



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:11 PM GMT

PDB ID : 4O1Z
Title : Crystal Structure of Ovine Cyclooxygenase-1 Complex with Meloxicam
Authors : Xu, S.; Hermanson, D.J.; Banerjee, S.; Ghebreselasie, K.; Clayton, G.M.;
Garavito, R.M.; Marnett, L.J.
Deposited on : 2013-12-16
Resolution : 2.40 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

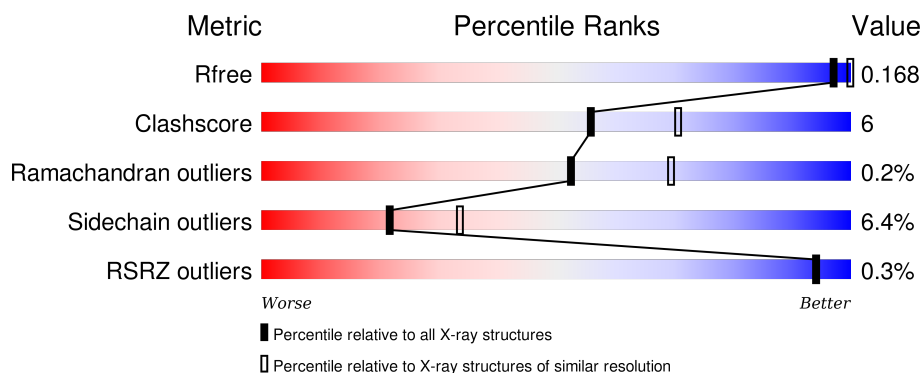
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	569	 80% 15% . .
1	B	569	 80% 15% . .

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	NAG	B	806	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9615 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.

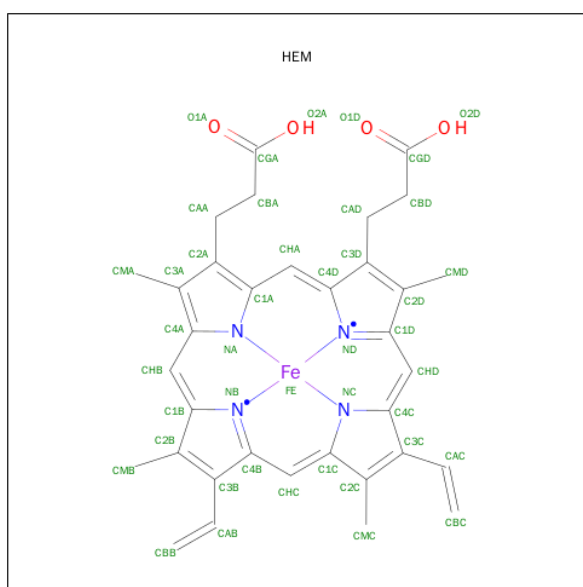
- Molecule 1 is a protein called Prostaglandin G/H synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4492	2912	760	792	28			
1	B	553	Total	C	N	O	S	0	0	0
			4492	2912	760	792	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	LEU	MET	SEE REMARK 999	UNP P05979
B	92	LEU	MET	SEE REMARK 999	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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

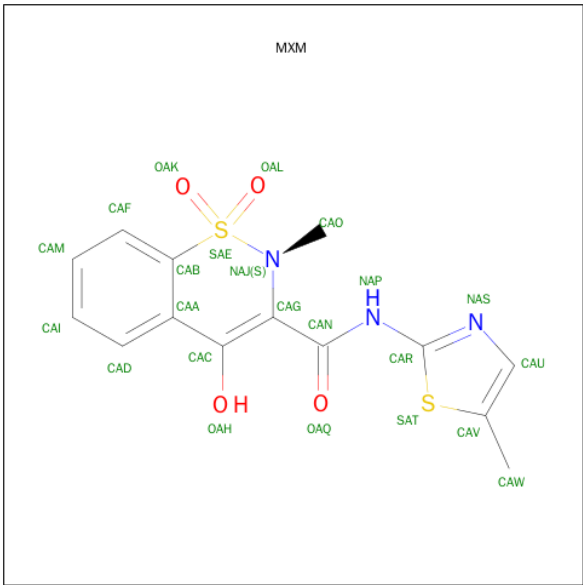


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

- Molecule 5 is 4-HYDROXY-2-METHYL-N-(5-METHYL-1,3-THIAZOL-2-YL)-2H-1,2-BENZOTHAZINE-3-CARBOXAMIDE 1,1-DIOXIDE (three-letter code: MXM) (formula: $C_{14}H_{13}N_3O_4S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	1
			46	28	6	8	4		
5	B	1	Total	C	N	O	S	0	1
			46	28	6	8	4		

