



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:57 PM GMT

PDB ID : 6COX  
Title : CYCLOOXYGENASE-2 (PROSTAGLANDIN SYNTHASE-2) COM-  
PLEXED WITH A SELECTIVE INHIBITOR, SC-558 IN I222 SPACE  
GROUP  
Authors : Kurumbail, R.; Stallings, W.  
Deposited on : 1996-12-18  
Resolution : 2.80 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

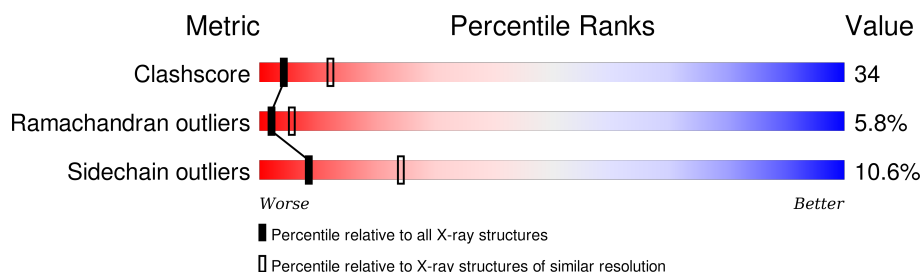
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

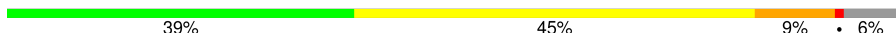

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	587	 39% 45% 9% • 6%
1	B	587	 40% 45% 9% • 6%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9168 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			

There are 4 discrepancies between the modelled and reference sequences:

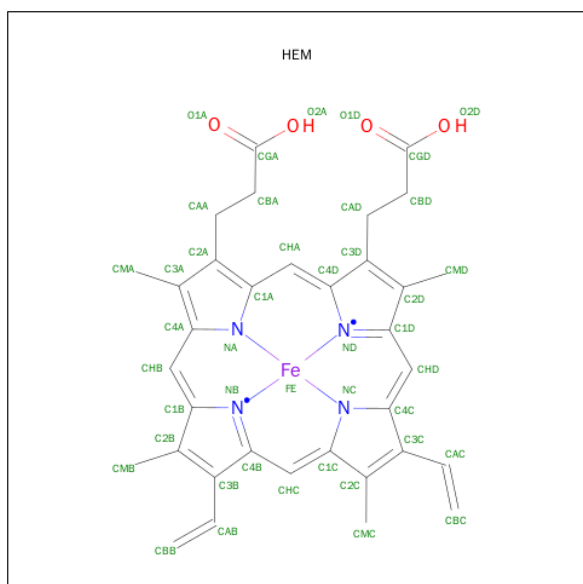
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	CONFLICT	UNP Q05769
A	333	LYS	ARG	CONFLICT	UNP Q05769
B	310	GLN	ASN	CONFLICT	UNP Q05769
B	333	LYS	ARG	CONFLICT	UNP Q05769

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



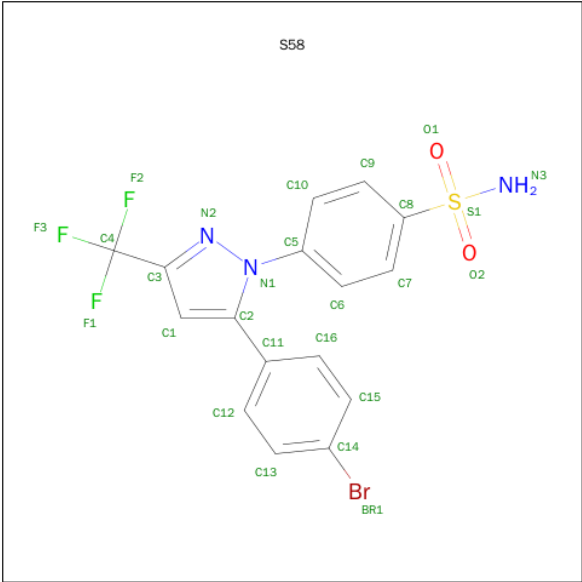
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 4 is 1-PHENYLSULFONAMIDE-3-TRIFLUOROMETHYL-5-PARABROMOPHENYLPYRAZOLE (three-letter code: S58) (formula:  $C_{16}H_{11}BrF_3N_3O_2S$ ).



