Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:50 AM GMT

PDB ID	:	3N8X
Title	:	Crystal Structure of Cyclooxygenase-1 in Complex with Nimesulide
Authors	:	Lee, J.Y.
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
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:

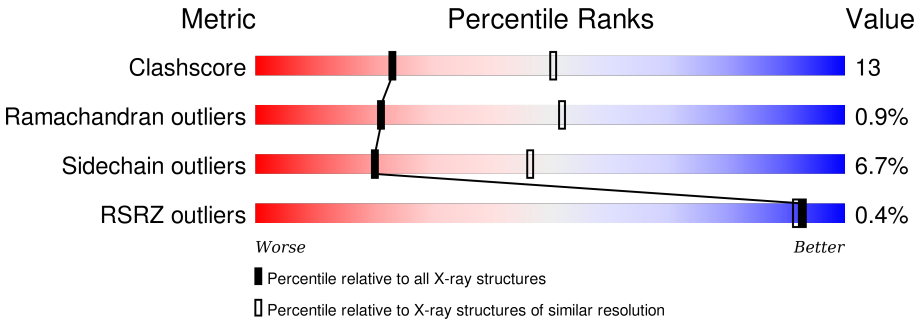
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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))
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 >=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	68% 29% .
1	B	553	70% 27% .

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
7	BOG	B	1751	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9315 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.

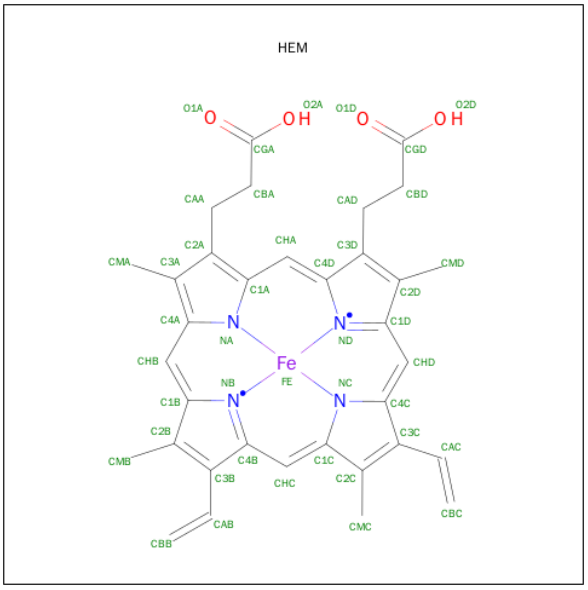
- Molecule 1 is a protein called Prostaglandin G/H synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4437	2876	746	788	27			
1	B	553	Total	C	N	O	S	0	1	0
			4438	2876	747	787	28			

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		

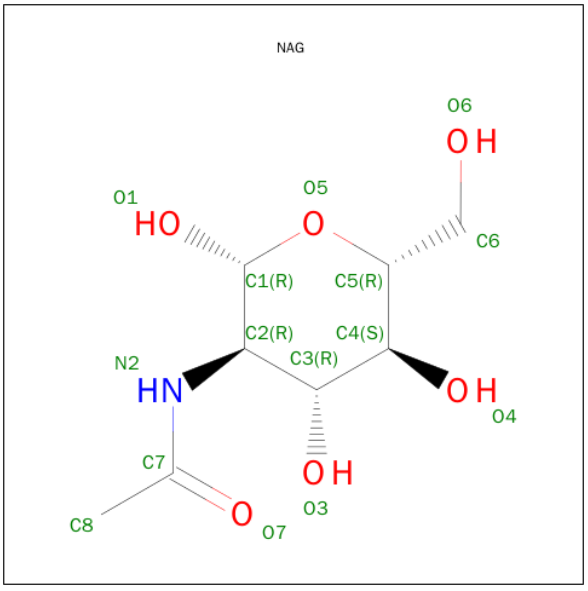
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

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

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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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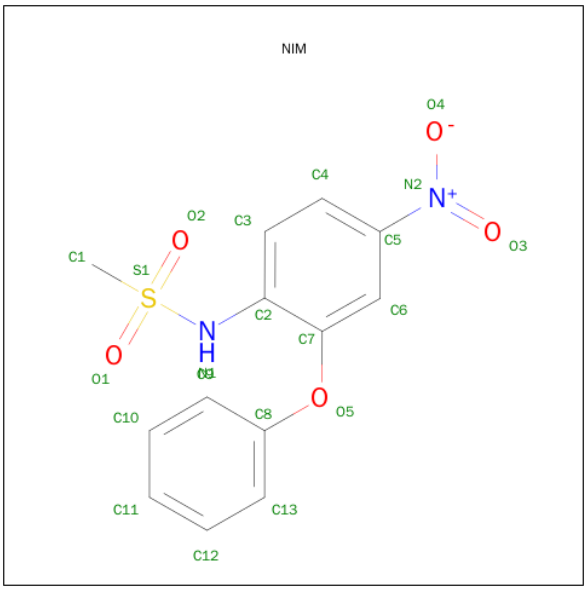
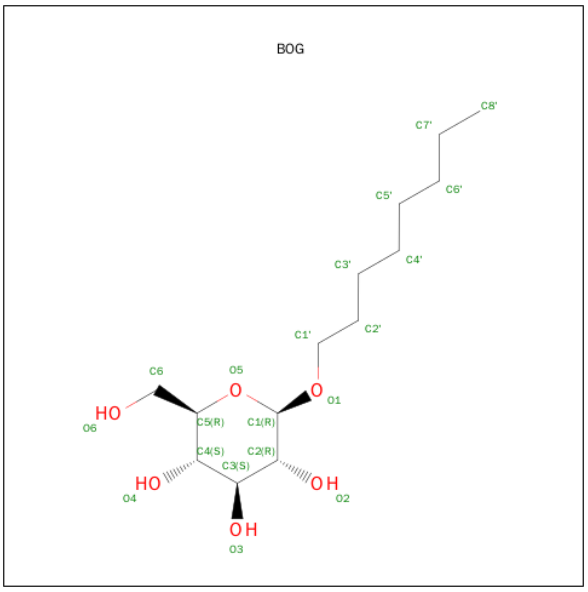
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is 4-NITRO-2-PHENOXYMETHANESULFONANILIDE (three-letter code: NIM) (formula: $C_{13}H_{12}N_2O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			21	13	2	5	1		
6	B	1	Total	C	N	O	S	0	0
			21	13	2	5	1		

- Molecule 7 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 8 is water.