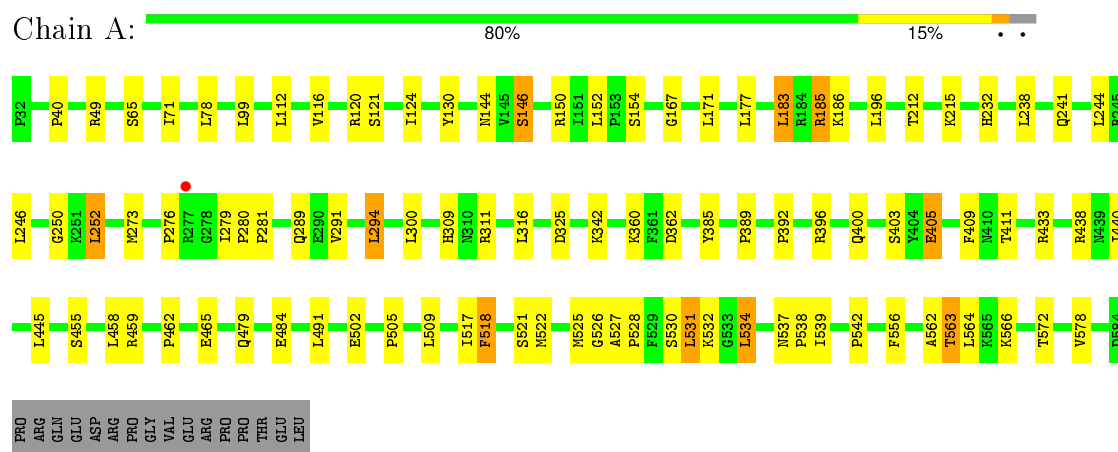
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	161	Total	O	0	0
			161	161		
6	B	152	Total	O	0	0
			152	152		

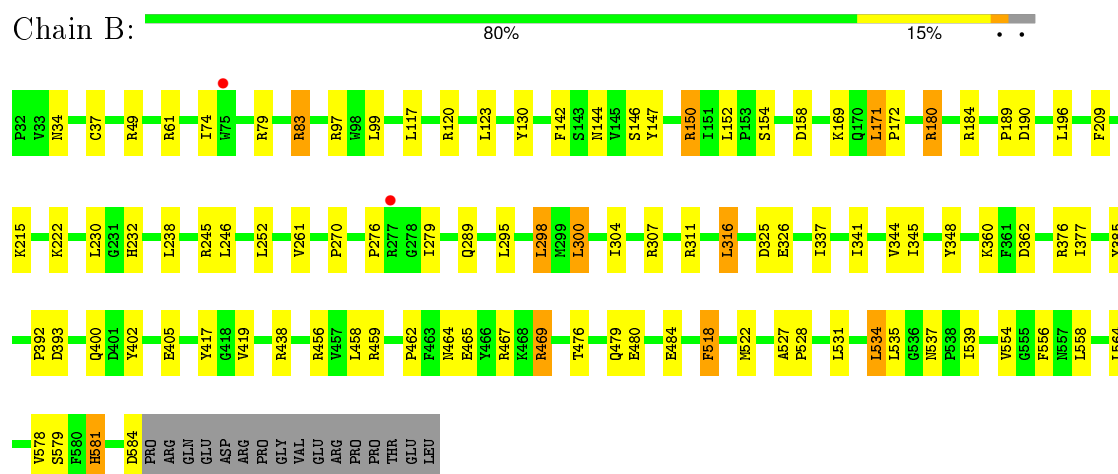
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Prostaglandin G/H synthase 1



• Molecule 1: 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	181.33Å 181.33Å 103.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.55 – 2.40 43.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.55-2.40) 99.6 (43.55-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.150 , 0.173 0.149 , 0.168	Depositor DCC
R_{free} test set	3013 reflections (4.18%)	DCC
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.3	EDS
Estimated twinning fraction	0.436 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 75189 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9615	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: HEM, MXM, NAG

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	0/4631	0.47	1/6286 (0.0%)
1	B	0.38	0/4631	0.47	0/6286
All	All	0.35	0/9262	0.47	1/12572 (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	A	531	LEU	CA-CB-CG	5.12	127.07	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	4492	0	4395	51	0
1	B	4492	0	4395	55	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
3	A	14	0	13	1	0
3	B	14	0	13	0	0
4	A	56	0	50	2	0
4	B	56	0	50	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	46	0	24	2	0
5	B	46	0	24	3	0
6	A	161	0	0	14	0
6	B	152	0	0	8	0
All	All	9615	0	9024	113	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 6.

