



Full wwPDB X-ray Structure Validation Report

Nov 18, 2014 – 10:56 PM EST

PDB ID : 4PH9
Title : The structure of Ibuprofen bound to cyclooxygenase-2
Authors : Orlando, B.J.; Lucido, M.J.; Malkowski, M.G.
Deposited on : 2014-05-05
Resolution : 1.81 Å(reported)

This is a full wwPDB validation 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>

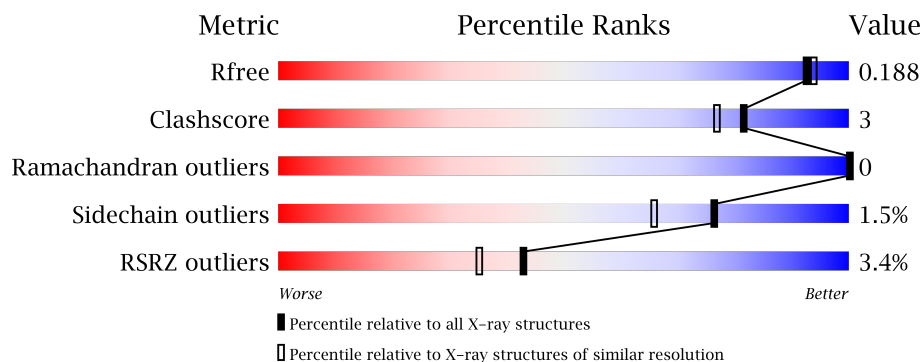
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24195
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24195

1 Overall quality at a glance

The reported resolution of this entry is 1.81 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	4101 (1.84-1.80)
Clashscore	79885	5140 (1.84-1.80)
Ramachandran outliers	78287	5077 (1.84-1.80)
Sidechain outliers	78261	5077 (1.84-1.80)
RSRZ outliers	66119	4103 (1.84-1.80)

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 ≥ 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	551	
1	B	551	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	BOG	A	604	-	X
4	BOG	B	603	-	X
5	NAG	A	605	-	X
5	NAG	A	608	-	X
5	NAG	B	609	-	X
7	AKR	A	609	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
7	AKR	B	611	-	X
8	EDO	A	611	-	X
8	EDO	A	613	-	X
8	EDO	A	615	-	X
8	EDO	B	612	-	X
8	EDO	B	614	-	X
8	EDO	B	615	-	X
8	EDO	B	617	-	X

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 10527 atoms, of which 0 are hydrogen 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.

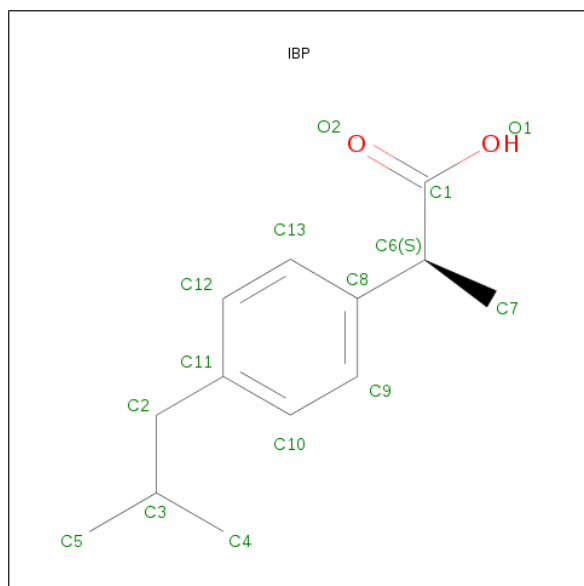
- Molecule 1 is a protein called Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	5	0
			4515	2909	759	821	26			
1	B	551	Total	C	N	O	S	0	3	0
			4500	2901	757	816	26			

There are 4 discrepancies between the modelled and reference sequences:

