



wwPDB X-ray Structure Validation Summary Report i

May 6, 2014 – 12:53 AM EDT

PDB ID : 4M10
Title : Crystal Structure of Murine Cyclooxygenase-2 Complex with Isoxicam
Authors : Xu, S.; Hermanson, D.J.; Banerjee, S.; Ghebrelasie, K.; Marnett, L.J.
Deposited on : 2013-08-02
Resolution : 2.01 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

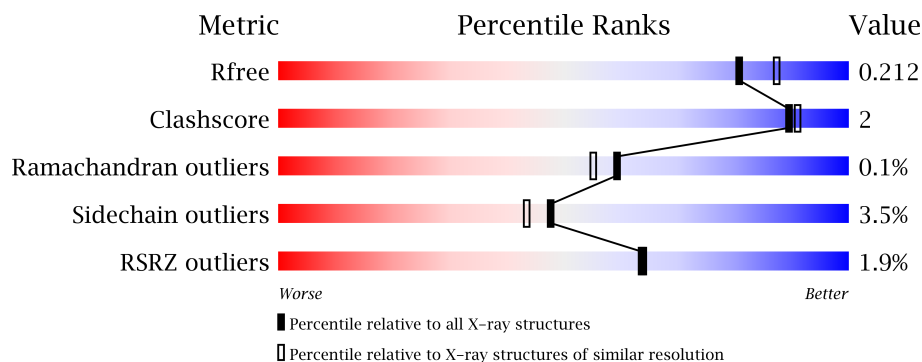
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable22978
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22978

1 Overall quality at a glance





The reported resolution of this entry is 2.01 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	587	
1	B	587	
1	C	587	
1	D	587	

2 Entry composition i

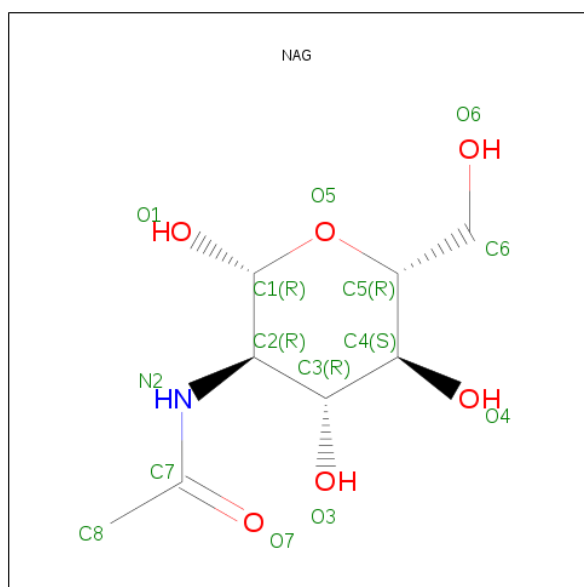
There are 7 unique types of molecules in this entry. The entry contains 20207 atoms, of which 0 are hydrogen and 0 are deuterium.

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	552	Total	C	N	O	S	0	1	0
			4480	2889	750	816	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	C	551	Total	C	N	O	S	0	0	0
			4465	2880	748	812	25			
1	D	552	Total	C	N	O	S	0	1	0
			4482	2890	753	814	25			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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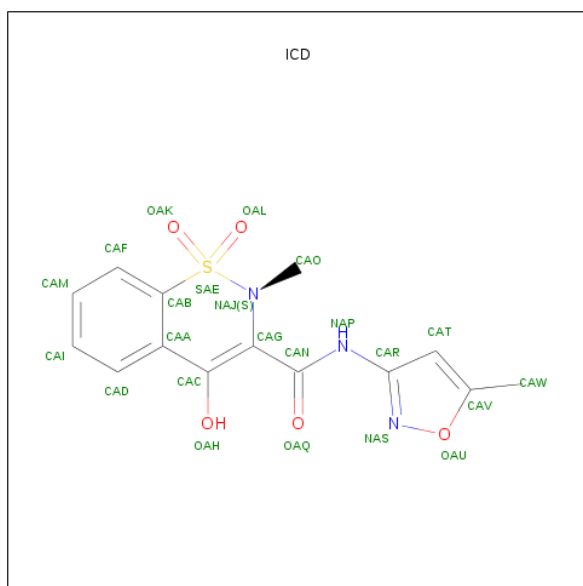
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0

