Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:50 AM GMT

PDB ID	:	3N8V
Title	:	Crystal Structure of Unoccupied Cyclooxygenase-1
Authors	:	Sidhu, R.S.
Deposited on	:	2010-05-28
Resolution	:	3.05 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

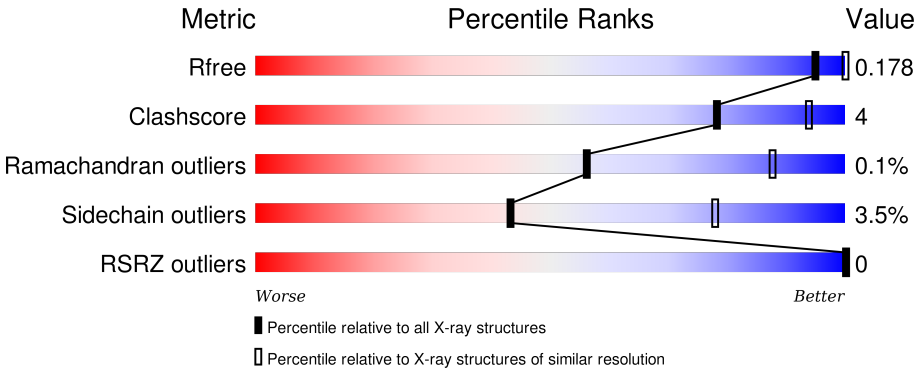
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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 <=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	91% 8%
1	B	553	86% 13%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9500 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.

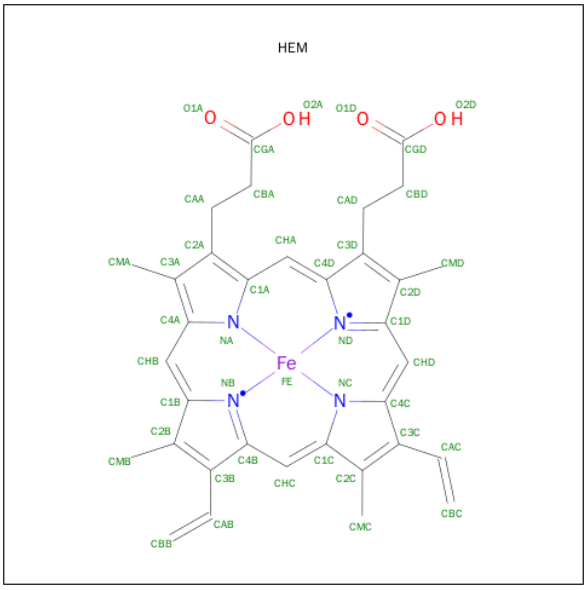
- Molecule 1 is a protein called Prostaglandin G/H synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	5	0	0
			4447	2882	745	792	28			
1	B	553	Total	C	N	O	S	0	0	0
			4422	2869	741	785	27			

There are 2 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

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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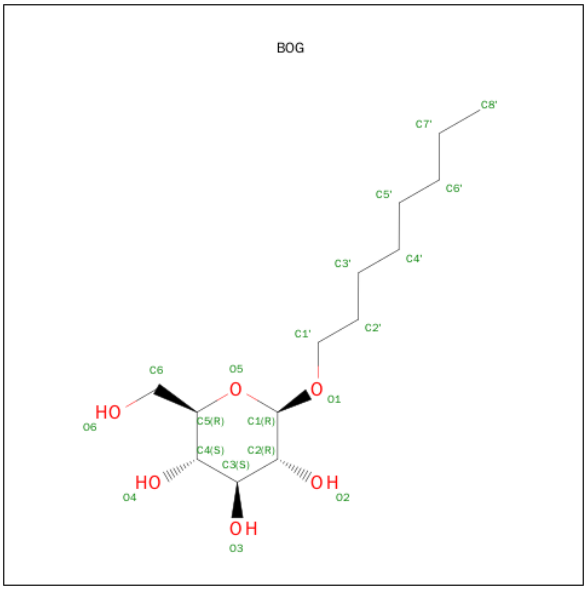
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is B-octylglucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			20	14	6			
3	A	1	Total	C	O		0	0
			12	6	6			
3	B	1	Total	C	O		5	0
			20	14	6			
3	B	1	Total	C	O		0	0
			20	14	6			
3	B	1	Total	C	O		0	0
			20	14	6			

