



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:43 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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

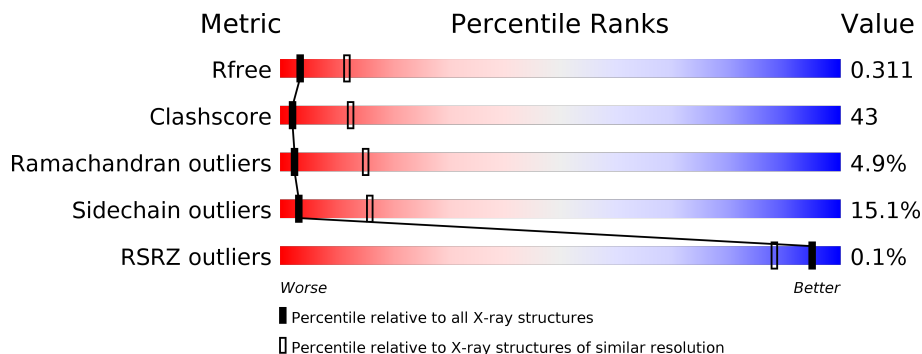
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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. 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	
1	B	587	
1	C	587	
1	D	587	

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	661	-	-	-	X
2	NAG	B	661	-	-	-	X
2	NAG	B	681	-	-	-	X
2	NAG	C	661	-	-	-	X
2	NAG	D	661	-	-	-	X
2	NAG	D	681	-	-	-	X
4	S58	A	701	-	-	X	-
4	S58	C	701	-	-	X	-
4	S58	D	701	-	-	X	-

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 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	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:

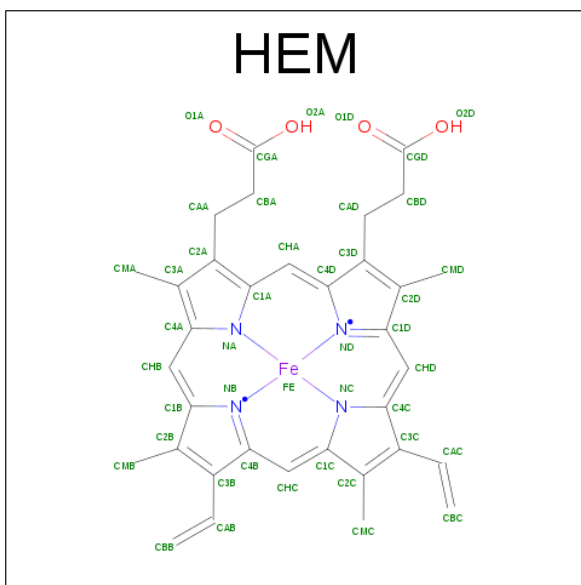
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	CONFLICT	UNP Q05769
A	333	LYS	ARG	CONFLICT	UNP Q05769
B	310	GLN	ASN	CONFLICT	UNP Q05769
B	333	LYS	ARG	CONFLICT	UNP Q05769
C	310	GLN	ASN	CONFLICT	UNP Q05769
C	333	LYS	ARG	CONFLICT	UNP Q05769
D	310	GLN	ASN	CONFLICT	UNP Q05769
D	333	LYS	ARG	CONFLICT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

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



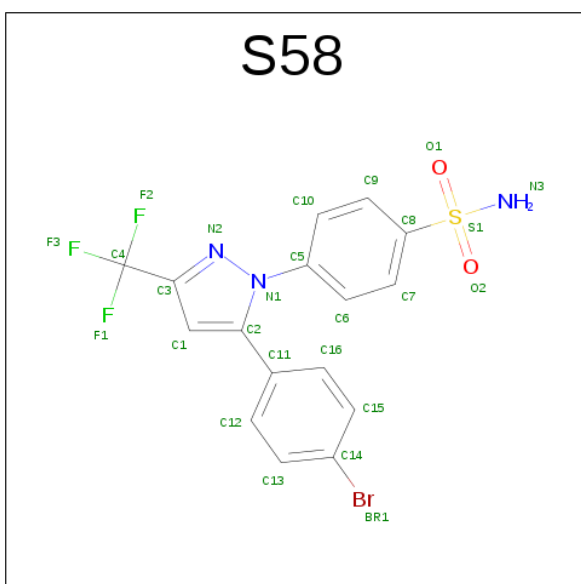
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	C	1	Total	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 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
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	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: $C_{16}H_{11}BrF_3N_3O_2S$).

