



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:00 PM GMT

PDB ID : 3QMO
Title : X-ray crystal structure of NS-398 bound to the cyclooxygenase channel of cyclooxygenase-2
Authors : Vecchio, A.J.; Malkowski, M.G.
Deposited on : 2011-02-04
Resolution : 3.00 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

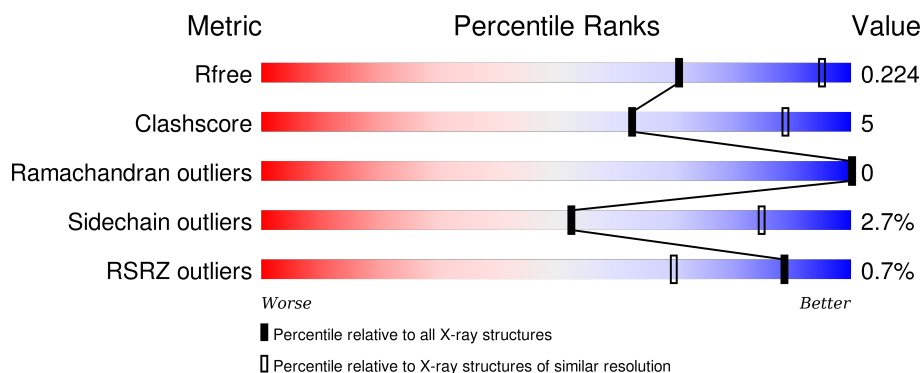
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	610	<div> <div></div> <div>80% 9% 10%</div> </div>
1	B	610	<div> <div></div> <div>80% 9% 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
2	GOL	A	7	-	-	-	X
2	GOL	B	2	-	-	-	X
7	NAG	A	681	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9237 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	3	0
			4392	2840	736	791	25			
1	B	551	Total	C	N	O	S	0	0	0
			4379	2838	729	787	25			

There are 14 discrepancies between the modelled and reference sequences:

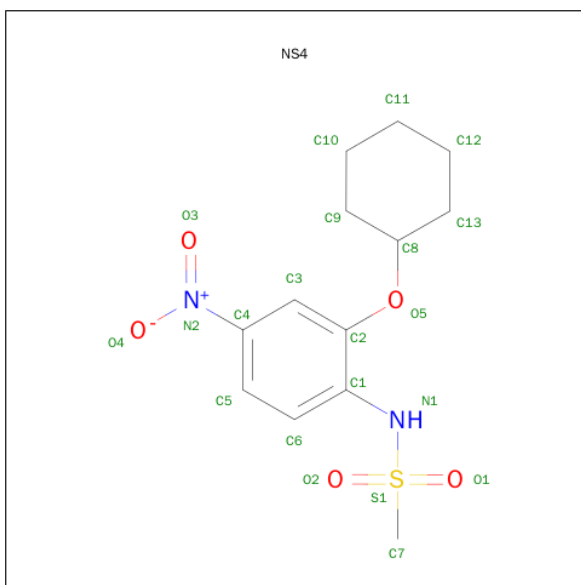
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	HIS	-	EXPRESSION TAG	UNP Q05769
A	30	HIS	-	EXPRESSION TAG	UNP Q05769
A	31	HIS	-	EXPRESSION TAG	UNP Q05769
A	32	HIS	-	EXPRESSION TAG	UNP Q05769
A	33	HIS	-	EXPRESSION TAG	UNP Q05769
A	34	HIS	-	EXPRESSION TAG	UNP Q05769
A	594	ALA	ASN	ENGINEERED MUTATION	UNP Q05769
B	29	HIS	-	EXPRESSION TAG	UNP Q05769
B	30	HIS	-	EXPRESSION TAG	UNP Q05769
B	31	HIS	-	EXPRESSION TAG	UNP Q05769
B	32	HIS	-	EXPRESSION TAG	UNP Q05769
B	33	HIS	-	EXPRESSION TAG	UNP Q05769
B	34	HIS	-	EXPRESSION TAG	UNP Q05769
B	594	ALA	ASN	ENGINEERED MUTATION	UNP Q05769