All (113) 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:123:LEU:O	1:B:469:ARG:NH2	2.21	0.74
4:A:806:NAG:O4	6:A:1052:HOH:O	2.06	0.73
2:A:801:HEM:HHD	2:A:801:HEM:HBC2	1.72	0.71
1:A:521:SER:O	6:A:1056:HOH:O	2.07	0.70
1:A:532:LYS:NZ	6:A:903:HOH:O	2.22	0.70
1:B:189:PRO:O	6:B:1049:HOH:O	2.11	0.69
1:A:525:MET:N	6:A:1056:HOH:O	2.22	0.69
1:A:563:THR:HG22	1:A:566:LYS:H	1.56	0.69
1:A:572:THR:O	6:A:969:HOH:O	2.09	0.69
1:B:79:ARG:HH11	1:B:83:ARG:NH2	1.93	0.66
1:B:180:ARG:O	1:B:438:ARG:NH1	2.28	0.66
5:B:807[B]:MXM:OAH	5:B:807[B]:MXM:NAP	2.22	0.65
5:A:807[B]:MXM:NAP	5:A:807[B]:MXM:OAH	2.21	0.65
1:B:79:ARG:HH11	1:B:83:ARG:HH21	1.46	0.64
2:B:801:HEM:HBC2	2:B:801:HEM:HHD	1.80	0.62
1:A:311:ARG:NH2	6:A:909:HOH:O	2.33	0.62
4:A:804:NAG:O4	6:A:1031:HOH:O	2.16	0.61
1:B:459:ARG:NH2	6:B:956:HOH:O	2.34	0.61
1:A:185:ARG:HE	1:A:438:ARG:HH11	1.49	0.60
1:B:196:LEU:HD21	1:B:392:PRO:HD3	1.83	0.60
1:B:245:ARG:NH2	1:B:325:ASP:OD2	2.35	0.59
1:B:97:ARG:NH2	6:B:994:HOH:O	2.12	0.59
1:B:579:SER:HG	1:B:581:HIS:HD1	1.51	0.58
1:A:522:MET:O	6:A:1056:HOH:O	2.17	0.58
1:B:196:LEU:HD11	1:B:392:PRO:HG3	1.86	0.58
1:B:150:ARG:HD3	1:B:152:LEU:O	2.04	0.58
1:B:462:PRO:HG2	1:B:465:GLU:HG2	1.87	0.57
2:A:801:HEM:HMB1	2:A:801:HEM:HBB2	1.86	0.57
1:A:462:PRO:HG2	1:A:465:GLU:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.45	0.56
1:A:196:LEU:HD11	1:A:392:PRO:HG3	1.87	0.56
1:B:345:ILE:HG13	1:B:534:LEU:HD12	1.86	0.56
1:A:563:THR:HB	1:A:566:LYS:HD3	1.88	0.55
1:B:518:PHE:CZ	5:B:807[B]:MXM:H2	2.41	0.55
1:A:518:PHE:CZ	5:A:807[B]:MXM:H2	2.41	0.55
1:B:190:ASP:O	6:B:911:HOH:O	2.17	0.54
1:A:130:TYR:HB2	1:A:150:ARG:HG3	1.88	0.54
1:A:342:LYS:HG2	1:A:562:ALA:HB3	1.91	0.53
1:A:526:GLY:N	6:A:1056:HOH:O	2.13	0.53
1:A:150:ARG:HD3	1:A:152:LEU:O	2.08	0.53
1:A:360:LYS:HE2	1:A:362:ASP:HB2	1.89	0.53
1:A:542:PRO:O	1:B:61:ARG:NH1	2.41	0.53
1:B:579:SER:OG	1:B:581:HIS:ND1	2.37	0.53
1:A:250:GLY:N	1:A:325:ASP:OD1	2.33	0.52
1:A:522:MET:C	6:A:1056:HOH:O	2.48	0.52
4:B:804:NAG:O4	6:B:1038:HOH:O	2.18	0.52
1:B:184:ARG:NH1	1:B:393:ASP:OD1	2.40	0.51
1:B:469:ARG:O	1:B:469:ARG:NE	2.37	0.50
1:A:185:ARG:HH21	1:A:438:ARG:NH1	2.08	0.50
1:B:400:GLN:NE2	4:B:806:NAG:O4	2.44	0.50
1:A:212:THR:OG1	2:A:801:HEM:O1D	2.30	0.50
1:B:479:GLN:HG3	6:B:1023:HOH:O	2.12	0.50
1:A:276:PRO:HD2	1:A:279:ILE:HD12	1.94	0.49
1:B:154:SER:HB2	1:B:459:ARG:HB2	1.93	0.49
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.95	0.49
1:A:154:SER:HB2	1:A:459:ARG:HB2	1.94	0.49
1:B:245:ARG:NH1	1:B:326:GLU:OE2	2.36	0.49
2:B:801:HEM:HMB2	2:B:801:HEM:HBB2	1.95	0.48
1:A:183:LEU:HG	1:A:445:LEU:HD22	1.95	0.48
1:B:402:TYR:OH	1:B:417:TYR:OH	2.19	0.48
