



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 06:46 AM GMT

PDB ID : 1CX2
Title : CYCLOOXYGENASE-2 (PROSTAGLANDIN SYNTHASE-2) COM-
PLEXED WITH A SELECTIVE INHIBITOR, SC-558
Authors : Kurumbail, R.; Stallings, W.
Deposited on : 1996-12-17
Resolution : 3.00 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>

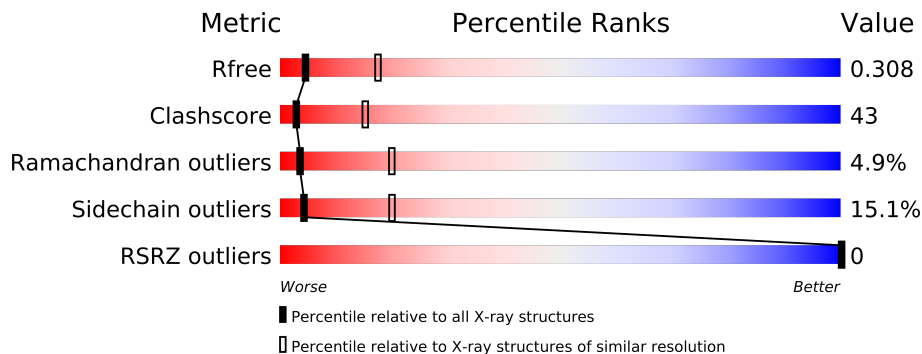
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
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)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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

There are 4 unique types of molecules in this entry. The entry contains 22376 atoms, of which 4040 are hydrogens 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 CYCLOOXYGENASE-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	552	Total	C	H	N	O	S	0	0	0
			5439	2886	966	748	814	25			
1	B	552	Total	C	H	N	O	S	0	0	0
			5439	2886	966	748	814	25			
1	C	552	Total	C	H	N	O	S	0	0	0
			5439	2886	966	748	814	25			
1	D	552	Total	C	H	N	O	S	0	0	0
			5439	2886	966	748	814	25			

There are 8 discrepancies between the modelled and reference sequences:

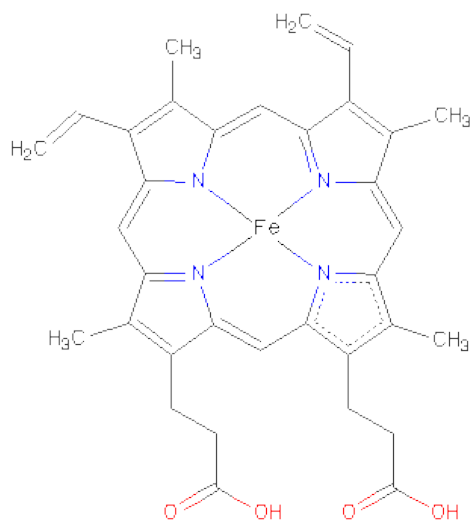
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	CONFLICT	UNP Q05769
A	333	LYS	ARG	CONFLICT	UNP Q05769
B	310	GLN	ASN	CONFLICT	UNP Q05769
B	333	LYS	ARG	CONFLICT	UNP Q05769
C	310	GLN	ASN	CONFLICT	UNP Q05769
C	333	LYS	ARG	CONFLICT	UNP Q05769
D	310	GLN	ASN	CONFLICT	UNP Q05769
D	333	LYS	ARG	CONFLICT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

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



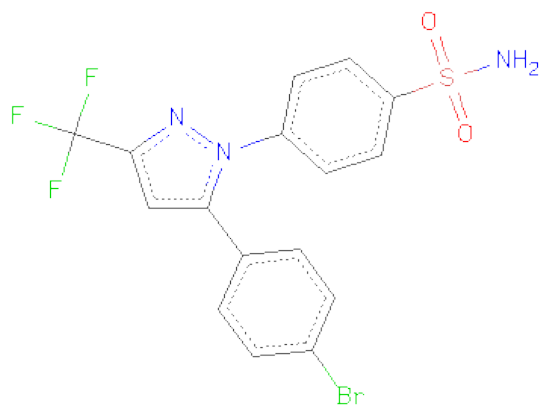
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