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



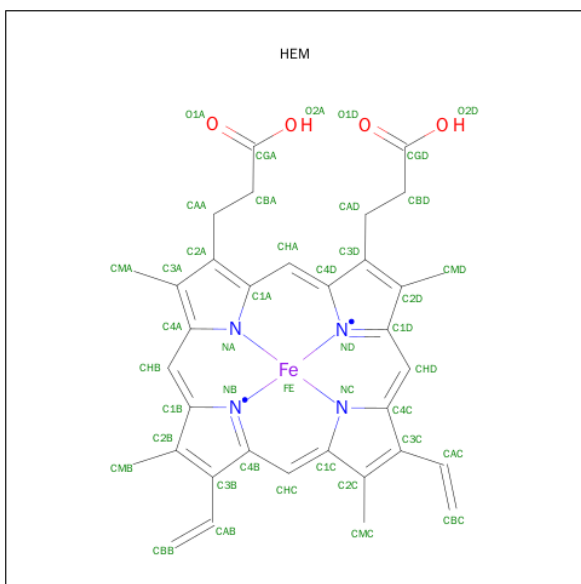
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is N-[2-(CYCLOHEXYLOXY)-4-NITROPHENYL]METHANESULFONAMIDE (three-letter code: NS4) (formula: $C_{13}H_{18}N_2O_5S$).



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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

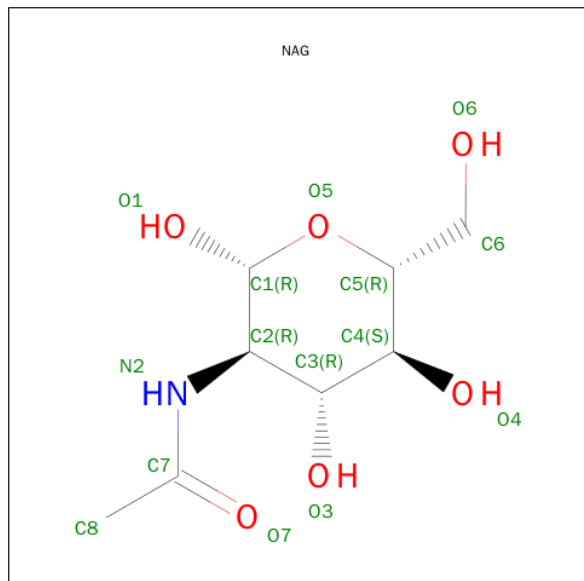
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

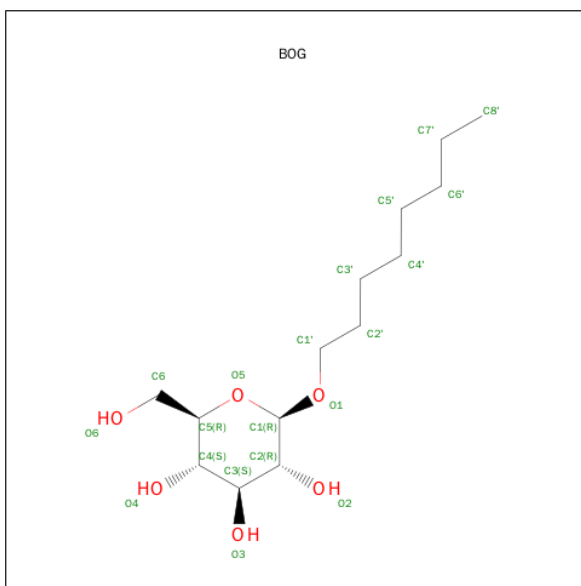
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



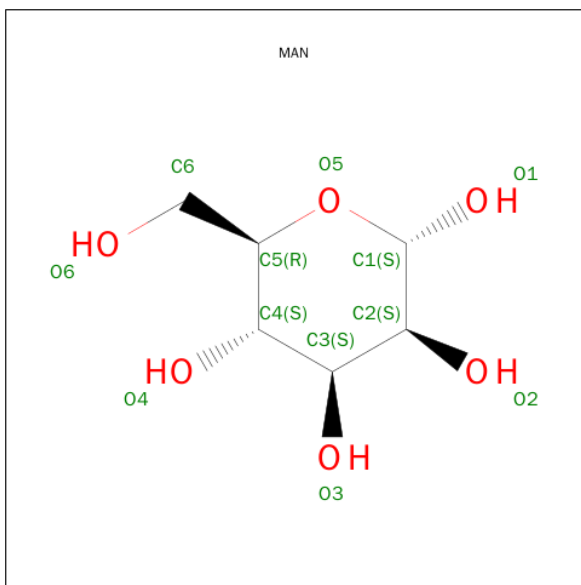
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 9 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			11	6	5		

