



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:34 PM GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

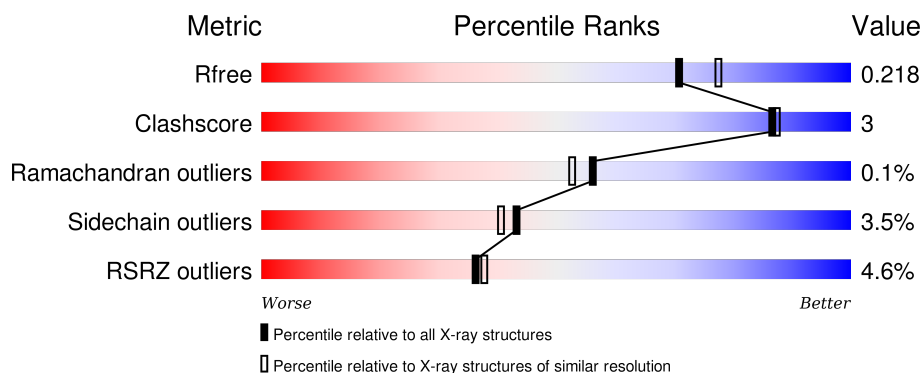
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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  $\geq 3$ , 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	587	<div> <div>5%</div> <div>88%</div> <div>5%</div> <div>6%</div> </div>
1	B	587	<div> <div>4%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>
1	C	587	<div> <div>4%</div> <div>86%</div> <div>7%</div> <div>6%</div> </div>
1	D	587	<div> <div>4%</div> <div>88%</div> <div>6%</div> <div>6%</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	NAG	A	701	-	-	-	X
2	NAG	B	701	-	-	-	X
2	NAG	D	701	-	-	-	X
6	BOG	B	708	-	-	-	X

## 2 Entry composition [i](#)

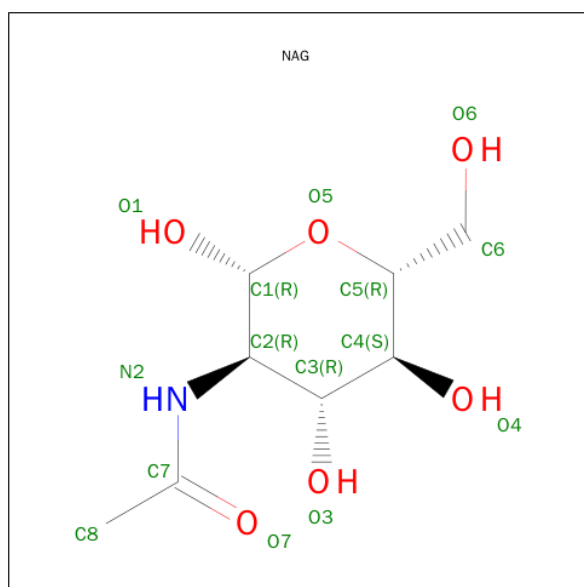
There are 7 unique types of molecules in this entry. The entry contains 20207 atoms, of which 0 are hydrogens and 0 are deuteriums.

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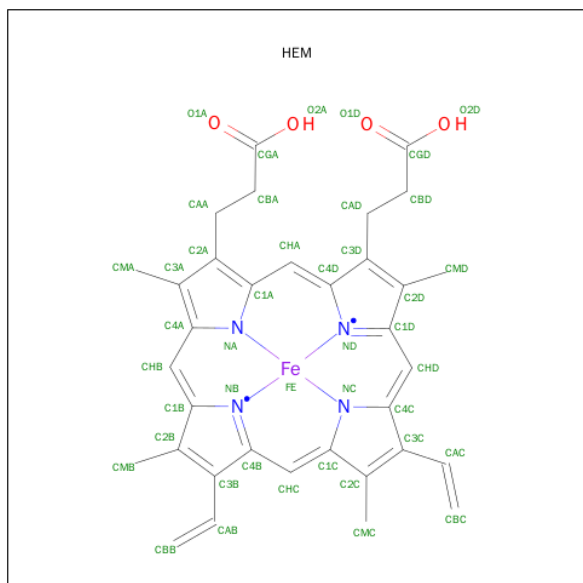
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
	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

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

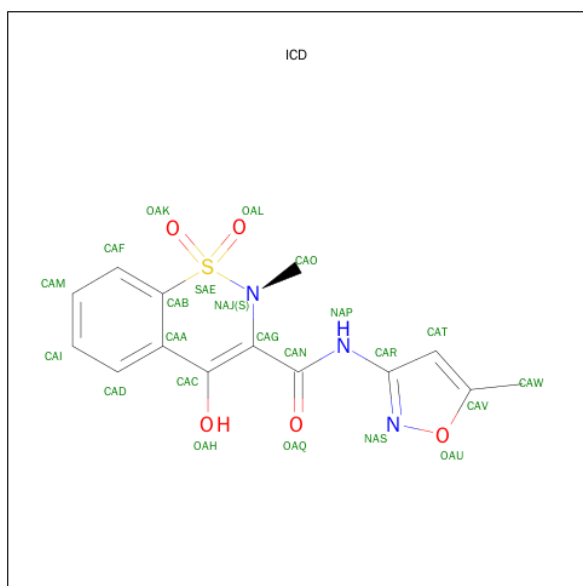
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

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



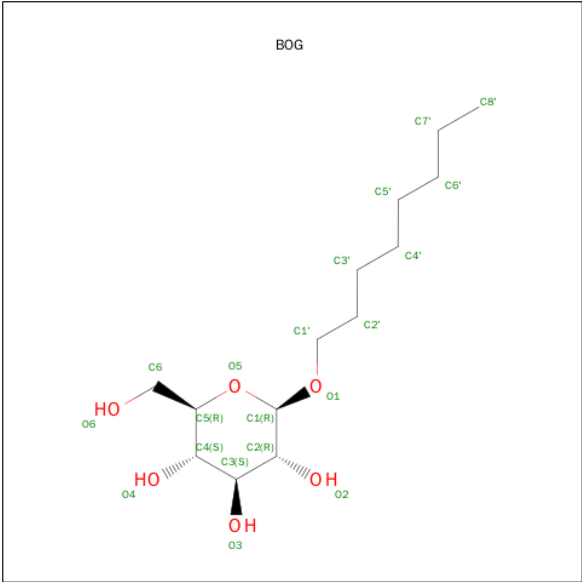
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is 4-HYDROXY-2-METHYL-N-(5-METHYL-1,2-OXAZOL-3-YL)-2H-1,2-BENZOTHAZINE-3-CARBOXAMIDE 1,1-DIOXIDE (three-letter code: ICD) (formula:  $C_{14}H_{13}N_3O_5S$ ).