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

-
- Chemical structure of HEM (Heme) is shown. The structure features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The side chains are labeled with green text: C1A, C2A, C3A, C4A, C1B, C2B, C3B, C4B, C1C, C2C, C3C, C4C, C1D, C2D, C3D, C4D, C1E, C2E, C3E, C4E, C1F, C2F, C3F, C4F, C1G, C2G, C3G, C4G, C1H, C2H, C3H, C4H, C1I, C2I, C3I, C4I, C1J, C2J, C3J, C4J, C1K, C2K, C3K, C4K, C1L, C2L, C3L, C4L, C1M, C2M, C3M, C4M, C1N, C2N, C3N, C4N, C1O, C2O, C3O, C4O, C1P, C2P, C3P, C4P, C1Q, C2Q, C3Q, C4Q, C1R, C2R, C3R, C4R, C1S, C2S, C3S, C4S, C1T, C2T, C3T, C4T, C1U, C2U, C3U, C4U, C1V, C2V, C3V, C4V, C1W, C2W, C3W, C4W, C1X, C2X, C3X, C4X, C1Y, C2Y, C3Y, C4Y, C1Z, C2Z, C3Z, C4Z, C1AA, C2AA, C3AA, C4AA, C1AB, C2AB, C3AB, C4AB, C1AC, C2AC, C3AC, C4AC, C1AD, C2AD, C3AD, C4AD, C1AE, C2AE, C3AE, C4AE, C1AF, C2AF, C3AF, C4AF, C1AG, C2AG, C3AG, C4AG, C1AH, C2AH, C3AH, C4AH, C1AI, C2AI, C3AI, C4AI, C1AJ, C2AJ, C3AJ, C4AJ, C1AK, C2AK, C3AK, C4AK, C1AL, C2AL, C3AL, C4AL, C1AM, C2AM, C3AM, C4AM, C1AN, C2AN, C3AN, C4AN, C1AO, C2AO, C3AO, C4AO, C1AP, C2AP, C3AP, C4AP, C1AQ, C2AQ, C3AQ, C4AQ, C1AR, C2AR, C3AR, C4AR, C1AS, C2AS, C3AS, C4AS, C1AT, C2AT, C3AT, C4AT, C1AU, C2AU, C3AU, C4AU, C1AV, C2AV, C3AV, C4AV, C1AW, C2AW, C3AW, C4AW, C1AX, C2AX, C3AX, C4AX, C1AY, C2AY, C3AY, C4AY, C1AZ, C2AZ, C3AZ, C4AZ, C1BA, C2BA, C3BA, C4BA, C1BB, C2BB, C3BB, C4BB, C1BC, C2BC, C3BC, C4BC, C1BD, C2BD, C3BD, C4BD, C1BE, C2BE, C3BE, C4BE, C1BF, C2BF, C3BF, C4BF, C1BG, C2BG, C3BG, C4BG, C1BH, C2BH, C3BH, C4BH, C1BI, C2BI, C3BI, C4BI, C1BJ, C2BJ, C3BJ, C4BJ, C1BK, C2BK, C3BK, C4BK, C1BL, C2BL, C3BL, C4BL, C1BM, C2BM, C3BM, C4BM, C1BN, C2BN, C3BN, C4BN, C1BO, C2BO, C3BO, C4BO, C1BP, C2BP, C3BP, C4BP, C1BQ, C2BQ, C3BQ, C4BQ, C1BR, C2BR, C3BR, C4BR, C1BS, C2BS, C3BS, C4BS, C1