



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:28 PM GMT

PDB ID : 3HS7
Title : X-ray crystal structure of docosahexaenoic acid bound to the cyclooxygenase channel of cyclooxygenase-2
Authors : Vecchio, A.J.; Simmons, D.M.; Malkowski, M.G.
Deposited on : 2009-06-10
Resolution : 2.65 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>

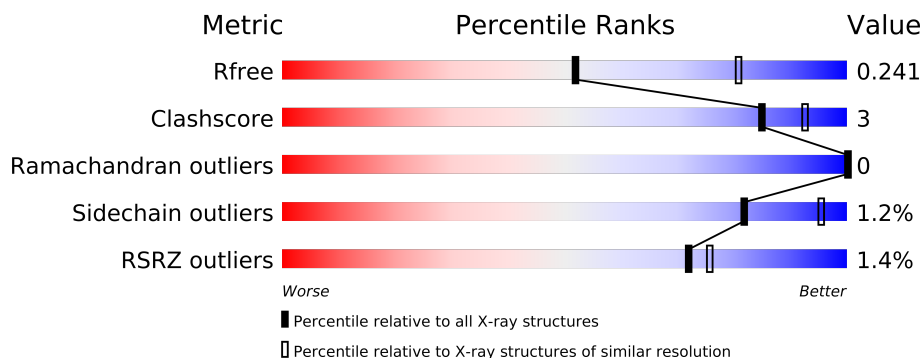
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 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 2.65 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	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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	591	
1	B	591	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9565 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.

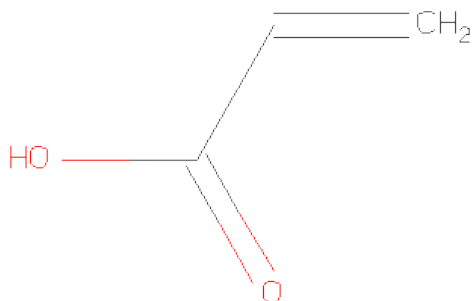
- Molecule 1 is a protein called Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	2	0
			4441	2873	738	805	25			
1	B	552	Total	C	N	O	S	0	2	0
			4422	2856	739	802	25			

There are 14 discrepancies between the modelled and reference sequences:

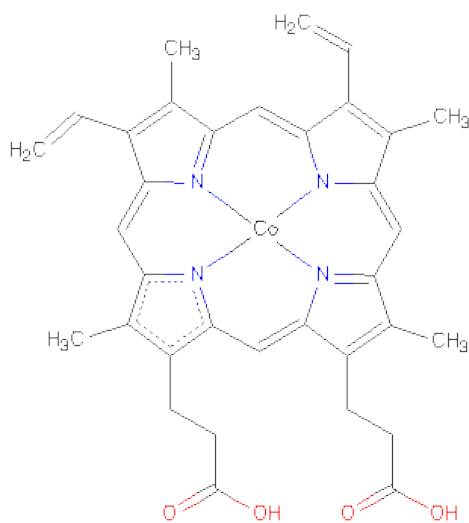
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	HIS	-	EXPRESSION TAG	UNP Q05769
A	30	HIS	-	EXPRESSION TAG	UNP Q05769
A	31	HIS	-	EXPRESSION TAG	UNP Q05769
A	32	HIS	-	EXPRESSION TAG	UNP Q05769
A	33	HIS	-	EXPRESSION TAG	UNP Q05769
A	34	HIS	-	EXPRESSION TAG	UNP Q05769
A	594	ALA	ASN	ENGINEERED	UNP Q05769
B	29	HIS	-	EXPRESSION TAG	UNP Q05769
B	30	HIS	-	EXPRESSION TAG	UNP Q05769
B	31	HIS	-	EXPRESSION TAG	UNP Q05769
B	32	HIS	-	EXPRESSION TAG	UNP Q05769
B	33	HIS	-	EXPRESSION TAG	UNP Q05769
B	34	HIS	-	EXPRESSION TAG	UNP Q05769
B	594	ALA	ASN	ENGINEERED	UNP Q05769

- Molecule 2 is ACRYLIC ACID (three-letter code: AKR) (formula: C₃H₄O₂).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING CO (three-letter code: COH) (formula: $C_{34}H_{32}CoN_4O_4$).