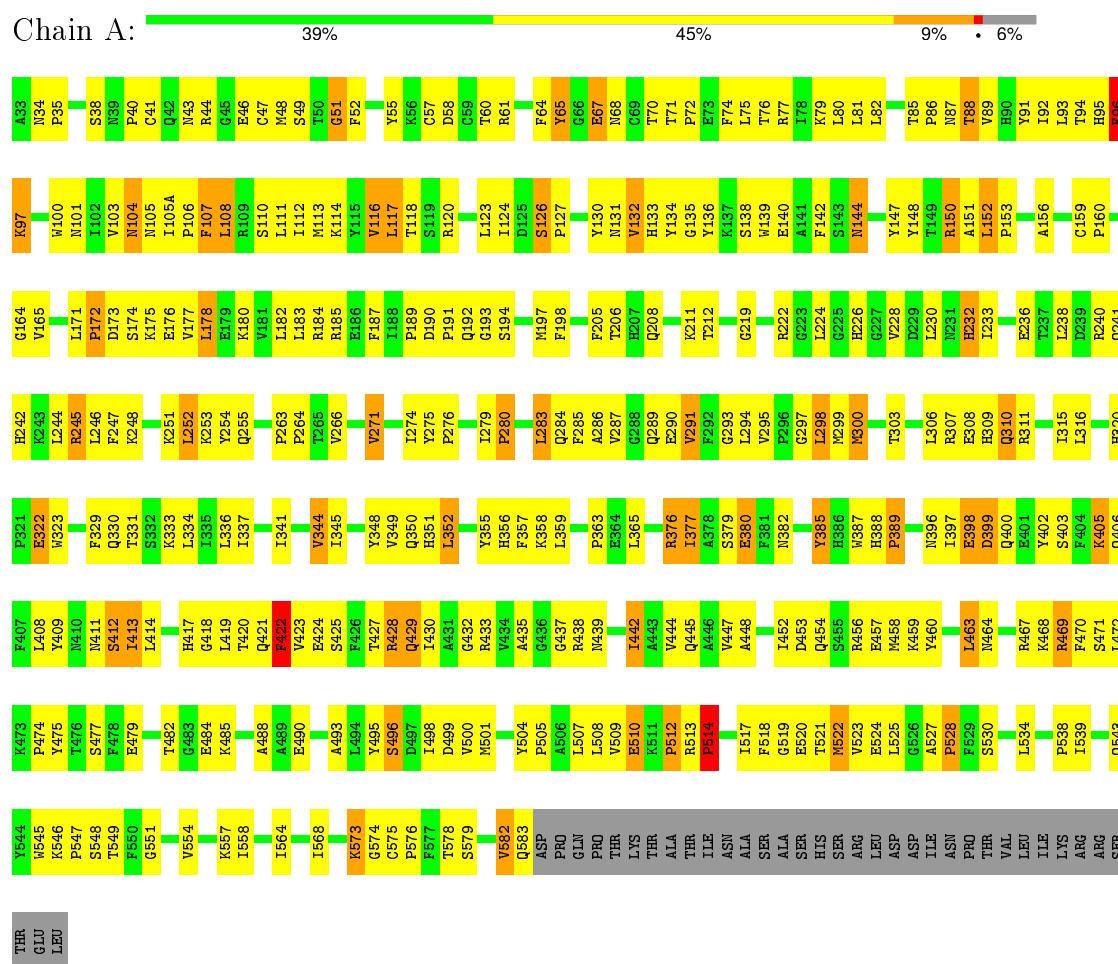
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Br	C	F	N	O	S		
4	A	1	26	1	16	3	3	2	1	0	0
4	B	1	26	1	16	3	3	2	1	0	0

### 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.

Note EDS was not executed.

