



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:36 PM GMT

PDB ID : 4COX  
Title : CYCLOOXYGENASE-2 (PROSTAGLANDIN SYNTHASE-2) COM-  
PLEXED WITH A NON-SELECTIVE INHIBITOR, INDOMETHACIN  
Authors : Kurumbail, R.; Stallings, W.  
Deposited on : 1996-12-18  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

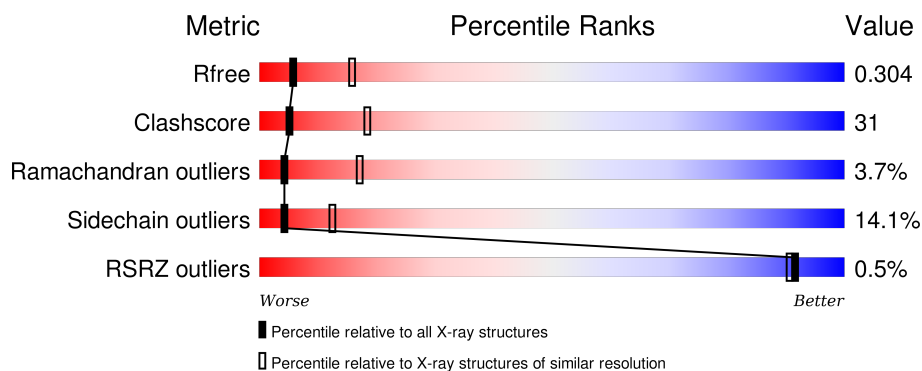
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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>%</div> <div> <div></div> <div>41%</div> <div>42%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	587	<div> <div>43%</div> <div>42%</div> <div>9%</div> <div>6%</div> </div>
1	C	587	<div> <div>41%</div> <div>44%</div> <div>9%</div> <div>6%</div> </div>
1	D	587	<div> <div>%</div> <div>42%</div> <div>43%</div> <div>8%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	681	-	-	-	X
2	NAG	C	661	-	-	-	X
2	NAG	C	681	-	-	-	X
4	IMN	B	701	-	-	X	X
4	IMN	D	701	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18332 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 CYCLOOXYGENASE-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			

There are 8 discrepancies between the modelled and reference sequences:

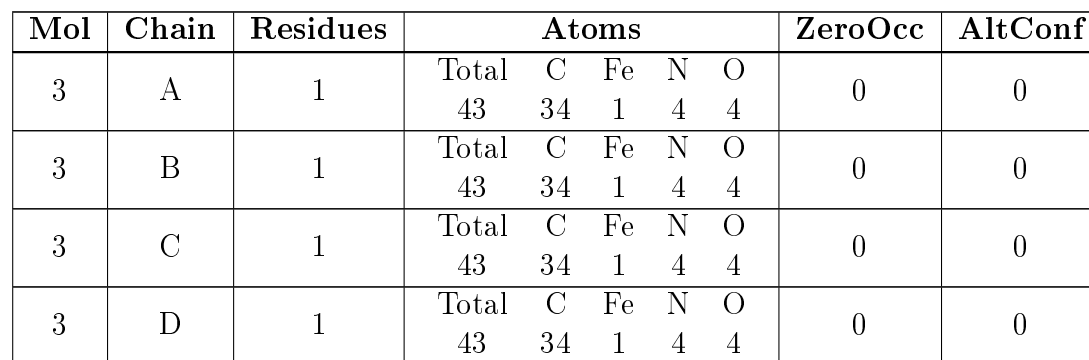
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	CONFLICT	UNP Q05769
A	333	LYS	ARG	CONFLICT	UNP Q05769
B	310	GLN	ASN	CONFLICT	UNP Q05769
B	333	LYS	ARG	CONFLICT	UNP Q05769
C	310	GLN	ASN	CONFLICT	UNP Q05769
C	333	LYS	ARG	CONFLICT	UNP Q05769
D	310	GLN	ASN	CONFLICT	UNP Q05769
D	333	LYS	ARG	CONFLICT	UNP Q05769