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:  $C_{14}H_{28}O_6$ ).



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		



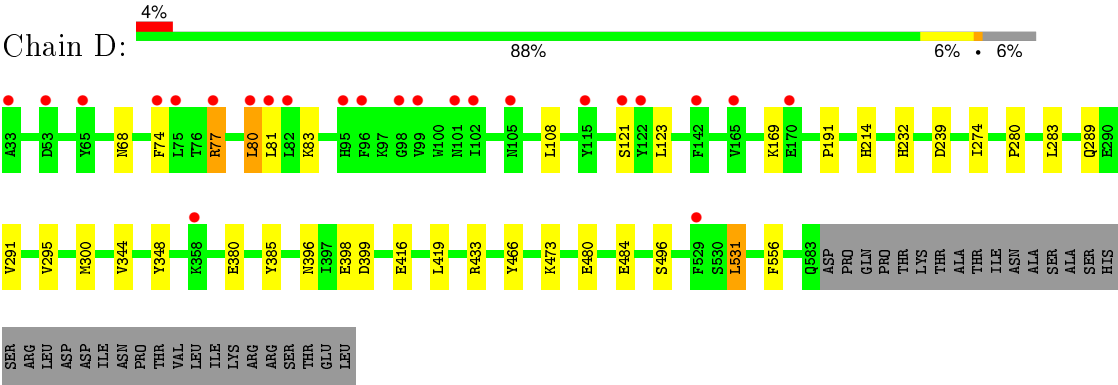
- Molecule 1: Prostaglandin G/H synthase 2





HIS  
SER  
ARG  
LEU  
ASP  
ASP  
ILE  
ASN  
PRO  
THR  
VAL  
LEU  
LEU  
LYS  
ARG  
ARG  
SER  
THR  
GLU  
LEU

● Molecule 1: Prostaglandin G/H synthase 2



SER  
ARG  
LEU  
ASP  
ASP  
ILE  
ASN  
PRO  
THR  
VAL  
LEU  
LEU  
LYS  
ARG  
ARG  
SER  
THR  
GLU  
LEU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.82 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.189 , 0.220 0.189 , 0.218	Depositor DCC
$R_{free}$ test set	9849 reflections (5.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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 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	4480	0	4379	17	0
1	B	4474	0	4373	32	0
1	C	4465	0	4364	17	0
1	D	4482	0	4386	16	0
2	A	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	26	5	0
2	C	28	0	26	1	0
2	D	28	0	26	1	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	4	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	12	3	0
5	B	23	0	12	2	0
5	C	23	0	12	2	0
5	D	23	0	12	2	0
6	B	40	0	56	9	0
6	C	20	0	28	1	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	4	0
7	D	451	0	0	3	0
All	All	20207	0	17986	98	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 3.