1:B:295:LEU:HB2	1:B:298:LEU:HD22	1.95	0.48
1:B:341:ILE:HG23	1:B:534:LEU:HD13	1.96	0.48
1:A:518:PHE:CD2	1:A:522:MET:HG2	2.48	0.47
1:B:360:LYS:HE2	1:B:362:ASP:HB2	1.97	0.47
1:B:311:ARG:NH2	6:B:1033:HOH:O	2.47	0.47
1:B:537:ASN:OD1	1:B:539:ILE:HG12	2.14	0.47
1:A:40:PRO:HB3	3:A:802:NAG:H62	1.97	0.47
1:A:241:GLN:OE1	6:A:968:HOH:O	2.21	0.46
1:A:294:LEU:HD12	1:A:409:PHE:HD1	1.81	0.45
1:A:491:LEU:HD11	1:A:509:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:SER:N	1:A:71:ILE:O	2.48	0.45
1:B:230:LEU:HD13	1:B:337:ILE:HG12	1.99	0.45
1:B:222:LYS:HB3	1:B:222:LYS:HE2	1.71	0.45
1:B:518:PHE:CD2	1:B:522:MET:HG2	2.52	0.44
1:A:389:PRO:HG3	1:A:440:ILE:HG12	1.99	0.44
1:B:476:THR:OG1	1:B:480:GLU:OE2	2.26	0.44
1:A:144:ASN:OD1	1:A:146:SER:HB2	2.16	0.44
1:B:300:LEU:HD21	1:B:419:VAL:HG13	2.00	0.44
1:A:112:LEU:O	1:A:116:VAL:HG23	2.18	0.44
1:B:531:LEU:HD23	5:B:807[B]:MXM:OAL	2.17	0.44
1:A:538:PRO:HG3	1:B:142:PHE:CE2	2.53	0.44
1:A:403:SER:OG	1:A:405:GLU:HG2	2.17	0.44
1:A:167:GLY:O	6:A:948:HOH:O	2.21	0.44
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.99	0.43
1:A:537:ASN:OD1	1:A:539:ILE:HG12	2.18	0.43
1:A:49:ARG:HG3	6:A:964:HOH:O	2.19	0.43
1:B:79:ARG:NH1	1:B:83:ARG:HH21	2.16	0.43
1:B:172:PRO:O	1:B:456:ARG:NH2	2.44	0.42
1:B:171:LEU:HD12	1:B:171:LEU:HA	1.87	0.42
1:A:252:LEU:HD22	1:A:309:HIS:CD2	2.55	0.42
1:B:464:ASN:HA	1:B:467:ARG:HG3	2.01	0.42
1:A:289:GLN:OE1	1:A:291:VAL:HG22	2.19	0.42
1:A:279:ILE:HD13	1:A:411:THR:HG21	2.02	0.42
1:A:273:MET:O	6:A:912:HOH:O	2.22	0.42
1:A:502:GLU:HB2	1:A:505:PRO:HG2	2.02	0.41
1:B:209:PHE:HB2	1:B:377:ILE:HG13	2.02	0.41
1:B:34:ASN:HB2	1:B:158:ASP:OD2	2.20	0.41
1:A:433:ARG:HG3	1:A:517:ILE:HA	2.02	0.41
1:A:121:SER:HB3	1:A:531:LEU:HD11	2.03	0.41
1:B:130:TYR:HB2	1:B:150:ARG:HG3	2.03	0.41
1:B:276:PRO:HD2	1:B:279:ILE:HD12	2.01	0.41
1:B:261:VAL:O	1:B:307:ARG:NH1	2.54	0.41
1:B:300:LEU:O	1:B:304:ILE:HG13	2.20	0.41
1:B:144:ASN:OD1	1:B:146:SER:HB2	2.21	0.41
1:B:316:LEU:HD12	1:B:316:LEU:HA	1.86	0.41
1:A:530:SER:O	1:A:534:LEU:HD22	2.21	0.41
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.83	0.41
1:B:169:LYS:HD3	1:B:169:LYS:HA	1.90	0.41
1:A:124:ILE:HD11	1:A:528:PRO:HB2	2.02	0.40
1:A:396:ARG:HG3	1:A:400:GLN:O	2.22	0.40
1:B:558:LEU:HD23	1:B:558:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:TYR:HB2	6:B:974:HOH:O	2.20	0.40
1:B:344:VAL:O	1:B:348:TYR:HB3	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	551/569 (97%)	529 (96%)	22 (4%)	0	100	100
1	B	551/569 (97%)	523 (95%)	26 (5%)	2 (0%)	39	56
All	All	1102/1138 (97%)	1052 (96%)	48 (4%)	2 (0%)	52	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	PRO
1	B	74	ILE