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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	HIS	-	EXPRESSION TAG	UNP Q05769
A	30	HIS	-	EXPRESSION TAG	UNP Q05769
A	31	HIS	-	EXPRESSION TAG	UNP Q05769
A	32	HIS	-	EXPRESSION TAG	UNP Q05769
A	33	HIS	-	EXPRESSION TAG	UNP Q05769
A	34	HIS	-	EXPRESSION TAG	UNP Q05769
A	594	ALA	ASN	ENGINEERED	UNP Q05769
B	29	HIS	-	EXPRESSION TAG	UNP Q05769
B	30	HIS	-	EXPRESSION TAG	UNP Q05769
B	31	HIS	-	EXPRESSION TAG	UNP Q05769
B	32	HIS	-	EXPRESSION TAG	UNP Q05769
B	33	HIS	-	EXPRESSION TAG	UNP Q05769
B	34	HIS	-	EXPRESSION TAG	UNP Q05769
B	594	ALA	ASN	ENGINEERED	UNP Q05769
B	29	HIS	-	EXPRESSION TAG	UNP Q05769
B	30	HIS	-	EXPRESSION TAG	UNP Q05769
B	31	HIS	-	EXPRESSION TAG	UNP Q05769
B	32	HIS	-	EXPRESSION TAG	UNP Q05769
B	33	HIS	-	EXPRESSION TAG	UNP Q05769
B	34	HIS	-	EXPRESSION TAG	UNP Q05769
B	594	ALA	ASN	ENGINEERED	UNP Q05769

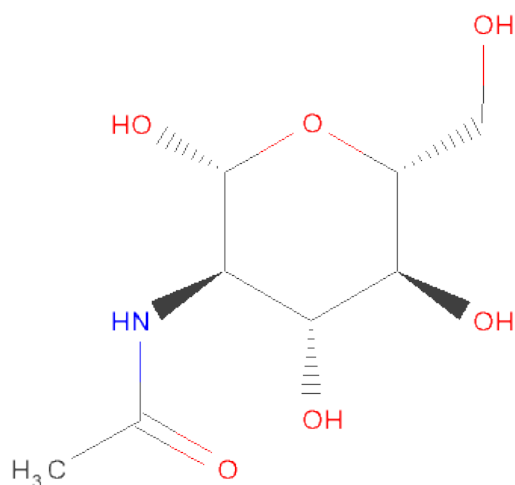
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

There are 7 discrepancies between the modelled and reference sequences:

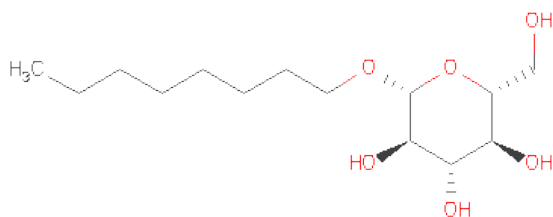
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	HIS	-	EXPRESSION TAG	UNP Q05769
A	30	HIS	-	EXPRESSION TAG	UNP Q05769
A	31	HIS	-	EXPRESSION TAG	UNP Q05769
A	32	HIS	-	EXPRESSION TAG	UNP Q05769
A	33	HIS	-	EXPRESSION TAG	UNP Q05769
A	34	HIS	-	EXPRESSION TAG	UNP Q05769
A	594	ALA	ASN	ENGINEERED	UNP Q05769

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



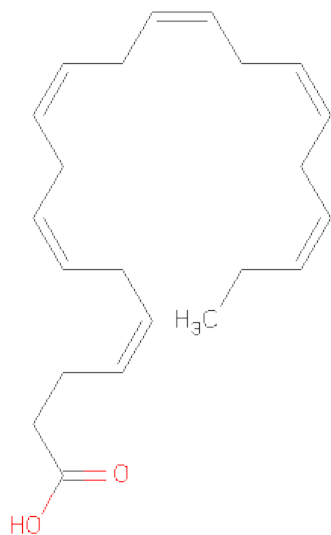
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 8 is DOCOSA-4,7,10,13,16,19-HEXAENOICACID (three-letter code: HXA) (formula: $C_{22}H_{32}O_2$).