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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		
2	A	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	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	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		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

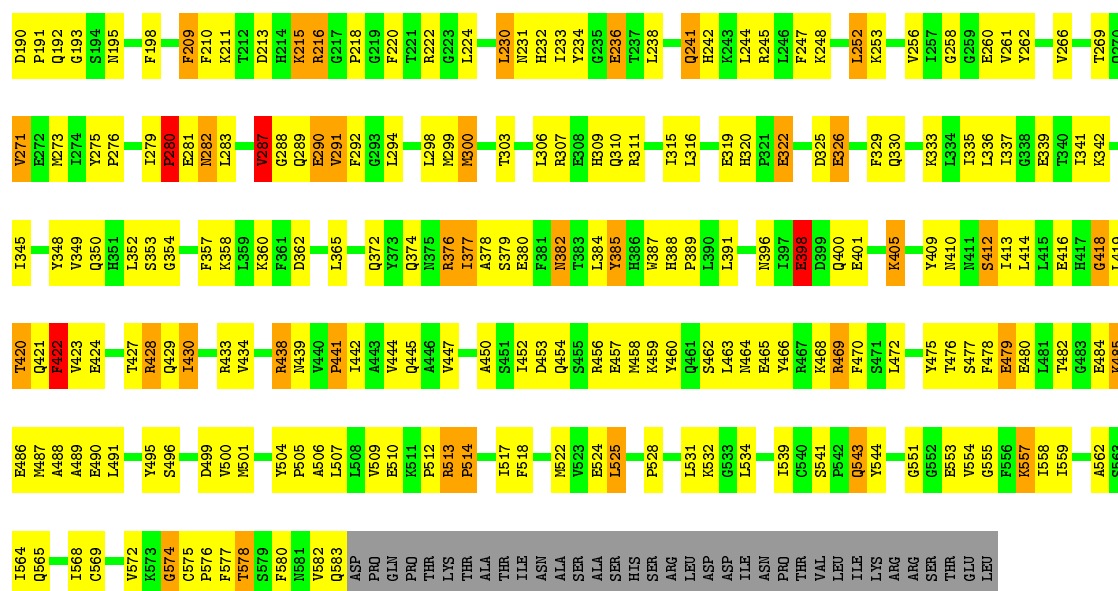


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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			25	19	1	1	4		
4	B	1	Total	C	Cl	N	O	0	0
			25	19	1	1	4		
4	C	1	Total	C	Cl	N	O	0	0
			25	19	1	1	4		
4	D	1	Total	C	Cl	N	O	0	0
			25	19	1	1	4		