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	488/503 (97%)	458 (94%)	30 (6%)	23	36
1	B	488/503 (97%)	456 (93%)	32 (7%)	21	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	976/1006 (97%)	914 (94%)	62 (6%)	22	34

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	99	LEU
1	A	120	ARG
1	A	146	SER
1	A	171	LEU
1	A	177	LEU
1	A	183	LEU
1	A	185	ARG
1	A	186	LYS
1	A	215	LYS
1	A	232	HIS
1	A	238	LEU
1	A	244	LEU
1	A	246	LEU
1	A	252	LEU
1	A	294	LEU
1	A	300	LEU
1	A	316	LEU
1	A	385	TYR
1	A	405	GLU
1	A	455	SER
1	A	458	LEU
1	A	479	GLN
1	A	484	GLU
1	A	518	PHE
1	A	534	LEU
1	A	556	PHE
1	A	563	THR
1	A	564	LEU
1	A	578	VAL
1	B	49	ARG
1	B	83	ARG
1	B	99	LEU
1	B	117	LEU
1	B	120	ARG
1	B	150	ARG
1	B	171	LEU

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Mol	Chain	Res	Type
1	B	180	ARG
1	B	215	LYS
1	B	232	HIS
1	B	238	LEU
1	B	246	LEU
1	B	252	LEU
1	B	289	GLN
1	B	298	LEU
1	B	300	LEU
1	B	316	LEU
1	B	376	ARG
1	B	385	TYR
1	B	405	GLU
1	B	458	LEU
1	B	469	ARG
1	B	484	GLU
1	B	518	PHE
1	B	534	LEU
1	B	535	LEU
1	B	554	VAL
1	B	556	PHE
1	B	564	LEU
1	B	578	VAL
1	B	581	HIS
1	B	584	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	HIS
1	A	388	HIS
1	A	557	ASN
1	B	400	GLN

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 ⓘ

8 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	803	1,4	14,14,15	0.39	0	15,19,21	0.66	0
4	NAG	A	804	4	14,14,15	0.44	0	15,19,21	0.37	0
4	NAG	A	805	1,4	14,14,15	0.97	2 (14%)	15,19,21	0.48	0
4	NAG	A	806	4	14,14,15	0.20	0	15,19,21	0.51	0
4	NAG	B	803	1,4	14,14,15	0.79	1 (7%)	15,19,21	0.94	0
4	NAG	B	804	4	14,14,15	0.99	0	15,19,21	1.14	1 (6%)
4	NAG	B	805	1,4	14,14,15	0.97	2 (14%)	15,19,21	0.48	0
4	NAG	B	806	4	14,14,15	0.46	0	15,19,21	1.93	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	803	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	804	4	-	0/6/23/26	0/1/1/1
4	NAG	A	805	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	806	4	-	0/6/23/26	0/1/1/1
4	NAG	B	803	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	804	4	-	0/6/23/26	0/1/1/1
4	NAG	B	805	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	806	4	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	805	NAG	O5-C1	-2.71	1.39	1.43
4	A	805	NAG	O5-C1	-2.69	1.39	1.43
4	B	805	NAG	C1-C2	2.13	1.55	1.52
4	A	805	NAG	C1-C2	2.13	1.55	1.52
4	B	803	NAG	C1-C2	2.69	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	804	NAG	O5-C5-C6	2.12	111.93	107.35
4	B	806	NAG	C4-C3-C2	2.70	115.43	111.23
4	B	806	NAG	C1-O5-C5	6.49	120.49	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	804	NAG	1	0
4	A	806	NAG	1	0
4	B	804	NAG	1	0
4	B	806	NAG	1	0

5.6 Ligand geometry ⓘ

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	801	1	30,50,50	2.19	10 (33%)	24,82,82	2.18	5 (20%)
3	NAG	A	802	1	14,14,15	0.20	0	15,19,21	0.47	0
5	MXM	A	807[A]	-	23,25,25	6.53	10 (43%)	31,38,38	4.81	16 (51%)
5	MXM	A	807[B]	-	23,25,25	5.59	10 (43%)	31,38,38	4.88	16 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	801	1	30,50,50	2.20	7 (23%)	24,82,82	2.23	7 (29%)
3	NAG	B	802	1	14,14,15	0.17	0	15,19,21	0.51	0
5	MXM	B	807[A]	-	23,25,25	6.88	10 (43%)	31,38,38	4.97	14 (45%)
5	MXM	B	807[B]	-	23,25,25	5.62	10 (43%)	31,38,38	5.06	14 (45%)