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

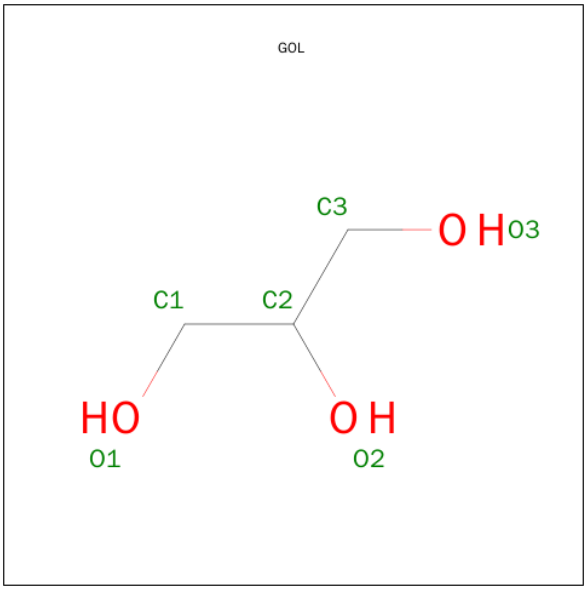
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

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

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- 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		

- 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		

- Molecule 10 is water.

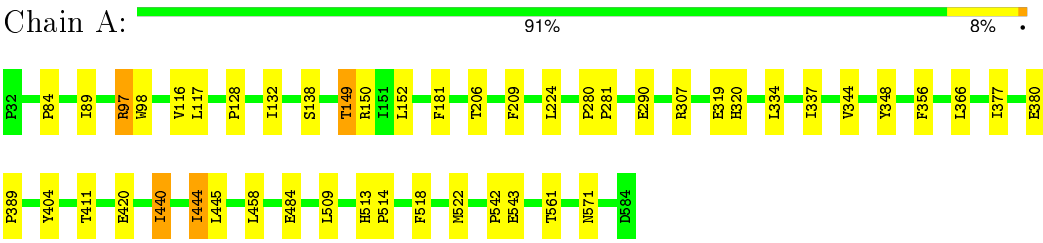
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	116	Total O 116 116	0	0
10	B	108	Total O 108 108	0	0

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 (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.

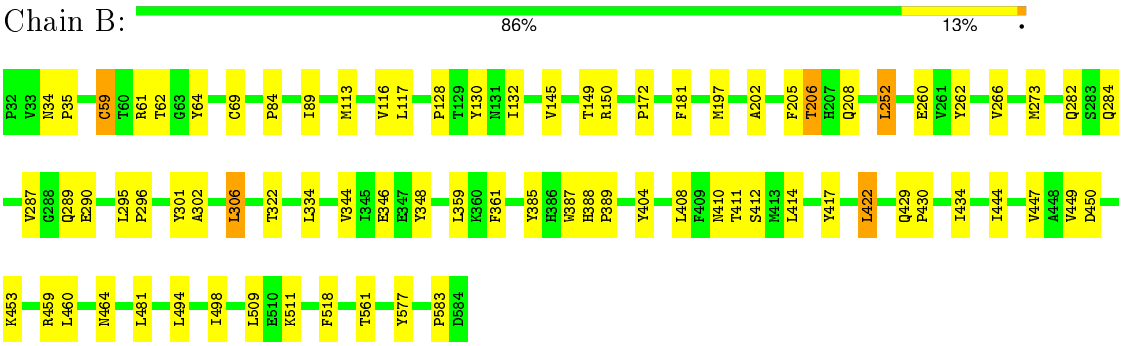
- Molecule 1: Prostaglandin G/H synthase 1

Chain A:



- Molecule 1: Prostaglandin G/H synthase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	181.91Å 181.91Å 102.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.20 – 3.05 40.20 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.20-3.05) 99.7 (40.20-3.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.203 , 0.235 0.155 , 0.178	Depositor DCC
R_{free} test set	1500 reflections (4.25%)	DCC
Wilson B-factor (Å^2)	66.5	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 25.2	EDS
Estimated twinning fraction	0.512 for H, K, L 0.488 for -H-K, K, -L 0.106 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.512 for H, K, L 0.488 for -H-K, K, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 36850 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9500	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, 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	0.33	0/4585	0.47	0/6236
1	B	0.33	0/4560	0.47	0/6206
All	All	0.33	0/9145	0.47	0/12442

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4447	0	4291	27	0
1	B	4422	0	4256	39	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	32	0	39	1	0
3	B	60	0	80	1	0
4	A	28	0	25	1	0
4	B	28	0	25	0	0
5	A	28	0	25	0	0
6	A	61	0	52	0	0
7	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	28	0	25	0	0
9	B	50	0	43	0	0
10	A	116	0	0	1	0
10	B	108	0	0	4	0
All	All	9500	0	8929	65	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 4.

All (65) 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:97:ARG:H	1:A:98:TRP:HB2	1.30	0.97
1:A:543:GLU:HB2	10:B:655:HOH:O	1.74	0.87
1:B:59:CYS:HB3	1:B:69:CYS:SG	2.24	0.77
1:A:97:ARG:N	1:A:98:TRP:HB2	2.00	0.76
1:A:388:HIS:HB3	1:A:440:ILE:HD13	1.74	0.69
1:A:97:ARG:H	1:A:98:TRP:CB	2.03	0.68
1:B:130:TYR:HB2	1:B:150:ARG:HB2	1.80	0.63
1:B:128:PRO:HB3	1:B:149:THR:HG21	1.83	0.61
1:A:209:PHE:HB2	1:A:377:ILE:HG13	1.83	0.61
1:B:172:PRO:HB3	1:B:494:LEU:HD12	1.84	0.60
1:A:344:VAL:HA	1:A:348:TYR:HB3	1.84	0.58
1:B:273:MET:HG2	1:B:290:GLU:HA	1.87	0.56
1:A:128:PRO:HB3	1:A:149:THR:HG21	1.88	0.54
1:A:388:HIS:N	1:A:389:PRO:CD	2.71	0.54
1:B:150:ARG:HH22	1:B:460:LEU:HA	1.72	0.54
1:A:132:ILE:HD12	1:A:458:LEU:HD23	1.90	0.53
1:B:84:PRO:HG2	1:B:89:ILE:HD11	1.93	0.51
1:B:287:VAL:HG11	1:B:302:ALA:HB1	1.93	0.50
1:B:346:GLU:HG2	1:B:359:LEU:O	2.11	0.50
1:A:97:ARG:CA	1:A:98:TRP:HB2	2.42	0.50
1:B:181:PHE:HB3	1:B:509:LEU:HD21	1.95	0.49
1:B:266:VAL:HG23	1:B:284:GLN:HB3	1.95	0.48
1:B:344:VAL:HA	1:B:348:TYR:HB3	1.96	0.47
1:A:116:VAL:HG22	3:A:751:BOG:H2'2	1.96	0.47
1:B:417:TYR:HB2	1:B:422:LEU:HD13	1.96	0.47
1:B:388:HIS:N	1:B:389:PRO:CD	2.78	0.47
1:B:410:ASN:OD1	1:B:412:SER:N	2.48	0.47
1:B:344:VAL:O	1:B:348:TYR:HB3	2.15	0.47
1:B:577:TYR:CE2	1:B:583:PRO:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ARG:HG2	1:A:152:LEU:O	2.15	0.46
1:A:97:ARG:HG2	1:A:356:PHE:CE1	2.51	0.46
1:B:387:TRP:HB3	1:B:434:ILE:HG12	1.97	0.46
1:B:481:LEU:O	1:B:511:LYS:HG2	2.17	0.45
1:A:84:PRO:HG2	1:A:89:ILE:HD11	1.98	0.45
1:A:181:PHE:HB3	1:A:509:LEU:HD21	1.98	0.45
1:B:361:PHE:HB2	10:B:626:HOH:O	2.17	0.44
1:B:346:GLU:HG3	10:B:626:HOH:O	2.18	0.44
1:A:404:TYR:HE1	1:A:444:ILE:HD11	1.83	0.44
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.92	0.43
1:A:484:GLU:HB3	10:A:654:HOH:O	2.18	0.43
1:A:319:GLU:HG3	1:A:320:HIS:CD2	2.53	0.43
1:B:62:THR:HG23	1:B:64:TYR:H	1.84	0.43
1:B:205:PHE:O	1:B:208:GLN:HG2	2.18	0.43
1:A:542:PRO:O	1:B:61:ARG:NH1	2.51	0.43
1:B:410:ASN:OD1	1:B:411:THR:N	2.51	0.43
1:A:404:TYR:CE1	1:A:444:ILE:HD11	2.53	0.43
1:B:197:MET:SD	1:B:301:TYR:OH	2.73	0.42
1:B:464:ASN:HD21	1:B:498:ILE:HG13	1.83	0.42
1:B:34:ASN:HA	1:B:35:PRO:HD3	1.93	0.42
1:B:295:LEU:HA	1:B:296:PRO:HD3	1.93	0.42
1:B:116:VAL:HA	3:B:1751:BOG:H1'1	2.01	0.42
1:B:459:ARG:HD3	10:B:605:HOH:O	2.20	0.42
1:B:449:VAL:HG12	1:B:453:LYS:HE2	2.01	0.42
1:B:202:ALA:O	1:B:206:THR:HB	2.19	0.42
1:B:429:GLN:HA	1:B:430:PRO:HD3	1.89	0.42
4:A:661:NAG:H61	4:A:662:NDG:C7	2.50	0.42
1:A:138:SER:HA	1:B:334:LEU:HD11	2.03	0.41
1:A:117:LEU:HB3	1:A:366:LEU:HD21	2.02	0.41
1:A:290:GLU:H	1:A:290:GLU:CD	2.24	0.41
1:A:307:ARG:HD2	1:A:571:ASN:HB3	2.01	0.41
1:B:260:GLU:HB2	1:B:262:TYR:CE2	2.56	0.40
1:B:388:HIS:CE1	1:B:447:VAL:HG11	2.56	0.40
1:B:252:LEU:HD13	1:B:306:LEU:HD22	2.03	0.40
1:A:334:LEU:HA	1:A:337:ILE:HD12	2.04	0.40
1:B:404:TYR:O	1:B:408:LEU:HB2	2.21	0.40