BT, C2BT, C3BT, C4BT, C1BU, C2BU, C3BU, C4BU, C1BV, C2BV, C3BV, C4BV, C1BW, C2BW, C3BW, C4BW, C1BX, C2BX, C3BX, C4BX, C1BY, C2BY, C3BY, C4BY, C1BZ, C2BZ, C3BZ, C4BZ, C1CA, C2CA, C3CA, C4CA, C1CB, C2CB, C3CB, C4CB, C1CC, C2CC, C3CC, C4CC, C1CD, C2CD, C3CD, C4CD, C1CE, C2CE, C3CE, C4CE, C1CF, C2CF, C3CF, C4CF, C1CG, C2CG, C3CG, C4CG, C1CH, C2CH, C3CH, C4CH, C1CI, C2CI, C3CI, C4CI, C1CJ, C2CJ, C3CJ, C4CJ, C1CK, C2CK, C3CK, C4CK, C1CL, C2CL, C3CL, C4CL, C1CM, C2CM, C3CM, C4CM, C1CN, C2CN, C3CN, C4CN, C1CO, C2CO, C3CO, C4CO, C1CP, C2CP, C3CP, C4CP, C1CQ, C2CQ, C3CQ, C4CQ, C1CR, C2CR, C3CR, C4CR, C1CS, C2CS, C3CS, C4CS, C1CT, C2CT, C3CT, C4CT, C1CU, C2CU, C3CU, C4CU, C1CV, C2CV, C3CV, C4CV, C1CW, C2CW, C3CW, C4CW, C1CX, C2CX, C3CX, C4CX, C1CY, C2CY, C3CY, C4CY, C1CZ, C2CZ, C3CZ, C4CZ, C1DA, C2DA, C3DA, C4DA, C1DB, C2DB, C3DB, C4DB, C1DC, C2DC, C3DC, C4DC, C1DD, C2DD, C3DD, C4DD, C1DE, C2DE, C3DE, C4DE, C1DF, C2DF, C3DF, C4DF, C1DG, C2DG, C3DG, C4DG, C1DH, C2DH, C3DH, C4DH, C1DI, C2DI, C3DI, C4DI, C1DJ, C2DJ, C3DJ, C4DJ, C1DK, C2DK, C3DK, C4DK, C1DL, C2DL, C3DL, C4DL, C1DM, C2DM, C3DM, C4DM, C1DN, C2DN, C3DN, C4DN, C1DO, C2DO, C3DO, C4DO, C1DP, C2DP, C3DP, C4DP, C1DQ, C2DQ, C3DQ, C4DQ, C1DR, C2DR, C3DR, C4DR, C1DS, C2DS, C3DS, C4DS, C1DT, C2DT, C3DT, C4DT, C1DU, C2DU, C3DU, C4DU, C1DV, C2DV, C3DV, C4DV, C1DW, C2DW, C3DW, C4DW, 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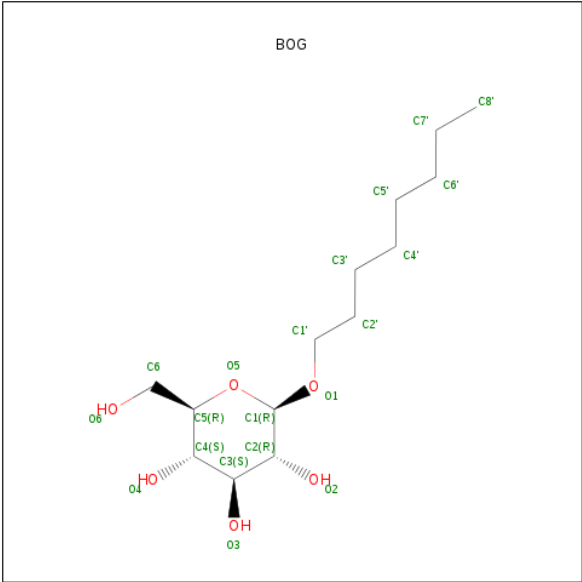
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is 4-HYDROXY-2-METHYL-N-(5-METHYL-1,2-OXAZOL-3-YL)-2H-1,2-BENZOTHAZINE-3-CARBOXAMIDE1,1-DIOXIDE (three-letter code: ICD) (formula: C₁₄H₁₃N₃O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			23	14	3	5	1		
5	B	1	Total	C	N	O	S	0	0
			23	14	3	5	1		
5	C	1	Total	C	N	O	S	0	0
			23	14	3	5	1		
5	D	1	Total	C	N	O	S	0	0
			23	14	3	5	1		