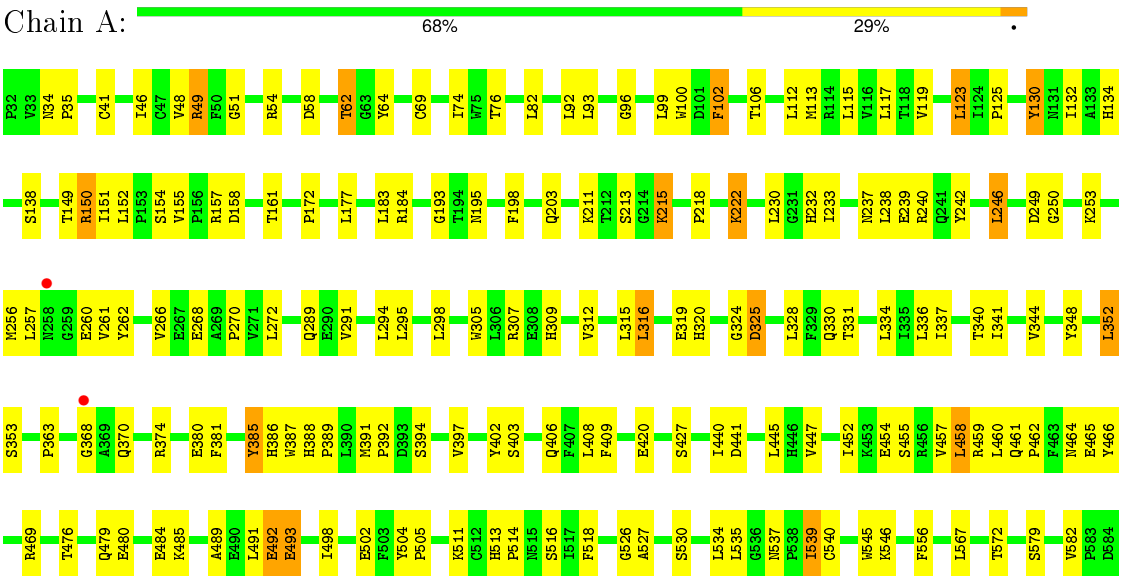
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	45	Total O 45 45	0	0
8	B	54	Total O 54 54	0	0

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.

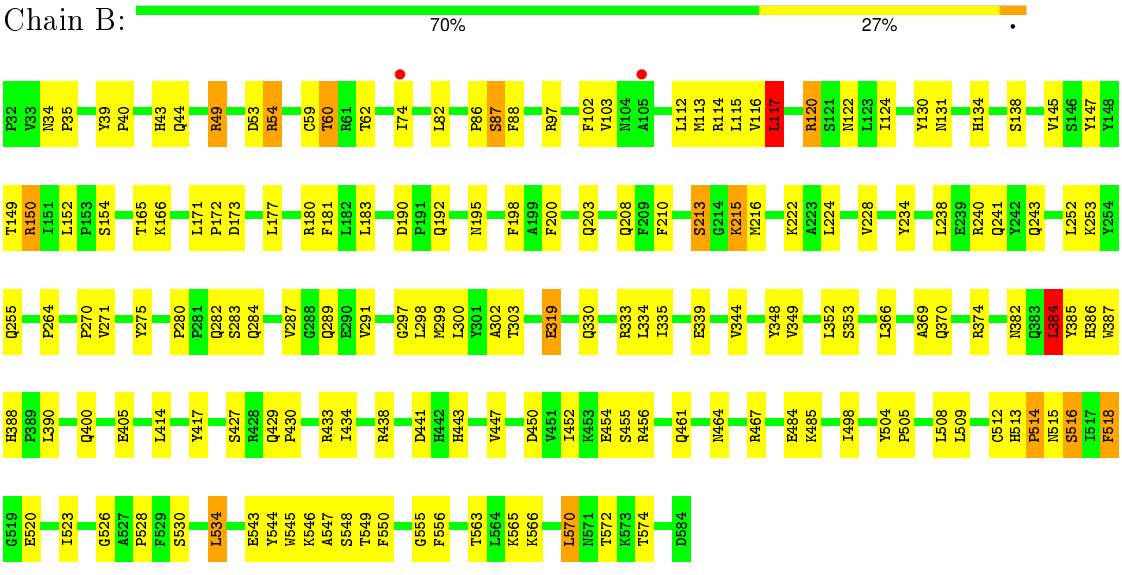
- Molecule 1: Prostaglandin G/H synthase 1

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	181.71Å 181.71Å 103.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.60 – 2.75 29.60 – 2.76	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.60-2.75) 97.2 (29.60-2.76)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.181 , 0.227 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	57.5	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 30.9	EDS
Estimated twinning fraction	0.504 for H, K, L 0.496 for -H-K, K, -L 0.074 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.504 for H, K, L 0.496 for -H-K, K, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 48920 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9315	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: BOG, HEM, BMA, NAG, NIM

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	0.60	0/4575	0.72	1/6223 (0.0%)
1	B	0.62	0/4577	0.72	2/6223 (0.0%)
All	All	0.61	0/9152	0.72	3/12446 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	41	CYS	CA-CB-SG	-6.73	101.88	114.00
1	B	384	LEU	CA-CB-CG	6.05	129.22	115.30
1	B	117	LEU	CA-CB-CG	5.08	126.98	115.30

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	4437	0	4285	130	0
1	B	4438	0	4293	121	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	28	0	25	1	0
3	B	56	0	50	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	61	0	52	2	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	21	0	12	4	0
6	B	21	0	12	1	0
7	B	40	0	56	5	0
8	A	45	0	0	8	0
8	B	54	0	0	9	0
All	All	9315	0	8871	243	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 13.

