



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:52 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 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 ⓘ 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

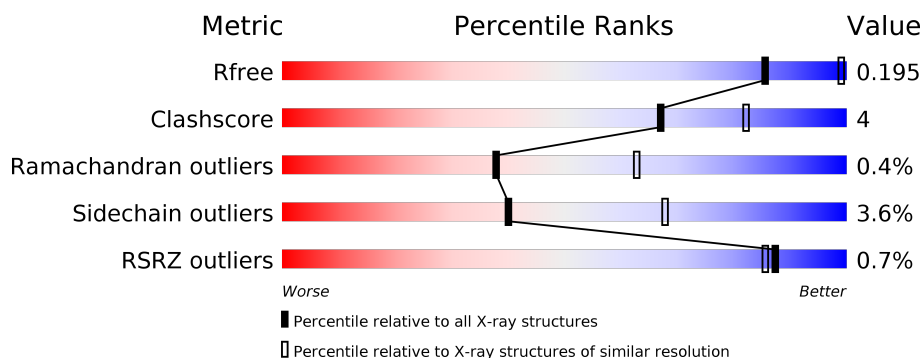
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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. 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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 89%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 89% 10% </div> </div>
2	B	553	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 89%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 89% 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	DIF	B	585[B]	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9465 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	5	0
			4427	2870	742	787	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	3	4	0
			4443	2887	740	789	27			

There are 2 discrepancies between the modelled and reference sequences:

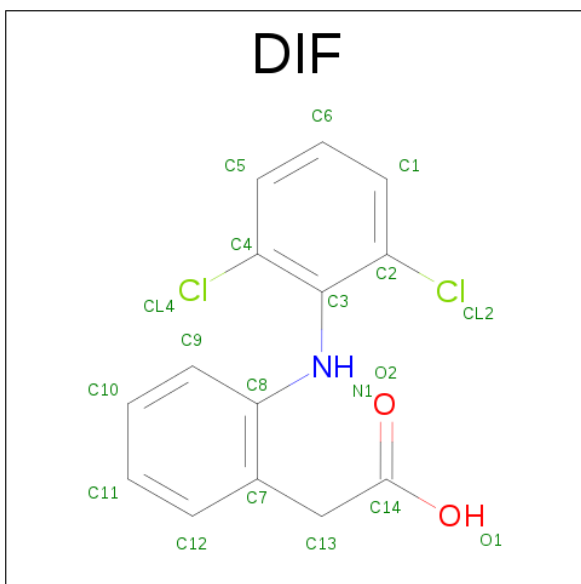
Chain	Residue	Modelled	Actual	Comment	Reference
B	92	LEU	MET	CONFLICT	UNP P05979
B	530	OAS	SER	MICROHETEROGENEITY	UNP P05979

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 2-[2,6-DICHLOROPHENYL)AMINO]BENZENEACETIC ACID (three-letter code: DIF) (formula: $C_{14}H_{11}Cl_2NO_2$).



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

Continued on next page...

Continued from previous page...

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

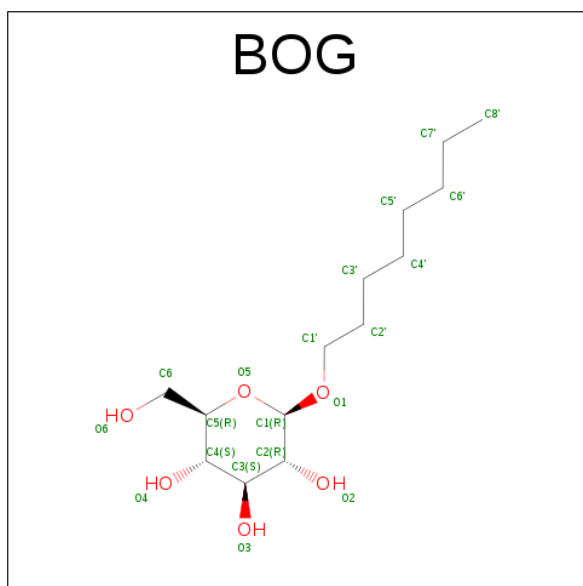
- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

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

- 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		
			61	34	2	25		
							0	0

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



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

Continued on next page...