- Molecule 6 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	403	Total	O	0	0
			403	403		
7	B	412	Total	O	0	0
			412	412		
7	C	472	Total	O	0	0
			472	472		
7	D	451	Total	O	0	0
			451	451		

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.61Å 134.08Å 180.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 2.01 49.27 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.27-2.01) 89.0 (49.27-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.189 , 0.220 0.182 , 0.212	Depositor DCC
R_{free} test set	8801 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	6 of 196354 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20207	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.26 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.9866e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ICD, NAG, BOG

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	0.48	0/4610	0.55	0/6251
1	B	0.48	0/4601	0.55	0/6239
1	C	0.50	0/4592	0.57	1/6227 (0.0%)
1	D	0.51	0/4612	0.56	1/6253 (0.0%)
All	All	0.49	0/18415	0.56	2/24970 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	306	LEU	CA-CB-CG	6.71	130.74	115.30
1	D	531	LEU	CA-CB-CG	6.62	130.52	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4480	0	0	3	0
1	B	4474	0	0	13	0
1	C	4465	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4482	0	0	6	0
2	A	28	0	26	0	0
2	B	28	0	26	4	0
2	C	28	0	26	1	0
2	D	28	0	26	0	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
3	C	28	0	25	1	0
3	D	28	0	25	0	0
4	A	43	0	30	3	0
4	B	43	0	30	2	0
4	C	43	0	30	1	0
4	D	43	0	30	3	0
5	A	23	0	0	1	0
5	B	23	0	0	1	0
5	C	23	0	0	1	0
5	D	23	0	0	1	0
6	B	40	0	56	4	0
6	C	20	0	28	0	0
6	D	20	0	28	0	0
7	A	403	0	0	1	0
7	B	412	0	0	2	0
7	C	472	0	0	2	0
7	D	451	0	0	3	0
All	All	20207	0	436	40	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

The worst 5 of 40 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:410:ASN:CG	2:B:704:NAG:C1	2.38	0.90
1:B:410:ASN:OD1	2:B:704:NAG:C1	2.31	0.78
1:D:53:ASP:N	7:D:1245:HOH:O	2.21	0.72
5:B:706:ICD:OAH	5:B:706:ICD:NAP	2.22	0.71
4:A:705:HEM:HHD	4:A:705:HEM:HBC2	1.80	0.64

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	551/587 (94%)	534 (97%)	17 (3%)	0	100	100
1	B	550/587 (94%)	529 (96%)	19 (4%)	2 (0%)	43	36
1	C	549/587 (94%)	535 (97%)	14 (3%)	0	100	100
1	D	551/587 (94%)	536 (97%)	15 (3%)	0	100	100
All	All	2201/2348 (94%)	2134 (97%)	65 (3%)	2 (0%)	59	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	LEU
1	B	81	LEU

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	494/525 (94%)	483 (98%)	11 (2%)	64	65
1	B	493/525 (94%)	471 (96%)	22 (4%)	38	31
1	C	492/525 (94%)	473 (96%)	19 (4%)	43	38
1	D	494/525 (94%)	477 (97%)	17 (3%)	49	45
All	All	1973/2100 (94%)	1904 (96%)	69 (4%)	48	43