#### • Molecule 1: CYCLOOXYGENASE-2



#### • Molecule 1: CYCLOOXYGENASE-2

Chain B: 



ARG SER THR GLU LEU	I539	F470	S403	E322	L246	P172	W100
	S471	S471	F404	W323	F247	D173	M101
	L472	L472	R405	L328	K248	S174	I102
	K473	K473	Q406	F329	K251	E176	N103
	P474	P474	Y409	Q330	L252	V177	N104
	Y475	Y475	R410	T331	K253	L178	N105
	T476	T476	M411	S332	Y254	E179	I105A
	S477	S477	S412	K333	Q255	K180	P106
	F478	F478	I413	L334	P263	V181	F107
	E479	E479	L414	L337	P264	L182	L108
	T482	T482	H417	L341	P265	L183	M109
	G483	G483	G418	K342	T266	R184	S110
	E484	E484	L419	T343	T269	R185	L111
	K485	K485	T420	V344	V271	P189	M112
	A488	A488	Q421	L345	Q270	D190	M113
	A489	A489	V423	V348	V271	P191	K114
	E490	E490	E424	Y349	I274	Q192	V116
	A493	A493	S425	Q350	Y275	G193	L117
	L494	L494	F426	K350	P276	S194	T118
	Y495	Y495	T427	H351	P277	M195	S119
	S496	S496	R428	L352	H278	M196	S120
	D497	D497	Q429	Y355	I279	M197	
	T498	T498	I430	H356	P280	F198	L123
	D499	D499	A431	F357	L283	A202	I124
	V500	V500	R432	K358	Q284	F205	D125
	M501	M501	V434	L359	F285	T206	P127
	Y504	Y504	A435	K360	A286	H207	Y130
ASP	P505	P505	G436	L365	V287	Q208	M131
GLU	A506	A506	G437	L366	G288	F209	V132
PRO	L507	L507	R438	F367	Q289	F210	H133
THR	L508	L508	N439	K368	E290	K211	Y134
LYS	V509	V509	I442	Q369	V291	T212	G135
THR	E510	E510	A443	Q370	F292		Y136
ALA	V511	V511	V444	F371	G293	G219	K137
THR	P512	P512	Q445		L294		S138
ILE	R513	R513	A446	K376	V295	R222	W139
ASN	P514	P514	V447	L377	P296		N144
ALA				A378	G297	H226	
SER	I517	I517	S451	A378	L298	G227	Y147
ALA	P518	P518	I452	S379	M299	V228	Y148
SER	G519	G519	D453	E380	M300	D229	T149
HIS	E520	E520	Q454	F381	T303	N231	R150
SER	T521	T521	S455	K382		H232	A151
ARG	M522	M522	R456	Y385	L306	L233	L152
LEU	V523	V523	E457		R307		P153
ASP	E524	E524	M458	H388	E308	E236	
ASP	L525	L525	R459	P389	H309	T237	A156
ILE	G526	G526	Y460	N396	Q310	L238	C159
ASN	A527	A527	L463	I397	R311	D239	P160
PRO	P528	P528	M464	K398	I315	Q241	G164
THR	F529	F529	R467	D399	L316	H242	V165
VAL	S530	S530	K468	Q400	H320	L244	
LEU			R469	Y402	P321	R245	L171
ILE	L534	L534					
LYS							
ARG	P538	P538					

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.17Å 132.81Å 122.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	88.5 (8.00-2.80)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.220 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP



## 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, S58

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	0.65	0/4600	0.84	1/6237 (0.0%)
1	B	0.65	1/4600 (0.0%)	0.85	2/6237 (0.0%)
All	All	0.65	1/9200 (0.0%)	0.85	3/12474 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	479	GLU	CB-CG	5.55	1.62	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	VAL	N-CA-C	5.54	125.97	111.00
1	B	287	VAL	N-CA-C	5.29	125.28	111.00
1	B	437	GLY	N-CA-C	-5.17	100.17	113.10

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	4473	0	4375	324	0
1	B	4473	0	4375	301	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	42	0	39	1	0
2	B	42	0	39	0	0
3	A	43	0	30	2	0
3	B	43	0	30	1	0
4	A	26	0	11	3	0
4	B	26	0	11	2	0
All	All	9168	0	8910	607	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 34.