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	801	1	-	0/10/54/54	0/0/8/8
3	NAG	A	802	1	-	0/6/23/26	0/1/1/1
5	MXM	A	807[A]	-	-	0/6/32/32	0/3/3/3
5	MXM	A	807[B]	-	-	0/6/32/32	0/3/3/3
2	HEM	B	801	1	-	0/10/54/54	0/0/8/8
3	NAG	B	802	1	-	0/6/23/26	0/1/1/1
5	MXM	B	807[A]	-	-	0/6/32/32	0/3/3/3
5	MXM	B	807[B]	-	-	0/6/32/32	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	807[A]	MXM	SAE-NAJ	-22.21	1.41	1.64
5	A	807[A]	MXM	CAB-SAE	-21.52	1.50	1.76
5	B	807[A]	MXM	CAB-SAE	-17.93	1.54	1.76
5	A	807[B]	MXM	CAB-SAE	-16.68	1.56	1.76
5	A	807[A]	MXM	SAE-NAJ	-15.78	1.48	1.64
5	B	807[B]	MXM	SAE-NAJ	-15.14	1.48	1.64
5	B	807[B]	MXM	CAB-SAE	-14.75	1.58	1.76
5	A	807[B]	MXM	SAE-NAJ	-12.37	1.51	1.64
5	B	807[B]	MXM	CAV-SAT	-8.10	1.59	1.74
5	A	807[B]	MXM	CAV-SAT	-7.78	1.59	1.74
2	A	801	HEM	C3B-C4B	-7.46	1.45	1.51
5	B	807[A]	MXM	CAG-NAJ	-7.34	1.36	1.44
2	B	801	HEM	C3B-C4B	-7.18	1.45	1.51
5	A	807[A]	MXM	CAG-NAJ	-6.38	1.37	1.44
2	B	801	HEM	C3D-C4D	-5.57	1.44	1.51
5	A	807[B]	MXM	CAG-NAJ	-5.34	1.38	1.44
5	B	807[B]	MXM	CAG-NAJ	-5.24	1.38	1.44
5	B	807[A]	MXM	CAV-SAT	-4.93	1.65	1.74
5	A	807[A]	MXM	CAV-SAT	-4.91	1.65	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3D-C4D	-4.84	1.45	1.51
5	B	807[A]	MXM	CAA-CAB	-4.16	1.36	1.40
2	B	801	HEM	C2C-C1C	-4.11	1.44	1.52
5	A	807[A]	MXM	CAA-CAB	-4.02	1.36	1.40
2	A	801	HEM	C2C-C1C	-3.89	1.45	1.52
5	A	807[B]	MXM	CAA-CAB	-3.87	1.36	1.40
5	B	807[B]	MXM	CAA-CAB	-3.72	1.37	1.40
5	B	807[A]	MXM	CAG-CAN	-3.43	1.39	1.46
5	A	807[A]	MXM	CAG-CAN	-3.28	1.39	1.46
5	A	807[B]	MXM	CAG-CAN	-3.18	1.39	1.46
5	A	807[A]	MXM	CAA-CAC	-2.89	1.40	1.45
5	B	807[B]	MXM	CAG-CAN	-2.84	1.40	1.46
5	B	807[A]	MXM	CAA-CAC	-2.79	1.41	1.45
5	A	807[B]	MXM	CAA-CAC	-2.70	1.41	1.45
5	B	807[B]	MXM	CAA-CAC	-2.48	1.41	1.45
2	B	801	HEM	C2B-C1B	-2.19	1.44	1.51
2	A	801	HEM	C2D-C1D	-2.02	1.45	1.51
2	A	801	HEM	FE-NB	2.01	2.08	1.97
2	B	801	HEM	C3C-CAC	2.05	1.55	1.51
2	A	801	HEM	C1C-NC	2.17	1.38	1.36
2	A	801	HEM	C4C-NC	2.21	1.38	1.36
2	B	801	HEM	C3B-CAB	2.24	1.55	1.51
2	A	801	HEM	C3C-CAC	2.27	1.55	1.51
2	B	801	HEM	C4C-NC	2.28	1.38	1.36
2	A	801	HEM	C3B-CAB	2.28	1.55	1.51
2	A	801	HEM	FE-ND	2.30	2.09	1.97
5	A	807[A]	MXM	CAG-CAC	5.10	1.43	1.36
5	B	807[A]	MXM	CAG-CAC	5.22	1.43	1.36
5	A	807[B]	MXM	CAG-CAC	5.32	1.43	1.36
5	B	807[B]	MXM	CAG-CAC	5.61	1.43	1.36
5	B	807[A]	MXM	OAK-SAE	6.61	1.51	1.43
5	B	807[B]	MXM	OAK-SAE	6.98	1.52	1.43
5	A	807[B]	MXM	OAK-SAE	7.49	1.53	1.43
5	A	807[A]	MXM	OAK-SAE	7.76	1.53	1.43
5	B	807[B]	MXM	OAL-SAE	8.33	1.54	1.43
5	A	807[A]	MXM	OAL-SAE	8.42	1.54	1.43
5	A	807[B]	MXM	OAL-SAE	8.59	1.54	1.43
5	B	807[A]	MXM	OAL-SAE	8.64	1.54	1.43