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

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

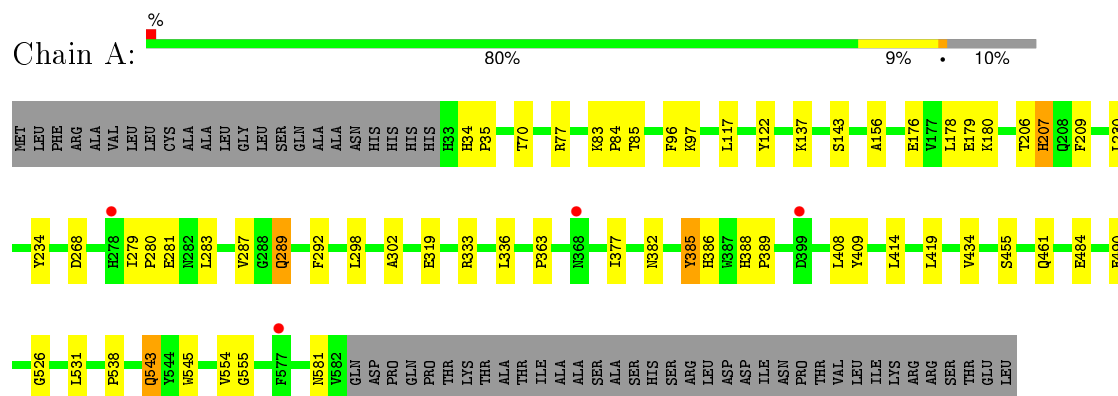
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	57	Total	O	0	0
			57	57		
11	B	63	Total	O	0	0
			63	63		

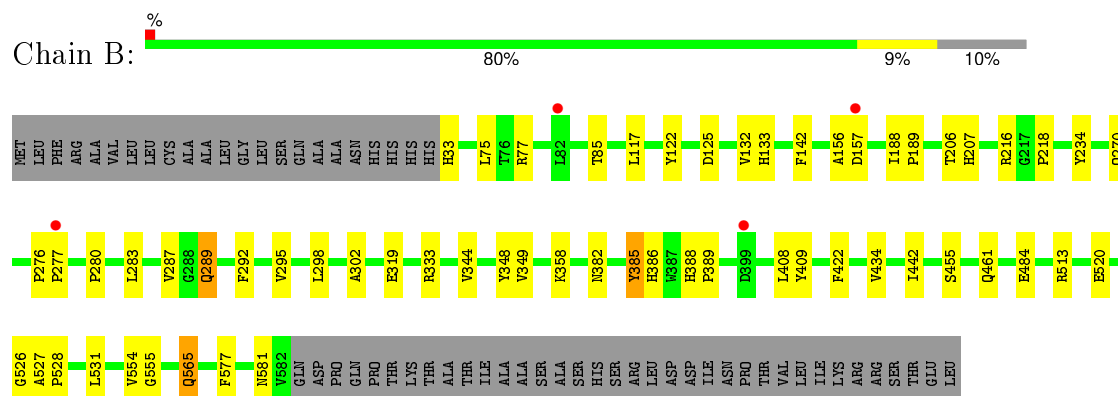
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Prostaglandin G/H synthase 2