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	556	PHE
1	C	123	LEU

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Mol	Chain	Res	Type
1	D	385	TYR
1	B	583	GLN
1	C	101	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z > 2$
3	NAG	A	702	1,3	12,14,15	0.38	0	15,19,21	0.68	0
3	NAG	A	703	3	12,14,15	0.39	0	15,19,21	0.30	0
3	NAG	B	702	1,3	12,14,15	0.40	0	15,19,21	0.50	0
3	NAG	B	703	3	12,14,15	0.38	0	15,19,21	0.36	0
3	NAG	C	702	1,3	12,14,15	0.44	0	15,19,21	0.70	0
3	NAG	C	703	3	12,14,15	0.38	0	15,19,21	0.40	0
3	NAG	D	702	1,3	12,14,15	0.51	0	15,19,21	0.75	0
3	NAG	D	703	3	12,14,15	0.48	0	15,19,21	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	702	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	703	3	-	0/6/23/26	0/1/1/1
3	NAG	B	702	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	703	3	-	0/6/23/26	0/1/1/1
3	NAG	C	702	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	703	3	-	0/6/23/26	0/1/1/1
3	NAG	D	702	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	703	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

20 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	NAG	A	701	1	12,14,15	0.53	0	15,19,21	0.48	0
2	NAG	A	704	1	12,14,15	0.42	0	15,19,21	0.52	0
4	HEM	A	705	1,7	42,50,50	3.56	15 (35%)	27,82,82	1.67	4 (14%)
5	ICD	A	706	-	25,25,25	4.86	14 (56%)	36,38,38	4.44	19 (52%)
2	NAG	B	701	1	12,14,15	0.92	1 (8%)	15,19,21	1.01	2 (13%)
2	NAG	B	704	1	12,14,15	0.42	0	15,19,21	0.55	0
4	HEM	B	705	1,7	42,50,50	3.53	15 (35%)	27,82,82	1.33	2 (7%)
5	ICD	B	706	-	25,25,25	4.43	14 (56%)	36,38,38	4.46	18 (50%)
6	BOG	B	707	-	20,20,20	0.80	1 (5%)	25,25,25	1.58	5 (20%)
6	BOG	B	708	-	20,20,20	1.01	1 (5%)	25,25,25	1.20	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	701	1	12,14,15	0.43	0	15,19,21	1.32	2 (13%)
2	NAG	C	704	1	12,14,15	0.40	0	15,19,21	0.53	0
4	HEM	C	705	1,7	42,50,50	3.63	14 (33%)	27,82,82	1.43	2 (7%)
5	ICD	C	706	-	25,25,25	3.87	12 (48%)	36,38,38	4.77	20 (55%)
6	BOG	C	707	-	20,20,20	1.03	1 (5%)	25,25,25	1.05	1 (4%)
2	NAG	D	701	1	12,14,15	0.54	0	15,19,21	0.55	0
2	NAG	D	704	1	12,14,15	0.44	0	15,19,21	0.39	0
4	HEM	D	705	1	42,50,50	3.57	13 (30%)	27,82,82	1.61	2 (7%)
5	ICD	D	706	-	25,25,25	3.87	14 (56%)	36,38,38	5.07	19 (52%)
6	BOG	D	707	-	20,20,20	1.01	1 (5%)	25,25,25	1.11	2 (8%)

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	NAG	A	701	1	-	0/6/23/26	0/1/1/1
2	NAG	A	704	1	-	0/6/23/26	0/1/1/1
4	HEM	A	705	1,7	-	0/14/114/114	0/0/8/8
5	ICD	A	706	-	-	0/6/32/32	0/3/3/3
2	NAG	B	701	1	-	0/6/23/26	0/1/1/1
2	NAG	B	704	1	-	0/6/23/26	0/1/1/1
4	HEM	B	705	1,7	-	0/14/114/114	0/0/8/8
5	ICD	B	706	-	-	0/6/32/32	0/3/3/3
6	BOG	B	707	-	-	0/11/31/31	0/1/1/1
6	BOG	B	708	-	-	0/11/31/31	0/1/1/1
2	NAG	C	701	1	-	0/6/23/26	0/1/1/1
2	NAG	C	704	1	-	0/6/23/26	0/1/1/1
4	HEM	C	705	1,7	-	0/14/114/114	0/0/8/8
5	ICD	C	706	-	-	0/6/32/32	0/3/3/3
6	BOG	C	707	-	-	0/11/31/31	0/1/1/1
2	NAG	D	701	1	-	0/6/23/26	0/1/1/1
2	NAG	D	704	1	-	0/6/23/26	0/1/1/1
4	HEM	D	705	1	-	0/14/114/114	0/0/8/8
5	ICD	D	706	-	-	0/6/32/32	0/3/3/3
6	BOG	D	707	-	-	0/11/31/31	0/1/1/1