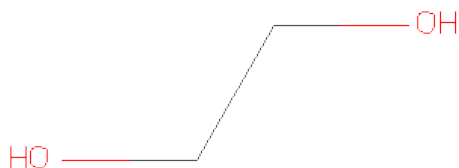
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			24	22	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			24	22	2		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 10 is water.

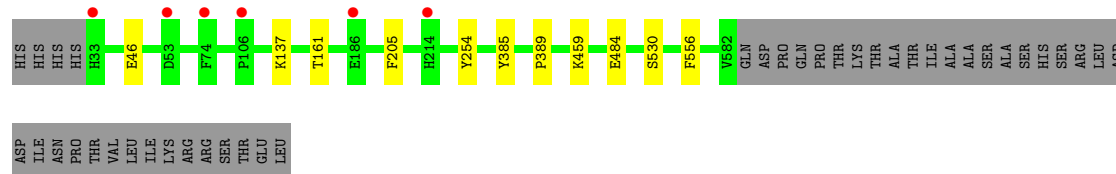
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	173	Total 173	O 173	0	0
10	B	157	Total 157	O 157	0	0

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.

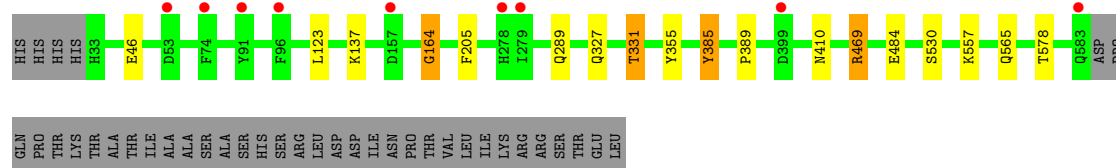
- Molecule 1: Prostaglandin G/H synthase 2

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	119.29Å 131.71Å 179.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 20.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.65) 100.0 (20.00-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.67Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.181 , 0.234 0.194 , 0.241	Depositor DCC
R_{free} test set	2074 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 10.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 41204 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9565	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: HXA, NAG, AKR, EDO, COH, 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	0.40	0/4577	0.49	0/6218
1	B	0.41	1/4558 (0.0%)	0.51	0/6194
All	All	0.40	1/9135 (0.0%)	0.50	0/12412

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	B	0	1
4	B	1	0
All	All	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	GLY	C-N	-5.03	1.22	1.34

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	661	NAG	C5

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	164	GLY	Mainchain

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	4441	0	0	6	0
1	B	4422	0	0	10	0
2	A	5	0	3	0	0
2	B	10	0	6	0	0
3	A	43	0	30	0	0
3	B	43	0	30	0	0
4	A	28	0	25	3	0
4	B	56	0	50	0	0
5	A	39	0	34	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
7	A	20	0	28	0	62
7	B	20	0	28	0	62
8	A	24	0	31	5	0
8	B	24	0	31	10	0
9	A	20	0	30	1	0
9	B	12	0	18	0	0
10	A	173	0	0	1	0
10	B	157	0	0	0	0
All	All	9565	0	370	27	62