All (243) 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:B:387:TRP:HB2	2:B:601:HEM:HBC2	1.42	1.01
1:B:387:TRP:HB2	2:B:601:HEM:CBC	1.97	0.95
1:A:51:GLY:HA3	1:A:54:ARG:NH1	1.83	0.92
1:B:115:LEU:HD23	7:B:1751:BOG:H4'1	1.58	0.86
1:A:215:LYS:HD2	1:A:222:LYS:HE2	1.56	0.86
1:B:49:ARG:HH11	1:B:49:ARG:HG2	1.43	0.83
1:A:294:LEU:HD12	1:A:409:PHE:HD2	1.44	0.82
1:A:49:ARG:HG2	1:A:49:ARG:HH11	1.46	0.81
1:A:246:LEU:HD12	1:A:253:LYS:HA	1.63	0.80
1:B:49:ARG:HH11	1:B:49:ARG:CG	1.94	0.79
1:A:530:SER:O	1:A:534:LEU:HD22	1.83	0.78
1:A:132:ILE:HD13	1:A:458:LEU:HD12	1.65	0.77
1:A:106:THR:HB	8:A:612:HOH:O	1.89	0.72
1:A:218:PRO:HG2	1:A:457:VAL:HG11	1.71	0.72
1:A:294:LEU:HD12	1:A:409:PHE:CD2	2.24	0.71
1:A:150:ARG:HD3	1:A:152:LEU:O	1.89	0.71
1:B:54[A]:ARG:HB2	1:B:54[A]:ARG:HH11	1.53	0.71
1:A:334:LEU:HD11	1:B:138:SER:HA	1.73	0.70
1:B:112:LEU:O	1:B:116:VAL:HG23	1.92	0.69
1:A:34:ASN:HB2	1:A:158:ASP:OD2	1.93	0.69
1:A:388:HIS:N	1:A:389:PRO:HD2	2.07	0.68
1:A:312:VAL:HA	1:A:315:LEU:HD12	1.75	0.68
1:B:43:HIS:O	1:B:62:THR:HG23	1.95	0.67
1:A:49:ARG:HG2	1:A:49:ARG:NH1	2.09	0.67
1:B:181:PHE:HB3	1:B:509:LEU:HD21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.77	0.65
1:B:563:THR:HG23	8:B:593:HOH:O	1.95	0.65
1:A:316:LEU:HB3	1:A:328:LEU:HD23	1.80	0.64
1:B:550:PHE:O	1:B:555:GLY:HA3	1.99	0.63
1:B:572:THR:OG1	1:B:574:THR:O	2.15	0.63
1:B:43:HIS:O	1:B:44:GLN:HB2	1.97	0.63
1:A:238:LEU:HD21	1:A:242:TYR:CE2	2.34	0.62
1:B:222:LYS:HD2	8:B:585:HOH:O	1.98	0.62
1:A:238:LEU:HD21	1:A:242:TYR:CZ	2.34	0.62
1:A:154:SER:HB2	1:A:459:ARG:HB2	1.82	0.62
1:A:462:PRO:HG2	1:A:465:GLU:HG2	1.80	0.62
1:A:193:GLY:O	1:A:582:VAL:HG22	2.00	0.61
1:B:87:SER:HB2	7:B:1752:BOG:O2	2.00	0.61
1:A:479:GLN:HE21	1:A:485:LYS:HA	1.66	0.61
1:B:382:ASN:OD1	1:B:386:HIS:HE1	1.84	0.61
1:A:51:GLY:HA3	1:A:54:ARG:HH11	1.63	0.60
1:A:539:ILE:HG13	1:A:540:CYS:N	2.17	0.60
1:B:433:ARG:NH2	1:B:512:CYS:HB2	2.16	0.60
1:A:340:THR:O	1:A:344:VAL:HG23	2.02	0.60
1:B:210:PHE:CE1	1:B:382:ASN:HA	2.37	0.59
1:B:49:ARG:HG2	1:B:49:ARG:NH1	2.12	0.58
1:B:54[A]:ARG:CB	1:B:54[A]:ARG:HH11	2.16	0.58
1:A:370:GLN:NE2	1:B:369:ALA:O	2.35	0.58
1:A:125:PRO:HD2	1:A:151:ILE:HD12	1.84	0.58
1:A:215:LYS:CD	1:A:222:LYS:HE2	2.33	0.57
1:A:344:VAL:O	1:A:348:TYR:HB3	2.04	0.57
1:A:386:HIS:HD2	1:A:388:HIS:HE1	1.50	0.57
1:A:397:VAL:HB	1:A:402:TYR:HE2	1.70	0.57
1:B:518:PHE:HE2	1:B:523:ILE:HD13	1.70	0.56
1:A:240:ARG:NH1	1:A:272:LEU:O	2.37	0.56
1:A:386:HIS:CD2	1:A:388:HIS:HE1	2.23	0.56
1:A:374:ARG:HB3	1:B:374:ARG:NH1	2.20	0.56
1:A:211:LYS:HE3	1:A:289:GLN:NE2	2.21	0.56
1:B:173:ASP:O	1:B:177:LEU:HD23	2.05	0.56
1:B:172:PRO:HB3	1:B:177:LEU:HD21	1.88	0.56
1:B:234:TYR:CE2	1:B:333:ARG:HG3	2.40	0.56
1:A:363:PRO:HG2	1:A:545:TRP:CE2	2.40	0.56
1:B:344:VAL:HA	1:B:348:TYR:HB3	1.87	0.56
1:B:547:ALA:O	1:B:548:SER:C	2.44	0.55
1:A:330:GLN:HB3	1:B:138:SER:HB2	1.89	0.55
1:A:238:LEU:CD2	1:A:242:TYR:CE2	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:SER:HB2	1:B:330:GLN:HB3	1.88	0.55
1:B:299:MET:HG3	1:B:414:LEU:HD23	1.89	0.55
1:B:116:VAL:O	1:B:120:ARG:HB2	2.07	0.54
1:A:125:PRO:HD2	1:A:151:ILE:CD1	2.38	0.54
1:A:230:LEU:HG	1:A:233:ILE:HD12	1.88	0.54
1:B:115:LEU:HD23	7:B:1751:BOG:C4'	2.35	0.54
1:B:518:PHE:CE2	1:B:523:ILE:HD13	2.42	0.54
1:A:184:ARG:NH1	1:A:391:MET:O	2.39	0.54
1:B:319:GLU:HG2	8:B:625:HOH:O	2.07	0.54
1:B:450:ASP:O	1:B:454:GLU:N	2.40	0.54
1:A:489:ALA:HA	1:A:492:GLU:HB2	1.89	0.54
1:B:49:ARG:HH12	1:B:53:ASP:HA	1.73	0.53
1:A:152:LEU:HB2	1:A:466:TYR:CZ	2.44	0.53
1:A:537:ASN:OD1	1:A:539:ILE:HG23	2.09	0.53
1:B:400:GLN:HG3	1:B:417:TYR:OH	2.07	0.53
1:B:280:PRO:HB2	1:B:283:SER:HB2	1.90	0.53