• Molecule 1: Prostaglandin G/H synthase 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.43Å 131.21Å 179.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.99-3.00) 99.8 (19.99-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.176 , 0.225 0.175 , 0.224	Depositor DCC
R_{free} test set	1452 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 28678 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9237	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, NDG, HEM, BOG, NS4, 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	0.52	0/4527	0.59	0/6158
1	B	0.51	0/4508	0.59	1/6130 (0.0%)
All	All	0.52	0/9035	0.59	1/12288 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	LEU	CA-CB-CG	5.44	127.82	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4392	0	4171	45	0
1	B	4379	0	4172	43	0
2	A	18	0	24	3	0
2	B	18	0	24	3	0
3	A	21	0	18	4	0
3	B	21	0	18	4	0
4	A	43	0	30	2	0
4	B	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	28	0	25	1	0
5	B	28	0	25	0	0
6	A	28	0	24	1	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
8	A	20	0	28	1	0
9	B	11	0	10	0	0
10	B	39	0	34	4	0
11	A	57	0	0	5	0
11	B	63	0	0	7	0
All	All	9237	0	8659	94	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (94) 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:137[B]:LYS:H	1:A:137[B]:LYS:CD	1.51	1.18
1:A:137[B]:LYS:HD2	1:A:137[B]:LYS:N	1.50	1.14
4:A:620:HEM:HBA1	4:A:620:HEM:HHA	1.43	0.95
1:B:156:ALA:H	2:B:3:GOL:H32	1.33	0.91
1:A:543[A]:GLN:HA	1:A:543[A]:GLN:OE1	1.71	0.90
1:A:137[B]:LYS:H	1:A:137[B]:LYS:HD2	0.74	0.89
1:A:137[B]:LYS:HD3	11:B:663:HOH:O	1.84	0.77
3:A:619:NS4:O2	3:A:619:NS4:H6	1.90	0.71
1:A:319:GLU:HG3	1:A:554:VAL:HG11	1.73	0.69
1:B:319:GLU:HG3	1:B:554:VAL:HG11	1.75	0.67
1:B:526:GLY:HA3	3:B:1:NS4:H12	1.77	0.66
4:B:619:HEM:HBC2	4:B:619:HEM:HHD	1.77	0.66
1:B:295:VAL:HG21	4:B:619:HEM:HBB2	1.79	0.64
1:A:179:GLU:HB3	8:A:703:BOG:H3'1	1.81	0.63
1:A:156:ALA:H	2:A:1:GOL:H32	1.64	0.63
1:A:287:VAL:HG11	1:A:302:ALA:HB1	1.80	0.62
10:B:620:BMA:H61	11:B:635:HOH:O	2.01	0.60
1:B:216:ARG:NH1	10:B:672:NAG:H83	2.16	0.60
1:A:389:PRO:HB2	1:A:434:VAL:HA	1.83	0.60
1:B:289:GLN:HG2	1:B:292:PHE:CE1	2.38	0.58
1:B:287:VAL:HG11	1:B:302:ALA:HB1	1.86	0.57
1:A:382:ASN:O	1:A:386:HIS:HD2	1.88	0.57
1:A:77:ARG:NH1	11:A:673:HOH:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLN:HG2	1:A:292:PHE:CE1	2.40	0.56
1:A:268:ASP:CG	11:A:650:HOH:O	2.45	0.55
1:A:414:LEU:HD11	1:A:419:LEU:HD12	1.89	0.54
1:B:389:PRO:HB2	1:B:434:VAL:HA	1.90	0.53
1:B:218:PRO:HD2	11:B:666:HOH:O	2.10	0.52
1:B:77:ARG:NH1	11:B:680:HOH:O	2.43	0.51
1:A:143:SER:O	2:A:7:GOL:H12	2.10	0.51
3:B:1:NS4:H6	3:B:1:NS4:O2	2.10	0.51
1:A:531:LEU:HD11	3:A:619:NS4:H7	1.94	0.50
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.47	0.50
1:B:382:ASN:O	1:B:386:HIS:HD2	1.95	0.49
1:B:531:LEU:HD11	3:B:1:NS4:H7	1.92	0.49