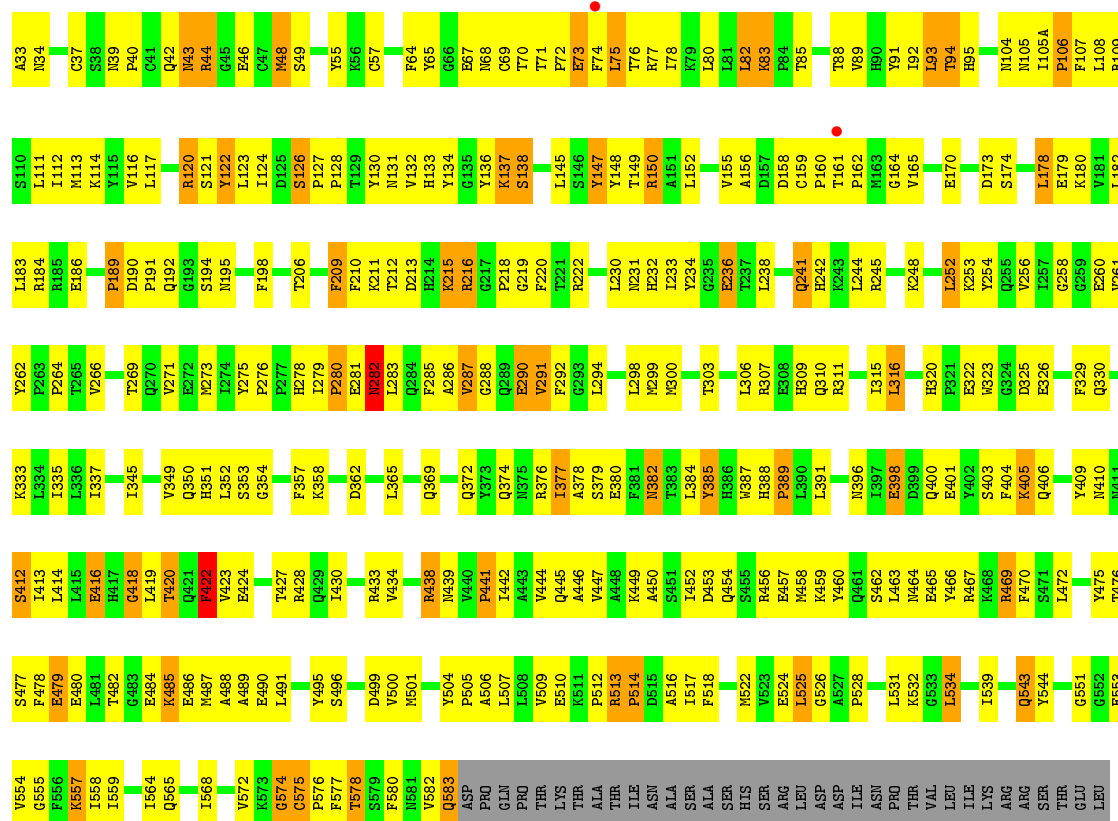






### • Molecule 1: CYCLOOXYGENASE-2

Chain C: 41% 44% 9% 6%



### • Molecule 1: CYCLOOXYGENASE-2

Chain D: 42% 43% 8% 6%

F556	T482	E416	K342	T269	D190	Y115	A33
K557	G483	H417	G418	Q270	P191	V116	N34
I558	E484	L419	I345	V271	Q192	L117	C37
A562	K485	T420	Y348	Y275	N195	R120	S38
S563	K487	Q421	Y349	P276	F198	S121	R39
I564	A488	E422	Q350	P277	A199	Y122	P40
I568	A489	E424	H351	H278	A199	L123	C41
V572	E490		L352	I279	T206	I124	Q42
V573	L491		S353	P280		D125	N43
K573		T427	G354	E281		S126	R44
G574	L494	R428		N282	F209	P127	G45
C575	Y495	Q429	F357	L283	F210	P128	E46
P576	S496	I430	K358	Q284	K211	T129	S49
F577	D497	A431		F285	T212	Y130	T50
T578	L498	G432	L366	A286	D213	N131	
S579	D499	R433	F367	V287	H214	V132	K56
F580	V500	V434	N368	G288	K215	H133	C57
	M501		Q369	Q289	R216	Y134	
M581		R438		E290	G217	G135	
V582	Y504	M439	Q372	V291	P218	Y136	F64
Q583	P505	V440	Y373	G292	G219	K137	
ASP	A506	P441	Q374	G293	F220	S138	
PRO		I442	R375	L294	T221		C69
	V509	A443	R376		R222	F142	T70
GLN	E510	V444	L377	L298			T71
THR	K511	Q445	A378	M299	L230	L145	P72
LYS	P512	A446	S379	N300	N231	S146	E73
THR	R513	V447	E380		H232	Y147	F74
ALA	P514		F381	T303	I233	Y148	L75
THR	D515	A450	N382		Y234	T149	T76
ILE	A516	S451	T383	L306	G235	R150	R77
ASN	L517	I452	L384	R307	E236		I78
SER		Q454	Y385	E308	T237	V155	L82
ALA	M522	S455	H386	H309	L238	A156	K83
SER	V523		K387	Q310		D157	P84
ALA	E524	R456	H388	R311	Q241	D158	T85
HIS	L525	E457	P389		H242	C159	
SER	G526	M458	L390	I315	K243	P160	T88
A527	ARG	K459	L391	L316	L244	T161	V89
LEU	P528				R245	P162	H90
ASP	F529	S462	T394	E319	L246	H163	Y91
ASP	S530	L463	F395	H320	F247	G164	I92
ILE	L531	M464	N396	P321	K248	V165	L93
ASN	K532	E465	I397	E322			T94
PRO	G533	Y466	E398		L252	E170	H95
THR	L534	R467	N399	D325	K253		F96
VAL		K468	Q400	E326	Y254	D173	
LEU	L539	R469	E401		Q255		N104
ILE	C540	F470	Y402	F329	V256	L178	N105
LYS	S541	S471		Q330	I257	E179	I105A
ARG	P542	L472	K405	K333	G258	K180	P106
ARG	Q543				G259	V181	F107
SER	Y544	Y475	Y409		E260	L182	L108
THR		T476	N410	L336	V261	L183	R109
GLU	G551	S477	N411	I337	Y262	R184	
LEU	E552	F478	S412	G338		R185	S110
	E553	E479	I413	E339	V266	E186	L111
	V554	E480	L414	T340	K267	L112	I112
	G555	L491	L415	T241	D268	K143	K144
						P189	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.80 Å   133.60 Å   118.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	8.00 – 2.90 19.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	68.0 (8.00-2.90) 75.7 (19.94-2.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.88 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.219   ,   0.309 0.225   ,   0.304	Depositor DCC
$R_{free}$ test set	4670 reflections (11.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 58.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 48216 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	18332	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	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 30.54 % 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 1.2860e-03. 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, NAG, IMN