1:B:255:GLN:HG2	1:B:264:PRO:HA	1.89	0.53
1:A:183:LEU:HD13	1:A:445:LEU:HD22	1.90	0.53
1:B:438:ARG:NH1	8:B:590:HOH:O	2.39	0.53
1:A:49:ARG:CG	1:A:49:ARG:HH11	2.17	0.53
1:A:452:ILE:O	1:A:455:SER:HB3	2.09	0.52
1:B:289:GLN:OE1	1:B:291:VAL:HG22	2.09	0.52
1:A:157:ARG:HG3	1:A:459:ARG:CZ	2.40	0.52
1:B:124:ILE:HD11	1:B:528:PRO:HB2	1.91	0.52
1:A:461:GLN:HB3	1:A:462:PRO:HD2	1.92	0.52
1:A:374:ARG:HB3	1:B:374:ARG:HH12	1.75	0.52
1:B:275:TYR:CG	1:B:284:GLN:HG2	2.44	0.52
1:B:145:VAL:HG23	1:B:224:LEU:HD22	1.91	0.51
1:A:195:ASN:ND2	1:A:427:SER:HA	2.26	0.51
1:A:291:VAL:O	1:A:294:LEU:CD2	2.58	0.51
1:A:260:GLU:HB2	1:A:262:TYR:CE1	2.45	0.51
1:B:335:ILE:O	1:B:339:GLU:HG3	2.10	0.51
1:B:563:THR:HG22	1:B:565:LYS:N	2.26	0.51
4:A:674:BMA:O6	4:A:675:BMA:H4	2.10	0.51
1:B:113:MET:O	1:B:117:LEU:HD13	2.10	0.51
1:A:157:ARG:HG3	1:A:459:ARG:NH1	2.26	0.50
1:A:381:PHE:O	1:A:385:TYR:HB2	2.11	0.50
1:B:563:THR:CG2	8:B:593:HOH:O	2.55	0.50
1:A:381:PHE:CE1	1:A:385:TYR:CD1	3.00	0.50
1:A:527:ALA:HA	1:A:530:SER:HB3	1.92	0.50
1:A:172:PRO:HB2	1:A:177:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:GLN:OE1	1:B:228:VAL:HA	2.12	0.50
1:A:237:ASN:OD1	1:A:239:GLU:HB2	2.13	0.49
1:A:256:MET:O	1:A:257:LEU:HD23	2.11	0.49
1:B:530:SER:O	1:B:534:LEU:HD22	2.13	0.49
1:B:287:VAL:HG11	1:B:302:ALA:HB1	1.93	0.49
1:A:250:GLY:HA2	1:A:325:ASP:OD1	2.13	0.49
1:B:130:TYR:HB3	1:B:134:HIS:O	2.13	0.49
1:A:403:SER:HB3	1:A:406:GLN:HG3	1.94	0.49
1:A:389:PRO:HD3	1:A:440:ILE:HG12	1.95	0.49
1:B:243:GLN:HG3	1:B:270:PRO:HD2	1.93	0.48
1:A:155:VAL:O	1:A:459:ARG:HD2	2.14	0.48
1:B:172:PRO:O	1:B:456:ARG:NH2	2.46	0.48
1:B:213:SER:OG	1:B:215:LYS:NZ	2.46	0.48
1:A:130:TYR:HB3	1:A:134:HIS:O	2.13	0.48
1:A:352:LEU:HD23	6:A:701:NIM:C8	2.43	0.48
1:A:93:LEU:HD23	1:A:100:TRP:CH2	2.49	0.48
1:B:352:LEU:HD21	1:B:387:TRP:HH2	1.78	0.48
1:B:384:LEU:HD11	1:B:526:GLY:HA2	1.95	0.48
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.96	0.48
1:B:513:HIS:C	1:B:514:PRO:O	2.51	0.48
1:B:390:LEU:HD21	1:B:434:ILE:HD11	1.96	0.47
1:A:198:PHE:CZ	1:A:352:LEU:HD13	2.49	0.47
1:B:352:LEU:HD21	1:B:387:TRP:CH2	2.49	0.47
1:B:190:ASP:HA	1:B:433:ARG:HB2	1.97	0.47
4:A:672:NAG:C3	4:A:672:NAG:O7	2.62	0.47
1:B:299:MET:HG3	1:B:414:LEU:CD2	2.45	0.47
1:A:250:GLY:N	1:A:325:ASP:OD1	2.46	0.47
1:B:544:TYR:O	1:B:546:LYS:N	2.42	0.47
1:A:58:ASP:OD2	1:B:546:LYS:HB3	2.15	0.47
1:B:287:VAL:HA	8:B:594:HOH:O	2.15	0.47
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.51	0.46
1:B:198:PHE:C	1:B:198:PHE:CD2	2.88	0.46
1:A:268:GLU:HG3	8:A:597:HOH:O	2.15	0.46
1:B:54[A]:ARG:CB	1:B:54[A]:ARG:NH1	2.78	0.46
1:A:363:PRO:HG2	1:A:545:TRP:CD2	2.49	0.46
1:A:387:TRP:HB2	2:A:601:HEM:HAC	1.97	0.46
1:A:203:GLN:HA	2:A:601:HEM:HBC2	1.98	0.46
1:A:502:GLU:HB2	1:A:505:PRO:HG2	1.98	0.46
1:B:484:GLU:HG2	1:B:485:LYS:H	1.80	0.46
1:A:403:SER:HB3	1:A:406:GLN:HE21	1.81	0.46
1:A:392:PRO:HG2	1:A:394:SER:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:O	1:A:113:MET:C	2.52	0.45
1:B:300:LEU:O	1:B:303:THR:HB	2.16	0.45
1:B:441:ASP:OD1	1:B:443:HIS:ND1	2.39	0.45
1:B:334:LEU:HD13	1:B:549:THR:HG22	1.98	0.45
1:A:215:LYS:HD2	1:A:222:LYS:CE	2.36	0.45
1:A:388:HIS:N	1:A:389:PRO:CD	2.76	0.45
1:B:120:ARG:HA	7:B:1751:BOG:H62	1.97	0.45
1:A:184:ARG:NH1	1:A:441:ASP:HB2	2.31	0.45
1:B:203:GLN:NE2	2:B:601:HEM:C4B	2.85	0.45
1:A:408:LEU:HB3	1:A:409:PHE:CD1	2.51	0.45
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.51	0.45
1:B:113:MET:HE3	1:B:117:LEU:CD1	2.47	0.45
1:A:344:VAL:HG11	1:A:534:LEU:HD11	1.99	0.45
1:A:291:VAL:O	1:A:294:LEU:HD22	2.17	0.45
1:A:198:PHE:C	1:A:198:PHE:CD2	2.91	0.44