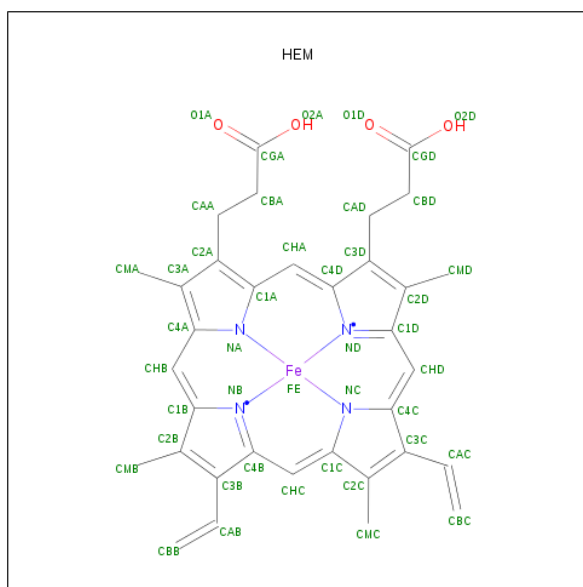
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	HIS	-	expression tag	UNP Q05769
A	34	HIS	-	expression tag	UNP Q05769
B	33	HIS	-	expression tag	UNP Q05769
B	34	HIS	-	expression tag	UNP Q05769

- Molecule 2 is IBUPROFEN (three-letter code: IBP) (formula: $C_{13}H_{18}O_2$).



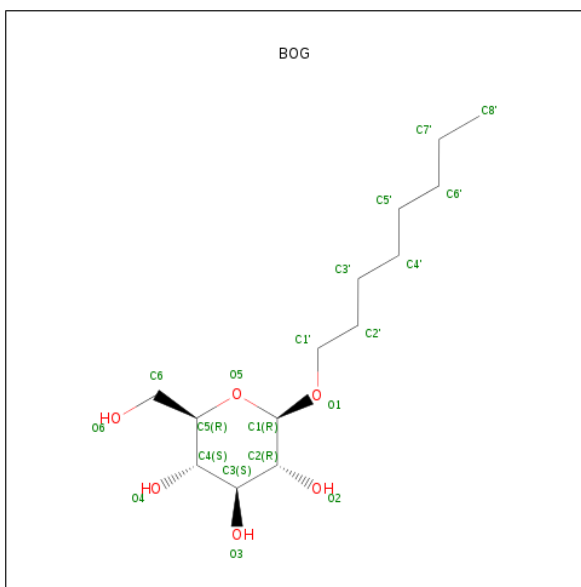
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 15	C 13	O 2	0	0
2	B	1	Total 15	C 13	O 2	0	0

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



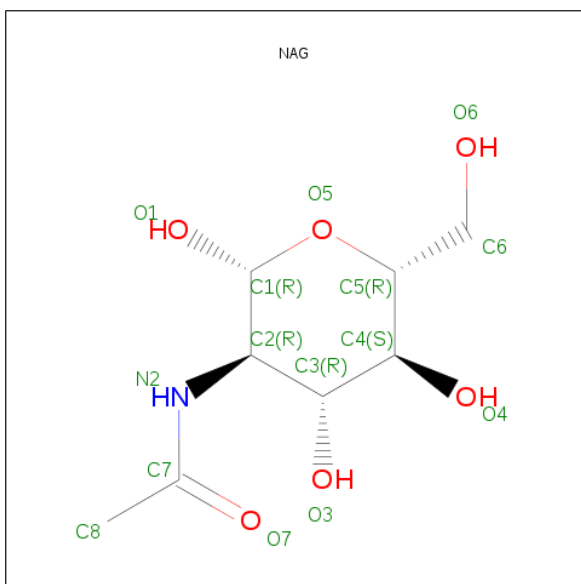
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