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%)	524 (95%)	26 (5%)	1 (0%)	52 84
1	B	551/553 (100%)	524 (95%)	27 (5%)	0	100 100
All	All	1102/1106 (100%)	1048 (95%)	53 (5%)	1 (0%)	56 88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	PRO

5.3.2 Protein sidechains (i)

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	478/488 (98%)	463 (97%)	15 (3%)	47 80
1	B	472/488 (97%)	454 (96%)	18 (4%)	40 75
All	All	950/976 (97%)	917 (96%)	33 (4%)	43 78

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	149	THR
1	A	206	THR
1	A	224	LEU
1	A	380	GLU

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Mol	Chain	Res	Type
1	A	385	TYR
1	A	411	THR
1	A	420	GLU
1	A	440	ILE
1	A	444	ILE
1	A	445	LEU
1	A	513	HIS
1	A	518	PHE
1	A	522	MET
1	A	561	THR
1	B	59	CYS
1	B	113	MET
1	B	117	LEU
1	B	132	ILE
1	B	145	VAL
1	B	206	THR
1	B	252	LEU
1	B	282	GLN
1	B	289	GLN
1	B	306	LEU
1	B	322	THR
1	B	385	TYR
1	B	414	LEU
1	B	422	LEU
1	B	444	ILE
1	B	450	ASP
1	B	518	PHE
1	B	561	THR

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 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 (i)