Continued from previous page...

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

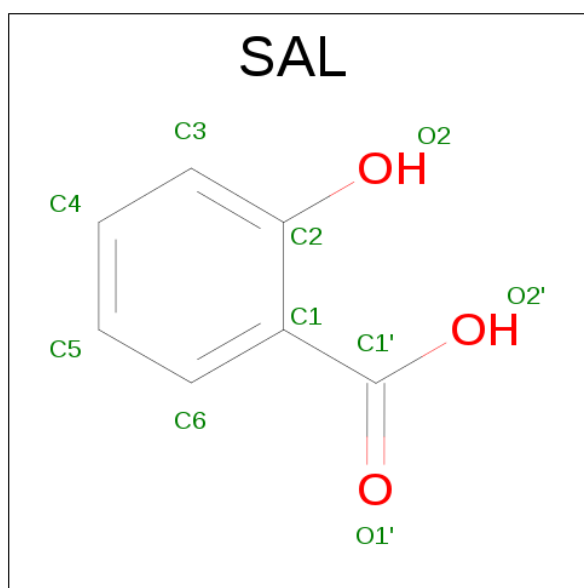
- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

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

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



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

- Molecule 11 is water.

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

Continued on next page...

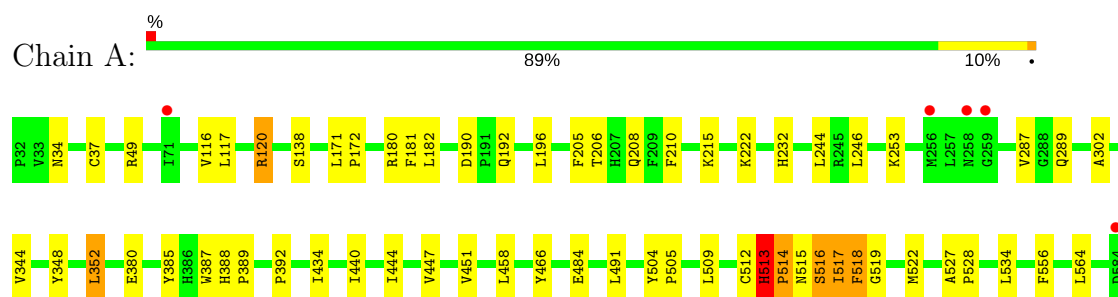
Continued from previous page...

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

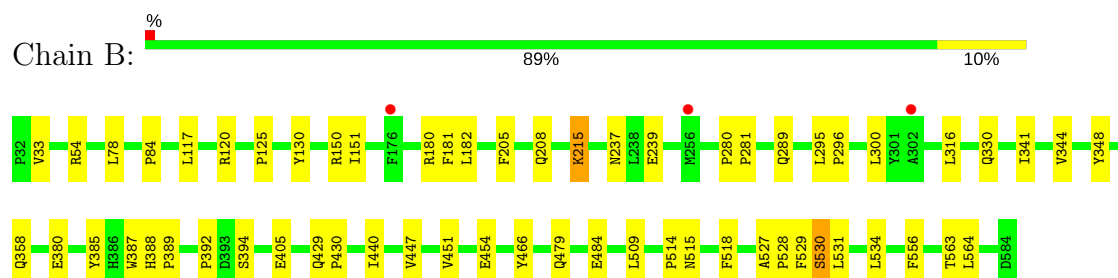
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($RSRZ > 2$). 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	182.33Å 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)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.184 , 0.200 0.183 , 0.195	Depositor DCC
R_{free} test set	1595 reflections (2.76%)	DCC
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.501 for H, K, L 0.499 for -H-K, K, -L	Depositor
Outliers	0 of 59356 reflections	Xtriage
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

Xtriage'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.