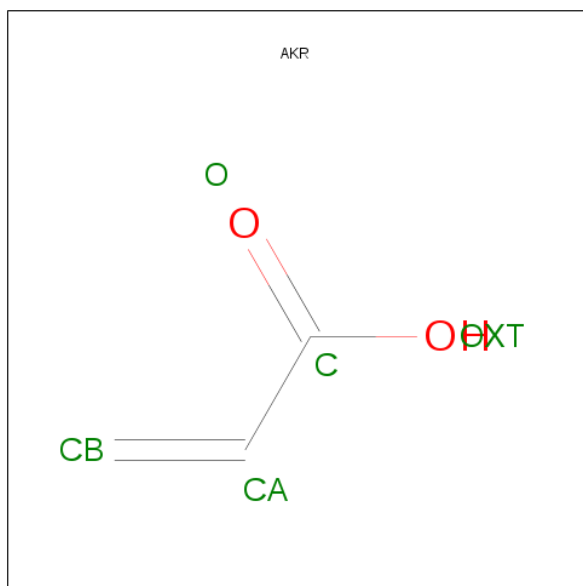


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

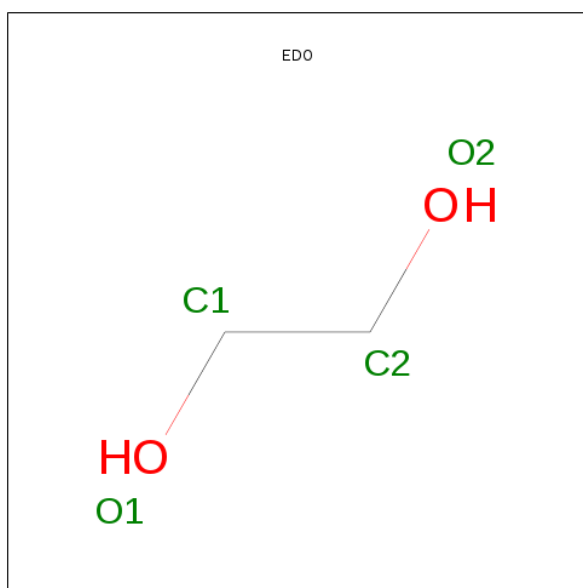
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is ACRYLIC ACID (three-letter code: AKR) (formula: $C_3H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			5	3	2		
7	A	1	Total	C	O	0	0
			5	3	2		
7	B	1	Total	C	O	0	0
			5	3	2		
7	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 is water.

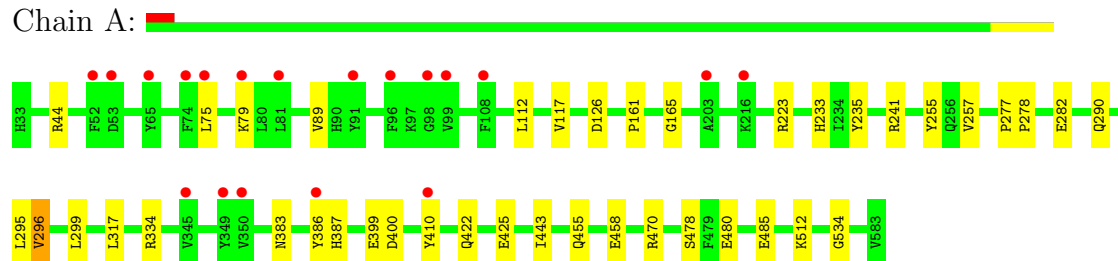
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	545	Total	O	0	0
			545	545		
10	B	582	Total	O	0	0
			582	582		

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.

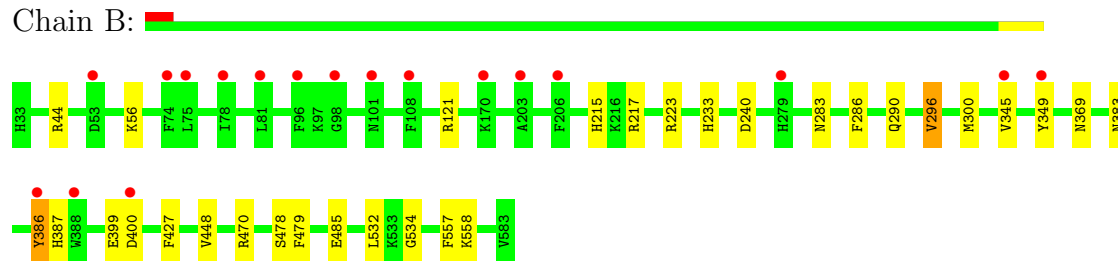
- Molecule 1: Prostaglandin G/H synthase 2

Chain A:



- Molecule 1: Prostaglandin G/H synthase 2

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.94Å 132.23Å 180.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.55 – 1.81 38.56 – 1.81	Depositor EDS
% Data completeness (in resolution range)	98.0 (35.55-1.81) 88.2 (38.56-1.81)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.160 , 0.197 0.153 , 0.188	Depositor DCC
R_{free} test set	5796 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 128525 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10527	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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: NAG, AKR, EDO, IBP, HEM, BOG, MAN

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	0.56	0/4644	0.62	0/6295
1	B	0.58	0/4629	0.64	0/6275
All	All	0.57	0/9273	0.63	0/12570

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4515	0	4402	32	0
1	B	4500	0	4393	24	0
2	A	15	0	17	0	0
2	B	15	0	17	0	0
3	A	43	0	30	2	0
3	B	43	0	30	3	0
4	A	40	0	56	3	0
4	B	20	0	28	0	0
5	A	28	0	26	0	0
5	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	28	0	25	0	0
6	B	28	0	25	0	0
7	A	10	0	6	6	0
7	B	10	0	6	7	0
8	A	24	0	36	3	0
8	B	28	0	42	3	0
9	B	39	0	34	1	0
10	A	545	0	0	8	1
10	B	582	0	0	4	1
All	All	10527	0	9186	60	1

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 3.

All (60) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:215:HIS:ND1	10:B:1238:HOH:O	2.11	0.84
1:A:126:ASP:OD2	10:A:1087:HOH:O	2.00	0.79
1:B:479:PHE:H	7:B:611:AKR:HA1	1.49	0.78
1:A:295:LEU:HG	1:A:296:VAL:HG12	1.69	0.75
1:A:241:ARG:HH11	7:A:610:AKR:HA1	1.56	0.70
1:B:223:ARG:NH2	10:B:1246:HOH:O	2.14	0.65
1:B:44[B]:ARG:HD3	1:B:470:ARG:HD2	1.78	0.64
1:A:455:GLN:NE2	10:A:1129:HOH:O	2.31	0.63
1:A:480:GLU:HB2	7:A:609:AKR:HB3	1.85	0.58
1:A:443:ILE:HD11	4:A:603:BOG:H6'2	1.86	0.56
1:A:223:ARG:NH1	10:A:994:HOH:O	2.39	0.56
1:A:117:VAL:HG22	4:A:604:BOG:H3'1	1.88	0.55
1:B:479:PHE:N	7:B:611:AKR:HA1	2.22	0.54
1:B:217:ARG:NH1	9:B:607:NAG:O7	2.40	0.54
1:A:399:GLU:HG2	1:A:422:GLN:OE1	2.08	0.53
1:A:44[B]:ARG:HD3	1:A:470:ARG:HD2	1.91	0.53
1:B:383:ASN:O	1:B:387:HIS:HD2	1.93	0.52
3:A:602:HEM:HHD	3:A:602:HEM:HBC2	1.91	0.51
1:A:480:GLU:H	7:A:609:AKR:CA	2.24	0.51
3:B:602:HEM:HBB2	3:B:602:HEM:HMB1	1.92	0.51
1:B:240:ASP:HB3	7:B:610:AKR:HB3	1.93	0.50
1:A:255:TYR:CZ	8:A:614:EDO:H21	2.46	0.50
1:A:480:GLU:H	7:A:609:AKR:HA1	1.76	0.50
1:B:478:SER:HB2	7:B:611:AKR:HA1	1.93	0.49
1:A:383:ASN:O	1:A:387:HIS:HD2	1.95	0.49
10:A:1163:HOH:O	8:B:615:EDO:H21	2.11	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:479:PHE:H	7:B:611:AKR:CA	2.20	0.49
1:A:295:LEU:CG	1:A:296:VAL:HG12	2.42	0.48
1:A:425:GLU:OE1	10:A:975:HOH:O	2.20	0.48
1:A:400:ASP:OD1	1:A:400:ASP:N	2.48	0.47
1:A:534:GLY:HA3	8:A:616:EDO:O2	2.15	0.47
1:A:480:GLU:HG3	7:A:609:AKR:HA1	1.97	0.47
1:A:512:LYS:NZ	10:A:872:HOH:O	2.47	0.47
1:B:448:VAL:HG13	3:B:602:HEM:HBA1	1.97	0.47
1:A:295:LEU:HA	1:A:410:TYR:CE1	2.50	0.46
1:A:161:PRO:HD2	1:A:165:GLY:O	2.15	0.46
1:A:235:TYR:CE2	1:A:334:ARG:HG3	2.51	0.46
1:A:89:VAL:HG11	4:A:604:BOG:H4'2	1.98	0.46
1:A:257:VAL:O	10:A:701:HOH:O	2.20	0.46
1:B:121:ARG:HG3	1:B:532:LEU:HD12	1.97	0.45
1:A:75:LEU:O	1:A:79:LYS:HG2	2.16	0.45
1:B:44[B]:ARG:HD2	10:B:1031:HOH:O	2.18	0.44
1:B:345:VAL:HA	1:B:349:TYR:HB3	2.00	0.44
1:A:296:VAL:HG13	1:A:299:LEU:HD12	2.00	0.43
1:A:296:VAL:HG22	1:A:299:LEU:H	1.82	0.43
1:B:534:GLY:HA3	8:B:616:EDO:O2	2.18	0.43
1:A:458[B]:GLU:OE1	10:A:1229:HOH:O	2.21	0.43
1:A:478:SER:HB2	7:A:609:AKR:CB	2.49	0.43
1:B:478:SER:HB2	7:B:611:AKR:CA	2.48	0.43
1:B:478:SER:CA	7:B:611:AKR:HA1	2.50	0.42
1:B:427:PHE:HA	1:B:427:PHE:HD1	1.71	0.42
1:B:369:ASN:HB3	10:B:1257:HOH:O	2.19	0.42
3:A:602:HEM:HMB2	3:A:602:HEM:HBB2	2.02	0.41
1:B:399:GLU:HB3	1:B:400:ASP:H	1.56	0.41
8:A:613:EDO:H11	1:B:56:LYS:HG2	2.02	0.41
1:B:386:TYR:HH	8:B:618:EDO:C2	2.33	0.41
1:A:317:LEU:HA	1:A:317:LEU:HD23	1.89	0.41
1:A:277:PRO:HA	1:A:278:PRO:HD3	1.94	0.40
1:B:286:PHE:HD2	1:B:300[A]:MET:HG2	1.87	0.40
1:B:296:VAL:HG21	3:B:602:HEM:CBB	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:A:749:HOH:O	10:B:737:HOH:O[7_555]	2.16	0.04