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:B:1:HXA:C13	8:B:1:HXA:H8	1.76	1.15
8:B:1:HXA:C12	8:B:1:HXA:H8	2.03	0.86
4:A:662:NAG:C3	4:A:662:NAG:O7	2.30	0.80
1:A:205:PHE:CE2	8:A:1:HXA:H17	2.26	0.70
1:B:123:LEU:O	1:B:469:ARG:NH2	2.25	0.68
1:B:205:PHE:CE2	8:B:1:HXA:H17	2.28	0.68
1:A:530:SER:OG	8:A:1:HXA:H152	1.93	0.68
4:A:662:NAG:H3	4:A:662:NAG:O7	1.93	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:A:1:HXA:H32	8:A:1:HXA:C7	2.36	0.55
1:B:327:GLN:O	1:B:331:THR:CG2	2.55	0.54
1:B:530[B]:SER:OG	8:B:1:HXA:H152	2.07	0.53
8:B:1:HXA:H122	8:B:1:HXA:H8	1.90	0.52
4:A:662:NAG:O3	4:A:662:NAG:O7	2.29	0.50
1:B:355:TYR:CE2	8:B:1:HXA:H22	2.48	0.48
8:A:1:HXA:H7	8:A:1:HXA:H32	1.96	0.48
1:B:565:GLN:OE1	1:B:578:THR:N	2.47	0.48
1:B:46:GLU:OE1	1:B:137:LYS:NZ	2.47	0.47
8:B:1:HXA:C13	8:B:1:HXA:C8	2.70	0.47
8:B:1:HXA:C12	8:B:1:HXA:C8	2.80	0.46
1:A:46:GLU:OE1	1:A:137:LYS:NZ	2.51	0.44
1:B:385:TYR:CE2	8:B:1:HXA:H151	2.53	0.43
1:B:205:PHE:CE2	8:B:1:HXA:C17	3.01	0.43
8:A:1:HXA:C8	8:A:1:HXA:H122	2.50	0.42
1:A:459:LYS:NZ	10:A:754:HOH:O	2.53	0.41
1:A:254:TYR:CE2	9:A:3:EDO:H21	2.56	0.40

All (62) 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)
7:A:703:BOG:C6'	7:B:703:BOG:C7'[6_554]	0.07	2.13
7:A:703:BOG:C5	7:B:703:BOG:C5[6_554]	0.09	2.11
7:A:703:BOG:O5	7:B:703:BOG:O5[6_554]	0.09	2.11
7:A:703:BOG:C6	7:B:703:BOG:C6[6_554]	0.10	2.10
7:A:703:BOG:O6	7:B:703:BOG:O6[6_554]	0.12	2.08
7:A:703:BOG:C1	7:B:703:BOG:C1[6_554]	0.14	2.06
7:A:703:BOG:C4	7:B:703:BOG:C4[6_554]	0.14	2.06
7:A:703:BOG:C3	7:B:703:BOG:C3[6_554]	0.16	2.04
7:A:703:BOG:O4	7:B:703:BOG:O4[6_554]	0.16	2.04
7:A:703:BOG:O1	7:B:703:BOG:O1[6_554]	0.17	2.03
7:A:703:BOG:C2	7:B:703:BOG:C2[6_554]	0.20	2.00
7:A:703:BOG:C1'	7:B:703:BOG:C1'[6_554]	0.20	2.00
7:A:703:BOG:O3	7:B:703:BOG:O3[6_554]	0.24	1.96
7:A:703:BOG:O2	7:B:703:BOG:O2[6_554]	0.33	1.87
7:A:703:BOG:C2'	7:B:703:BOG:C2'[6_554]	0.39	1.81
7:A:703:BOG:C3'	7:B:703:BOG:C3'[6_554]	0.59	1.61
7:A:703:BOG:C4'	7:B:703:BOG:C4'[6_554]	0.59	1.61
7:A:703:BOG:C5'	7:B:703:BOG:C6'[6_554]	0.83	1.37
7:A:703:BOG:C3'	7:B:703:BOG:C4'[6_554]	0.95	1.25
7:A:703:BOG:C7'	7:B:703:BOG:C8'[6_554]	1.03	1.17