1:B:234:TYR:CE2	1:B:333:ARG:HG3	2.48	0.48
1:A:137[B]:LYS:CD	11:B:663:HOH:O	2.54	0.48
1:B:565:GLN:OE1	1:B:577:PHE:HA	2.13	0.48
1:B:531:LEU:HD11	3:B:1:NS4:C7	2.44	0.48
1:A:408:LEU:O	1:A:409:TYR:HB2	2.14	0.47
1:A:531:LEU:HD11	3:A:619:NS4:C7	2.45	0.47
1:A:137[B]:LYS:CD	1:A:137[B]:LYS:N	2.29	0.47
1:A:554:VAL:HG13	1:A:555:GLY:N	2.30	0.47
2:A:6:GOL:H32	4:A:620:HEM:NA	2.30	0.46
1:B:554:VAL:HG13	1:B:555:GLY:N	2.29	0.46
1:A:117:LEU:HD23	1:A:531:LEU:HD13	1.98	0.46
1:B:207:HIS:O	1:B:289:GLN:NE2	2.49	0.46
1:B:388:HIS:N	1:B:389:PRO:CD	2.80	0.45
6:A:671:NAG:H82	11:A:637:HOH:O	2.15	0.45
1:A:543[A]:GLN:HG3	1:B:125:ASP:OD1	2.16	0.45
1:B:216:ARG:HG2	10:B:672:NAG:H81	1.98	0.45
1:A:382:ASN:O	1:A:386:HIS:CD2	2.68	0.45
1:B:513:ARG:HH21	1:B:520:GLU:HG3	1.81	0.45
1:B:206:THR:HG21	1:B:385:TYR:CE2	2.51	0.45
1:A:268:ASP:CB	11:A:656:HOH:O	2.64	0.45
1:B:280:PRO:HG2	1:B:283:LEU:HD12	1.99	0.45
1:B:117:LEU:HD23	1:B:531:LEU:HD13	1.99	0.44
1:B:358:LYS:HB3	1:B:358:LYS:HE2	1.76	0.44
1:B:289:GLN:HG2	1:B:292:PHE:CZ	2.52	0.44
1:A:292:PHE:CD1	1:A:298:LEU:HD13	2.53	0.44
5:A:662:NDG:H2	5:A:662:NDG:H8C1	1.84	0.43
1:B:527:ALA:HB3	1:B:528:PRO:HD3	2.01	0.43
1:B:270:GLN:HA	1:B:270:GLN:HE21	1.84	0.43
1:A:280:PRO:HG2	1:A:283:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:HA	1:A:280:PRO:HD2	1.84	0.43
1:B:156:ALA:N	2:B:3:GOL:H32	2.15	0.42
1:A:538:PRO:HG3	1:B:142:PHE:CE2	2.54	0.42
1:A:363:PRO:HG2	1:A:545:TRP:CD2	2.54	0.42
2:B:4:GOL:H31	4:B:619:HEM:C1A	2.54	0.42
1:A:77:ARG:CZ	11:A:673:HOH:O	2.67	0.42
1:B:77:ARG:NH2	11:B:658:HOH:O	2.53	0.42
1:B:344:VAL:HA	1:B:348:TYR:HB3	2.01	0.42
1:A:34:HIS:HA	1:A:35:PRO:HD3	1.96	0.42
1:B:216:ARG:HH11	10:B:672:NAG:H83	1.83	0.42
1:A:96:PHE:O	1:A:97:LYS:C	2.57	0.42
1:A:230:LEU:CD2	1:A:336:LEU:HB3	2.50	0.41
1:A:83:LYS:HA	1:A:84:PRO:HD3	1.96	0.41
1:A:209:PHE:HB2	1:A:377:ILE:HG13	2.02	0.41
1:A:388:HIS:N	1:A:389:PRO:CD	2.84	0.41
1:B:388:HIS:N	1:B:389:PRO:HD2	2.35	0.41
1:B:132:VAL:HG13	1:B:133:HIS:CD2	2.55	0.41
1:B:333:ARG:NH1	11:B:637:HOH:O	2.50	0.41
1:A:207:HIS:O	1:A:289:GLN:NE2	2.54	0.41
1:B:276:PRO:HA	1:B:277:PRO:HD3	1.91	0.41
1:A:538:PRO:HG3	1:B:142:PHE:CZ	2.56	0.40
1:B:344:VAL:O	1:B:349:VAL:HG23	2.21	0.40
1:B:442:ILE:H	1:B:442:ILE:HD12	1.85	0.40
1:A:526:GLY:HA3	3:A:619:NS4:H12	2.03	0.40
1:B:292:PHE:CD1	1:B:298:LEU:HD13	2.56	0.40
1:B:408:LEU:O	1:B:409:TYR:HB2	2.21	0.40
1:B:188:ILE:HA	1:B:189:PRO:HD2	1.87	0.40
1:A:206:THR:HG21	1:A:385:TYR:CE2	2.56	0.40
1:A:176:GLU:HG2	1:A:180:LYS:HD2	2.03	0.40
1:A:180:LYS:HE3	1:A:490:GLU:OE1	2.22	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	552/610 (90%)	530 (96%)	22 (4%)	0	100	100
1	B	549/610 (90%)	529 (96%)	20 (4%)	0	100	100
All	All	1101/1220 (90%)	1059 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	461/542 (85%)	447 (97%)	14 (3%)	48	83
1	B	460/542 (85%)	448 (97%)	12 (3%)	54	85
All	All	921/1084 (85%)	895 (97%)	26 (3%)	52	84