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	554/551 (100%)	541 (98%)	13 (2%)	0	100	100
1	B	552/551 (100%)	539 (98%)	13 (2%)	0	100	100
All	All	1106/1102 (100%)	1080 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	498/493 (101%)	491 (99%)	7 (1%)	78	69
1	B	496/493 (101%)	488 (98%)	8 (2%)	75	63
All	All	994/986 (101%)	979 (98%)	15 (2%)	76	66

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	233	HIS
1	A	282	GLU
1	A	290	GLN
1	A	296	VAL
1	A	386	TYR
1	A	485	GLU
1	B	233	HIS
1	B	283	ASN

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Mol	Chain	Res	Type
1	B	290	GLN
1	B	296	VAL
1	B	386	TYR
1	B	485	GLU
1	B	557	PHE
1	B	558	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

7 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	$\# Z > 2$
6	NAG	A	606	1,6	12,14,15	0.53	0	15,19,21	0.57	0
6	NAG	A	607	6	12,14,15	0.45	0	15,19,21	0.56	0
6	NAG	B	604	1,6	12,14,15	0.44	0	15,19,21	0.52	0
6	NAG	B	605	6	12,14,15	0.35	0	15,19,21	0.32	0
9	NAG	B	606	1,9	12,14,15	0.44	0	15,19,21	0.66	0
9	NAG	B	607	9	12,14,15	0.57	0	15,19,21	0.74	0
9	MAN	B	608	9	10,11,12	0.84	0	11,15,17	1.13	2 (18%)

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
6	NAG	A	606	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	607	6	-	0/6/23/26	0/1/1/1
6	NAG	B	604	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	605	6	-	0/6/23/26	0/1/1/1
9	NAG	B	606	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	607	9	-	0/6/23/26	0/1/1/1
9	MAN	B	608	9	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	608	MAN	O2-C2-C3	-2.56	104.68	110.10
9	B	608	MAN	C4-C3-C2	-2.30	108.04	110.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