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	0.67	0/4600	0.84	6/6237 (0.1%)
1	B	0.70	0/4600	0.85	5/6237 (0.1%)
1	C	0.68	0/4600	0.84	5/6237 (0.1%)
1	D	0.68	0/4600	0.84	5/6237 (0.1%)
All	All	0.68	0/18400	0.84	21/24948 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	418	GLY	N-CA-C	6.00	128.09	113.10
1	D	418	GLY	N-CA-C	5.97	128.02	113.10
1	B	258	GLY	N-CA-C	-5.97	98.19	113.10
1	C	418	GLY	N-CA-C	5.92	127.90	113.10
1	D	258	GLY	N-CA-C	-5.85	98.48	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	TYR	Sidechain
1	A	466	TYR	Sidechain
1	C	147	TYR	Sidechain
1	D	147	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4473	0	4375	284	0
1	B	4473	0	4375	277	0
1	C	4473	0	4375	278	0
1	D	4473	0	4375	283	0
2	A	42	0	39	1	0
2	B	42	0	39	1	0
2	C	42	0	39	1	0
2	D	42	0	39	0	0
3	A	43	0	30	4	0
3	B	43	0	30	5	0
3	C	43	0	30	5	0
3	D	43	0	30	5	0
4	A	25	0	15	8	0
4	B	25	0	15	9	0
4	C	25	0	15	8	0
4	D	25	0	15	9	0
All	All	18332	0	17836	1109	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 31.

The worst 5 of 1109 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:477:SER:HB2	1:B:479:GLU:HG2	1.37	1.07
1:A:579:SER:HB2	1:D:267:LYS:HZ1	1.23	1.03
1:C:477:SER:HB2	1:C:479:GLU:HG2	1.41	1.01
1:B:183:LEU:HD22	1:B:442:ILE:HD13	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:574:GLY:O	1:D:576:PRO:HD3	1.63	0.97

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	550/587 (94%)	456 (83%)	74 (14%)	20 (4%)	4	18
1	B	550/587 (94%)	455 (83%)	74 (14%)	21 (4%)	4	16
1	C	550/587 (94%)	454 (82%)	78 (14%)	18 (3%)	5	20
1	D	550/587 (94%)	451 (82%)	76 (14%)	23 (4%)	3	13
All	All	2200/2348 (94%)	1816 (82%)	302 (14%)	82 (4%)	4	17