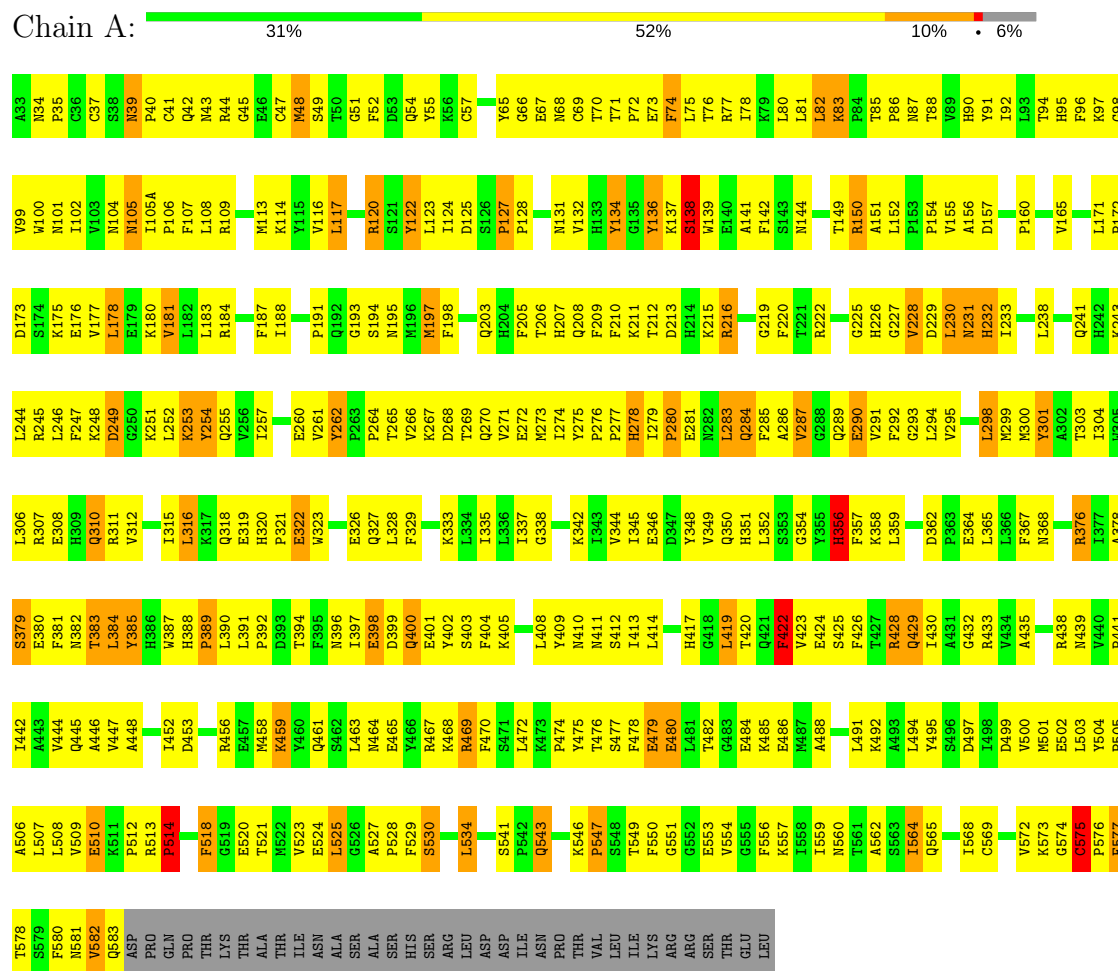


Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
4	A	1	Total	Br	C	F	H	N	O	S	0	0
			28	1	16	3	2	3	2	1		
4	B	1	Total	Br	C	F	H	N	O	S	0	0
			28	1	16	3	2	3	2	1		
4	C	1	Total	Br	C	F	H	N	O	S	0	0
			28	1	16	3	2	3	2	1		
4	D	1	Total	Br	C	F	H	N	O	S	0	0
			28	1	16	3	2	3	2	1		

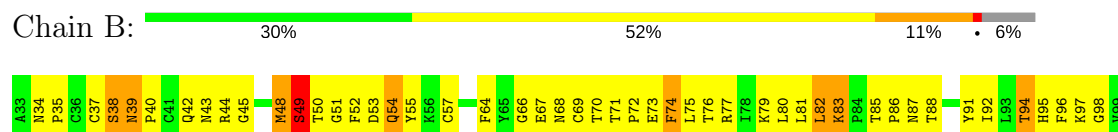
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

• Molecule 1: CYCLOOXYGENASE-2



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K573	A493	G432	L365	M300	R240	S174	W100
G574	L494	R433	L366	Y301	Q241	K175	N101
C575	Y495	V434	F367	A302	H242	E176	
P576	S496	A435	N368	T303	K243	V177	M105
F577	D497		Q369		L244	L178	N104
T578	L498	R438			R245	E179	L105A
S579	D499	V439	K374	L306	R246	P106	
F580	V500	L440	N375	R307	L247	K180	F107
N581	M501	P441	R376	E308	F247	V181	
S582	E502	L442	L377	H309	K248	L183	L108
G583	L503	K443	A378	Q310	D249	L183	L109
ASP	Y504	V444	S379	R311	G250	R184	S110
PRO	P505	Q445	S379	V312	K251		L111
GLN	A506	A446	E380	C313	L252	F187	L112
PRO	L507	V447	N381	D314	K253	L188	K114
THR	L508	A448	T383	L316	Q255	D190	Y115
THR	V509	K449	L384	K317	V256	P191	V116
THR	E510	A450	S385	Q318	T257	Q192	L117
ALA	R511	S451	R386	E319	G259	G193	
THR	P512	L452	N387	H320	K259	S194	
ILE	R513	D453	H388	P321	E260	N195	
ASN	P514	Q454	R389	E322	V261	M196	Y121