All (98) 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:410:ASN:HD21	2:B:704:NAG:C1	1.16	1.58
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:B:185:ARG:HE	6:B:707:BOG:H62	1.53	0.73
1:B:185:ARG:HH21	6:B:707:BOG:H62	1.55	0.70
1:B:88:THR:HG23	6:B:708:BOG:H4'1	1.74	0.69
1:D:280:PRO:HG2	1:D:283:LEU:HD12	1.76	0.68
1:B:294:LEU:HG	1:B:295:VAL:HG12	1.76	0.66
5:B:706:ICD:NAP	5:B:706:ICD:OAH	2.22	0.65
4:A:705:HEM:HBC2	4:A:705:HEM:HHD	1.80	0.64
1:C:447:VAL:HG13	4:C:705:HEM:HBA1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ARG:NH1	3:C:703:NAG:O7	2.34	0.60
1:B:222:ARG:NH2	1:B:290:GLU:OE2	2.34	0.60
4:D:705:HEM:HBC2	4:D:705:HEM:HHD	1.84	0.58
1:C:531:LEU:HD13	5:C:706:ICD:CAM	2.35	0.57
5:C:706:ICD:OAH	5:C:706:ICD:NAP	2.31	0.56
4:B:705:HEM:HBB2	4:B:705:HEM:HMB2	1.87	0.55
1:A:274:ILE:HD12	1:A:291:VAL:HG12	1.88	0.55
1:B:411:ASN:ND2	7:B:1065:HOH:O	2.40	0.55
1:C:294:LEU:HD22	1:C:409:TYR:CD1	2.42	0.55
5:D:706:ICD:NAP	5:D:706:ICD:OAH	2.28	0.55
1:B:185:ARG:NH2	6:B:707:BOG:H62	2.22	0.54
1:B:185:ARG:NE	6:B:707:BOG:H62	2.24	0.53
1:D:274:ILE:HD12	1:D:291:VAL:HG12	1.91	0.53
1:A:386:HIS:HE1	7:A:1193:HOH:O	1.91	0.52
1:D:191:PRO:HD2	1:D:433[A]:ARG:HD3	1.92	0.51
1:A:531:LEU:HD13	5:A:706:ICD:CAM	2.41	0.51
1:C:88:THR:HG23	6:C:707:BOG:H3'1	1.92	0.51
1:C:181:VAL:HG21	1:C:491:LEU:HD21	1.92	0.51
5:A:706:ICD:OAH	5:A:706:ICD:NAP	2.32	0.50
1:B:80:LEU:O	1:B:82:LEU:N	2.41	0.50
1:B:294:LEU:HA	1:B:409:TYR:CE1	2.47	0.49
1:A:214:HIS:NE2	4:A:705:HEM:O1A	2.41	0.49
1:C:274:ILE:HD12	1:C:291:VAL:HG12	1.95	0.48
2:C:701:NAG:H61	7:C:1245:HOH:O	2.12	0.48
1:D:380:GLU:HG2	1:D:466:TYR:CE1	2.49	0.48
1:C:34:ASN:HB3	1:C:37:CYS:SG	2.54	0.48
1:B:410:ASN:ND2	2:B:704:NAG:O5	2.41	0.47
1:B:449:LYS:NZ	1:B:453:ASP:OD2	2.46	0.47
1:C:120:ARG:HD3	7:C:1195:HOH:O	2.13	0.47
4:D:705:HEM:HMB2	4:D:705:HEM:HBB2	1.97	0.46
1:B:185:ARG:HE	6:B:707:BOG:C6	2.25	0.46
1:B:230:LEU:HG	1:B:233:ILE:HD12	1.97	0.46
1:C:382:ASN:O	1:C:386:HIS:HD2	1.99	0.46
1:D:396:ASN:HB3	7:D:1037:HOH:O	2.14	0.46
1:B:80:LEU:C	1:B:82:LEU:H	2.18	0.46
4:A:705:HEM:HBB2	4:A:705:HEM:HMB2	1.98	0.46
1:B:87:ASN:HB2	6:B:708:BOG:H62	1.98	0.45
1:B:382:ASN:O	1:B:386:HIS:HD2	2.00	0.45
1:B:406:GLN:O	1:B:410:ASN:OD1	2.35	0.45
1:D:214:HIS:NE2	4:D:705:HEM:O1A	2.49	0.45
1:D:473:LYS:NZ	7:D:1134:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LEU:HD23	1:A:419:LEU:HA	1.77	0.45
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.52	0.45
1:A:300:MET:HG3	1:A:419:LEU:CD2	2.46	0.45
1:D:398:GLU:HB3	1:D:399:ASP:H	1.63	0.45
1:D:68:ASN:HD22	2:D:701:NAG:H83	1.82	0.44
1:A:531:LEU:HD12	1:A:535:MET:HG2	1.99	0.44
1:A:382:ASN:O	1:A:386:HIS:HD2	2.01	0.44
1:C:411:ASN:ND2	7:C:1171:HOH:O	2.51	0.43
1:A:294:LEU:HA	1:A:409:TYR:CE1	2.53	0.43
1:D:80:LEU:HD12	1:D:80:LEU:HA	1.86	0.43
1:D:300:MET:HG3	1:D:419:LEU:HD22	2.01	0.43
1:D:74:PHE:O	1:D:77:ARG:HG3	2.18	0.43
1:A:452:ILE:O	1:A:456:ARG:HG3	2.18	0.43
1:A:181:VAL:HG21	1:A:491:LEU:HD21	2.01	0.43
1:A:389:PRO:HB2	1:A:434:VAL:HA	2.00	0.43
1:C:75:LEU:HA	1:C:78:ILE:HD12	1.99	0.43
1:D:83:LYS:HB2	1:D:83:LYS:HE3	1.89	0.43
1:C:317:LYS:HB2	7:C:1229:HOH:O	2.19	0.43
1:B:77:ARG:O	1:B:81:LEU:HG	2.18	0.43
1:A:78:ILE:O	1:A:82:LEU:HG	2.18	0.42
5:B:706:ICD:HAT	5:B:706:ICD:OAQ	2.19	0.42
1:D:191:PRO:CD	1:D:433[A]:ARG:HD3	2.48	0.42
1:D:480:GLU:OE1	7:D:1134:HOH:O	2.21	0.42
1:A:295:VAL:HG11	4:A:705:HEM:CBB	2.50	0.42
1:B:307:ARG:NH1	1:B:419:LEU:HD12	2.34	0.42
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.86	0.42
1:C:90:HIS:CE1	1:C:513:ARG:HG2	2.55	0.42
4:B:705:HEM:HBC2	4:B:705:HEM:HHD	2.01	0.42
1:B:454:GLN:HA	1:B:457:GLU:HB2	2.02	0.42
1:A:191:PRO:HD2	1:A:433:ARG:HD3	2.02	0.42
6:B:708:BOG:H7'1	6:B:708:BOG:H4'2	1.86	0.41
1:B:398:GLU:HB3	1:B:399:ASP:H	1.66	0.41
1:B:181:VAL:HG21	1:B:491:LEU:HD21	2.02	0.41
6:B:707:BOG:H2'2	6:B:707:BOG:H5'1	1.77	0.41
1:B:442:ILE:HG13	7:B:847:HOH:O	2.20	0.41
5:A:706:ICD:OAQ	5:A:706:ICD:HAT	2.21	0.41
1:C:398:GLU:HB3	1:C:399:ASP:H	1.63	0.41
1:C:380:GLU:HG2	1:C:466:TYR:CE1	2.55	0.41
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.61	0.41
1:B:410:ASN:OD1	2:B:704:NAG:C2	2.68	0.41
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:VAL:HA	1:D:348:TYR:HB3	2.03	0.41
1:B:349:VAL:HA	1:B:352:LEU:HG	2.01	0.41
1:B:78:ILE:O	1:B:82:LEU:HG	2.21	0.40
1:C:78:ILE:O	1:C:82:LEU:HG	2.21	0.40
5:D:706:ICD:HAT	5:D:706:ICD:OAQ	2.22	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	551/587 (94%)	534 (97%)	17 (3%)	0	100	100
1	B	550/587 (94%)	529 (96%)	19 (4%)	2 (0%)	39	33
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%)	56	53