All (72) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	807[A]	MXM	CAG-NAJ-SAE	-9.84	98.59	113.17
5	B	807[B]	MXM	CAG-NAJ-SAE	-9.66	98.86	113.17
5	B	807[A]	MXM	CAB-CAA-CAC	-9.66	115.22	120.53
5	A	807[A]	MXM	CAG-NAJ-SAE	-9.51	99.07	113.17
5	A	807[B]	MXM	CAG-NAJ-SAE	-9.44	99.17	113.17
5	B	807[B]	MXM	CAB-CAA-CAC	-9.02	115.57	120.53
5	A	807[B]	MXM	CAB-CAA-CAC	-8.70	115.74	120.53
5	A	807[A]	MXM	CAB-CAA-CAC	-8.55	115.82	120.53
5	B	807[A]	MXM	OAL-SAE-OAK	-8.07	107.59	118.63
5	A	807[A]	MXM	OAL-SAE-OAK	-7.89	107.83	118.63
5	B	807[B]	MXM	OAL-SAE-OAK	-7.87	107.86	118.63
5	A	807[B]	MXM	OAL-SAE-OAK	-7.79	107.97	118.63
5	B	807[B]	MXM	CAA-CAB-SAE	-7.31	108.40	117.21
5	B	807[A]	MXM	CAA-CAB-SAE	-7.14	108.61	117.21
5	A	807[B]	MXM	OAH-CAC-CAG	-7.11	116.57	122.80
5	B	807[B]	MXM	OAH-CAC-CAG	-7.00	116.67	122.80
5	A	807[A]	MXM	CAA-CAB-SAE	-6.60	109.26	117.21
5	A	807[B]	MXM	CAA-CAB-SAE	-6.56	109.31	117.21
5	B	807[A]	MXM	OAH-CAC-CAG	-6.43	117.17	122.80
5	A	807[A]	MXM	OAH-CAC-CAG	-6.28	117.30	122.80
5	B	807[B]	MXM	OAK-SAE-NAJ	-5.50	104.19	108.11
5	B	807[A]	MXM	CAC-CAG-NAJ	-4.48	117.40	120.92
5	A	807[B]	MXM	CAO-NAJ-CAG	-4.35	109.17	115.15
5	B	807[A]	MXM	OAK-SAE-NAJ	-4.31	105.04	108.11
5	B	807[B]	MXM	CAO-NAJ-CAG	-4.26	109.29	115.15
5	A	807[B]	MXM	OAK-SAE-NAJ	-3.95	105.30	108.11
5	A	807[A]	MXM	CAC-CAG-NAJ	-3.58	118.11	120.92
5	A	807[A]	MXM	CAO-NAJ-CAG	-3.52	110.31	115.15
5	B	807[A]	MXM	CAR-NAP-CAN	-2.83	118.30	127.24
5	A	807[A]	MXM	CAR-NAP-CAN	-2.80	118.38	127.24
5	A	807[A]	MXM	OAK-SAE-NAJ	-2.74	106.16	108.11
5	A	807[A]	MXM	OAK-SAE-CAB	-2.64	105.90	109.06
5	B	807[B]	MXM	CAC-CAG-NAJ	-2.38	119.05	120.92
5	A	807[B]	MXM	CAC-CAG-NAJ	-2.38	119.05	120.92
5	A	807[B]	MXM	CAC-CAG-CAN	-2.27	118.63	120.83
5	A	807[B]	MXM	OAK-SAE-CAB	-2.17	106.46	109.06
5	B	807[A]	MXM	CAO-NAJ-CAG	-2.08	112.29	115.15
2	B	801	HEM	C3B-C4B-CHC	2.04	126.03	123.16
2	B	801	HEM	C2D-C3D-C4D	2.29	105.38	101.50
5	A	807[A]	MXM	CAF-CAB-SAE	2.68	124.65	120.66
2	A	801	HEM	CMD-C2D-C3D	2.75	126.49	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CMD-C2D-C3D	2.92	127.26	114.35
5	B	807[B]	MXM	OAL-SAE-NAJ	3.14	110.35	108.11
5	A	807[B]	MXM	CAF-CAB-SAE	3.24	125.48	120.66
5	B	807[A]	MXM	CAF-CAB-SAE	3.53	125.92	120.66
2	A	801	HEM	CMC-C2C-C3C	3.67	125.70	116.53
2	B	801	HEM	CMC-C2C-C3C	3.76	125.92	116.53
5	A	807[A]	MXM	OAL-SAE-NAJ	3.77	110.80	108.11
5	B	807[B]	MXM	CAF-CAB-SAE	3.78	126.29	120.66
2	B	801	HEM	CAD-C3D-C4D	3.95	126.40	112.47
5	A	807[A]	MXM	CAA-CAC-CAG	3.97	124.67	122.57
5	B	807[A]	MXM	CAA-CAC-CAG	4.12	124.75	122.57
5	B	807[B]	MXM	CAW-CAV-SAT	4.32	124.38	119.72
5	A	807[B]	MXM	CAW-CAV-SAT	4.38	124.44	119.72
2	A	801	HEM	CAD-C3D-C4D	4.55	128.50	112.47
2	A	801	HEM	CAD-C3D-C2D	4.71	126.76	113.22
2	A	801	HEM	CMB-C2B-C3B	4.86	128.66	116.53
5	A	807[B]	MXM	OAL-SAE-NAJ	5.06	111.72	108.11
2	B	801	HEM	CMB-C2B-C3B	5.16	129.42	116.53
2	B	801	HEM	CAD-C3D-C2D	5.22	128.22	113.22
5	B	807[A]	MXM	CAW-CAV-SAT	6.07	126.26	119.72
5	A	807[A]	MXM	CAW-CAV-SAT	6.58	126.81	119.72
5	A	807[B]	MXM	CAA-CAC-CAG	6.76	126.14	122.57
5	B	807[B]	MXM	CAA-CAC-CAG	7.40	126.49	122.57
5	A	807[B]	MXM	CAB-SAE-NAJ	9.90	114.97	102.01
5	A	807[A]	MXM	CAB-SAE-NAJ	10.33	115.53	102.01
5	B	807[A]	MXM	CAB-SAE-NAJ	10.74	116.07	102.01
5	B	807[B]	MXM	CAB-SAE-NAJ	10.86	116.23	102.01
5	A	807[B]	MXM	CAO-NAJ-SAE	12.61	134.80	116.78
5	A	807[A]	MXM	CAO-NAJ-SAE	12.61	134.80	116.78
5	B	807[B]	MXM	CAO-NAJ-SAE	12.76	135.01	116.78
5	B	807[A]	MXM	CAO-NAJ-SAE	12.87	135.17	116.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	3	0
3	A	802	NAG	1	0
5	A	807[B]	MXM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HEM	2	0
5	B	807[B]	MXM	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	553/569 (97%)	-0.07	1 (0%) 95 95	30, 47, 69, 100	0
1	B	553/569 (97%)	-0.06	2 (0%) 93 93	31, 45, 72, 92	0
All	All	1106/1138 (97%)	-0.06	3 (0%) 94 94	30, 46, 71, 100	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	75	TRP	2.4
1	A	277	ARG	2.4
1	B	277	ARG	2.1