17 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	$\#\|Z\| > 2$
4	NAG	A	661	1,4	14,14,15	0.50	0	15,19,21	1.07	2 (13%)
4	NDG	A	662	4	14,14,15	0.43	0	15,19,21	1.41	1 (6%)
6	NAG	A	671	1,6	14,14,15	0.46	0	15,19,21	1.18	1 (6%)
6	NDG	A	672	6	14,14,15	0.62	0	15,19,21	1.74	3 (20%)
6	BMA	A	673	6	11,11,12	0.53	0	14,15,17	1.20	1 (7%)
6	MAN	A	674	6	11,11,12	0.50	0	14,15,17	1.70	2 (14%)
6	MAN	A	675	6	11,11,12	0.53	0	14,15,17	0.87	1 (7%)
5	NAG	A	681	1,5	14,14,15	0.48	0	15,19,21	0.67	0
5	NAG	A	682	5	14,14,15	0.47	0	15,19,21	0.90	1 (6%)
4	NAG	B	1661	1,4	14,14,15	0.56	0	15,19,21	1.09	2 (13%)
4	NDG	B	1662	4	14,14,15	0.47	0	15,19,21	1.20	1 (6%)
9	NAG	B	1671	1,9	14,14,15	1.36	1 (7%)	15,19,21	1.15	1 (6%)
9	NDG	B	1672	9	14,14,15	0.46	0	15,19,21	1.58	2 (13%)
9	BMA	B	1673	9	11,11,12	0.57	0	14,15,17	0.89	1 (7%)
9	BMA	B	1674	9	11,11,12	0.57	0	14,15,17	1.60	2 (14%)
8	NDG	B	1681	1,8	14,14,15	0.52	0	15,19,21	0.69	0
8	NAG	B	1682	8	14,14,15	0.58	0	15,19,21	1.56	2 (13%)

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	NAG	A	661	1,4	-	0/6/23/26	0/1/1/1
4	NDG	A	662	4	-	0/6/23/26	0/1/1/1
6	NAG	A	671	1,6	-	0/6/23/26	0/1/1/1
6	NDG	A	672	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	A	673	6	-	0/2/19/22	1/1/1/1
6	MAN	A	674	6	-	0/2/19/22	1/1/1/1
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
4	NAG	B	1661	1,4	-	0/6/23/26	0/1/1/1
4	NDG	B	1662	4	-	0/6/23/26	0/1/1/1
9	NAG	B	1671	1,9	-	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	1/1/1/1
8	NDG	B	1681	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1682	8	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1671	NAG	O5-C1	-4.82	1.35	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1661	NAG	C4-C3-C2	2.03	114.39	111.23
9	B	1673	BMA	C1-O5-C5	2.07	114.87	112.25
6	A	672	NDG	O4-C4-C5	2.08	114.76	109.24
4	B	1661	NAG	O4-C4-C3	2.12	115.11	110.34
6	A	675	MAN	C1-O5-C5	2.15	114.98	112.25
4	A	661	NAG	C1-O5-C5	2.30	115.16	112.25
6	A	674	MAN	C1-C2-C3	2.33	112.30	109.54
5	A	682	NAG	C1-O5-C5	2.37	115.26	112.25
4	A	661	NAG	O4-C4-C5	2.44	115.72	109.24
6	A	672	NDG	C2-N2-C7	2.54	126.31	123.04
9	B	1671	NAG	C4-C3-C2	2.91	115.76	111.23
9	B	1674	BMA	C1-C2-C3	2.94	113.02	109.54
9	B	1672	NDG	C2-N2-C7	3.02	126.91	123.04
4	B	1662	NDG	C1-O-C5	3.08	116.16	112.25
6	A	673	BMA	C1-O5-C5	3.34	116.49	112.25
8	B	1682	NAG	C3-C4-C5	3.50	116.30	110.20
8	B	1682	NAG	C4-C3-C2	3.94	117.36	111.23
6	A	671	NAG	C1-O5-C5	4.05	117.39	112.25
9	B	1672	NDG	C1-O-C5	4.23	117.62	112.25
9	B	1674	BMA	C1-O5-C5	4.78	118.31	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	672	NDG	C1-O-C5	4.80	118.34	112.25
4	A	662	NDG	C1-O-C5	4.94	118.52	112.25
6	A	674	MAN	C1-O5-C5	5.35	119.04	112.25

There are no chirality outliers.

There are no torsion outliers.