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

5.1 Standard geometry

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 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	4427	0	4236	41	0
2	B	4443	0	4258	33	0
3	A	43	0	30	2	0
3	B	43	0	30	1	0
4	A	19	0	10	0	0
4	B	19	0	10	14	0
5	A	50	0	43	0	0
5	B	50	0	43	0	0
6	A	61	0	52	0	0
7	A	40	0	56	0	0
7	B	40	0	56	1	0
8	B	28	0	25	0	0
9	B	50	0	43	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	8896	81	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 (81) 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:530[B]:OAS:OG	4:B:585[B]:DIF:O2	1.64	1.15
1:A:513[A]:HIS:HB2	1:A:514[A]:PRO:CD	1.86	1.05
1:A:513[A]:HIS:CB	1:A:514[A]:PRO:HD2	1.88	1.02
1:A:513[A]:HIS:HB2	1:A:514[A]:PRO:HD2	1.01	0.99
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
4:B:585[B]:DIF:C9	4:B:585[B]:DIF:CL2	2.70	0.77
1:A:512[B]:CYS:O	1:A:513[B]:HIS:CB	2.34	0.76
2:B:531[B]:LEU:CD2	4:B:585[B]:DIF:CL4	2.74	0.72
4:B:585[B]:DIF:HN1	4:B:585[B]:DIF:C14	2.09	0.65
2:B:531[B]:LEU:HD21	4:B:585[B]:DIF:CL4	2.36	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:585[B]:DIF:C2	4:B:585[B]:DIF:H9	2.30	0.60
2:B:215:LYS:H	2:B:215:LYS:HE2	1.67	0.60
2:B:387:TRP:HB2	3:B:601:HEM:HBC2	1.84	0.58
4:B:585[B]:DIF:C8	4:B:585[B]:DIF:CL2	2.89	0.57
1:A:387:TRP:HB2	3:A:601:HEM:HAC	1.85	0.57
1:A:344:VAL:HA	1:A:348:TYR:HB3	1.87	0.57
2:B:125:PRO:HD2	2:B:151:ILE:HD12	1.88	0.55
2:B:514:PRO:O	2:B:515:ASN:HB2	2.06	0.55
1:A:182:LEU:HB3	1:A:440:ILE:HD12	1.89	0.55
1:A:206:THR:HB	1:A:210:PHE:HD2	1.71	0.54
4:B:585[B]:DIF:C9	4:B:585[B]:DIF:C2	2.84	0.54
4:B:585[B]:DIF:O2	4:B:585[B]:DIF:C8	2.54	0.54
1:A:348:TYR:O	1:A:352:LEU:HD23	2.08	0.54
1:A:205:PHE:O	1:A:208:GLN:HG2	2.08	0.53
2:B:181:PHE:HB3	2:B:509:LEU:HD21	1.90	0.52
1:A:513[B]:HIS:O	1:A:514[B]:PRO:C	2.47	0.52
1:A:181:PHE:HB3	1:A:509:LEU:HD21	1.91	0.52
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.45	0.51
1:A:352:LEU:HD12	1:A:518:PHE:HZ	1.76	0.51
1:A:388:HIS:HE1	3:A:601:HEM:ND	2.03	0.50
2:B:530[B]:OAS:O	2:B:531[B]:LEU:C	2.48	0.50
1:A:206:THR:HB	1:A:210:PHE:CD2	2.46	0.50
1:A:518:PHE:CD1	1:A:522:MET:HG2	2.46	0.50
1:A:116:VAL:O	1:A:120:ARG:HB2	2.11	0.50
2:B:388:HIS:N	2:B:389:PRO:CD	2.75	0.50