27 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	IBP	A	601	-	15,15,15	0.68	0	20,20,20	1.02	2 (10%)
3	HEM	A	602	1,10	42,50,50	3.66	14 (33%)	27,82,82	1.54	4 (14%)
4	BOG	A	603	-	20,20,20	0.88	1 (5%)	25,25,25	1.16	1 (4%)
4	BOG	A	604	-	20,20,20	0.92	1 (5%)	25,25,25	1.07	2 (8%)
5	NAG	A	605	1	12,14,15	0.29	0	15,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	608	1	12,14,15	0.42	0	15,19,21	0.53	0
7	AKR	A	609	-	4,4,4	0.92	0	4,4,4	1.27	0
7	AKR	A	610	-	4,4,4	1.07	0	4,4,4	1.47	1 (25%)
8	EDO	A	611	-	3,3,3	0.82	0	2,2,2	0.54	0
8	EDO	A	612	-	3,3,3	0.47	0	2,2,2	0.52	0
8	EDO	A	613	-	3,3,3	0.57	0	2,2,2	0.44	0
8	EDO	A	614	-	3,3,3	0.59	0	2,2,2	0.43	0
8	EDO	A	615	-	3,3,3	0.66	0	2,2,2	0.67	0
8	EDO	A	616	-	3,3,3	0.59	0	2,2,2	0.37	0
2	IBP	B	601	-	15,15,15	0.57	0	20,20,20	0.95	1 (5%)
3	HEM	B	602	1,10	42,50,50	3.54	12 (28%)	27,82,82	1.54	3 (11%)
4	BOG	B	603	-	20,20,20	0.91	1 (5%)	25,25,25	1.02	0
5	NAG	B	609	1	12,14,15	0.40	0	15,19,21	0.76	1 (6%)
7	AKR	B	610	-	4,4,4	1.32	0	4,4,4	1.04	0
7	AKR	B	611	-	4,4,4	1.34	0	4,4,4	1.48	1 (25%)
8	EDO	B	612	-	3,3,3	0.70	0	2,2,2	0.66	0
8	EDO	B	613	-	3,3,3	0.61	0	2,2,2	0.42	0
8	EDO	B	614	-	3,3,3	0.69	0	2,2,2	0.58	0
8	EDO	B	615	-	3,3,3	0.63	0	2,2,2	0.49	0
8	EDO	B	616	-	3,3,3	0.61	0	2,2,2	0.40	0
8	EDO	B	617	-	3,3,3	0.55	0	2,2,2	0.29	0
8	EDO	B	618	-	3,3,3	0.39	0	2,2,2	0.96	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
2	IBP	A	601	-	-	0/12/12/12	0/1/1/1
3	HEM	A	602	1,10	-	0/14/114/114	0/0/8/8
4	BOG	A	603	-	-	0/11/31/31	0/1/1/1
4	BOG	A	604	-	-	0/11/31/31	0/1/1/1
5	NAG	A	605	1	-	0/6/23/26	0/1/1/1
5	NAG	A	608	1	-	0/6/23/26	0/1/1/1
7	AKR	A	609	-	-	0/2/2/2	0/0/0/0
7	AKR	A	610	-	-	0/2/2/2	0/0/0/0
8	EDO	A	611	-	-	0/1/1/1	0/0/0/0
8	EDO	A	612	-	-	0/1/1/1	0/0/0/0
8	EDO	A	613	-	-	0/1/1/1	0/0/0/0
8	EDO	A	614	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	A	615	-	-	0/1/1/1	0/0/0/0
8	EDO	A	616	-	-	0/1/1/1	0/0/0/0
2	IBP	B	601	-	-	0/12/12/12	0/1/1/1
3	HEM	B	602	1,10	-	0/14/114/114	0/0/8/8
4	BOG	B	603	-	-	0/11/31/31	0/1/1/1
5	NAG	B	609	1	-	0/6/23/26	0/1/1/1
7	AKR	B	610	-	-	0/2/2/2	0/0/0/0
7	AKR	B	611	-	-	0/2/2/2	0/0/0/0
8	EDO	B	612	-	-	0/1/1/1	0/0/0/0
8	EDO	B	613	-	-	0/1/1/1	0/0/0/0
8	EDO	B	614	-	-	0/1/1/1	0/0/0/0
8	EDO	B	615	-	-	0/1/1/1	0/0/0/0
8	EDO	B	616	-	-	0/1/1/1	0/0/0/0
8	EDO	B	617	-	-	0/1/1/1	0/0/0/0
8	EDO	B	618	-	-	0/1/1/1	0/0/0/0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	C3C-C2C	-14.98	1.33	1.45
3	B	602	HEM	C3C-C2C	-13.35	1.35	1.45
3	B	602	HEM	C3B-C2B	-10.68	1.35	1.45
3	A	602	HEM	C3B-C2B	-10.23	1.35	1.45
3	B	602	HEM	CMB-C2B	6.52	1.56	1.45
3	A	602	HEM	CMB-C2B	6.28	1.55	1.45
3	A	602	HEM	CMC-C2C	5.73	1.54	1.45
3	B	602	HEM	CMD-C2D	5.50	1.54	1.45
3	B	602	HEM	CMC-C2C	5.09	1.53	1.45
3	A	602	HEM	CMD-C2D	4.87	1.53	1.45
3	A	602	HEM	C3B-CAB	4.53	1.55	1.40
3	B	602	HEM	FE-NB	4.51	2.11	1.95
3	B	602	HEM	C3B-CAB	4.49	1.55	1.40
3	A	602	HEM	C3C-CAC	4.48	1.55	1.40
3	B	602	HEM	C3C-CAC	4.39	1.54	1.40
3	A	602	HEM	FE-ND	3.72	2.10	1.95
3	B	602	HEM	C3D-C2D	3.41	1.52	1.43
3	A	602	HEM	C3D-C2D	3.28	1.52	1.43
3	A	602	HEM	FE-NB	3.19	2.06	1.95
3	B	602	HEM	FE-ND	2.97	2.07	1.95
4	B	603	BOG	O5-C1	2.94	1.49	1.41
4	A	604	BOG	O5-C1	2.78	1.48	1.41
4	A	603	BOG	O5-C1	2.71	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	HEM	C1C-NC	2.57	1.40	1.33
3	A	602	HEM	C4C-NC	2.40	1.39	1.33
3	A	602	HEM	C1C-NC	2.36	1.39	1.33
3	A	602	HEM	C4A-NA	2.28	1.40	1.36
3	A	602	HEM	CHC-C4B	-2.18	1.37	1.39
3	B	602	HEM	C1D-ND	2.10	1.39	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	HEM	CBD-CAD-C3D	-5.59	102.37	114.51
3	A	602	HEM	CBD-CAD-C3D	-5.17	103.29	114.51
4	A	603	BOG	C1'-O1-C1	3.78	120.59	113.91
3	B	602	HEM	CBA-CAA-C2A	-2.69	108.15	112.63
2	B	601	IBP	C12-C13-C8	-2.69	118.43	121.20
3	A	602	HEM	CBA-CAA-C2A	-2.67	108.18	112.63
3	A	602	HEM	CAD-CBD-CGD	-2.36	109.07	113.53
2	A	601	IBP	O1-C1-O2	-2.30	118.89	124.05
7	A	610	AKR	OXT-C-CA	2.22	121.00	113.75
3	A	602	HEM	C3A-C4A-NA	-2.13	108.07	109.50
4	A	604	BOG	C1'-O1-C1	-2.13	110.15	113.91
5	B	609	NAG	O5-C5-C4	-2.13	107.95	110.65
4	A	604	BOG	O5-C1-C2	2.11	114.63	110.30
3	B	602	HEM	C4A-C3A-C2A	2.11	108.46	107.00
7	B	611	AKR	OXT-C-CA	2.05	120.44	113.75
2	A	601	IBP	C12-C13-C8	-2.00	119.13	121.20