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	705	HEM	C3C-C2C	-14.44	1.34	1.45
4	D	705	HEM	C3C-C2C	-14.13	1.34	1.45
4	A	705	HEM	C3C-C2C	-13.89	1.34	1.45
4	B	705	HEM	C3C-C2C	-13.25	1.35	1.45
5	A	706	ICD	CAB-SAE	-12.98	1.60	1.76

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	706	ICD	CAO-NAJ-SAE	14.17	137.66	116.91
5	B	706	ICD	CAO-NAJ-SAE	13.70	136.98	116.91
5	C	706	ICD	CAO-NAJ-SAE	13.36	136.49	116.91
5	A	706	ICD	CAO-NAJ-SAE	13.12	136.13	116.91
5	C	706	ICD	CAV-OAU-NAS	-12.79	103.50	107.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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, 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	552/587 (94%)	0.01	10 (1%) 65 66	16, 27, 51, 71	0
1	B	552/587 (94%)	-0.06	13 (2%) 56 56	15, 29, 53, 89	0
1	C	551/587 (93%)	-0.12	11 (1%) 62 62	14, 25, 45, 72	0
1	D	552/587 (94%)	-0.10	8 (1%) 72 72	13, 24, 49, 71	0
All	All	2207/2348 (93%)	-0.07	42 (1%) 64 64	13, 26, 51, 89	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	LEU	9.4
1	B	409	TYR	4.3
1	A	74	PHE	4.2
1	B	33	ALA	4.1
1	C	74	PHE	4.0

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	702	14/15	0.07	-	19,26,34,38	0
3	NAG	D	702	14/15	0.10	-	21,28,33,37	0
3	NAG	A	703	14/15	0.13	-	37,48,56,60	0
3	NAG	C	703	14/15	0.18	-	44,54,57,60	0
3	NAG	D	703	14/15	0.13	-	39,45,53,60	0
3	NAG	A	702	14/15	0.11	-	17,29,37,38	0
3	NAG	B	703	14/15	0.19	-	37,41,49,54	0
3	NAG	C	702	14/15	0.10	-	16,27,33,39	0

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	HEM	A	705	43/43	0.12	-	16,22,39,57	0
6	BOG	B	708	20/20	0.28	-	46,62,65,66	20
6	BOG	C	707	20/20	0.25	-	51,54,56,58	9
5	ICD	C	706	23/23	0.13	-	21,25,29,33	0
2	NAG	C	704	14/15	0.24	-	35,45,52,54	0
4	HEM	D	705	43/43	0.12	-	14,20,42,55	0
5	ICD	D	706	23/23	0.14	-	22,26,31,32	0
6	BOG	B	707	20/20	0.17	-	29,36,53,53	10
6	BOG	D	707	20/20	0.12	-	22,26,46,46	7
2	NAG	D	704	14/15	0.12	-	33,45,50,56	0
4	HEM	B	705	43/43	0.12	-	15,22,43,56	0
2	NAG	B	704	14/15	0.23	-	44,52,56,56	0
2	NAG	C	701	14/15	0.23	-	43,54,58,60	0
2	NAG	D	701	14/15	0.24	-	40,50,56,60	0
2	NAG	A	701	14/15	0.16	-	41,53,57,58	0
2	NAG	B	701	14/15	0.26	-	42,55,61,63	0
5	ICD	B	706	23/23	0.14	-	18,29,38,41	0
5	ICD	A	706	23/23	0.15	-	24,28,32,33	0
4	HEM	C	705	43/43	0.13	-	15,21,45,62	0
2	NAG	A	704	14/15	0.12	-	31,42,46,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.