ALA		S455	L390	K323	Y262	M197	L123
SER	F518	R456	L391	G324	P263	F198	
ALA	G519	E457	P392	D325	P264		R120
SER	E520	N458	D393	E326	T265	F201	Y121
HIS	T521	K459	T394	Q327	V266	A202	S126
SER	M522	Y460	F395	L328	K267	Q203	P128
ARG	V523	Q461	N396	F329	D268	H204	
LEU	E524	S462	L397		T269	F205	N131
ASP	L525	L463	E398	K333	Q270	T206	V132
ASP	G526	N464	D399	L334	V271	H207	H133
ILE	A527	E465	Q400	L335	E272	Q208	Y134
ASN	P528	V466	E401	L336	K273	F209	G135
PRO	F529	R467	Y402	L337	T274	F210	Y136
THR	S530	K468		G338	Y275	K211	K137
VAL		R469	K405		P276	T212	S138
LEU	L534	F470	Q406	K342	P277	D213	
ILE	L471	S471	F407	L343	H278	H214	A141
LYS	P538	L472	L408	V344	L279	K215	F142
ARG		K473	Y409	L345	P280	R216	S143
ARG	Q543	P474	N410	E346	E281		N144
SER		Y475	N411	D347	H282		
THR	K546	T476	S412	F348	L283	G219	T149
GLU	P547	S477	I413	V349	Q284	T221	R150
LEU	S548	F478		Q350	F285	R222	L152
	T549	E479	H417	H351	A286		F153
	F550	E480	G418	L352	V287	H226	P154
	G551	L481	L419	S353	G288	G227	V155
	V554	G483	T420	G354	Q289	V228	A156
		E484	Q421	Y355	E290	D229	D157
	L559	K485	F422	H356	V291	T230	
		E486	V423	F357	F292	N231	P160
	L564	A487	E424	K358	G293	H232	
		N488	S425	L359	L294	L233	V165
	F568	L489	F426	K360	V295	Y234	
		E490	T427	F361	T296	G235	
	C569	L491	R428	D362	G297		L171
		V493	Q429	P363	N299	L238	P172
	V570			F324		D239	D173