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	551/551 (100%)	-0.12	19 (3%)	43	35	16, 28, 48, 67	0
1	B	551/551 (100%)	-0.17	18 (3%)	44	36	16, 26, 41, 70	0
All	All	1102/1102 (100%)	-0.14	37 (3%)	43	35	16, 27, 45, 70	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	PHE	4.8
1	A	75	LEU	4.2
1	B	75	LEU	4.2
1	A	108	PHE	4.0
1	B	74	PHE	3.5
1	A	99	VAL	3.4
1	A	81	LEU	3.3
1	A	98	GLY	3.1
1	A	96	PHE	3.0
1	B	108	PHE	2.9
1	A	79	LYS	2.8
1	A	65	TYR	2.7
1	B	81	LEU	2.7
1	A	349	TYR	2.6
1	B	206	PHE	2.5
1	A	410	TYR	2.5
1	A	91	TYR	2.5
1	A	52	PHE	2.5
1	B	78	ILE	2.5
1	B	349	TYR	2.5
1	B	279	HIS	2.5
1	B	53	ASP	2.4
1	B	101	ASN	2.4
1	B	386	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	350	VAL	2.4
1	A	53	ASP	2.4
1	B	98	GLY	2.4
1	B	203	ALA	2.3
1	A	203	ALA	2.3
1	A	216	LYS	2.3
1	B	388	TRP	2.2
1	A	345	VAL	2.2
1	B	170	LYS	2.2
1	B	400	ASP	2.2
1	B	345	VAL	2.1
1	A	386	TYR	2.1
1	B	96	PHE	2.1