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:A:703:BOG:C2'	7:B:703:BOG:C3'[6_554]	1.19	1.01
7:A:703:BOG:C5'	7:B:703:BOG:C5'[6_554]	1.23	0.97
7:A:703:BOG:O1	7:B:703:BOG:C1'[6_554]	1.31	0.89
7:A:703:BOG:C1	7:B:703:BOG:O1[6_554]	1.32	0.88
7:A:703:BOG:C2	7:B:703:BOG:O2[6_554]	1.32	0.88
7:A:703:BOG:O4	7:B:703:BOG:C4[6_554]	1.32	0.88
7:A:703:BOG:C5	7:B:703:BOG:O5[6_554]	1.36	0.84
7:A:703:BOG:C6	7:B:703:BOG:O6[6_554]	1.37	0.83
7:A:703:BOG:C3	7:B:703:BOG:C2[6_554]	1.39	0.81
7:A:703:BOG:O3	7:B:703:BOG:C3[6_554]	1.39	0.81
7:A:703:BOG:C2	7:B:703:BOG:C1[6_554]	1.41	0.79
7:A:703:BOG:C4	7:B:703:BOG:C3[6_554]	1.41	0.79
7:A:703:BOG:C1'	7:B:703:BOG:C2'[6_554]	1.41	0.79
7:A:703:BOG:C1	7:B:703:BOG:O5[6_554]	1.42	0.78
7:A:703:BOG:O5	7:B:703:BOG:C1[6_554]	1.44	0.76
7:A:703:BOG:C6'	7:B:703:BOG:C6'[6_554]	1.46	0.74
7:A:703:BOG:C6	7:B:703:BOG:C5[6_554]	1.49	0.71
7:A:703:BOG:C3	7:B:703:BOG:O3[6_554]	1.50	0.70
7:A:703:BOG:O5	7:B:703:BOG:C5[6_554]	1.50	0.70
7:A:703:BOG:O6	7:B:703:BOG:C6[6_554]	1.50	0.70
7:A:703:BOG:C6'	7:B:703:BOG:C8'[6_554]	1.50	0.70
7:A:703:BOG:C5	7:B:703:BOG:C4[6_554]	1.51	0.69
7:A:703:BOG:O1	7:B:703:BOG:C1[6_554]	1.54	0.66
7:A:703:BOG:C4	7:B:703:BOG:O4[6_554]	1.54	0.66
7:A:703:BOG:C4	7:B:703:BOG:C5[6_554]	1.55	0.65
7:A:703:BOG:C1'	7:B:703:BOG:O1[6_554]	1.55	0.65
7:A:703:BOG:C5	7:B:703:BOG:C6[6_554]	1.56	0.64
7:A:703:BOG:C5'	7:B:703:BOG:C7'[6_554]	1.56	0.64
7:A:703:BOG:C7'	7:B:703:BOG:C7'[6_554]	1.56	0.64
7:A:703:BOG:O2	7:B:703:BOG:C2[6_554]	1.57	0.63
7:A:703:BOG:C1	7:B:703:BOG:C2[6_554]	1.63	0.57
7:A:703:BOG:C4'	7:B:703:BOG:C5'[6_554]	1.63	0.57
7:A:703:BOG:C3	7:B:703:BOG:C4[6_554]	1.64	0.56
7:A:703:BOG:C2	7:B:703:BOG:C3[6_554]	1.66	0.54
7:A:703:BOG:C2'	7:B:703:BOG:C1'[6_554]	1.67	0.53
7:A:703:BOG:C5'	7:B:703:BOG:C4'[6_554]	1.74	0.46
7:A:703:BOG:C8'	7:B:703:BOG:C8'[6_554]	1.78	0.42
7:A:703:BOG:C3'	7:B:703:BOG:C2'[6_554]	1.90	0.30
7:A:703:BOG:C7'	7:B:703:BOG:C6'[6_554]	1.90	0.30
7:A:703:BOG:C3'	7:B:703:BOG:C5'[6_554]	2.00	0.20
7:A:703:BOG:C4'	7:B:703:BOG:C3'[6_554]	2.08	0.12
7:A:703:BOG:C2'	7:B:703:BOG:C4'[6_554]	2.12	0.08

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	551/591 (93%)	538 (98%)	13 (2%)	0	100	100
1	B	552/591 (93%)	540 (98%)	12 (2%)	0	100	100
All	All	1103/1182 (93%)	1078 (98%)	25 (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	478/529 (90%)	474 (99%)	4 (1%)	89	97
1	B	470/529 (89%)	463 (98%)	7 (2%)	76	94
All	All	948/1058 (90%)	937 (99%)	11 (1%)	82	95

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	THR
1	A	385	TYR
1	A	484	GLU
1	A	556	PHE
1	B	289	GLN
1	B	331	THR
1	B	385	TYR
1	B	410	ASN
1	B	469	ARG
1	B	484	GLU
1	B	557	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 ⓘ