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	282	ASN
1	A	398	GLU
1	A	514	PRO
1	B	138	SER

### 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	493/525 (94%)	423 (86%)	70 (14%)	4	12
1	B	493/525 (94%)	421 (85%)	72 (15%)	4	12
1	C	493/525 (94%)	424 (86%)	69 (14%)	4	12
1	D	493/525 (94%)	426 (86%)	67 (14%)	5	13
All	All	1972/2100 (94%)	1694 (86%)	278 (14%)	4	12

5 of 278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	412	SER
1	C	120	ARG
1	D	382	ASN
1	B	441	PRO
1	B	583	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	133	HIS
1	C	282	ASN
1	D	374	GLN
1	C	232	HIS
1	C	351	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 ⓘ

There are no carbohydrates in this entry.

## 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	661	1	14,14,15	0.58	0	15,19,21	0.59	0
2	NAG	A	671	1	14,14,15	0.56	0	15,19,21	1.06	1 (6%)
2	NAG	A	681	1	14,14,15	0.44	0	15,19,21	0.94	1 (6%)
3	HEM	A	682	1	30,50,50	3.15	11 (36%)	24,82,82	2.10	6 (25%)
4	IMN	A	701	-	21,27,27	2.44	9 (42%)	26,39,39	1.33	3 (11%)
2	NAG	B	661	1	14,14,15	0.80	0	15,19,21	0.89	1 (6%)
2	NAG	B	671	1	14,14,15	0.69	0	15,19,21	1.17	2 (13%)
2	NAG	B	681	1	14,14,15	0.45	0	15,19,21	0.88	1 (6%)
3	HEM	B	682	1	30,50,50	2.98	9 (30%)	24,82,82	2.10	7 (29%)
4	IMN	B	701	-	21,27,27	2.38	10 (47%)	26,39,39	1.24	3 (11%)
2	NAG	C	661	1	14,14,15	0.79	0	15,19,21	0.96	2 (13%)
2	NAG	C	671	1	14,14,15	0.84	0	15,19,21	1.29	2 (13%)
2	NAG	C	681	1	14,14,15	0.48	0	15,19,21	0.80	0
3	HEM	C	682	1	30,50,50	3.19	9 (30%)	24,82,82	2.11	7 (29%)
4	IMN	C	701	-	21,27,27	2.40	9 (42%)	26,39,39	1.33	3 (11%)
2	NAG	D	661	1	14,14,15	0.73	0	15,19,21	0.91	1 (6%)
2	NAG	D	671	1	14,14,15	0.62	0	15,19,21	1.31	3 (20%)
2	NAG	D	681	1	14,14,15	0.77	0	15,19,21	0.99	0
3	HEM	D	682	1	30,50,50	3.03	11 (36%)	24,82,82	2.06	7 (29%)
4	IMN	D	701	-	21,27,27	2.42	7 (33%)	26,39,39	1.33	4 (15%)

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	661	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	671	1	-	0/6/23/26	0/1/1/1
2	NAG	A	681	1	-	0/6/23/26	0/1/1/1
3	HEM	A	682	1	-	0/10/54/54	0/0/8/8
4	IMN	A	701	-	-	0/8/14/14	0/3/3/3
2	NAG	B	661	1	-	0/6/23/26	0/1/1/1
2	NAG	B	671	1	-	0/6/23/26	0/1/1/1
2	NAG	B	681	1	-	0/6/23/26	0/1/1/1
3	HEM	B	682	1	-	0/10/54/54	0/0/8/8
4	IMN	B	701	-	-	0/8/14/14	0/3/3/3
2	NAG	C	661	1	-	0/6/23/26	0/1/1/1
2	NAG	C	671	1	-	0/6/23/26	0/1/1/1
2	NAG	C	681	1	-	0/6/23/26	0/1/1/1
3	HEM	C	682	1	-	0/10/54/54	0/0/8/8
4	IMN	C	701	-	-	0/8/14/14	0/3/3/3
2	NAG	D	661	1	-	0/6/23/26	0/1/1/1
2	NAG	D	671	1	-	0/6/23/26	0/1/1/1
2	NAG	D	681	1	-	0/6/23/26	0/1/1/1
3	HEM	D	682	1	-	0/10/54/54	0/0/8/8
4	IMN	D	701	-	-	0/8/14/14	0/3/3/3