All (2) Ramachandran outliers are listed below:

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

### 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	494/525 (94%)	483 (98%)	11 (2%)	60	62
1	B	493/525 (94%)	471 (96%)	22 (4%)	34	29
1	C	492/525 (94%)	473 (96%)	19 (4%)	39	35
1	D	494/525 (94%)	477 (97%)	17 (3%)	44	41
All	All	1973/2100 (94%)	1904 (96%)	69 (4%)	43	40

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	102	ILE
1	A	107	PHE
1	A	123	LEU
1	A	232	HIS
1	A	289	GLN
1	A	295	VAL
1	A	385	TYR
1	A	422	PHE
1	A	473	LYS
1	A	484	GLU
1	B	81	LEU
1	B	82	LEU
1	B	101	ASN
1	B	107	PHE
1	B	123	LEU
1	B	169	LYS
1	B	176	GLU
1	B	183	LEU
1	B	232	HIS
1	B	239	ASP
1	B	271	VAL
1	B	289	GLN
1	B	295	VAL
1	B	318	GLN
1	B	358	LYS
1	B	385	TYR
1	B	410	ASN
1	B	416	GLU
1	B	484	GLU
1	B	485	LYS

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Mol	Chain	Res	Type
1	B	556	PHE
1	B	583	GLN
1	C	80	LEU
1	C	81	LEU
1	C	101	ASN
1	C	107	PHE
1	C	111	LEU
1	C	123	LEU
1	C	169	LYS
1	C	232	HIS
1	C	239	ASP
1	C	272	GLU
1	C	289	GLN
1	C	306	LEU
1	C	318	GLN
1	C	364	GLU
1	C	385	TYR
1	C	408	LEU
1	C	416	GLU
1	C	422	PHE
1	C	484	GLU
1	D	77	ARG
1	D	80	LEU
1	D	81	LEU
1	D	108	LEU
1	D	121	SER
1	D	123	LEU
1	D	169	LYS
1	D	232	HIS
1	D	239	ASP
1	D	289	GLN
1	D	295	VAL
1	D	385	TYR
1	D	416	GLU
1	D	484	GLU
1	D	496	SER
1	D	531	LEU
1	D	556	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	410	ASN
1	C	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 ⓘ

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	14,14,15	0.29	0	15,19,21	0.53	0
3	NAG	A	703	3	14,14,15	0.38	0	15,19,21	0.22	0
3	NAG	B	702	1,3	14,14,15	0.22	0	15,19,21	0.40	0
3	NAG	B	703	3	14,14,15	0.48	0	15,19,21	0.36	0
3	NAG	C	702	1,3	14,14,15	0.35	0	15,19,21	0.43	0
3	NAG	C	703	3	14,14,15	0.34	0	15,19,21	0.53	0
3	NAG	D	702	1,3	14,14,15	0.23	0	15,19,21	0.64	0
3	NAG	D	703	3	14,14,15	0.50	0	15,19,21	0.32	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	703	NAG	1	0

## 5.6 Ligand geometry [i](#)

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	14,14,15	0.31	0	15,19,21	0.73	0
2	NAG	A	704	1	14,14,15	0.27	0	15,19,21	0.21	0
4	HEM	A	705	1,7	30,50,50	2.42	10 (33%)	24,82,82	2.48	9 (37%)
5	ICD	A	706	-	21,25,25	5.28	12 (57%)	30,38,38	4.50	16 (53%)
2	NAG	B	701	1	14,14,15	0.98	1 (7%)	15,19,21	1.30	2 (13%)
2	NAG	B	704	1	14,14,15	0.91	1 (7%)	15,19,21	0.42	0
4	HEM	B	705	1,7	30,50,50	2.26	6 (20%)	24,82,82	2.29	8 (33%)
5	ICD	B	706	-	21,25,25	4.42	13 (61%)	30,38,38	4.56	15 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BOG	B	707	-	20,20,20	0.81	1 (5%)	25,25,25	1.58	5 (20%)
6	BOG	B	708	-	20,20,20	1.02	1 (5%)	25,25,25	1.21	2 (8%)
2	NAG	C	701	1	14,14,15	1.28	2 (14%)	15,19,21	2.36	3 (20%)
2	NAG	C	704	1	14,14,15	0.25	0	15,19,21	0.37	0
4	HEM	C	705	1,7	30,50,50	2.44	12 (40%)	24,82,82	2.34	8 (33%)
5	ICD	C	706	-	21,25,25	4.23	10 (47%)	30,38,38	4.51	17 (56%)
6	BOG	C	707	-	20,20,20	1.04	1 (5%)	25,25,25	1.05	1 (4%)
2	NAG	D	701	1	14,14,15	0.58	0	15,19,21	0.55	0
2	NAG	D	704	1	14,14,15	0.31	0	15,19,21	0.18	0
4	HEM	D	705	1	30,50,50	2.30	10 (33%)	24,82,82	2.49	8 (33%)
5	ICD	D	706	-	21,25,25	4.24	13 (61%)	30,38,38	4.87	17 (56%)
6	BOG	D	707	-	20,20,20	1.02	1 (5%)	25,25,25	1.12	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	-	0/10/54/54	0/0/8/8
5	ICD	A	706	-	-	0/6/32/32	0/2/3/3
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	-	0/10/54/54	0/0/8/8
5	ICD	B	706	-	-	0/6/32/32	0/2/3/3
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	-	0/10/54/54	0/0/8/8
5	ICD	C	706	-	-	0/6/32/32	0/2/3/3
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	-	0/10/54/54	0/0/8/8
5	ICD	D	706	-	-	0/6/32/32	0/2/3/3
6	BOG	D	707	-	-	0/11/31/31	0/1/1/1