9 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	$\# Z > 2$
4	NAG	A	661	1,4	12,14,15	0.60	0	15,19,21	1.19	1 (6%)
4	NAG	A	662	4	12,14,15	0.90	1 (8%)	15,19,21	1.47	2 (13%)
5	NAG	A	671	1,5	12,14,15	0.70	0	15,19,21	0.68	0
5	NAG	A	672	5	12,14,15	0.60	0	15,19,21	1.04	0
5	MAN	A	673	5	10,11,12	0.66	0	11,15,17	0.86	0
4	NAG	B	661	1,4	12,14,15	0.61	0	15,19,21	1.05	1 (6%)
4	NAG	B	662	4	12,14,15	0.67	0	15,19,21	1.16	1 (6%)
4	NAG	B	671	1,4	12,14,15	0.61	0	15,19,21	0.67	0
4	NAG	B	672	4	12,14,15	0.62	0	15,19,21	1.26	2 (13%)

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
4	NAG	A	661	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	662	4	-	1/6/23/26	0/1/1/1
5	NAG	A	671	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	672	5	-	0/6/23/26	0/1/1/1
5	MAN	A	673	5	-	0/2/19/22	0/1/1/1
4	NAG	B	661	1,4	1/1/5/7	0/6/23/26	1/1/1/1
4	NAG	B	662	4	-	0/6/23/26	0/1/1/1
4	NAG	B	671	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	672	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	662	NAG	O5-C5	-2.00	1.41	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	662	NAG	O5-C5-C6	3.65	110.81	106.98
4	A	661	NAG	O5-C5-C6	3.52	110.68	106.98
4	B	672	NAG	O5-C5-C6	2.98	110.10	106.98
4	A	662	NAG	C3-C4-C5	2.54	114.75	110.20
4	B	662	NAG	C3-C4-C5	2.33	114.36	110.20
4	B	661	NAG	O5-C5-C6	2.28	109.38	106.98
4	B	672	NAG	C3-C2-N2	-2.18	108.44	111.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	661	NAG	C5

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	662	NAG	C3-C2-N2-C7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	661	NAG	C1-C2-C3-C4-C5-O5