1:A:388:HIS:N	1:A:389:PRO:CD	2.75	0.49
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.93	0.49
2:B:344:VAL:HA	2:B:348:TYR:HB3	1.94	0.49
2:B:130:TYR:HB2	2:B:150:ARG:HG3	1.94	0.49
4:B:585[B]:DIF:O2	4:B:585[B]:DIF:CL4	2.67	0.49
1:A:512[B]:CYS:HA	1:A:519:GLY:HA2	1.95	0.49
2:B:388:HIS:N	2:B:389:PRO:HD2	2.27	0.49
2:B:344:VAL:O	2:B:348:TYR:HB3	2.13	0.48
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.54	0.48
1:A:287:VAL:HG11	1:A:302:ALA:HB1	1.97	0.47
2:B:205:PHE:O	2:B:208:GLN:HG2	2.15	0.47
2:B:237:ASN:OD1	2:B:239:GLU:HG2	2.15	0.47
2:B:182:LEU:HB3	2:B:440:ILE:HD12	1.97	0.47
1:A:352:LEU:HD12	1:A:518:PHE:CZ	2.50	0.46
2:B:84:PRO:HA	7:B:1750:BOG:H6'2	1.96	0.46
2:B:447:VAL:O	2:B:451:VAL:HG23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:SER:HB2	2:B:330:GLN:HB3	1.98	0.46
1:A:513[A]:HIS:CB	1:A:514[A]:PRO:CD	2.62	0.46
2:B:341:ILE:HG23	2:B:534:LEU:HD12	1.98	0.45
2:B:358[B]:GLN:OE1	2:B:358[B]:GLN:HA	2.16	0.45
2:B:405:GLU:H	2:B:405:GLU:CD	2.20	0.45
2:B:280:PRO:HA	2:B:281:PRO:HD3	1.87	0.44
2:B:527:ALA:HB3	2:B:528:PRO:HD3	1.98	0.44
1:A:388:HIS:N	1:A:389:PRO:HD2	2.34	0.43
2:B:392:PRO:HG2	2:B:394:SER:O	2.18	0.43
2:B:531[B]:LEU:HD23	4:B:585[B]:DIF:CL4	2.53	0.43
2:B:514:PRO:O	2:B:515:ASN:CB	2.66	0.43
1:A:196:LEU:HD11	1:A:392:PRO:HG3	2.00	0.43
2:B:380:GLU:HG2	2:B:466:TYR:CE1	2.54	0.43
2:B:531[B]:LEU:HG	4:B:585[B]:DIF:CL4	2.55	0.43
1:A:512[A]:CYS:HA	1:A:519:GLY:HA2	2.01	0.42
2:B:429:GLN:HA	2:B:430:PRO:HD3	1.93	0.42
1:A:388:HIS:HB3	1:A:444:ILE:HD12	2.00	0.42
1:A:171:LEU:HD12	1:A:172:PRO:HD2	2.02	0.42
1:A:515[B]:ASN:O	1:A:516[B]:SER:HB3	2.20	0.42
1:A:190:ASP:OD2	1:A:192:GLN:HB2	2.19	0.41
1:A:344:VAL:O	1:A:348:TYR:HB3	2.20	0.41
1:A:246:LEU:HG	1:A:253:LYS:HA	2.02	0.41
1:A:491:LEU:HD11	1:A:509:LEU:HD13	2.02	0.41
2:B:295:LEU:HA	2:B:296:PRO:HD3	1.96	0.41
1:A:208:GLN:HB3	1:A:232:HIS:CG	2.56	0.40
1:A:527:ALA:HB3	1:A:528:PRO:HD3	2.03	0.40
1:A:447:VAL:O	1:A:451:VAL:HG23	2.21	0.40
1:A:434:ILE:HD12	1:A:517:ILE:HG21	2.02	0.40
1:A:389:PRO:HB2	1:A:434:ILE:HA	2.04	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	556/553 (100%)	534 (96%)	16 (3%)	6 (1%)	17	35
2	B	553/553 (100%)	533 (96%)	19 (3%)	1 (0%)	51	76
All	All	1109/1106 (100%)	1067 (96%)	35 (3%)	7 (1%)	38	53