1:A:238:LEU:CD1	3:B:1671:NAG:H4	2.48	0.44
1:A:319:GLU:HB3	1:A:320:HIS:CD2	2.52	0.44
1:B:238:LEU:O	1:B:241:GLN:HB3	2.18	0.44
1:A:324:GLY:HA3	8:A:17:HOH:O	2.18	0.44
1:A:511:LYS:HA	8:A:606:HOH:O	2.18	0.44
1:A:513:HIS:HB2	1:A:516:SER:OG	2.18	0.44
1:B:195:ASN:ND2	1:B:427:SER:HA	2.32	0.44
1:A:462:PRO:HB2	8:A:596:HOH:O	2.16	0.44
1:B:504:TYR:CZ	1:B:508:LEU:HD11	2.53	0.43
1:B:114:ARG:HA	1:B:117:LEU:HD22	2.00	0.43
1:A:353:SER:HA	6:A:701:NIM:N2	2.33	0.43
1:A:353:SER:HA	6:A:701:NIM:C5	2.48	0.43
1:A:469:ARG:HH11	1:A:469:ARG:HG3	1.84	0.43
1:B:102:PHE:O	1:B:103:VAL:C	2.56	0.43
1:B:240:ARG:HG3	1:B:271:VAL:HG11	1.99	0.43
1:B:88:PHE:HB2	7:B:1752:BOG:H3'1	2.01	0.43
1:B:566:LYS:HG3	8:B:600:HOH:O	2.17	0.43
1:B:117:LEU:HB3	1:B:366:LEU:HD21	2.01	0.43
1:B:384:LEU:HD11	1:B:526:GLY:CA	2.47	0.43
1:B:452:ILE:O	1:B:455:SER:HB3	2.18	0.43
1:A:289:GLN:HG2	8:A:609:HOH:O	2.19	0.43
1:A:291:VAL:O	1:A:294:LEU:HD23	2.18	0.43
1:A:113:MET:O	1:A:117:LEU:HD13	2.19	0.43
1:B:382:ASN:HB3	8:B:608:HOH:O	2.19	0.42
1:A:370:GLN:HE22	1:B:369:ALA:C	2.21	0.42
1:B:498:ILE:O	1:B:498:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ASN:HA	1:B:35:PRO:HD2	1.86	0.42
1:B:464:ASN:HA	1:B:467:ARG:HG3	2.01	0.42
1:A:305:TRP:HE3	1:A:336:LEU:HD23	1.83	0.42
1:A:119:VAL:O	1:A:123:LEU:HD23	2.19	0.42
1:A:250:GLY:CA	1:A:325:ASP:OD1	2.68	0.42
1:B:200:PHE:CD1	1:B:297:GLY:HA3	2.54	0.42
1:B:353:SER:HA	6:B:1701:NIM:N2	2.34	0.42
1:B:192:GLN:HG2	1:B:515:ASN:O	2.20	0.42
1:A:341:ILE:HG23	1:A:534:LEU:HB3	2.02	0.42
1:A:502:GLU:HG2	8:A:12:HOH:O	2.20	0.42
1:A:125:PRO:HB3	1:B:543:GLU:CD	2.40	0.42
1:B:130:TYR:O	1:B:149:THR:HA	2.20	0.42
1:A:34:ASN:HA	1:A:35:PRO:HD3	1.83	0.42
1:B:59:CYS:O	1:B:60:THR:C	2.58	0.42
1:B:166:LYS:HA	1:B:166:LYS:HD3	1.89	0.42
1:B:131:ASN:HB2	1:B:147:TYR:CD1	2.55	0.42
1:A:316:LEU:HD21	1:A:331:THR:HG22	2.02	0.42
1:A:526:GLY:HA3	6:A:701:NIM:H10	2.01	0.42
1:A:334:LEU:HA	1:A:337:ILE:HD12	2.01	0.42
1:B:253:LYS:HB3	1:B:264:PRO:HG3	2.01	0.42
1:A:62:THR:HG22	1:A:64:TYR:N	2.35	0.42
1:A:316:LEU:HB3	1:A:328:LEU:CD2	2.48	0.41
1:B:39:TYR:N	1:B:40:PRO:HD3	2.35	0.41
1:B:344:VAL:O	1:B:348:TYR:HB3	2.19	0.41
1:B:513:HIS:O	1:B:516:SER:HB2	2.20	0.41
1:A:464:ASN:HD21	1:A:498:ILE:HG13	1.86	0.41
1:A:309:HIS:CD2	1:A:309:HIS:C	2.93	0.41
1:B:49:ARG:NH1	1:B:49:ARG:CG	2.64	0.41
1:A:238:LEU:HD13	3:B:1671:NAG:H4	2.02	0.41
1:B:215:LYS:HD2	1:B:216:MET:HG3	2.03	0.41
1:A:261:VAL:H	1:A:307:ARG:HH21	1.68	0.41
1:A:149:THR:OG1	1:A:150:ARG:N	2.54	0.41
1:B:388:HIS:CE1	1:B:447:VAL:HG11	2.55	0.41
1:B:344:VAL:O	1:B:349:VAL:HG23	2.21	0.41
1:B:384:LEU:C	1:B:384:LEU:HD23	2.41	0.41
1:A:368:GLY:HA2	1:B:370:GLN:NE2	2.35	0.41
1:B:429:GLN:HA	1:B:430:PRO:HD3	1.90	0.41
1:B:113:MET:CE	1:B:117:LEU:CD1	2.99	0.41
1:B:514:PRO:HA	8:B:18:HOH:O	2.21	0.41
1:A:113:MET:O	1:A:117:LEU:CD1	2.69	0.41
1:A:46:ILE:HG22	1:A:48:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:TYR:CD2	1:B:284:GLN:HG2	2.56	0.41
1:A:102:PHE:C	1:A:102:PHE:CD1	2.95	0.41
1:A:370:GLN:NE2	1:B:369:ALA:C	2.74	0.40
3:A:661:NAG:H61	3:A:662:NAG:C7	2.52	0.40
1:B:150:ARG:NH1	1:B:154:SER:HB3	2.36	0.40
1:B:566:LYS:O	1:B:570:LEU:HB2	2.21	0.40
1:A:491:LEU:O	1:A:493:GLU:N	2.55	0.40
1:A:161:THR:HB	8:A:20:HOH:O	2.21	0.40
1:B:280:PRO:C	1:B:282:GLN:N	2.74	0.40
1:A:420:GLU:CD	1:A:572:THR:HB	2.41	0.40
1:A:260:GLU:HB2	1:A:262:TYR:HE1	1.85	0.40
1:B:152:LEU:HD13	1:B:461:GLN:OE1	2.22	0.40
1:A:266:VAL:O	1:A:270:PRO:HA	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%)	496 (90%)	49 (9%)	6 (1%)	17	46
1	B	552/553 (100%)	500 (91%)	48 (9%)	4 (1%)	26	59
All	All	1103/1106 (100%)	996 (90%)	97 (9%)	10 (1%)	21	52