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	706	ICD	CAB-SAE	-13.52	1.60	1.76
5	A	706	ICD	SAE-NAJ	-11.89	1.52	1.64
5	D	706	ICD	SAE-NAJ	-10.30	1.53	1.64
5	C	706	ICD	CAB-SAE	-10.16	1.64	1.76
5	B	706	ICD	SAE-NAJ	-9.70	1.54	1.64
5	B	706	ICD	CAB-SAE	-8.03	1.66	1.76
4	A	705	HEM	C3B-C4B	-7.75	1.44	1.51
4	C	705	HEM	C3B-C4B	-7.71	1.45	1.51
4	D	705	HEM	C3B-C4B	-7.59	1.45	1.51
4	B	705	HEM	C3B-C4B	-7.39	1.45	1.51
5	D	706	ICD	CAB-SAE	-7.39	1.67	1.76
5	C	706	ICD	SAE-NAJ	-6.60	1.57	1.64
4	A	705	HEM	C3D-C4D	-5.99	1.43	1.51
4	C	705	HEM	C3D-C4D	-5.81	1.44	1.51
4	D	705	HEM	C3D-C4D	-5.32	1.44	1.51
4	B	705	HEM	C3D-C4D	-5.31	1.44	1.51
4	C	705	HEM	C2C-C1C	-4.50	1.44	1.52
4	A	705	HEM	C2C-C1C	-4.42	1.44	1.52
4	B	705	HEM	C2C-C1C	-4.33	1.44	1.52
4	D	705	HEM	C2C-C1C	-3.86	1.45	1.52
5	B	706	ICD	OAH-CAC	-3.21	1.24	1.33
5	D	706	ICD	OAH-CAC	-3.04	1.24	1.33
5	D	706	ICD	CAA-CAB	-3.04	1.37	1.40
5	D	706	ICD	CAR-NAP	-2.93	1.34	1.40
5	B	706	ICD	CAR-NAP	-2.93	1.34	1.40
5	A	706	ICD	OAH-CAC	-2.85	1.25	1.33
5	C	706	ICD	CAR-NAP	-2.83	1.34	1.40
5	C	706	ICD	OAH-CAC	-2.76	1.25	1.33
5	B	706	ICD	CAG-NAJ	-2.63	1.41	1.44
5	C	706	ICD	CAA-CAB	-2.60	1.38	1.40
5	A	706	ICD	CAR-NAP	-2.59	1.35	1.40
6	C	707	BOG	O2-C2	-2.54	1.36	1.43
6	D	707	BOG	O2-C2	-2.52	1.36	1.43
5	A	706	ICD	CAG-NAJ	-2.50	1.41	1.44
2	B	701	NAG	C1-C2	-2.49	1.49	1.52
6	B	708	BOG	O2-C2	-2.49	1.37	1.43
5	D	706	ICD	CAG-NAJ	-2.42	1.41	1.44
5	A	706	ICD	CAA-CAB	-2.37	1.38	1.40
5	B	706	ICD	CAA-CAC	-2.29	1.41	1.45
5	B	706	ICD	CAT-CAV	-2.25	1.33	1.39
5	D	706	ICD	CAT-CAV	-2.22	1.34	1.39
4	A	705	HEM	C2D-C1D	-2.20	1.44	1.51
5	B	706	ICD	CAA-CAB	-2.20	1.38	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	707	BOG	O2-C2	-2.19	1.37	1.43
4	C	705	HEM	C2B-C1B	-2.16	1.44	1.51
2	C	701	NAG	C1-C2	-2.16	1.49	1.52
5	D	706	ICD	CAA-CAC	-2.11	1.42	1.45
4	C	705	HEM	C2D-C1D	-2.10	1.45	1.51
5	A	706	ICD	CAT-CAV	-2.08	1.34	1.39
4	D	705	HEM	C2D-C1D	-2.01	1.45	1.51
4	A	705	HEM	FE-NB	2.01	2.08	1.97
4	D	705	HEM	FE-ND	2.03	2.08	1.97
4	A	705	HEM	C4C-NC	2.10	1.38	1.36
4	D	705	HEM	FE-NB	2.11	2.08	1.97
4	C	705	HEM	C3C-CAC	2.20	1.55	1.51
4	C	705	HEM	FE-NB	2.32	2.09	1.97
4	D	705	HEM	C3B-CAB	2.32	1.55	1.51
4	B	705	HEM	C3B-CAB	2.33	1.55	1.51
4	A	705	HEM	C3C-CAC	2.33	1.55	1.51
4	C	705	HEM	FE-ND	2.34	2.09	1.97
4	B	705	HEM	C4C-NC	2.35	1.38	1.36
4	C	705	HEM	C3B-CAB	2.41	1.55	1.51
4	D	705	HEM	C4C-NC	2.42	1.39	1.36
4	D	705	HEM	FE-NC	2.54	2.05	1.95
4	C	705	HEM	FE-NC	2.57	2.06	1.95
4	D	705	HEM	C1C-NC	2.61	1.39	1.36
4	B	705	HEM	C1C-NC	2.62	1.39	1.36
4	A	705	HEM	C3B-CAB	2.66	1.56	1.51
4	C	705	HEM	C4C-NC	2.71	1.39	1.36
4	A	705	HEM	C1C-NC	2.81	1.39	1.36
5	C	706	ICD	CAW-CAV	2.92	1.52	1.48
5	D	706	ICD	CAW-CAV	3.13	1.52	1.48
4	C	705	HEM	C1C-NC	3.15	1.39	1.36
4	A	705	HEM	FE-NC	3.16	2.08	1.95
2	B	704	NAG	C1-C2	3.30	1.57	1.52
5	B	706	ICD	CAW-CAV	3.82	1.53	1.48
5	A	706	ICD	CAW-CAV	3.87	1.53	1.48
2	C	701	NAG	O5-C1	4.15	1.50	1.43
5	C	706	ICD	OAK-SAE	5.13	1.50	1.43
5	D	706	ICD	OAK-SAE	5.80	1.50	1.43
5	C	706	ICD	OAQ-CAN	6.01	1.35	1.23
5	D	706	ICD	OAQ-CAN	6.10	1.35	1.23
5	B	706	ICD	OAQ-CAN	6.15	1.35	1.23
5	B	706	ICD	OAK-SAE	6.17	1.51	1.43
5	D	706	ICD	OAL-SAE	6.22	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	706	ICD	OAK-SAE	6.49	1.51	1.43
5	A	706	ICD	OAQ-CAN	6.85	1.36	1.23
5	D	706	ICD	CAG-CAC	6.96	1.45	1.36
5	B	706	ICD	CAG-CAC	7.21	1.46	1.36
5	A	706	ICD	CAG-CAC	7.36	1.46	1.36
5	C	706	ICD	CAG-CAC	7.62	1.46	1.36
5	C	706	ICD	OAL-SAE	7.76	1.53	1.43
5	B	706	ICD	OAL-SAE	7.76	1.53	1.43
5	A	706	ICD	OAL-SAE	7.96	1.53	1.43