All (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
1	A	516[A]	SER
1	A	516[B]	SER

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%)	36	64
2	B	471/487 (97%)	455 (97%)	16 (3%)	42	69
All	All	942/975 (97%)	907 (96%)	35 (4%)	40	66

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	117	LEU
1	A	120	ARG
1	A	180	ARG
1	A	215	LYS
1	A	222	LYS
1	A	244	LEU
1	A	289	GLN
1	A	352	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	385	TYR
1	A	458	LEU
1	A	484	GLU
1	A	513[A]	HIS
1	A	513[B]	HIS
1	A	517	ILE
1	A	518	PHE
1	A	534	LEU
1	A	556	PHE
1	A	564	LEU
2	B	54	ARG
2	B	78	LEU
2	B	117	LEU
2	B	120	ARG
2	B	180	ARG
2	B	215	LYS
2	B	289	GLN
2	B	300	LEU
2	B	316	LEU
2	B	385	TYR
2	B	454	GLU
2	B	484	GLU
2	B	518	PHE
2	B	556	PHE
2	B	563	THR
2	B	564	LEU

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 ⓘ

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	2.33	3 (37%)	6,9,11	2.21	2 (33%)
2	OAS	B	530[B]	2	5,5,9	0.75	0	1,5,11	1.58	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
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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	530[A]	OAS	C2A-C1A	-4.80	1.32	1.49
2	B	530[A]	OAS	OG-C1A	2.60	1.46	1.33
2	B	530[A]	OAS	OAC-C1A	3.45	1.33	1.20

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	530[A]	OAS	O-C-CA	-2.41	118.37	125.02
2	B	530[A]	OAS	OG-CB-CA	4.01	119.96	108.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	530[B]	OAS	3	0

5.5 Carbohydrates

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	14,14,15	0.56	0	15,19,21	0.94	1 (6%)
6	NDG	A	672	6	14,14,15	0.55	0	15,19,21	1.71	3 (20%)
6	BMA	A	673	6	11,11,12	0.55	0	13,15,17	1.66	1 (7%)
6	MAN	A	674	6	11,11,12	0.58	0	13,15,17	1.23	1 (7%)
6	MAN	A	675	6	11,11,12	0.59	0	13,15,17	0.72	0
5	NAG	A	681	1,5	14,14,15	0.48	0	15,19,21	0.79	0
5	NAG	A	682	5	14,14,15	0.44	0	15,19,21	0.99	0
5	BMA	A	683	5	11,11,12	0.54	0	13,15,17	1.82	1 (7%)
5	BMA	A	684	5	11,11,12	0.53	0	13,15,17	1.79	2 (15%)
8	NAG	B	1661	8,2	14,14,15	1.45	1 (7%)	15,19,21	1.19	1 (6%)
8	NDG	B	1662	8	14,14,15	0.49	0	15,19,21	1.01	1 (6%)
9	NAG	B	1671	9,2	14,14,15	0.54	0	15,19,21	1.09	2 (13%)
9	NDG	B	1672	9	14,14,15	0.76	1 (7%)	15,19,21	1.98	4 (26%)
9	BMA	B	1673	9	11,11,12	0.60	0	13,15,17	0.91	0
9	BMA	B	1674	9	11,11,12	0.52	0	13,15,17	1.74	2 (15%)
5	NAG	B	1681	2,5	14,14,15	0.53	0	15,19,21	0.91	1 (6%)
5	NAG	B	1682	5	14,14,15	0.47	0	15,19,21	1.04	2 (13%)
5	BMA	B	1683	5	11,11,12	0.59	0	13,15,17	1.33	2 (15%)
5	BMA	B	1684	5	11,11,12	0.60	0	13,15,17	1.09	2 (15%)