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	545	TRP
1	A	96	GLY
1	A	492	GLU
1	A	69	CYS
1	A	249	ASP

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Mol	Chain	Res	Type
1	B	60	THR
1	A	514	PRO
1	A	579	SER
1	B	86	PRO
1	B	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	476/488 (98%)	440 (92%)	36 (8%)	16	39
1	B	476/488 (98%)	447 (94%)	29 (6%)	23	52
All	All	952/976 (98%)	887 (93%)	65 (7%)	20	46

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	62	THR
1	A	74	ILE
1	A	76	THR
1	A	82	LEU
1	A	92	LEU
1	A	99	LEU
1	A	102	PHE
1	A	115	LEU
1	A	123	LEU
1	A	130	TYR
1	A	150	ARG
1	A	213	SER
1	A	215	LYS
1	A	222	LYS
1	A	232	HIS
1	A	246	LEU
1	A	295	LEU

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Mol	Chain	Res	Type
1	A	298	LEU
1	A	316	LEU
1	A	325	ASP
1	A	352	LEU
1	A	385	TYR
1	A	454	GLU
1	A	458	LEU
1	A	460	LEU
1	A	476	THR
1	A	480	GLU
1	A	484	GLU
1	A	493	GLU
1	A	518	PHE
1	A	535	LEU
1	A	539	ILE
1	A	546	LYS
1	A	556	PHE
1	A	567	LEU
1	B	49	ARG
1	B	54[A]	ARG
1	B	54[B]	ARG
1	B	74	ILE
1	B	82	LEU
1	B	87	SER
1	B	97	ARG
1	B	117	LEU
1	B	120	ARG
1	B	122	ASN
1	B	150	ARG
1	B	165	THR
1	B	171	LEU
1	B	180	ARG
1	B	183	LEU
1	B	213	SER
1	B	215	LYS
1	B	252	LEU
1	B	298	LEU
1	B	319	GLU
1	B	384	LEU
1	B	385	TYR
1	B	405	GLU
1	B	516	SER

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Mol	Chain	Res	Type
1	B	518	PHE
1	B	520	GLU
1	B	534	LEU
1	B	556	PHE
1	B	570	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	284	GLN
1	A	382	ASN
1	A	406	GLN
1	A	442	HIS
1	A	479	GLN
1	B	122	ASN
1	B	134	HIS
1	B	370	GLN
1	B	386	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

11 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	$\#\|Z\|>2$
3	NAG	A	661	1,3	14,14,15	0.64	0	15,19,21	1.11	2 (13%)
3	NAG	A	662	3	14,14,15	0.61	0	15,19,21	1.19	1 (6%)
4	NAG	A	671	1,4	14,14,15	0.77	0	15,19,21	1.78	2 (13%)
4	NAG	A	672	4	14,14,15	0.60	0	15,19,21	1.29	2 (13%)
4	BMA	A	673	4	11,11,12	0.75	0	14,15,17	1.38	2 (14%)
4	BMA	A	674	4	11,11,12	0.73	0	14,15,17	0.70	0
4	BMA	A	675	4	11,11,12	0.65	0	14,15,17	1.09	1 (7%)
3	NAG	B	1671	1,3	14,14,15	0.85	0	15,19,21	1.92	4 (26%)
3	NAG	B	1672	3	14,14,15	0.74	0	15,19,21	0.96	1 (6%)
3	NAG	B	1681	1,3	14,14,15	0.56	0	15,19,21	1.01	0
3	NAG	B	1682	3	14,14,15	0.63	0	15,19,21	1.32	1 (6%)