• Molecule 1: CYCLOOXYGENASE-2

Chain C: 33% 51% 10% 6%

L507	Q445	T383	H509	L244	S174	M101	A33
V508	A446	L384	Q310	R245	K175	M101	N34
V509	V447	V385	R311	L246	E176	M104	N35
E510	A448	H386	V312	F247	V177	M105	C36
K511	K449	H387	C313	K248	L178	I105A	C37
P512	A450	H388	C514		E179	P106	S36
E513	S451	P389	L315	K251	K180	P107	N39
P514	L452	L430	L316	L252	L181	L108	P40
F518	D453	L391	K317	K253	L182	L109	C41
E519	A454	P392	Q318	Q254	L183	S110	C42
E520	S455	V393	E319	Q255	L184	L111	N43
	A456	T394	H320		R185	I112	N44
T521	E457	F395	P321	E260	E186	M113	C47
E524	M458	N396	E322	V261	F187	K114	M48
L525	K459	L397	V323	Y262	L188	Y115	
G526	V460	E398	G324	P263	P189	V116	S49
A527	D461	D399	D325	P264	D190	L117	G51
P528	S462	Q400	E326	T265	P191		F52
F529	M464	E401	Q327	V266	Q192	R120	D53
S530	E465	V402	L328	K267	G193	S121	Q54
	S530	F403	F329	D268	S194	Y122	Y55
L531	V466	F404		T269	N195	L123	K56
	K467		K333	Q270	M196	I124	
L534	K468		L334	V271	M197	D125	C57
	E469	L408	L335	E272	F198	S126	G66
Q543	F470	V409	L336	K273		P127	E67
K546	S471	N410	L337	L274	Q203	P128	N68
P547	K473	N411		Y275	D204		C69
S548	P474	S413	V344	P276	F205	M131	T70
T549	V475	L414	L345	P277	T206	V132	T71
F550	T476	L415	Y348	H278	H207	H133	P72
G551	S477	E416	V349	L279	Q208	Y134	P73
	F478	H417	Q350	E280	F209	G135	E74
	E479	G418	H351	E281	F210	Y136	F74
V554	E480	L419	L352	V282	K211	K137	L75
	L481	T420	S353	L283	T212	S138	T77
I559	T482	Q421	G354	Q284	D213		T78
L564	G483	F422	V355	A286	K215	F142	K79
E568	E484	V423	H356	V287	R216	S143	L80
C569	K485	F424	F357	G288		M144	L81
	E486	S425	K358	Q289	Q219		L82
	P487	F426	L359	E290	F220	T149	K83
V572	A488	T427	K360	V291	T221	R150	P84
K573		R428		G292	R222	A151	T85
G574	L491	L429	E364	F293	V228	L152	P86
P576	K492	T430	L365	L294	D229	D157	N87
F577	A493	A431	L366	V295	G225	P153	T88
T578	L494	G432	F367	P296	G227	V155	V89
S579	V495	R433	N368	G297	V228	A156	H90
F580	S496	V434		L298	D230	D158	N91
N581	D497	A435	Q374	M299	L231	C159	I92
			N375	M300	N230	T331	L93
	V500	R438	R376	Y301	H232	P160	T94
Q583	M501	N439	L377	A302	L233		H95
ASP	E502	V440	A378	T303	L238	V165	F96
PRO	L503	P441	S379	L304	Q241	L171	G97
GLN	Y504	L442	E380		P172		N98
PRO	P505	V443	F381		D169		G99
PRO	A506	L444	N382	R307			V99
			F308				V100