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

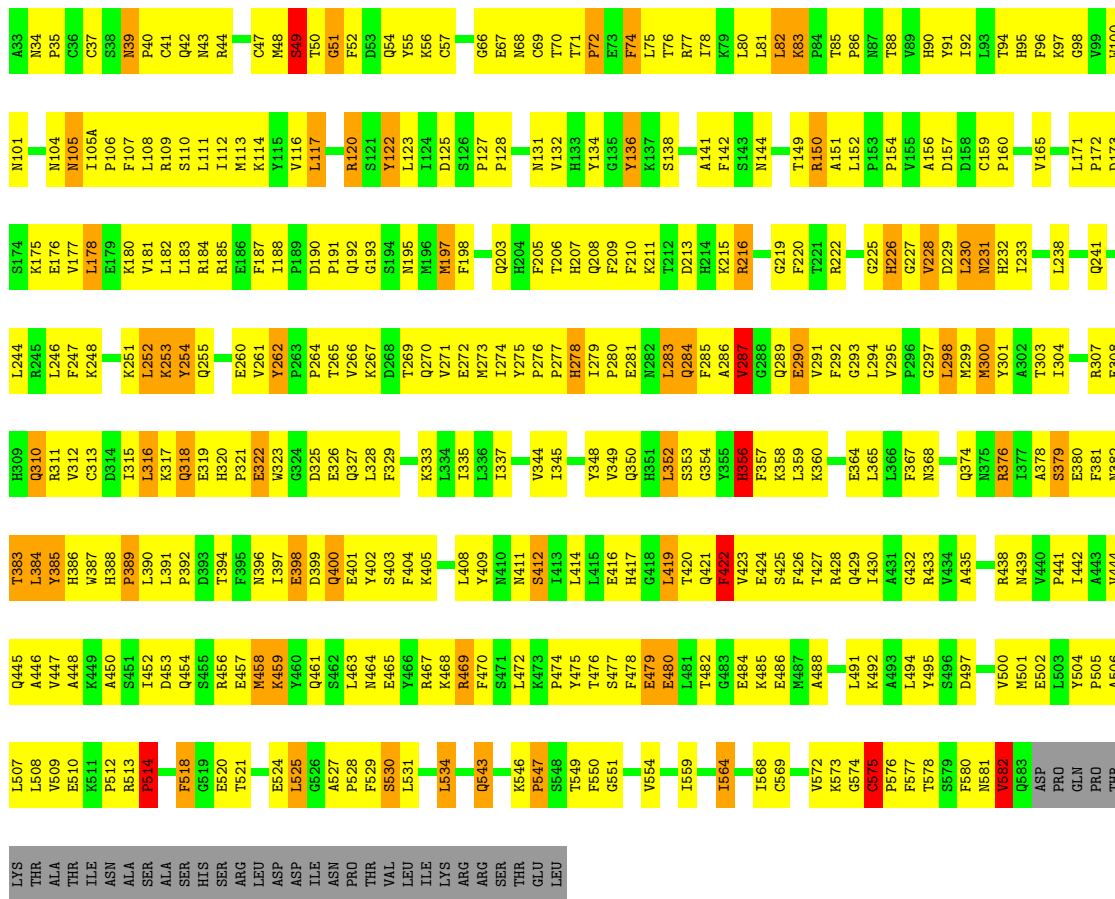


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

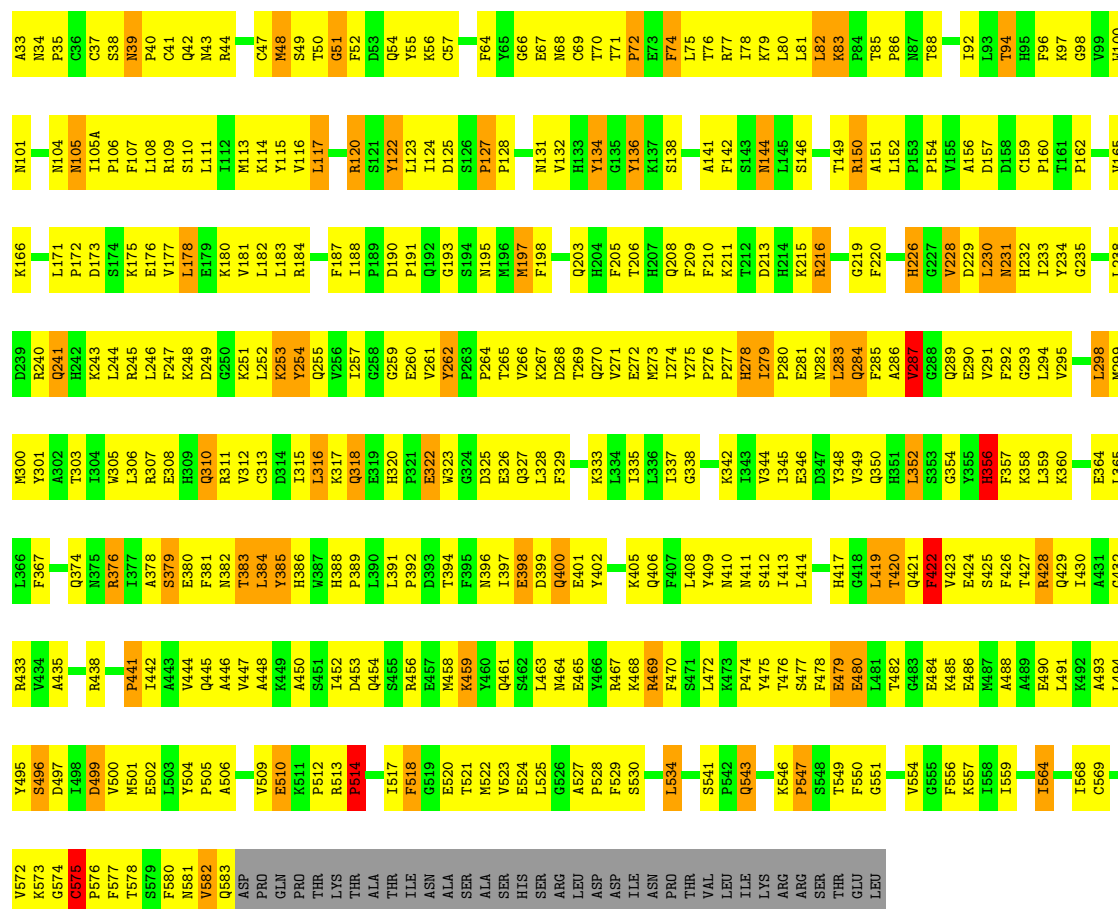
- Molecule 4 is 1-PHENYLSULFONAMIDE-3-TRIFLUOROMETHYL-5-PARABROMOPHENYLPYRAZOLE (three-letter code: S58) (formula: $C_{16}H_{11}BrF_3N_3O_2S$).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
4	A	1	Total	Br	C	F	H	N	O	S	0	0
			28	1	16	3	2	3	2	1		
4	B	1	Total	Br	C	F	H	N	O	S	0	0
			28	1	16	3	2	3	2	1		
4	C	1	Total	Br	C	F	H	N	O	S	0	0
			28	1	16	3	2	3	2	1		
4	D	1	Total	Br	C	F	H	N	O	S	0	0
			28	1	16	3	2	3	2	1		



Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	180.34Å 133.92Å 121.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	54.0 (8.00-3.00) 61.9 (20.00-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.98Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.216 , 0.218 0.232 , 0.308	Depositor DCC
R_{free} test set	3652 reflections (11.09%)	DCC
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.960	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 36581 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	22376	wwPDB-VP
Average B, all atoms (Å ²)	9.0	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 39.14 % 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 3.3164e-04. 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, 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	0.71	0/4600	0.88	4/6237 (0.1%)
1	B	0.71	0/4600	0.88	4/6237 (0.1%)
1	C	0.69	0/4600	0.88	3/6237 (0.0%)
1	D	0.72	0/4600	0.89	3/6237 (0.0%)
All	All	0.71	0/18400	0.88	14/24948 (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	3
1	B	0	2
1	C	0	2
1	D	0	4
All	All	0	11