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	1674	BMA	C1-C2-C3-C4-C5-O5
6	A	674	MAN	C1-C2-C3-C4-C5-O5
6	A	673	BMA	C1-C2-C3-C4-C5-O5

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	661	NAG	1	0
4	A	662	NDG	1	0

5.6 Ligand geometry (i)

8 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	BOG	A	751	-	20,20,20	0.49	0	25,25,25	0.75	0
3	BOG	A	755	-	12,12,20	0.49	0	17,17,25	0.93	1 (5%)
2	HEM	A	801	-	30,50,50	2.18	11 (36%)	24,82,82	2.33	12 (50%)
3	BOG	B	1750	-	20,20,20	2.02	1 (5%)	25,25,25	1.01	2 (8%)
3	BOG	B	1751	-	20,20,20	0.54	0	25,25,25	0.60	0
3	BOG	B	1752	-	20,20,20	0.55	0	25,25,25	0.60	0
2	HEM	B	1801	-	30,50,50	2.11	9 (30%)	24,82,82	2.32	11 (45%)
7	GOL	B	851	-	5,5,5	0.34	0	5,5,5	0.19	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	BOG	A	751	-	-	0/11/31/31	0/1/1/1
3	BOG	A	755	-	-	0/2/22/31	0/1/1/1
2	HEM	A	801	-	-	0/10/54/54	0/0/8/8
3	BOG	B	1750	-	-	0/11/31/31	0/1/1/1
3	BOG	B	1751	-	-	0/11/31/31	0/1/1/1
3	BOG	B	1752	-	-	0/11/31/31	0/1/1/1
2	HEM	B	1801	-	-	0/10/54/54	0/0/8/8
7	GOL	B	851	-	-	0/4/4/4	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1750	BOG	C4'-C3'	-8.76	1.00	1.51
2	A	801	HEM	C3B-C4B	-6.82	1.45	1.51
2	B	1801	HEM	C3B-C4B	-6.42	1.46	1.51
2	A	801	HEM	C3D-C4D	-4.84	1.45	1.51
2	B	1801	HEM	C3D-C4D	-4.81	1.45	1.51
2	B	1801	HEM	C2C-C1C	-3.50	1.45	1.52
2	A	801	HEM	C2C-C1C	-3.49	1.46	1.52
2	A	801	HEM	C2D-C1D	-2.02	1.45	1.51
2	A	801	HEM	C3C-CAC	2.02	1.55	1.51
2	A	801	HEM	C3B-CAB	2.02	1.55	1.51
2	B	1801	HEM	C3B-CAB	2.06	1.55	1.51
2	B	1801	HEM	C3C-CAC	2.12	1.55	1.51
2	A	801	HEM	C1C-NC	2.18	1.38	1.36
2	B	1801	HEM	C1C-NC	2.23	1.38	1.36
2	B	1801	HEM	C4C-NC	2.30	1.38	1.36
2	A	801	HEM	CAA-C2A	2.32	1.56	1.52
2	A	801	HEM	C4C-NC	2.40	1.39	1.36
2	A	801	HEM	FE-NC	2.50	2.05	1.95
2	B	1801	HEM	FE-NC	2.53	2.05	1.95
2	B	1801	HEM	FE-ND	2.70	2.11	1.97
2	A	801	HEM	FE-ND	3.13	2.14	1.97