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(Å ²)	Q<0.9
4	NAG	B	806	14/15	0.76	0.25	3.29	53,74,99,106	0
4	NAG	B	805	14/15	0.90	0.17	1.14	51,60,68,71	0
4	NAG	A	803	14/15	0.98	0.14	0.60	20,37,44,47	0
4	NAG	A	805	14/15	0.93	0.14	-0.32	51,60,68,71	0
4	NAG	B	803	14/15	0.98	0.13	-1.08	26,41,48,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	804	14/15	0.96	0.12	-	39,48,62,69	0
4	NAG	A	806	14/15	0.95	0.14	-	55,67,77,87	0
4	NAG	B	804	14/15	0.96	0.07	-	39,48,62,69	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
5	MXM	A	807[B]	23/23	0.96	0.19	1.24	50,63,74,84	0
5	MXM	A	807[A]	23/23	0.96	0.19	1.19	51,63,72,77	23
3	NAG	B	802	14/15	0.89	0.14	0.77	53,67,91,97	0
2	HEM	A	801	43/43	0.98	0.17	0.74	30,46,56,118	0
2	HEM	B	801	43/43	0.97	0.17	0.66	32,48,64,101	0
3	NAG	A	802	14/15	0.88	0.15	0.39	57,70,91,104	0
5	MXM	B	807[B]	23/23	0.95	0.17	0.27	47,65,71,78	0
5	MXM	B	807[A]	23/23	0.95	0.17	0.23	48,63,70,74	23

6.5 Other polymers [i](#)

There are no such residues in this entry.