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, 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
6	NAG	B	604	14/15	0.17	3.50	41,49,60,67	0
6	NAG	A	607	14/15	0.24	2.94	37,47,55,58	0
6	NAG	A	606	14/15	0.07	0.50	25,29,35,39	0
9	NAG	B	606	14/15	0.07	-0.07	24,31,34,40	0
9	NAG	B	607	14/15	0.13	-0.14	37,41,52,61	0
6	NAG	B	605	14/15	0.32	-	68,72,77,82	0
9	MAN	B	608	11/12	0.38	-	64,68,73,78	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, 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
8	EDO	B	614	4/4	0.25	14.48	30,35,36,41	0
8	EDO	A	615	4/4	0.20	12.21	30,32,35,41	0
8	EDO	B	612	4/4	0.20	11.92	24,27,30,35	0
8	EDO	B	615	4/4	0.30	11.03	34,37,39,54	0
8	EDO	A	613	4/4	0.39	9.09	38,38,41,43	0
8	EDO	B	617	4/4	0.22	8.00	37,41,44,44	0
5	NAG	A	605	14/15	0.27	7.75	48,54,61,64	0
8	EDO	A	611	4/4	0.19	5.70	28,31,31,37	0
7	AKR	B	611	5/5	0.23	4.53	30,31,42,44	0
7	AKR	A	609	5/5	0.34	4.48	28,41,46,47	0
4	BOG	B	603	20/20	0.15	2.75	41,44,47,49	0
4	BOG	A	604	20/20	0.14	2.48	42,48,52,53	0
5	NAG	A	608	14/15	0.26	2.41	44,51,58,59	0
5	NAG	B	609	14/15	0.23	2.31	34,39,46,46	0
7	AKR	B	610	5/5	0.21	1.95	36,38,39,45	0
7	AKR	A	610	5/5	0.17	1.22	32,35,43,43	0
2	IBP	A	601	15/15	0.17	0.63	24,28,31,33	0
8	EDO	A	614	4/4	0.09	0.59	26,27,31,32	0
2	IBP	B	601	15/15	0.17	0.49	22,24,29,29	0
4	BOG	A	603	20/20	0.09	0.28	27,32,38,40	0
8	EDO	A	612	4/4	0.10	0.15	25,28,30,32	0
3	HEM	A	602	43/43	0.12	0.10	20,24,34,54	0
3	HEM	B	602	43/43	0.12	-0.12	18,23,35,56	0
8	EDO	A	616	4/4	0.12	-0.58	26,28,29,32	0
8	EDO	B	616	4/4	0.12	-0.68	23,28,28,31	0
8	EDO	B	613	4/4	0.08	-0.79	22,26,28,29	0
8	EDO	B	618	4/4	0.15	-1.54	27,29,31,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.