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	NAG	A	661	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	662	3	-	0/6/23/26	0/1/1/1
4	NAG	A	671	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	672	4	-	0/6/23/26	0/1/1/1
4	BMA	A	673	4	-	0/2/19/22	0/1/1/1
4	BMA	A	674	4	-	0/2/19/22	0/1/1/1
4	BMA	A	675	4	-	0/2/19/22	1/1/1/1
3	NAG	B	1671	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1672	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1681	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1682	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1682	NAG	C2-N2-C7	-4.26	117.56	123.04
3	B	1671	NAG	O7-C7-C8	-2.67	117.16	122.06
4	A	671	NAG	O4-C4-C3	-2.47	104.77	110.34
3	B	1671	NAG	C4-C3-C2	-2.32	107.62	111.23
3	B	1671	NAG	C2-N2-C7	-2.18	120.24	123.04
4	A	672	NAG	C4-C3-C2	-2.18	107.85	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	673	BMA	C6-C5-C4	2.04	118.05	113.02
3	B	1672	NAG	O3-C3-C2	2.05	113.17	109.11
3	A	661	NAG	C4-C3-C2	2.09	114.48	111.23
4	A	675	BMA	C1-O5-C5	2.22	115.06	112.25
3	A	662	NAG	C4-C3-C2	2.39	114.95	111.23
3	A	661	NAG	C3-C4-C5	2.61	114.75	110.20
4	A	672	NAG	C3-C2-N2	2.75	117.14	110.56
4	A	673	BMA	C1-O5-C5	3.15	116.25	112.25
3	B	1671	NAG	C1-O5-C5	5.14	118.77	112.25
4	A	671	NAG	C1-O5-C5	5.40	119.09	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	675	BMA	C1-C2-C3-C4-C5-O5

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	661	NAG	1	0
3	A	662	NAG	1	0
4	A	672	NAG	1	0
4	A	674	BMA	1	0
4	A	675	BMA	1	0
3	B	1671	NAG	2	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	$\#\|Z\|>2$
2	HEM	A	601	1	30,50,50	2.15	10 (33%)	24,82,82	2.47	10 (41%)
5	NAG	A	681	1	14,14,15	0.72	0	15,19,21	1.63	4 (26%)
6	NIM	A	701	-	20,22,22	2.97	4 (20%)	29,31,31	1.96	5 (17%)
5	NAG	B	1661	1	14,14,15	0.58	0	15,19,21	0.97	0
6	NIM	B	1701	-	20,22,22	2.66	5 (25%)	29,31,31	1.77	3 (10%)
7	BOG	B	1751	-	20,20,20	0.74	0	25,25,25	2.20	7 (28%)
7	BOG	B	1752	-	20,20,20	0.79	1 (5%)	25,25,25	1.44	5 (20%)
2	HEM	B	601	1,8	30,50,50	2.16	9 (30%)	24,82,82	2.43	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
2	HEM	A	601	1	-	0/10/54/54	0/0/8/8
5	NAG	A	681	1	-	0/6/23/26	0/1/1/1
6	NIM	A	701	-	-	0/13/13/13	0/2/2/2
5	NAG	B	1661	1	-	0/6/23/26	0/1/1/1
6	NIM	B	1701	-	-	0/13/13/13	0/2/2/2
7	BOG	B	1751	-	-	0/11/31/31	0/1/1/1
7	BOG	B	1752	-	-	0/11/31/31	0/1/1/1
2	HEM	B	601	1,8	-	0/10/54/54	0/0/8/8

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C3B-C4B	-7.08	1.45	1.51
2	A	601	HEM	C3B-C4B	-6.59	1.46	1.51
6	B	1701	NIM	C2-N1	-5.54	1.32	1.42
2	A	601	HEM	C3D-C4D	-5.51	1.44	1.51
2	B	601	HEM	C3D-C4D	-5.24	1.44	1.51
6	A	701	NIM	C2-N1	-5.23	1.33	1.42
2	B	601	HEM	C2C-C1C	-3.48	1.46	1.52
2	A	601	HEM	C2C-C1C	-3.32	1.46	1.52
2	A	601	HEM	C2B-C1B	-2.42	1.43	1.51
2	B	601	HEM	C2B-C1B	-2.31	1.44	1.51
6	B	1701	NIM	S1-N1	-2.25	1.60	1.63
2	B	601	HEM	CMA-C3A	2.03	1.55	1.51
7	B	1752	BOG	O1-C1	2.05	1.43	1.40
2	B	601	HEM	FE-NC	2.10	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C4C-NC	2.15	1.38	1.36
2	A	601	HEM	C3B-CAB	2.17	1.55	1.51
2	A	601	HEM	C1C-NC	2.18	1.38	1.36
2	A	601	HEM	CAA-C2A	2.20	1.55	1.52
2	A	601	HEM	CMA-C3A	2.26	1.56	1.51
2	B	601	HEM	C3C-CAC	2.28	1.55	1.51
2	B	601	HEM	C3B-CAB	2.28	1.55	1.51
2	B	601	HEM	C4C-NC	2.67	1.39	1.36
2	A	601	HEM	FE-ND	2.72	2.11	1.97
6	A	701	NIM	O2-S1	3.09	1.49	1.43
6	B	1701	NIM	O1-S1	3.14	1.50	1.43
6	A	701	NIM	O1-S1	3.28	1.50	1.43
6	B	1701	NIM	O2-S1	3.52	1.50	1.43
6	B	1701	NIM	O3-N2	8.66	1.39	1.22
6	A	701	NIM	O3-N2	10.93	1.44	1.22