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	THR
1	A	85	THR
1	A	122	TYR
1	A	178	LEU
1	A	207	HIS
1	A	281	GLU
1	A	289	GLN
1	A	385	TYR
1	A	455	SER
1	A	461	GLN
1	A	484	GLU
1	A	543[A]	GLN
1	A	543[B]	GLN
1	A	581	ASN
1	B	33	HIS

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Mol	Chain	Res	Type
1	B	85	THR
1	B	122	TYR
1	B	157	ASP
1	B	289	GLN
1	B	385	TYR
1	B	422	PHE
1	B	455	SER
1	B	461	GLN
1	B	484	GLU
1	B	565	GLN
1	B	581	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	270	GLN
1	B	168	ASN
1	B	207	HIS
1	B	270	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

9 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	661	1,5	14,14,15	0.61	0	15,19,21	1.43	3 (20%)
5	NDG	A	662	5	14,14,15	0.74	1 (7%)	15,19,21	2.19	6 (40%)
6	NAG	A	671	1,6	14,14,15	0.70	0	15,19,21	1.29	2 (13%)
6	NAG	A	672	9,6	14,14,15	0.54	0	15,19,21	1.37	2 (13%)
10	BMA	B	620	10	11,11,12	0.83	0	14,15,17	2.07	3 (21%)
5	NAG	B	661	1,5	14,14,15	0.60	0	15,19,21	0.67	0
5	NDG	B	662	5	14,14,15	0.51	0	15,19,21	0.90	1 (6%)
10	NAG	B	671	1,10	14,14,15	1.89	1 (7%)	15,19,21	2.64	5 (33%)
10	NAG	B	672	10	14,14,15	0.67	0	15,19,21	2.63	5 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	661	1,5	-	0/6/23/26	0/1/1/1
5	NDG	A	662	5	-	0/6/23/26	0/1/1/1
6	NAG	A	671	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	672	9,6	-	0/6/23/26	0/1/1/1
10	BMA	B	620	10	-	0/2/19/22	1/1/1/1
5	NAG	B	661	1,5	-	0/6/23/26	0/1/1/1
5	NDG	B	662	5	-	0/6/23/26	0/1/1/1
10	NAG	B	671	1,10	-	0/6/23/26	0/1/1/1
10	NAG	B	672	10	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	671	NAG	O5-C1	-6.49	1.32	1.43
5	A	662	NDG	C1-C2	2.34	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	671	NAG	C1-O5-C5	-8.27	101.76	112.25
5	A	662	NDG	C3-C4-C5	-5.26	101.03	110.20
10	B	672	NAG	C3-C4-C5	-4.49	102.37	110.20
10	B	672	NAG	C4-C3-C2	-4.36	104.45	111.23
5	A	661	NAG	C3-C4-C5	-3.19	104.63	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	672	NAG	C2-N2-C7	-2.61	119.69	123.04
10	B	671	NAG	C2-N2-C7	-2.49	119.84	123.04
10	B	671	NAG	C3-C4-C5	-2.09	106.55	110.20
5	A	662	NDG	C6-C5-C4	2.06	118.09	113.02
5	B	662	NDG	C1-O-C5	2.06	114.86	112.25
6	A	671	NAG	O7-C7-N2	2.14	126.23	121.86
5	A	662	NDG	C8-C7-N2	2.20	120.32	116.11
5	A	662	NDG	O-C5-C6	2.30	112.32	107.35
5	A	661	NAG	O5-C5-C6	2.36	112.47	107.35
5	A	661	NAG	O4-C4-C3	2.55	116.08	110.34
10	B	671	NAG	O4-C4-C5	2.56	116.01	109.24
5	A	662	NDG	O4-C4-C5	2.59	116.11	109.24
6	A	672	NAG	C1-O5-C5	2.86	115.88	112.25
10	B	620	BMA	O2-C2-C1	3.32	115.86	109.21
6	A	671	NAG	C2-N2-C7	3.37	127.37	123.04
5	A	662	NDG	C1-O-C5	3.54	116.74	112.25
10	B	671	NAG	O5-C5-C6	3.60	115.15	107.35
10	B	620	BMA	C1-C2-C3	3.71	113.93	109.54
10	B	672	NAG	O4-C4-C3	4.24	119.87	110.34
10	B	672	NAG	O5-C5-C6	4.26	116.58	107.35
10	B	672	NAG	O4-C4-C5	4.48	121.12	109.24
10	B	620	BMA	C1-O5-C5	5.12	118.74	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	620	BMA	C1-C2-C3-C4-C5-O5

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	662	NDG	1	0
6	A	671	NAG	1	0
10	B	620	BMA	1	0
10	B	672	NAG	3	0

5.6 Ligand geometry [i](#)

14 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	GOL	A	1	-	5,5,5	0.56	0	5,5,5	0.39	0
2	GOL	A	6	-	5,5,5	0.39	0	5,5,5	0.39	0
3	NS4	A	619	-	20,22,22	2.99	4 (20%)	26,31,31	1.88	3 (11%)
4	HEM	A	620	1	30,50,50	2.11	9 (30%)	24,82,82	2.29	9 (37%)
7	NAG	A	681	1	14,14,15	1.48	2 (14%)	15,19,21	0.83	1 (6%)
2	GOL	A	7	-	5,5,5	0.26	0	5,5,5	0.42	0
8	BOG	A	703	-	20,20,20	1.14	2 (10%)	25,25,25	1.02	1 (4%)
3	NS4	B	1	-	20,22,22	2.96	4 (20%)	26,31,31	1.49	1 (3%)
2	GOL	B	2	-	5,5,5	0.49	0	5,5,5	0.39	0
2	GOL	B	3	-	5,5,5	0.25	0	5,5,5	0.27	0
2	GOL	B	4	-	5,5,5	0.51	0	5,5,5	0.26	0
4	HEM	B	619	1	30,50,50	2.33	7 (23%)	24,82,82	2.41	10 (41%)
9	MAN	B	673	6	11,11,12	0.88	1 (9%)	14,15,17	2.25	3 (21%)
7	NAG	B	681	1	14,14,15	0.74	0	15,19,21	2.08	5 (33%)