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	HEM	C3C-CAC-CBC	-2.64	120.40	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1750	BOG	C5'-C4'-C3'	-2.46	101.82	114.53
2	B	1801	HEM	C3B-CAB-CBB	-2.36	120.83	124.46
2	A	801	HEM	C3B-CAB-CBB	-2.35	120.86	124.46
2	B	1801	HEM	C3C-CAC-CBC	-2.15	121.16	124.46
2	B	1801	HEM	C3B-C4B-NB	-2.09	107.64	111.63
2	A	801	HEM	CMA-C3A-C4A	-2.08	124.92	128.36
2	A	801	HEM	C3B-C4B-NB	-2.03	107.74	111.63
3	A	755	BOG	C3-C4-C5	2.05	113.78	110.20
2	B	1801	HEM	C2C-C1C-CHC	2.14	126.94	123.68
2	B	1801	HEM	C2D-C3D-C4D	2.29	105.38	101.50
2	A	801	HEM	C2D-C3D-C4D	2.37	105.51	101.50
2	A	801	HEM	C2C-C1C-CHC	2.53	127.53	123.68
2	B	1801	HEM	C3B-C4B-CHC	2.82	127.13	123.16
3	B	1750	BOG	C4'-C3'-C2'	2.84	129.19	114.53
2	B	1801	HEM	CMD-C2D-C3D	2.89	127.14	114.35
2	A	801	HEM	CMD-C2D-C3D	2.91	127.23	114.35
2	A	801	HEM	C3B-C4B-CHC	2.92	127.27	123.16
2	A	801	HEM	CMC-C2C-C3C	3.59	125.49	116.53
2	B	1801	HEM	CMC-C2C-C3C	3.60	125.51	116.53
2	A	801	HEM	CMB-C2B-C3B	3.97	126.43	116.53
2	B	1801	HEM	CMB-C2B-C3B	4.00	126.52	116.53
2	A	801	HEM	CAD-C3D-C4D	4.22	127.36	112.47
2	B	1801	HEM	CAD-C3D-C4D	4.25	127.47	112.47
2	A	801	HEM	CAD-C3D-C2D	4.84	127.12	113.22
2	B	1801	HEM	CAD-C3D-C2D	4.85	127.15	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	751	BOG	1	0
3	B	1751	BOG	1	0

5.7 Other polymers (i)

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, 95^{th} 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%)	-0.54	0	100	100	57, 70, 86, 95	1 (0%)
1	B	553/553 (100%)	-0.50	0	100	100	57, 68, 82, 92	0
All	All	1106/1106 (100%)	-0.52	0	100	100	57, 69, 85, 95	1 (0%)

There are no RSRZ outliers to report.

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

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

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, 95^{th} 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
4	NAG	A	661	14/15	0.97	0.25	1.81	50,52,54,56	0
4	NAG	B	1661	14/15	0.97	0.25	0.67	50,53,54,56	0
8	NAG	B	1682	14/15	0.97	0.13	0.25	54,55,55,55	0
6	NAG	A	671	14/15	0.96	0.16	-0.42	47,49,50,52	0
5	NAG	A	681	14/15	0.98	0.15	-0.42	50,52,53,54	0
9	NAG	B	1671	14/15	0.96	0.18	-0.64	48,50,52,52	0
8	NDG	B	1681	14/15	0.97	0.10	-0.93	49,51,52,53	0
6	NDG	A	672	14/15	0.94	0.32	-	54,55,56,56	0
4	NDG	B	1662	14/15	0.94	0.27	-	57,58,59,59	0
6	MAN	A	674	11/12	0.94	0.28	-	60,60,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	A	682	14/15	0.95	0.21	-	55,56,57,57	0
9	NDG	B	1672	14/15	0.96	0.31	-	54,55,56,57	0
4	NDG	A	662	14/15	0.96	0.27	-	57,58,59,59	0
6	BMA	A	673	11/12	0.97	0.33	-	58,58,59,60	0
9	BMA	B	1673	11/12	0.95	0.31	-	59,60,61,62	0
9	BMA	B	1674	11/12	0.91	0.30	-	62,62,63,63	0
6	MAN	A	675	11/12	0.94	0.23	-	61,62,62,62	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
7	GOL	B	851	6/6	0.91	0.35	1.76	68,69,69,69	0
3	BOG	A	751	20/20	0.88	0.26	1.27	75,79,84,85	0
3	BOG	B	1751	20/20	0.91	0.21	0.61	70,73,77,79	0
2	HEM	B	1801	43/43	0.95	0.18	-0.14	66,71,76,77	0
2	HEM	A	801	43/43	0.95	0.17	-0.57	67,72,76,78	0
3	BOG	B	1752	20/20	0.92	0.25	-	75,79,83,84	0
3	BOG	B	1750	20/20	0.94	0.30	-	20,80,84,84	5
3	BOG	A	755	12/20	0.91	0.19	-	86,87,91,92	0

6.5 Other polymers

There are no such residues in this entry.