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	CYS	N-CA-C	-6.66	93.02	111.00
1	D	575	CYS	N-CA-C	-6.47	93.54	111.00
1	C	575	CYS	N-CA-C	-6.38	93.78	111.00
1	B	575	CYS	N-CA-C	-6.35	93.85	111.00
1	D	287	VAL	N-CA-C	5.94	127.03	111.00

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	TYR	Sidechain
1	A	262	TYR	Sidechain
1	A	348	TYR	Sidechain
1	B	262	TYR	Sidechain
1	B	348	TYR	Sidechain

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	4473	966	3415	395	0
1	B	4473	966	3415	406	0
1	C	4473	966	3415	384	0
1	D	4473	966	3415	391	0
2	A	42	42	0	0	0
2	B	42	42	0	4	0
2	C	42	42	0	0	0
2	D	42	42	0	8	0
3	A	43	0	30	3	0
3	B	43	0	30	6	0
3	C	43	0	30	7	0
3	D	43	0	30	5	0
4	A	26	2	9	9	0
4	B	26	2	9	5	0
4	C	26	2	9	11	0
4	D	26	2	9	8	0
All	All	18336	4040	13816	1540	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 43.

The worst 5 of 1540 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:52:PHE:N	1:D:322:GLU:HG2	1.80	0.96
1:C:322:GLU:HG2	1:D:52:PHE:N	1.83	0.93
1:A:275:TYR:CE2	1:A:284:GLN:HA	2.04	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:184:ARG:HA	1:C:438:ARG:O	1.71	0.89
1:C:275:TYR:CE2	1:C:284:GLN:HA	2.07	0.89

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	550/587 (94%)	439 (80%)	86 (16%)	25 (4%)	4	22
1	B	550/587 (94%)	438 (80%)	85 (16%)	27 (5%)	3	20
1	C	550/587 (94%)	439 (80%)	84 (15%)	27 (5%)	3	20
1	D	550/587 (94%)	444 (81%)	78 (14%)	28 (5%)	3	18
All	All	2200/2348 (94%)	1760 (80%)	333 (15%)	107 (5%)	3	20

5 of 107 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	A	138	SER
1	A	226	HIS
1	A	270	GLN
1	A	284	GLN

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%)	422 (86%)	71 (14%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	493/525 (94%)	411 (83%)	82 (17%)	3	16
1	C	493/525 (94%)	423 (86%)	70 (14%)	5	22
1	D	493/525 (94%)	418 (85%)	75 (15%)	4	20
All	All	1972/2100 (94%)	1674 (85%)	298 (15%)	4	20

5 of 298 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	428	ARG
1	C	150	ARG
1	D	412	SER
1	B	469	ARG
1	B	577	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	351	HIS
1	C	87	ASN
1	D	318	GLN
1	B	382	ASN
1	B	464	ASN

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 ⓘ

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	12,14,15	0.67	0	15,19,21	0.89	0
2	NAG	A	671	1	12,14,15	0.68	0	15,19,21	1.25	3 (20%)
2	NAG	A	681	1	12,14,15	0.90	0	15,19,21	0.90	0
3	HEM	A	682	1	49,50,50	2.03	8 (16%)	46,82,82	1.13	4 (8%)
4	S58	A	701	-	28,28,28	2.49	6 (21%)	43,43,43	1.65	10 (23%)
2	NAG	B	661	1	12,14,15	0.54	0	15,19,21	0.78	1 (6%)
2	NAG	B	671	1	12,14,15	0.59	0	15,19,21	0.99	2 (13%)
2	NAG	B	681	1	12,14,15	0.72	0	15,19,21	0.75	0
3	HEM	B	682	1	49,50,50	1.78	9 (18%)	46,82,82	1.13	4 (8%)
4	S58	B	701	-	28,28,28	2.57	8 (28%)	43,43,43	1.71	10 (23%)
2	NAG	C	661	1	12,14,15	0.78	0	15,19,21	0.72	0
2	NAG	C	671	1	12,14,15	0.58	0	15,19,21	1.22	2 (13%)
2	NAG	C	681	1	12,14,15	0.96	1 (8%)	15,19,21	0.73	0
3	HEM	C	682	1	49,50,50	2.37	8 (16%)	46,82,82	1.09	5 (10%)
4	S58	C	701	-	28,28,28	2.61	6 (21%)	43,43,43	1.55	9 (20%)
2	NAG	D	661	1	12,14,15	0.59	0	15,19,21	0.67	0
2	NAG	D	671	1	12,14,15	0.67	0	15,19,21	1.26	2 (13%)
2	NAG	D	681	1	12,14,15	0.58	0	15,19,21	0.75	0
3	HEM	D	682	1	49,50,50	2.40	9 (18%)	46,82,82	1.09	4 (8%)
4	S58	D	701	-	28,28,28	2.70	9 (32%)	43,43,43	1.64	9 (20%)