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	706	ICD	OAK-SAE-OAL	-9.45	105.70	118.63
5	B	706	ICD	CAG-NAJ-SAE	-9.10	99.69	113.17
5	A	706	ICD	OAK-SAE-OAL	-9.05	106.24	118.63
5	D	706	ICD	CAG-NAJ-SAE	-8.62	100.40	113.17
5	C	706	ICD	CAG-NAJ-SAE	-8.42	100.69	113.17
5	B	706	ICD	OAK-SAE-OAL	-8.17	107.45	118.63
5	A	706	ICD	CAG-NAJ-SAE	-7.84	101.55	113.17
5	C	706	ICD	OAK-SAE-OAL	-7.70	108.10	118.63
5	D	706	ICD	CAO-NAJ-CAG	-6.57	106.11	115.15
5	B	706	ICD	CAA-CAB-SAE	-6.34	109.57	117.21
5	C	706	ICD	CAA-CAB-SAE	-6.19	109.75	117.21
5	A	706	ICD	CAO-NAJ-CAG	-6.12	106.74	115.15
5	A	706	ICD	CAA-CAB-SAE	-6.06	109.91	117.21
5	D	706	ICD	CAA-CAB-SAE	-6.01	109.97	117.21
5	C	706	ICD	CAO-NAJ-CAG	-5.97	106.94	115.15
5	B	706	ICD	CAC-CAG-CAN	-5.78	115.23	120.83
4	A	705	HEM	CBA-CAA-C2A	-5.61	102.48	112.53
5	B	706	ICD	CAO-NAJ-CAG	-5.39	107.74	115.15
4	D	705	HEM	CBA-CAA-C2A	-5.14	103.31	112.53
5	D	706	ICD	OAH-CAC-CAG	-5.01	118.42	122.80
5	D	706	ICD	CAB-CAA-CAC	-4.97	117.79	120.53
5	B	706	ICD	CAB-CAA-CAC	-4.94	117.81	120.53
5	C	706	ICD	CAC-CAG-CAN	-4.76	116.22	120.83
5	B	706	ICD	OAH-CAC-CAG	-4.60	118.77	122.80
5	D	706	ICD	CAC-CAG-CAN	-4.24	116.72	120.83
5	C	706	ICD	OAK-SAE-CAB	-4.06	104.20	109.06
5	A	706	ICD	CAR-NAP-CAN	-4.01	122.98	128.36
6	B	707	BOG	O2-C2-C1	-3.94	101.38	110.02
5	B	706	ICD	CAR-NAP-CAN	-3.79	123.28	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	706	ICD	CAC-CAG-CAN	-3.74	117.21	120.83
5	C	706	ICD	OAH-CAC-CAG	-3.73	119.54	122.80
5	D	706	ICD	CAR-NAP-CAN	-3.59	123.55	128.36
4	C	705	HEM	CBA-CAA-C2A	-3.58	106.12	112.53
5	A	706	ICD	OAH-CAC-CAG	-3.56	119.68	122.80
5	C	706	ICD	CAR-NAP-CAN	-3.53	123.63	128.36
4	B	705	HEM	CBD-CAD-C3D	-3.26	104.05	113.55
5	A	706	ICD	CAB-CAA-CAC	-3.21	118.76	120.53
2	C	701	NAG	C4-C3-C2	-3.16	106.32	111.23
4	C	705	HEM	CBD-CAD-C3D	-2.96	104.95	113.55
5	A	706	ICD	OAK-SAE-NAJ	-2.88	106.06	108.11
5	C	706	ICD	CAB-CAA-CAC	-2.82	118.98	120.53
4	D	705	HEM	CBD-CAD-C3D	-2.80	105.40	113.55
4	B	705	HEM	CBA-CAA-C2A	-2.66	107.77	112.53
5	D	706	ICD	OAQ-CAN-CAG	-2.48	117.31	121.98
6	D	707	BOG	C1-O5-C5	-2.41	109.07	113.75
5	C	706	ICD	OAQ-CAN-CAG	-2.17	117.91	121.98
5	A	706	ICD	CAC-CAG-NAJ	-2.16	119.22	120.92
4	A	705	HEM	CAA-C2A-C1A	-2.07	124.76	127.01
5	D	706	ICD	OAK-SAE-NAJ	-2.04	106.66	108.11
4	A	705	HEM	CBD-CAD-C3D	-2.02	107.69	113.55
5	C	706	ICD	CAG-CAN-NAP	2.05	117.74	115.26
2	B	701	NAG	C3-C4-C5	2.08	113.83	110.20
4	C	705	HEM	C2D-C3D-C4D	2.15	105.15	101.50
4	D	705	HEM	C2D-C3D-C4D	2.17	105.17	101.50
5	A	706	ICD	CAF-CAB-SAE	2.22	123.97	120.66
4	A	705	HEM	C2D-C3D-C4D	2.28	105.36	101.50
5	D	706	ICD	CAN-CAG-NAJ	2.28	121.23	116.24
6	B	707	BOG	O3-C3-C2	2.32	115.55	110.34
4	B	705	HEM	C2D-C3D-C4D	2.40	105.57	101.50
6	B	707	BOG	C3-C4-C5	2.43	114.44	110.20
5	C	706	ICD	CAF-CAB-SAE	2.50	124.39	120.66
6	B	707	BOG	C1-O5-C5	2.51	118.62	113.75
5	D	706	ICD	OAL-SAE-CAB	2.55	112.10	109.06
5	A	706	ICD	CAN-CAG-NAJ	2.59	121.92	116.24
5	A	706	ICD	OAL-SAE-CAB	2.70	112.29	109.06
5	B	706	ICD	OAL-SAE-CAB	2.71	112.30	109.06