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	0/1/1/1
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1/1/1/1
5	BMA	A	684	5	-	0/2/19/22	1/1/1/1
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	1/1/1/1
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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1661	NAG	O5-C1	-5.18	1.35	1.43
9	B	1672	NDG	C1-C2	2.35	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1661	NAG	O5-C1-C2	-2.73	107.67	111.47
9	B	1671	NAG	O5-C1-C2	-2.07	108.59	111.47
9	B	1674	BMA	C1-C2-C3	2.05	112.25	109.65
9	B	1671	NAG	C1-O5-C5	2.09	115.05	112.17
5	B	1681	NAG	C4-C3-C2	2.10	114.09	111.02
5	B	1684	BMA	C1-O5-C5	2.19	115.18	112.17
5	B	1682	NAG	O4-C4-C5	2.42	115.37	109.28
5	B	1683	BMA	C1-C2-C3	2.43	112.73	109.65
8	B	1662	NDG	C1-O-C5	2.46	115.56	112.17
5	B	1682	NAG	C1-O5-C5	2.47	115.56	112.17
6	A	672	NDG	O4-C4-C3	2.57	115.94	110.36
6	A	671	NAG	C1-O5-C5	2.61	115.77	112.17
9	B	1672	NDG	C2-N2-C7	2.68	126.86	122.94
5	B	1684	BMA	C1-C2-C3	2.70	113.08	109.65
5	A	684	BMA	C1-C2-C3	2.73	113.11	109.65
9	B	1672	NDG	C4-C3-C2	2.95	115.35	111.02
9	B	1672	NDG	O-C1-C2	3.31	116.08	111.47
6	A	674	MAN	C1-O5-C5	3.46	116.93	112.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	672	NDG	C2-N2-C7	3.47	128.01	122.94
5	B	1683	BMA	C1-O5-C5	3.78	117.37	112.17
6	A	672	NDG	C1-O-C5	3.91	117.56	112.17
6	A	673	BMA	C1-O5-C5	4.83	118.82	112.17
9	B	1672	NDG	C1-O-C5	4.92	118.95	112.17
5	A	684	BMA	C1-O5-C5	5.41	119.62	112.17
9	B	1674	BMA	C1-O5-C5	5.41	119.63	112.17
5	A	683	BMA	C1-O5-C5	6.06	120.52	112.17

There are no chirality outliers.

There are no torsion outliers.

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	683	BMA	C1-C2-C3-C4-C5-O5
5	A	684	BMA	C1-C2-C3-C4-C5-O5
9	B	1674	BMA	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