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	GOL	A	1	-	-	0/4/4/4	0/0/0/0
2	GOL	A	6	-	-	0/4/4/4	0/0/0/0
3	NS4	A	619	-	-	0/13/21/21	0/2/2/2
4	HEM	A	620	1	-	2/10/54/54	0/0/8/8
7	NAG	A	681	1	-	0/6/23/26	0/1/1/1
2	GOL	A	7	-	-	0/4/4/4	0/0/0/0
8	BOG	A	703	-	-	0/11/31/31	0/1/1/1
3	NS4	B	1	-	-	0/13/21/21	0/2/2/2
2	GOL	B	2	-	-	0/4/4/4	0/0/0/0
2	GOL	B	3	-	-	0/4/4/4	0/0/0/0
2	GOL	B	4	-	-	0/4/4/4	0/0/0/0
4	HEM	B	619	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	B	673	6	-	0/2/19/22	0/1/1/1
7	NAG	B	681	1	-	0/6/23/26	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	619	HEM	C3B-C4B	-7.44	1.45	1.51
4	A	620	HEM	C3B-C4B	-7.04	1.45	1.51
3	B	1	NS4	C1-N1	-5.71	1.32	1.42
4	B	619	HEM	C3D-C4D	-5.31	1.44	1.51
3	A	619	NS4	C1-N1	-5.19	1.33	1.42
7	A	681	NAG	O5-C1	-4.46	1.36	1.43
4	A	620	HEM	C3D-C4D	-4.39	1.45	1.51
4	A	620	HEM	C2C-C1C	-3.85	1.45	1.52
4	B	619	HEM	C2C-C1C	-3.84	1.45	1.52
4	A	620	HEM	C2D-C1D	-2.09	1.45	1.51
4	B	619	HEM	C3C-CAC	2.01	1.55	1.51
4	A	620	HEM	C1C-NC	2.02	1.38	1.36
4	A	620	HEM	FE-NB	2.03	2.08	1.97
4	B	619	HEM	C4C-NC	2.10	1.38	1.36
9	B	673	MAN	C2-C3	2.15	1.55	1.52
4	A	620	HEM	C4C-NC	2.24	1.38	1.36
4	A	620	HEM	C3C-CAC	2.30	1.55	1.51
8	A	703	BOG	O5-C1	2.38	1.47	1.41
4	A	620	HEM	CAA-C2A	2.48	1.56	1.52
7	A	681	NAG	C1-C2	2.82	1.56	1.52
4	B	619	HEM	C1C-NC	2.87	1.39	1.36
3	A	619	NS4	O1-S1	3.12	1.49	1.43
3	A	619	NS4	O2-S1	3.56	1.50	1.43
3	B	1	NS4	O1-S1	3.62	1.51	1.43
8	A	703	BOG	O1-C1	3.64	1.46	1.40
3	B	1	NS4	O2-S1	3.72	1.51	1.43
4	B	619	HEM	FE-NC	4.44	2.13	1.95
3	B	1	NS4	O3-N2	10.41	1.43	1.22
3	A	619	NS4	O3-N2	10.96	1.44	1.22