5.6 Ligand geometry ⓘ

19 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$
8	HXA	A	1	-	23,23,23	1.74	7 (30%)	23,23,23	0.61	0
2	AKR	A	2	-	4,4,4	1.77	2 (50%)	4,4,4	1.22	0
9	EDO	A	3	-	3,3,3	0.62	0	2,2,2	0.25	0
9	EDO	A	5	-	3,3,3	0.61	0	2,2,2	0.34	0
3	COH	A	619	-	50,50,50	2.35	15 (30%)	60,82,82	1.17	3 (5%)
9	EDO	A	620	-	3,3,3	0.55	0	2,2,2	0.35	0
9	EDO	A	621	-	3,3,3	0.59	0	2,2,2	0.32	0
6	NAG	A	681	1	12,14,15	0.63	0	15,19,21	1.26	2 (13%)
7	BOG	A	703	-	20,20,20	0.44	0	25,25,25	0.55	0
9	EDO	A	8	-	3,3,3	0.55	0	2,2,2	0.36	0
8	HXA	B	1	-	23,23,23	1.74	5 (21%)	23,23,23	0.65	0
2	AKR	B	2	-	4,4,4	1.76	1 (25%)	4,4,4	0.90	0
2	AKR	B	3	-	4,4,4	1.79	2 (50%)	4,4,4	0.92	0
9	EDO	B	4	-	3,3,3	0.53	0	2,2,2	0.39	0
9	EDO	B	6	-	3,3,3	0.61	0	2,2,2	0.26	0
3	COH	B	619	1	50,50,50	2.37	16 (32%)	60,82,82	1.13	4 (6%)
6	NAG	B	681	-	12,14,15	0.64	0	15,19,21	0.75	0
9	EDO	B	7	-	3,3,3	0.57	0	2,2,2	0.37	0
7	BOG	B	703	-	20,20,20	0.40	0	25,25,25	0.64	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
8	HXA	A	1	-	-	0/21/21/21	0/0/0/0
2	AKR	A	2	-	-	0/2/2/2	0/0/0/0
9	EDO	A	3	-	-	0/1/1/1	0/0/0/0
9	EDO	A	5	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COH	A	619	-	-	0/10/54/54	0/0/8/8
9	EDO	A	620	-	-	0/1/1/1	0/0/0/0
9	EDO	A	621	-	-	0/1/1/1	0/0/0/0
6	NAG	A	681	1	-	0/6/23/26	0/1/1/1
7	BOG	A	703	-	-	0/11/31/31	0/1/1/1
9	EDO	A	8	-	-	0/1/1/1	0/0/0/0
8	HXA	B	1	-	-	0/21/21/21	0/0/0/0
2	AKR	B	2	-	-	0/2/2/2	0/0/0/0
2	AKR	B	3	-	-	0/2/2/2	0/0/0/0
9	EDO	B	4	-	-	0/1/1/1	0/0/0/0
9	EDO	B	6	-	-	0/1/1/1	0/0/0/0
3	COH	B	619	1	-	0/10/54/54	0/0/8/8
6	NAG	B	681	-	-	0/6/23/26	0/1/1/1
9	EDO	B	7	-	-	0/1/1/1	0/0/0/0
7	BOG	B	703	-	-	0/11/31/31	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	619	COH	C3B-CAB	6.48	1.55	1.49
3	A	619	COH	C3C-CAC	6.43	1.55	1.49
3	B	619	COH	C3C-CAC	6.36	1.55	1.49
3	A	619	COH	C3B-CAB	6.29	1.55	1.49
3	B	619	COH	C3D-C2D	5.59	1.54	1.37
3	A	619	COH	C3D-C2D	5.48	1.53	1.37
3	B	619	COH	C1B-C2B	4.44	1.45	1.40
3	A	619	COH	C1B-C2B	4.30	1.45	1.40
3	A	619	COH	C3B-C2B	-4.04	1.34	1.41
3	B	619	COH	C3C-C2C	-3.94	1.34	1.41
3	A	619	COH	C3C-C2C	-3.90	1.34	1.41
3	B	619	COH	C4D-ND	3.89	1.39	1.36
3	B	619	COH	C3B-C2B	-3.79	1.34	1.41
3	B	619	COH	C3B-C4B	3.76	1.46	1.40
3	A	619	COH	C4D-ND	3.61	1.39	1.36
3	A	619	COH	C3B-C4B	3.60	1.45	1.40
3	A	619	COH	C3C-C4C	3.28	1.45	1.40
3	A	619	COH	C1B-NB	3.27	1.39	1.36
3	B	619	COH	C3C-C4C	3.26	1.45	1.40
3	B	619	COH	C1B-NB	3.08	1.39	1.36
3	B	619	COH	C4B-NB	3.00	1.38	1.36
3	A	619	COH	C4B-NB	2.95	1.38	1.36
3	A	619	COH	C4C-NC	2.80	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	619	COH	C4C-NC	2.70	1.38	1.36
3	A	619	COH	CO-ND	2.59	2.11	1.95
8	B	1	HXA	C21-C20	-2.58	1.39	1.51
8	A	1	HXA	C21-C20	-2.54	1.39	1.51
3	A	619	COH	CO-NA	2.45	2.11	1.95
8	B	1	HXA	C3-C4	-2.45	1.39	1.50
3	B	619	COH	CO-ND	2.45	2.11	1.95
8	A	1	HXA	C3-C4	-2.41	1.39	1.50
3	A	619	COH	CO-NB	2.33	2.10	1.95
2	A	2	AKR	CA-C	-2.27	1.40	1.48
2	B	2	AKR	CA-C	-2.26	1.40	1.48
2	B	3	AKR	CA-C	-2.24	1.40	1.48
3	B	619	COH	CO-NA	2.21	2.09	1.95
3	B	619	COH	CO-NB	2.16	2.09	1.95
8	B	1	HXA	C6-C7	-2.15	1.39	1.51
8	A	1	HXA	C15-C16	-2.09	1.39	1.51
8	B	1	HXA	C15-C16	-2.05	1.39	1.51
3	B	619	COH	C1D-ND	2.05	1.39	1.36
8	B	1	HXA	C15-C14	-2.04	1.39	1.51
2	B	3	AKR	CB-CA	2.04	1.40	1.29
8	A	1	HXA	C15-C14	-2.03	1.39	1.51
8	A	1	HXA	C18-C19	-2.02	1.39	1.51
8	A	1	HXA	C18-C17	-2.01	1.39	1.51
2	A	2	AKR	CB-CA	2.01	1.39	1.29
8	A	1	HXA	C9-C8	-2.00	1.39	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	681	NAG	O5-C5-C4	-2.94	106.92	110.65
3	A	619	COH	C3B-CAB-CBB	-2.89	119.96	125.95
3	A	619	COH	C3C-CAC-CBC	-2.75	120.25	125.95
3	A	619	COH	C1D-C2D-C3D	-2.70	105.18	106.89
3	B	619	COH	C3C-CAC-CBC	-2.63	120.51	125.95
3	B	619	COH	C3B-CAB-CBB	-2.59	120.58	125.95
3	B	619	COH	C1D-C2D-C3D	-2.53	105.28	106.89
6	A	681	NAG	O5-C5-C6	2.45	109.55	106.98
3	B	619	COH	C4A-C3A-C2A	2.04	108.19	106.89