5.6 Ligand geometry

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	28,50,50	2.27	6 (21%)	17,82,82	1.33	2 (11%)
4	DIF	A	701	-	17,20,20	1.06	2 (11%)	24,27,27	1.09	2 (8%)
7	BOG	A	751	-	20,20,20	0.52	0	25,25,25	1.02	1 (4%)
7	BOG	A	754	-	20,20,20	0.53	0	25,25,25	0.59	0
7	BOG	B	1750	-	20,20,20	0.52	0	25,25,25	0.58	0
7	BOG	B	1751	-	20,20,20	0.44	0	25,25,25	0.69	0
4	DIF	B	585[B]	-	17,20,20	1.13	2 (11%)	24,27,27	1.11	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	B	601	2	28,50,50	2.24	7 (25%)	17,82,82	1.31	1 (5%)
10	SAL	B	900[A]	-	7,10,10	0.43	0	9,13,13	0.40	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	-	0/6/54/54	0/0/8/8
4	DIF	A	701	-	-	0/6/8/8	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]	-	-	0/6/8/8	0/2/2/2
3	HEM	B	601	2	-	0/6/54/54	0/0/8/8
10	SAL	B	900[A]	-	-	0/0/4/4	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	HEM	C3C-C2C	-4.49	1.34	1.40
3	B	601	HEM	C3B-C2B	-4.46	1.34	1.40
3	A	601	HEM	C3B-C2B	-4.44	1.34	1.40
3	B	601	HEM	C3C-C2C	-4.31	1.34	1.40
3	B	601	HEM	CAA-C2A	2.06	1.55	1.52
3	A	601	HEM	C4D-ND	2.55	1.39	1.36
4	A	701	DIF	C4-CL4	2.55	1.79	1.73
3	B	601	HEM	C4D-ND	2.59	1.39	1.36
4	B	585[B]	DIF	C4-CL4	2.60	1.79	1.73
4	B	585[B]	DIF	C2-CL2	2.62	1.79	1.73
4	A	701	DIF	C2-CL2	2.62	1.79	1.73
3	A	601	HEM	C3B-CAB	3.70	1.55	1.47
3	B	601	HEM	C3B-CAB	3.71	1.55	1.47
3	B	601	HEM	C3C-CAC	3.73	1.55	1.47
3	A	601	HEM	C3C-CAC	3.85	1.55	1.47
3	B	601	HEM	C3D-C2D	5.54	1.54	1.37
3	A	601	HEM	C3D-C2D	5.64	1.54	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	601	HEM	C1D-C2D-C3D	-2.43	105.30	107.00
3	A	601	HEM	CBA-CAA-C2A	-2.18	108.32	112.48
4	A	701	DIF	C14-C13-C7	-2.11	109.80	114.71
3	A	601	HEM	CMA-C3A-C4A	-2.03	125.35	128.46
4	B	585[B]	DIF	C4-C3-C2	2.16	119.92	116.26
4	A	701	DIF	C7-C8-N1	2.35	120.32	118.58
4	B	585[B]	DIF	C7-C8-N1	2.49	120.43	118.58
7	A	751	BOG	C3-C4-C5	2.62	114.83	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HEM	2	0
7	B	1750	BOG	1	0
4	B	585[B]	DIF	14	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%)	-0.47	5 (0%) 84 81	34, 47, 61, 68	1 (0%)
2	B	552/553 (99%)	-0.48	3 (0%) 90 89	34, 48, 61, 69	1 (0%)
All	All	1105/1106 (99%)	-0.48	8 (0%) 87 85	34, 47, 61, 69	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	256	MET	2.5
2	B	302	ALA	2.4
1	A	259	GLY	2.3
1	A	258	ASN	2.2
1	A	584	ASP	2.2
1	A	256	MET	2.1
1	A	71	ILE	2.0
2	B	176	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	OAS	B	530[B]	6/10	0.99	0.13	-	35,36,36,36	6
2	OAS	B	530[A]	9/10	0.99	0.13	-	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	NAG	B	1671	14/15	0.93	0.15	0.62	61,64,67,69	0
8	NAG	B	1661	14/15	0.90	0.20	0.38	58,59,66,73	0
5	NAG	B	1681	14/15	0.91	0.15	0.24	85,86,87,87	0
6	NAG	A	671	14/15	0.94	0.12	-0.69	58,60,60,62	0
5	NAG	A	681	14/15	0.96	0.08	-2.00	56,58,61,62	0
9	BMA	B	1673	11/12	0.93	0.48	-	71,75,81,83	0
5	BMA	A	683	11/12	0.89	0.28	-	67,76,86,87	0
5	BMA	A	684	11/12	0.72	0.41	-	88,97,116,117	0
6	MAN	A	674	11/12	0.78	0.25	-	68,69,71,71	0
5	BMA	B	1683	11/12	0.86	0.23	-	85,86,89,90	0
5	NAG	B	1682	14/15	0.89	0.27	-	84,85,86,87	0
5	BMA	B	1684	11/12	0.81	0.46	-	91,93,96,97	0
6	BMA	A	673	11/12	0.89	0.26	-	65,66,67,68	0
5	NAG	A	682	14/15	0.94	0.12	-	57,59,63,64	0
6	NDG	A	672	14/15	0.87	0.20	-	63,64,65,65	0
9	NDG	B	1672	14/15	0.89	0.25	-	65,66,68,68	0
6	MAN	A	675	11/12	0.87	0.24	-	69,71,72,73	0
9	BMA	B	1674	11/12	0.84	0.36	-	84,89,98,99	0
8	NDG	B	1662	14/15	0.93	0.23	-	60,66,72,79	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	BOG	A	754	20/20	0.93	0.21	1.60	46,46,46,46	0
4	DIF	B	585[B]	19/19	0.92	0.19	1.14	22,23,23,23	19
7	BOG	A	751	20/20	0.93	0.16	1.03	39,47,64,69	0
3	HEM	A	601	43/43	0.94	0.16	0.41	40,45,49,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	BOG	B	1750	20/20	0.92	0.15	0.13	42,43,44,44	0
3	HEM	B	601	43/43	0.95	0.16	0.04	41,45,50,51	0
7	BOG	B	1751	20/20	0.97	0.11	-0.46	35,37,38,38	0
10	SAL	B	900[A]	10/10	0.95	0.12	-1.25	34,34,35,35	10
4	DIF	A	701	19/19	0.96	0.11	-1.40	46,47,48,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.