112.32
8	B	1751	BOG	C4-C3-C2	-2.62	105.90	110.79
3	B	601	HEM	CMA-C3A-C4A	-2.28	124.59	128.36
3	B	601	HEM	C3B-C4B-NB	-2.03	107.75	111.63
8	B	1751	BOG	O5-C5-C4	-2.03	105.88	109.68
3	A	801	HEM	C3B-C4B-CHC	2.10	126.12	123.16
3	A	801	HEM	C2D-C3D-C4D	2.18	105.19	101.50
3	B	601	HEM	C2C-C1C-CHC	2.25	127.11	123.68
3	B	601	HEM	C2D-C3D-C4D	2.29	105.38	101.50
3	B	601	HEM	C3B-C4B-CHC	2.63	126.87	123.16
3	B	601	HEM	CMD-C2D-C3D	2.94	127.36	114.35
3	A	801	HEM	CMD-C2D-C3D	2.95	127.38	114.35
3	A	801	HEM	CMC-C2C-C3C	3.47	125.19	116.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	HEM	CMC-C2C-C3C	3.49	125.24	116.53
4	A	701	FLP	C7-C6-C11	3.61	119.49	115.90
3	A	801	HEM	CAD-C3D-C4D	4.07	126.81	112.47
3	B	601	HEM	CAD-C3D-C4D	4.17	127.17	112.47
3	B	601	HEM	CMB-C2B-C3B	4.27	127.19	116.53
3	A	801	HEM	CMB-C2B-C3B	4.29	127.23	116.53
3	B	601	HEM	CAD-C3D-C2D	4.95	127.45	113.22
3	A	801	HEM	CAD-C3D-C2D	5.14	127.99	113.22

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 ⓘ

### 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, 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%)	0.10	18 (3%)	50	43	43, 56, 71, 79	0
2	B	553/553 (100%)	0.05	17 (3%)	52	46	44, 58, 74, 81	0
All	All	1106/1106 (100%)	0.08	35 (3%)	51	44	43, 56, 72, 81	0

All (35) 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	3.3
1	A	107	PHE	3.3
2	B	483	GLY	3.1
2	B	489	ALA	3.1
1	A	281	PRO	3.1
1	A	75	TRP	2.9
1	A	493	GLU	2.9
1	A	261	VAL	2.8
2	B	75	TRP	2.8
2	B	265	SER	2.8
2	B	157	ARG	2.7
1	A	256	MET	2.7
2	B	491	LEU	2.6
2	B	107	PHE	2.6
2	B	32	PRO	2.6
1	A	243	GLN	2.4
1	A	91	PHE	2.4
2	B	487	MET	2.3
2	B	297	GLY	2.3
2	B	98	TRP	2.3
1	A	247	PHE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	493	GLU	2.3
1	A	489	ALA	2.2
2	B	496	GLY	2.2
1	A	270	PRO	2.2
1	A	267	GLU	2.2
1	A	246	LEU	2.1
1	A	98	TRP	2.1
1	A	268	GLU	2.0
2	B	181	PHE	2.0
1	A	126	SER	2.0
1	A	86	PRO	2.0

## 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
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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, 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
8	BOG	A	751	20/20	0.88	0.29	2.24	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.