6	B	708	BOG	O5-C5-C4	2.82	114.98	109.68
5	C	706	ICD	CAN-CAG-NAJ	2.84	122.45	116.24
5	B	706	ICD	CAN-CAG-NAJ	2.86	122.50	116.24
4	D	705	HEM	CMD-C2D-C3D	2.88	127.09	114.35
4	B	705	HEM	CMD-C2D-C3D	3.03	127.73	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	705	HEM	CMD-C2D-C3D	3.04	127.79	114.35
5	D	706	ICD	CAA-CAC-CAG	3.04	124.18	122.57
4	A	705	HEM	CMD-C2D-C3D	3.12	128.15	114.35
5	D	706	ICD	CAF-CAB-SAE	3.16	125.37	120.66
5	C	706	ICD	OAL-SAE-CAB	3.16	112.84	109.06
6	B	707	BOG	O5-C5-C4	3.17	115.63	109.68
5	B	706	ICD	CAA-CAC-CAG	3.18	124.25	122.57
2	C	701	NAG	C2-N2-C7	3.29	127.27	123.04
6	C	707	BOG	C1'-O1-C1	3.35	119.80	113.94
6	D	707	BOG	C1'-O1-C1	3.61	120.25	113.94
4	C	705	HEM	CMC-C2C-C3C	3.61	125.55	116.53
4	A	705	HEM	CMC-C2C-C3C	3.68	125.72	116.53
4	C	705	HEM	CAD-C3D-C4D	3.76	125.74	112.47
2	B	701	NAG	C1-O5-C5	3.80	117.07	112.25
4	B	705	HEM	CAD-C3D-C4D	3.86	126.08	112.47
5	B	706	ICD	CAF-CAB-SAE	3.92	126.50	120.66
4	A	705	HEM	CAD-C3D-C4D	3.99	126.53	112.47
4	D	705	HEM	CMC-C2C-C3C	4.02	126.58	116.53
4	D	705	HEM	CAD-C3D-C4D	4.20	127.28	112.47
4	B	705	HEM	CMC-C2C-C3C	4.20	127.02	116.53
5	B	706	ICD	OAL-SAE-NAJ	4.22	111.12	108.11
6	B	708	BOG	C1'-O1-C1	4.25	121.37	113.94
4	B	705	HEM	CMB-C2B-C3B	4.70	128.27	116.53
4	C	705	HEM	CMB-C2B-C3B	4.92	128.80	116.53
4	A	705	HEM	CMB-C2B-C3B	4.93	128.83	116.53
4	D	705	HEM	CAD-C3D-C2D	4.93	127.39	113.22
4	D	705	HEM	CMB-C2B-C3B	5.01	129.03	116.53
4	A	705	HEM	CAD-C3D-C2D	5.16	128.06	113.22
4	B	705	HEM	CAD-C3D-C2D	5.24	128.28	113.22
4	C	705	HEM	CAD-C3D-C2D	5.52	129.08	113.22
5	C	706	ICD	CAB-SAE-NAJ	5.95	109.80	102.01
5	D	706	ICD	CAB-SAE-NAJ	6.16	110.08	102.01
5	B	706	ICD	CAB-SAE-NAJ	6.28	110.24	102.01
5	A	706	ICD	CAB-SAE-NAJ	6.95	111.11	102.01
2	C	701	NAG	C1-O5-C5	7.45	121.70	112.25
5	A	706	ICD	OAL-SAE-NAJ	7.57	113.50	108.11
5	C	706	ICD	OAL-SAE-NAJ	7.89	113.73	108.11
5	D	706	ICD	OAL-SAE-NAJ	9.09	114.59	108.11
5	A	706	ICD	CAO-NAJ-SAE	13.54	136.13	116.78
5	C	706	ICD	CAO-NAJ-SAE	13.79	136.49	116.78
5	B	706	ICD	CAO-NAJ-SAE	14.14	136.98	116.78
5	D	706	ICD	CAO-NAJ-SAE	14.62	137.66	116.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	HEM	4	0
5	A	706	ICD	3	0
2	B	704	NAG	5	0
4	B	705	HEM	2	0
5	B	706	ICD	2	0
6	B	707	BOG	6	0
6	B	708	BOG	3	0
2	C	701	NAG	1	0
4	C	705	HEM	1	0
5	C	706	ICD	2	0
6	C	707	BOG	1	0
2	D	701	NAG	1	0
4	D	705	HEM	3	0
5	D	706	ICD	2	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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	552/587 (94%)	0.18	30 (5%) 29 31	16, 27, 51, 71	0
1	B	552/587 (94%)	0.10	26 (4%) 35 37	15, 29, 53, 89	0
1	C	551/587 (93%)	0.03	21 (3%) 44 45	14, 25, 45, 72	0
1	D	552/587 (94%)	0.10	24 (4%) 39 40	13, 24, 49, 71	0
All	All	2207/2348 (93%)	0.10	101 (4%) 36 38	13, 26, 51, 89	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	LEU	9.7
1	D	81	LEU	5.3
1	B	409	TYR	4.7
1	A	74	PHE	4.7
1	D	82	LEU	4.5
1	C	75	LEU	4.5
1	C	82	LEU	4.4
1	B	399	ASP	4.4
1	A	81	LEU	4.4
1	D	74	PHE	4.3
1	C	80	LEU	4.2
1	C	107	PHE	4.1
1	A	96	PHE	4.1