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	701	NIM	O2-S1-O1	-8.26	106.78	118.77
6	B	1701	NIM	O2-S1-O1	-6.52	109.29	118.77
7	B	1751	BOG	C4-C3-C2	-5.05	101.36	110.79
7	B	1751	BOG	O1-C1-C2	-5.01	101.71	108.04
7	B	1751	BOG	C1'-O1-C1	-4.92	105.35	113.94
2	A	601	HEM	C3C-CAC-CBC	-4.44	117.64	124.46
2	B	601	HEM	CBA-CAA-C2A	-3.85	105.63	112.53
7	B	1752	BOG	O5-C1-C2	-3.45	103.20	110.28
7	B	1752	BOG	O5-C5-C4	-3.04	103.98	109.68
7	B	1751	BOG	O5-C1-C2	-2.89	104.34	110.28
2	B	601	HEM	CAA-C2A-C1A	-2.50	124.30	127.01
2	B	601	HEM	CMA-C3A-C4A	-2.49	124.24	128.36
5	A	681	NAG	C3-C4-C5	-2.39	106.03	110.20
2	A	601	HEM	CAA-CBA-CGA	-2.39	108.37	112.75
7	B	1752	BOG	C3-C4-C5	-2.32	106.16	110.20
7	B	1751	BOG	O5-C5-C6	-2.20	100.79	106.36
2	B	601	HEM	CBD-CAD-C3D	-2.19	107.17	113.55
2	A	601	HEM	CAA-C2A-C1A	-2.16	124.66	127.01
7	B	1752	BOG	C4-C3-C2	-2.11	106.85	110.79
7	B	1752	BOG	O5-C1-O1	2.14	115.21	110.05
6	A	701	NIM	O1-S1-C1	2.21	112.30	108.37
2	A	601	HEM	C2C-C1C-CHC	2.23	127.07	123.68
2	A	601	HEM	C3B-C4B-CHC	2.24	126.31	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	681	NAG	C3-C2-N2	2.27	116.00	110.56
5	A	681	NAG	C1-O5-C5	2.28	115.15	112.25
7	B	1751	BOG	O2-C2-C3	2.31	115.53	110.34
6	A	701	NIM	C1-S1-N1	2.33	109.76	106.83
6	A	701	NIM	C7-O5-C8	2.56	124.45	117.77
7	B	1751	BOG	C1-O5-C5	2.59	118.77	113.75
2	A	601	HEM	CMD-C2D-C3D	2.70	126.28	114.35
2	B	601	HEM	CMD-C2D-C3D	2.74	126.47	114.35
2	B	601	HEM	C3B-C4B-CHC	2.76	127.05	123.16
2	B	601	HEM	CMC-C2C-C3C	3.16	124.42	116.53
6	B	1701	NIM	O1-S1-C1	3.16	113.98	108.37
5	A	681	NAG	O3-C3-C2	3.21	115.48	109.11
6	A	701	NIM	C6-C5-N2	3.54	121.91	118.80
2	B	601	HEM	CAD-C3D-C4D	3.93	126.33	112.47
2	A	601	HEM	CMC-C2C-C3C	4.11	126.78	116.53
2	A	601	HEM	CAD-C3D-C4D	4.15	127.09	112.47
2	A	601	HEM	CMB-C2B-C3B	4.25	127.13	116.53
2	B	601	HEM	CMB-C2B-C3B	4.83	128.60	116.53
6	B	1701	NIM	C1-S1-N1	4.86	112.96	106.83
2	A	601	HEM	CAD-C3D-C2D	5.24	128.29	113.22
2	B	601	HEM	CAD-C3D-C2D	5.43	128.82	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	2	0
6	A	701	NIM	4	0
6	B	1701	NIM	1	0
7	B	1751	BOG	3	0
7	B	1752	BOG	2	0
2	B	601	HEM	3	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%)	-0.45	2 (0%)	93	92	39, 57, 76, 82	0
1	B	553/553 (100%)	-0.43	2 (0%)	93	92	37, 54, 74, 85	0
All	All	1106/1106 (100%)	-0.44	4 (0%)	93	92	37, 55, 75, 85	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	ILE	3.1
1	A	368	GLY	2.1
1	B	105	ALA	2.1
1	A	258	ASN	2.0

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
3	NAG	A	661	14/15	0.91	0.18	0.27	84,90,92,92	0
3	NAG	B	1672	14/15	0.89	0.19	-0.22	57,61,64,66	0
3	NAG	B	1681	14/15	0.96	0.12	-0.47	68,71,75,80	0
3	NAG	B	1671	14/15	0.97	0.11	-0.67	40,44,48,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	A	671	14/15	0.96	0.10	-1.11	44,47,50,56	0
3	NAG	B	1682	14/15	0.94	0.14	-	83,85,86,88	0
4	BMA	A	675	11/12	0.93	0.20	-	93,96,97,98	0
4	BMA	A	673	11/12	0.94	0.19	-	71,74,76,82	0
4	NAG	A	672	14/15	0.94	0.20	-	60,63,68,68	0
4	BMA	A	674	11/12	0.88	0.14	-	84,88,91,94	0
3	NAG	A	662	14/15	0.93	0.19	-	91,95,99,99	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	BOG	B	1751	20/20	0.94	0.17	2.20	45,48,50,52	0
5	NAG	A	681	14/15	0.90	0.20	1.35	65,67,69,69	0
5	NAG	B	1661	14/15	0.95	0.18	0.56	71,75,78,78	0
2	HEM	B	601	43/43	0.95	0.15	0.21	48,54,63,68	0
7	BOG	B	1752	20/20	0.88	0.15	-0.04	65,70,73,74	0
2	HEM	A	601	43/43	0.95	0.15	-0.29	40,49,57,60	0
6	NIM	A	701	21/21	0.98	0.11	-0.71	55,59,65,66	0
6	NIM	B	1701	21/21	0.99	0.10	-0.83	49,53,57,60	0

6.5 Other polymers

There are no such residues in this entry.