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	551/591 (93%)	-0.31	6 (1%) 77 81	20, 35, 57, 83	0
1	B	552/591 (93%)	-0.26	9 (1%) 68 72	18, 37, 66, 95	0
All	All	1103/1182 (93%)	-0.29	15 (1%) 72 76	18, 36, 62, 95	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	ASP	3.6
1	B	91	TYR	3.3
1	B	279	ILE	2.8
1	B	278	HIS	2.6
1	B	53	ASP	2.5
1	B	74	PHE	2.3
1	B	96	PHE	2.3
1	B	157	ASP	2.2
1	B	583	GLN	2.2
1	A	106	PRO	2.2
1	A	74	PHE	2.1
1	A	53	ASP	2.1
1	A	214	HIS	2.1
1	A	186	GLU	2.1
1	A	33	HIS	2.0

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
5	MAN	A	673	11/12	0.36	-	57,60,61,61	0
4	NAG	A	662	14/15	0.42	-	57,60,61,62	0
4	NAG	B	671	14/15	0.12	-	25,29,31,36	0
5	NAG	A	671	14/15	0.11	-	27,31,34,39	0
5	NAG	A	672	14/15	0.18	-	44,48,50,54	0
4	NAG	A	661	14/15	0.31	-	40,47,49,54	0
4	NAG	B	661	14/15	0.32	-	48,55,57,61	0
4	NAG	B	662	14/15	0.39	-	64,66,67,67	0
4	NAG	B	672	14/15	0.27	-	40,43,44,44	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	HXA	B	1	24/24	0.28	-	57,64,69,70	0
7	BOG	A	703	20/20	0.19	-	64,66,66,66	20
6	NAG	B	681	14/15	0.26	-	92,93,93,93	0
2	AKR	B	3	5/5	0.24	-	62,62,62,62	0
2	AKR	B	2	5/5	0.40	-	76,76,76,76	0
3	COH	B	619	43/43	0.33	-	88,90,92,93	0
3	COH	A	619	43/43	0.26	-	99,101,102,102	0
9	EDO	A	621	4/4	0.23	-	61,61,61,61	0
2	AKR	A	2	5/5	0.32	-	74,74,74,74	0
7	BOG	B	703	20/20	0.20	-	37,40,41,41	20
8	HXA	A	1	24/24	0.29	-	62,63,66,66	0
6	NAG	A	681	14/15	0.33	-	40,44,46,46	0
9	EDO	A	5	4/4	0.21	-	72,72,72,72	0
9	EDO	B	6	4/4	0.24	-	54,54,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	EDO	B	7	4/4	0.25	-	70,71,71,71	0
9	EDO	A	620	4/4	0.34	-	52,53,54,54	0
9	EDO	B	4	4/4	0.32	-	57,57,57,57	0
9	EDO	A	8	4/4	0.19	-	50,50,50,50	0
9	EDO	A	3	4/4	0.28	-	39,40,40,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.