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

• Molecule 1: CYCLOOXYGENASE-2

Chain D: 31% 52% 11% 6%

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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 0.231 , 0.311	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 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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 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	966	4375	399	0
1	B	4473	966	4375	409	0
1	C	4473	966	4375	389	0
1	D	4473	966	4375	392	0
2	A	42	42	39	1	0
2	B	42	42	39	6	0
2	C	42	42	39	1	0
2	D	42	42	39	7	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	11	9	0
4	B	26	2	11	5	0
4	C	26	2	11	11	0
4	D	26	2	11	7	0
All	All	18336	4040	17820	1552	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 43.

The worst 5 of 1552 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: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	Interatomic distance (Å)	Clash overlap (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 [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%)	439 (80%)	86 (16%)	25 (4%)	3	17
1	B	550/587 (94%)	438 (80%)	85 (16%)	27 (5%)	2	15
1	C	550/587 (94%)	439 (80%)	84 (15%)	27 (5%)	2	15
1	D	550/587 (94%)	444 (81%)	78 (14%)	28 (5%)	2	14
All	All	2200/2348 (94%)	1760 (80%)	333 (15%)	107 (5%)	2	15

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 [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%)	422 (86%)	71 (14%)	4	18
1	B	493/525 (94%)	411 (83%)	82 (17%)	2	13
1	C	493/525 (94%)	423 (86%)	70 (14%)	4	18
1	D	493/525 (94%)	418 (85%)	75 (15%)	3	16
All	All	1972/2100 (94%)	1674 (85%)	298 (15%)	3	16

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 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	0.75	0	15,19,21	0.91	0
2	NAG	A	671	1	14,14,15	0.54	0	15,19,21	1.10	2 (13%)
2	NAG	A	681	1	14,14,15	0.82	0	15,19,21	1.02	1 (6%)
3	HEM	A	682	1	28,50,50	1.69	6 (21%)	17,82,82	1.21	1 (5%)
4	S58	A	701	-	27,28,28	2.50	6 (22%)	38,43,43	1.56	7 (18%)
2	NAG	B	661	1	14,14,15	0.61	0	15,19,21	0.89	1 (6%)
2	NAG	B	671	1	14,14,15	0.60	0	15,19,21	0.99	1 (6%)
2	NAG	B	681	1	14,14,15	0.68	0	15,19,21	0.85	0
3	HEM	B	682	1	28,50,50	1.93	5 (17%)	17,82,82	1.27	3 (17%)
4	S58	B	701	-	27,28,28	2.63	8 (29%)	38,43,43	1.58	8 (21%)
2	NAG	C	661	1	14,14,15	0.92	0	15,19,21	0.78	1 (6%)
2	NAG	C	671	1	14,14,15	0.88	1 (7%)	15,19,21	1.18	2 (13%)
2	NAG	C	681	1	14,14,15	0.87	1 (7%)	15,19,21	0.91	1 (6%)
3	HEM	C	682	1	28,50,50	1.70	5 (17%)	17,82,82	1.32	3 (17%)
4	S58	C	701	-	27,28,28	2.61	6 (22%)	38,43,43	1.46	6 (15%)
2	NAG	D	661	1	14,14,15	0.63	0	15,19,21	0.80	0
2	NAG	D	671	1	14,14,15	0.61	0	15,19,21	1.09	2 (13%)
2	NAG	D	681	1	14,14,15	0.55	0	15,19,21	0.96	1 (6%)
3	HEM	D	682	1	28,50,50	1.75	4 (14%)	17,82,82	1.15	2 (11%)
4	S58	D	701	-	27,28,28	2.71	9 (33%)	38,43,43	1.55	8 (21%)