1	B	33	ALA	4.0
1	A	80	LEU	3.9
1	A	82	LEU	3.8
1	B	74	PHE	3.8
1	C	81	LEU	3.8
1	A	115	TYR	3.7
1	C	74	PHE	3.7
1	C	115	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	75	LEU	3.5
1	B	52	PHE	3.5
1	B	377	ILE	3.4
1	D	80	LEU	3.3
1	C	399	ASP	3.3
1	A	534	LEU	3.2
1	B	53	ASP	3.1
1	B	115	TYR	3.1
1	D	65	TYR	3.1
1	B	75	LEU	3.1
1	D	77	ARG	2.9
1	D	33	ALA	2.9
1	B	111	LEU	2.8
1	B	65	TYR	2.8
1	C	65	TYR	2.7
1	B	80	LEU	2.7
1	B	105(A)	ILE	2.7
1	A	98	GLY	2.7
1	C	78	ILE	2.7
1	B	169	LYS	2.7
1	A	65	TYR	2.7
1	C	96	PHE	2.7
1	D	170	GLU	2.7
1	A	536	GLY	2.7
1	B	215	LYS	2.6
1	D	115	TYR	2.6
1	C	228	VAL	2.6
1	A	529	PHE	2.6
1	C	111	LEU	2.6
1	A	94	THR	2.6
1	B	70	THR	2.6
1	A	124	ILE	2.5
1	A	105	ASN	2.5
1	A	278	HIS	2.5
1	D	75	LEU	2.5
1	B	400	GLN	2.4
1	A	78	ILE	2.4
1	B	82	LEU	2.4
1	D	142	PHE	2.4
1	C	377	ILE	2.4
1	C	145	LEU	2.4
1	C	534	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	102	ILE	2.4
1	D	105	ASN	2.4
1	C	215	LYS	2.4
1	D	99	VAL	2.3
1	A	77	ARG	2.3
1	D	98	GLY	2.3
1	B	410	ASN	2.3
1	A	123	LEU	2.3
1	A	378	ALA	2.3
1	D	122	TYR	2.3
1	D	53	ASP	2.3
1	A	95	HIS	2.3
1	B	63	GLY	2.3
1	C	409	TYR	2.3
1	C	122	TYR	2.2
1	D	165	VAL	2.2
1	D	96	PHE	2.2
1	A	239	ASP	2.2
1	B	405	LYS	2.2
1	B	122	TYR	2.2
1	D	529	PHE	2.2
1	B	78	ILE	2.2
1	B	583	GLN	2.2
1	A	106	PRO	2.2
1	C	79	LYS	2.1
1	D	101	ASN	2.1
1	A	107	PHE	2.1
1	A	496	SER	2.1
1	A	145	LEU	2.1
1	D	95	HIS	2.1
1	B	64	PHE	2.1
1	C	91	TYR	2.1
1	A	97	LYS	2.1
1	A	525	LEU	2.1
1	A	91	TYR	2.1
1	D	358	LYS	2.0
1	D	121	SER	2.0
1	A	341	ILE	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	A	702	14/15	0.95	0.11	0.14	17,29,37,38	0
3	NAG	D	702	14/15	0.95	0.11	0.13	21,28,33,37	0
3	NAG	C	702	14/15	0.95	0.10	-0.46	16,27,33,39	0
3	NAG	B	702	14/15	0.96	0.07	-2.94	19,26,34,38	0
3	NAG	D	703	14/15	0.91	0.14	-	39,45,53,60	0
3	NAG	A	703	14/15	0.83	0.15	-	37,48,56,60	0
3	NAG	B	703	14/15	0.92	0.19	-	37,41,49,54	0
3	NAG	C	703	14/15	0.88	0.20	-	44,54,57,60	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	D	701	14/15	0.76	0.31	7.13	40,50,56,60	0
6	BOG	B	708	20/20	0.70	0.26	5.66	46,62,65,66	20
2	NAG	A	701	14/15	0.87	0.24	3.89	41,53,57,58	0
2	NAG	B	701	14/15	0.81	0.31	2.92	42,55,61,63	0
6	BOG	B	707	20/20	0.89	0.17	1.97	29,36,53,53	10
2	NAG	C	704	14/15	0.92	0.25	1.63	35,45,52,54	0
6	BOG	C	707	20/20	0.88	0.24	1.49	51,54,56,58	9
5	ICD	B	706	23/23	0.92	0.15	1.40	18,29,38,41	0
2	NAG	B	704	14/15	0.86	0.29	1.08	44,52,56,56	0
5	ICD	C	706	23/23	0.92	0.14	0.44	21,25,29,33	0
4	HEM	A	705	43/43	0.96	0.13	0.42	16,22,39,57	0
4	HEM	C	705	43/43	0.96	0.12	0.42	15,21,45,62	0
6	BOG	D	707	20/20	0.94	0.12	0.31	22,26,46,46	7
2	NAG	A	704	14/15	0.91	0.14	0.14	31,42,46,50	0
5	ICD	A	706	23/23	0.93	0.15	0.02	24,28,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	D	704	14/15	0.91	0.13	0.01	33,45,50,56	0
4	HEM	D	705	43/43	0.97	0.12	-0.02	14,20,42,55	0
4	HEM	B	705	43/43	0.97	0.12	-0.08	15,22,43,56	0
5	ICD	D	706	23/23	0.95	0.14	-0.27	22,26,31,32	0
2	NAG	C	701	14/15	0.76	0.25	-	43,54,58,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.