The worst 5 of 607 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD22	1:A:411:ASN:HB2	1.32	1.11
1:B:280:PRO:HD2	1:B:283:LEU:HD23	1.35	1.09
1:A:279:ILE:HG23	1:A:283:LEU:HG	1.32	1.08
1:B:279:ILE:HG23	1:B:283:LEU:HG	1.37	1.07
1:A:280:PRO:HD2	1:A:283:LEU:HD23	1.41	1.02

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%)	435 (79%)	84 (15%)	31 (6%)	2	6
1	B	550/587 (94%)	431 (78%)	86 (16%)	33 (6%)	2	5
All	All	1100/1174 (94%)	866 (79%)	170 (16%)	64 (6%)	2	5

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	348	TYR
1	A	398	GLU
1	A	510	GLU
1	A	514	PRO

### 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	493/525 (94%)	439 (89%)	54 (11%)	8	23
1	B	493/525 (94%)	442 (90%)	51 (10%)	9	26
All	All	986/1050 (94%)	881 (89%)	105 (11%)	8	24

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	469	ARG
1	B	101	ASN
1	B	442	ILE
1	A	484	GLU
1	A	557	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	43	ASN
1	B	95	HIS
1	B	417	HIS
1	A	417	HIS
1	A	565	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

10 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	0.64	0	15,19,21	0.55	0
2	NAG	A	671	1	14,14,15	0.43	0	15,19,21	0.91	1 (6%)
2	NAG	A	681	1	14,14,15	0.31	0	15,19,21	0.87	1 (6%)
3	HEM	A	682	1	30,50,50	3.11	11 (36%)	24,82,82	2.02	7 (29%)
4	S58	A	701	-	27,28,28	2.48	7 (25%)	40,43,43	2.06	10 (25%)
2	NAG	B	661	1	14,14,15	0.57	0	15,19,21	0.67	0
2	NAG	B	671	1	14,14,15	0.57	0	15,19,21	1.02	1 (6%)
2	NAG	B	681	1	14,14,15	0.68	0	15,19,21	0.80	1 (6%)
3	HEM	B	682	1	30,50,50	2.95	11 (36%)	24,82,82	1.94	7 (29%)
4	S58	B	701	-	27,28,28	2.43	7 (25%)	40,43,43	1.82	9 (22%)

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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	682	1	-	0/10/54/54	0/0/8/8
4	S58	A	701	-	-	0/20/20/20	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	S58	B	701	-	-	0/20/20/20	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	682	HEM	C3B-C4B	-7.46	1.45	1.51
3	B	682	HEM	C3B-CAB	-7.11	1.38	1.51
3	A	682	HEM	C3B-CAB	-6.89	1.38	1.51
3	A	682	HEM	C3C-CAC	-6.87	1.38	1.51
3	B	682	HEM	C3B-C4B	-6.82	1.45	1.51

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	S58	O2-S1-O1	-6.18	110.11	118.80
4	B	701	S58	O2-S1-O1	-5.31	111.34	118.80
2	B	671	NAG	C2-N2-C7	-3.19	118.94	123.04
2	A	671	NAG	C2-N2-C7	-2.93	119.28	123.04
4	B	701	S58	F2-C4-C3	-2.85	107.49	112.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	661	NAG	1	0
3	A	682	HEM	2	0
4	A	701	S58	3	0
3	B	682	HEM	1	0
4	B	701	S58	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.