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	619	NS4	O2-S1-O1	-7.91	107.28	118.77
3	B	1	NS4	O2-S1-O1	-6.46	109.39	118.77
4	B	619	HEM	C3B-CAB-CBB	-4.32	117.82	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	620	HEM	C3B-CAB-CBB	-2.70	120.31	124.46
7	B	681	NAG	C3-C2-N2	-2.45	104.69	110.56
4	A	620	HEM	CMA-C3A-C4A	-2.37	124.44	128.36
8	A	703	BOG	C1'-O1-C1	-2.36	109.81	113.94
4	B	619	HEM	CBD-CAD-C3D	-2.25	107.00	113.55
4	B	619	HEM	CMA-C3A-C4A	-2.10	124.89	128.36
4	B	619	HEM	CAA-CBA-CGA	-2.09	108.92	112.75
4	A	620	HEM	C3C-CAC-CBC	-2.08	121.27	124.46
9	B	673	MAN	O5-C5-C6	2.08	111.86	107.35
7	A	681	NAG	O5-C5-C6	2.20	112.12	107.35
4	B	619	HEM	C2D-C3D-C4D	2.38	105.54	101.50
4	A	620	HEM	CBA-CAA-C2A	2.56	117.11	112.53
7	B	681	NAG	C3-C4-C5	2.58	114.69	110.20
3	A	619	NS4	C7-S1-N1	2.64	110.15	106.83
3	A	619	NS4	C9-C8-C13	2.67	115.94	111.61
4	A	620	HEM	CMD-C2D-C3D	2.76	126.55	114.35
7	B	681	NAG	C1-O5-C5	2.76	115.75	112.25
4	B	619	HEM	CMD-C2D-C3D	2.86	127.00	114.35
9	B	673	MAN	C2-C3-C4	3.28	116.61	111.04
7	B	681	NAG	C2-N2-C7	3.46	127.49	123.04
4	A	620	HEM	CMC-C2C-C3C	3.62	125.56	116.53
4	B	619	HEM	CAD-C3D-C4D	3.80	125.86	112.47
4	B	619	HEM	CMC-C2C-C3C	3.99	126.50	116.53
4	A	620	HEM	CMB-C2B-C3B	4.00	126.52	116.53
4	B	619	HEM	CMB-C2B-C3B	4.22	127.07	116.53
4	A	620	HEM	CAD-C3D-C2D	4.54	126.27	113.22
4	A	620	HEM	CAD-C3D-C4D	4.75	129.22	112.47
7	B	681	NAG	C4-C3-C2	5.03	119.05	111.23
4	B	619	HEM	CAD-C3D-C2D	5.35	128.60	113.22
9	B	673	MAN	C1-C2-C3	6.64	117.39	109.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	620	HEM	C3A-C2A-CAA-CBA
4	A	620	HEM	C1A-C2A-CAA-CBA

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	GOL	1	0
2	A	6	GOL	1	0
3	A	619	NS4	4	0
4	A	620	HEM	2	0
2	A	7	GOL	1	0
8	A	703	BOG	1	0
3	B	1	NS4	4	0
2	B	3	GOL	2	0
2	B	4	GOL	1	0
4	B	619	HEM	3	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	551/610 (90%)	-0.56	4 (0%)	89 70	17, 33, 51, 60	0
1	B	551/610 (90%)	-0.51	4 (0%)	89 70	17, 33, 51, 60	0
All	All	1102/1220 (90%)	-0.53	8 (0%)	89 70	17, 33, 51, 60	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	HIS	2.7
1	A	577	PHE	2.6
1	B	157	ASP	2.6
1	A	399	ASP	2.4
1	B	277	PRO	2.3
1	A	368	ASN	2.1
1	B	82	LEU	2.1
1	B	399	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	A	671	14/15	0.93	0.20	1.17	32,36,38,43	0
5	NAG	A	661	14/15	0.95	0.32	1.12	59,61,65,69	0
10	NAG	B	671	14/15	0.96	0.15	-0.31	31,34,39,39	0
6	NAG	A	672	14/15	0.89	0.32	-	47,50,54,58	0
5	NDG	B	662	14/15	0.82	0.43	-	72,73,74,74	0
10	BMA	B	620	11/12	0.78	0.47	-	55,57,58,58	0
5	NDG	A	662	14/15	0.79	0.54	-	74,77,78,79	0
5	NAG	B	661	14/15	0.88	0.34	-	60,63,65,69	0
10	NAG	B	672	14/15	0.95	0.28	-	43,45,50,52	0

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	B	2	6/6	0.79	0.31	7.68	53,58,58,59	0
7	NAG	A	681	14/15	0.90	0.38	7.10	58,59,61,61	0
2	GOL	A	7	6/6	0.87	0.29	6.45	49,49,50,50	0
2	GOL	B	3	6/6	0.87	0.25	1.55	54,55,56,56	0
2	GOL	A	1	6/6	0.93	0.17	0.76	51,52,52,53	0
3	NS4	A	619	21/21	0.97	0.15	0.55	29,35,38,41	0
3	NS4	B	1	21/21	0.97	0.15	0.35	39,42,43,46	0
4	HEM	B	619	43/43	0.95	0.16	0.04	24,29,43,49	0
8	BOG	A	703	20/20	0.94	0.17	-0.24	49,51,53,54	0
4	HEM	A	620	43/43	0.97	0.14	-0.27	20,26,41,47	0
9	MAN	B	673	11/12	0.90	0.29	-	61,63,65,65	0
2	GOL	B	4	6/6	0.81	0.30	-	57,58,59,59	0
7	NAG	B	681	14/15	0.80	0.33	-	61,66,67,68	0
2	GOL	A	6	6/6	0.92	0.19	-	49,51,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.