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	-	0/6/54/54	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	-	0/6/54/54	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	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
4	S58	D	701	-	-	0/20/20/20	0/3/3/3

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	682	HEM	C3B-CAB	-5.28	1.37	1.47
4	B	701	S58	BR1-C14	-4.77	1.80	1.90
3	D	682	HEM	C3B-CAB	-4.71	1.38	1.47
3	B	682	HEM	C3C-CAC	-4.47	1.38	1.47
3	B	682	HEM	C3B-C2B	-4.45	1.34	1.40

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	S58	O2-S1-O1	-4.90	109.71	118.70
4	B	701	S58	O2-S1-O1	-4.73	110.02	118.70
4	D	701	S58	O2-S1-O1	-4.54	110.38	118.70
4	C	701	S58	O2-S1-O1	-3.90	111.55	118.70
4	B	701	S58	F2-C4-C3	-3.02	107.35	112.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	671	NAG	1	0
3	A	682	HEM	3	0
4	A	701	S58	9	0
2	B	661	NAG	2	0
2	B	681	NAG	4	0
3	B	682	HEM	6	0
4	B	701	S58	5	0
2	C	661	NAG	1	0
3	C	682	HEM	7	0
4	C	701	S58	11	0
2	D	661	NAG	5	0
2	D	681	NAG	2	0
3	D	682	HEM	5	0
4	D	701	S58	7	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, 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%)	-0.54	0 100 100	2, 6, 16, 30	0
1	B	552/587 (94%)	-0.57	1 (0%) 94 85	2, 6, 16, 27	0
1	C	552/587 (94%)	-0.54	0 100 100	2, 6, 16, 26	0
1	D	552/587 (94%)	-0.52	1 (0%) 94 85	2, 7, 17, 30	0
All	All	2208/2348 (94%)	-0.54	2 (0%) 95 88	2, 6, 16, 30	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	105	ASN	2.5
1	B	583	GLN	2.0

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, 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	C	661	14/15	0.80	0.31	6.62	12,17,21,22	0
2	NAG	A	661	14/15	0.80	0.30	5.08	12,17,20,21	0
2	NAG	D	681	14/15	0.84	0.43	4.83	12,17,20,24	0
2	NAG	D	661	14/15	0.88	0.31	4.55	15,17,19,21	0
2	NAG	B	681	14/15	0.80	0.30	2.63	11,17,22,24	0
2	NAG	B	661	14/15	0.89	0.30	2.61	15,17,19,20	0
2	NAG	C	681	14/15	0.85	0.29	1.93	11,17,21,22	0
3	HEM	B	682	43/43	0.94	0.18	0.51	2,3,7,9	0
2	NAG	A	681	14/15	0.89	0.23	0.32	7,17,18,21	0
3	HEM	D	682	43/43	0.94	0.17	0.07	2,3,7,9	0
3	HEM	A	682	43/43	0.94	0.17	-0.06	2,3,8,10	0
2	NAG	A	671	14/15	0.93	0.16	-0.31	4,12,17,17	0
2	NAG	D	671	14/15	0.92	0.15	-0.33	5,11,17,17	0
2	NAG	C	671	14/15	0.92	0.15	-0.47	7,13,17,17	0
2	NAG	B	671	14/15	0.93	0.17	-0.50	5,12,17,17	0
4	S58	C	701	26/26	0.97	0.13	-0.71	2,8,15,17	0
4	S58	A	701	26/26	0.98	0.13	-0.78	2,9,15,17	0
4	S58	D	701	26/26	0.97	0.12	-0.90	2,8,13,17	0
3	HEM	C	682	43/43	0.96	0.14	-0.91	2,3,7,8	0
4	S58	B	701	26/26	0.98	0.12	-1.45	2,8,14,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.