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	682	HEM	C3B-C4B	-8.89	1.43	1.51
3	D	682	HEM	C3C-CAC	-7.40	1.37	1.51
3	D	682	HEM	C3B-C4B	-7.35	1.45	1.51
3	A	682	HEM	C3B-C4B	-7.15	1.45	1.51
3	B	682	HEM	C3B-C4B	-6.98	1.45	1.51

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	671	NAG	C2-N2-C7	-3.12	119.03	123.04
2	D	671	NAG	C2-N2-C7	-2.81	119.42	123.04
2	B	671	NAG	C2-N2-C7	-2.65	119.64	123.04
2	B	661	NAG	C2-N2-C7	-2.58	119.72	123.04
2	D	661	NAG	C2-N2-C7	-2.56	119.75	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	661	NAG	1	0
3	A	682	HEM	4	0
4	A	701	IMN	8	0
2	B	661	NAG	1	0
3	B	682	HEM	5	0
4	B	701	IMN	9	0
2	C	661	NAG	1	0
3	C	682	HEM	5	0
4	C	701	IMN	8	0
3	D	682	HEM	5	0
4	D	701	IMN	9	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, 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%)	-0.26	5 (0%) 85 84	2, 10, 22, 35	0
1	B	552/587 (94%)	-0.26	0 100 100	2, 10, 22, 34	0
1	C	552/587 (94%)	-0.29	2 (0%) 93 92	2, 10, 22, 34	0
1	D	552/587 (94%)	-0.22	3 (0%) 91 90	2, 11, 24, 31	0
All	All	2208/2348 (94%)	-0.26	10 (0%) 91 90	2, 10, 22, 35	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	74	PHE	3.4
1	A	280	PRO	2.8
1	A	74	PHE	2.5
1	A	278	HIS	2.5
1	D	582	VAL	2.4

### 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](#)

There are no carbohydrates in this entry.

### 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, 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( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	661	14/15	0.87	0.27	6.17	20,23,29,30	0
2	NAG	C	681	14/15	0.85	0.38	4.14	19,26,28,32	0
2	NAG	A	681	14/15	0.86	0.25	3.85	18,24,27,32	0
4	IMN	B	701	25/25	0.90	0.21	2.17	5,18,24,25	0
4	IMN	D	701	25/25	0.90	0.20	1.92	8,22,23,26	0
2	NAG	B	681	14/15	0.87	0.24	1.73	14,27,29,31	0
2	NAG	D	661	14/15	0.85	0.26	1.04	16,22,29,29	0
2	NAG	D	681	14/15	0.87	0.23	0.72	19,27,29,33	0
4	IMN	C	701	25/25	0.93	0.17	0.49	3,20,23,24	0
2	NAG	B	671	14/15	0.92	0.19	0.40	2,8,19,24	0
2	NAG	B	661	14/15	0.82	0.28	0.34	15,22,29,31	0
3	HEM	B	682	43/43	0.94	0.17	0.28	2,10,20,33	0
2	NAG	D	671	14/15	0.88	0.20	0.26	2,10,17,21	0
2	NAG	C	671	14/15	0.90	0.17	0.16	2,10,20,25	0
2	NAG	A	671	14/15	0.91	0.18	0.10	2,8,20,24	0
4	IMN	A	701	25/25	0.94	0.16	0.09	2,18,21,22	0
3	HEM	A	682	43/43	0.94	0.16	-0.04	2,8,23,32	0
3	HEM	C	682	43/43	0.94	0.16	-0.09	2,7,19,27	0
3	HEM	D	682	43/43	0.95	0.15	-0.34	4,10,20,33	0
2	NAG	A	661	14/15	0.82	0.33	-	19,23,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.