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	-	0/14/114/114	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	-	0/14/114/114	0/0/8/8
4	S58	B	701	-	-	0/20/20/20	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	-	0/14/114/114	0/0/8/8
4	S58	C	701	-	-	0/20/20/20	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	-	0/14/114/114	0/0/8/8
4	S58	D	701	-	-	0/20/20/20	0/3/3/3

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	682	HEM	C2B-C1B	12.34	1.47	1.44
3	C	682	HEM	C2B-C1B	10.31	1.47	1.44
4	C	701	S58	C1-C3	8.05	1.50	1.39
4	D	701	S58	C1-C3	8.00	1.50	1.39
3	A	682	HEM	C2B-C1B	7.92	1.46	1.44

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	S58	O2-S1-O1	-5.22	109.71	118.78
4	B	701	S58	O2-S1-O1	-5.04	110.02	118.78
4	D	701	S58	O2-S1-O1	-4.83	110.38	118.78
4	C	701	S58	O2-S1-O1	-4.16	111.55	118.78
4	B	701	S58	C4-C3-N2	3.57	124.06	119.70

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%)	-0.34	0 100 100	2, 6, 16, 30	0
1	B	552/587 (94%)	-0.35	0 100 100	2, 6, 16, 27	0
1	C	552/587 (94%)	-0.34	0 100 100	2, 6, 16, 26	0
1	D	552/587 (94%)	-0.32	0 100 100	2, 7, 17, 30	0
All	All	2208/2348 (94%)	-0.34	0 100 100	2, 6, 16, 30	0

There are no RSRZ outliers to report.

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 ⓘ

There are no carbohydrates in this entry.

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(Å ²)	Q<0.9
4	S58	B	701	26/26	0.13	-	2,8,14,17	0
2	NAG	C	671	14/15	0.18	-	7,13,17,17	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	D	671	14/15	0.15	-	5,11,17,17	0
2	NAG	A	671	14/15	0.16	-	4,12,17,17	0
2	NAG	B	671	14/15	0.19	-	5,12,17,17	0
2	NAG	D	661	14/15	0.34	-	15,17,19,21	0
2	NAG	D	681	14/15	0.42	-	12,17,20,24	0
4	S58	C	701	26/26	0.13	-	2,8,15,17	0
2	NAG	B	681	14/15	0.31	-	11,17,22,24	0
2	NAG	C	661	14/15	0.32	-	12,17,21,22	0
2	NAG	B	661	14/15	0.32	-	15,17,19,20	0
3	HEM	B	682	43/43	0.19	-	2,3,7,9	0
2	NAG	C	681	14/15	0.29	-	11,17,21,22	0
3	HEM	D	682	43/43	0.17	-	2,3,7,9	0
4	S58	D	701	26/26	0.14	-	2,8,13,17	0
3	HEM	A	682	43/43	0.18	-	2,3,8,10	0
2	NAG	A	681	14/15	0.21	-	7,17,18,21	0
3	HEM	C	682	43/43	0.15	-	2,3,7,8	0
4	S58	A	701	26/26	0.13	-	2,9,15,17	0
2	NAG	A	661	14/15	0.30	-	12,17,20,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.