



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:01 PM GMT

PDB ID : 4E1G
Title : X-ray crystal structure of alpha-linolenic acid bound to the cyclooxygenase channel of cyclooxygenase-2
Authors : Vecchio, A.J.; Malkowski, M.G.
Deposited on : 2012-03-06
Resolution : 2.10 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

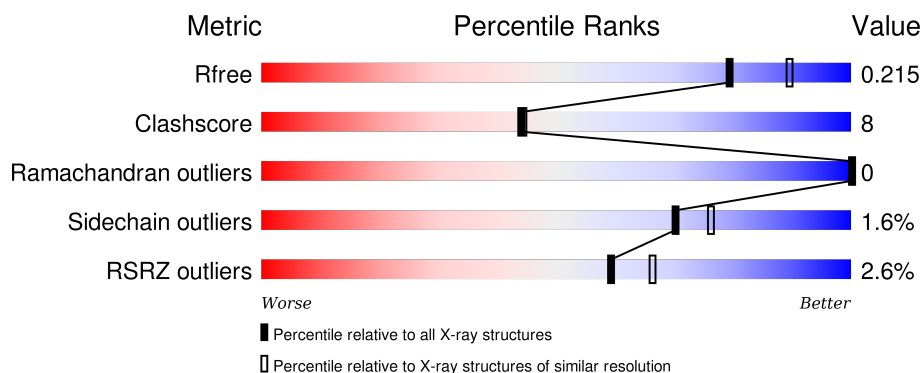
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	610	<div> <div></div> <div>80% 10% • 10%</div> </div>
1	B	610	<div> <div>4%</div> <div>80% 9% • 10%</div> </div>

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LNL	A	701	-	-	X	X
2	LNL	B	701	-	-	X	X
3	COH	A	702	-	-	-	X
3	COH	B	702	-	-	-	X
4	NAG	A	703	-	-	-	X
4	NAG	B	703	-	-	-	X
4	NAG	B	706	-	-	X	-
5	NAG	A	706	-	-	X	-
6	NAG	A	708	-	-	-	X
6	NAG	B	707	-	-	-	X
8	EDO	B	709	-	-	X	-
9	AKR	A	712	-	-	X	-
9	AKR	A	713	-	-	X	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9967 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

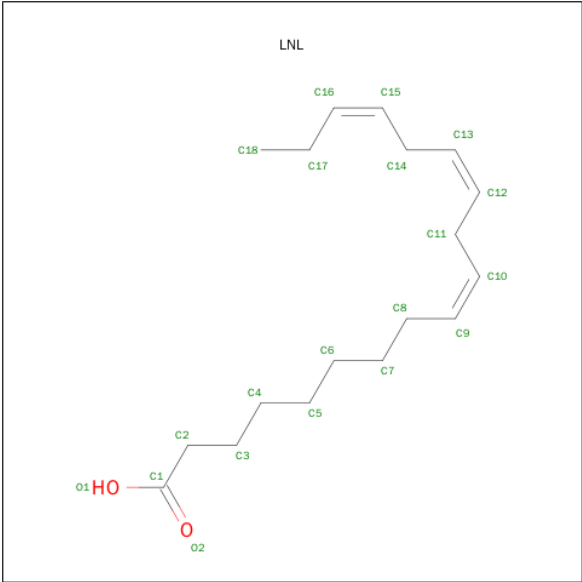
- Molecule 1 is a protein called Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	5	0
			4436	2871	737	802	26			
1	B	551	Total	C	N	O	S	0	4	0
			4450	2880	741	803	26			

There are 14 discrepancies between the modelled and reference sequences:

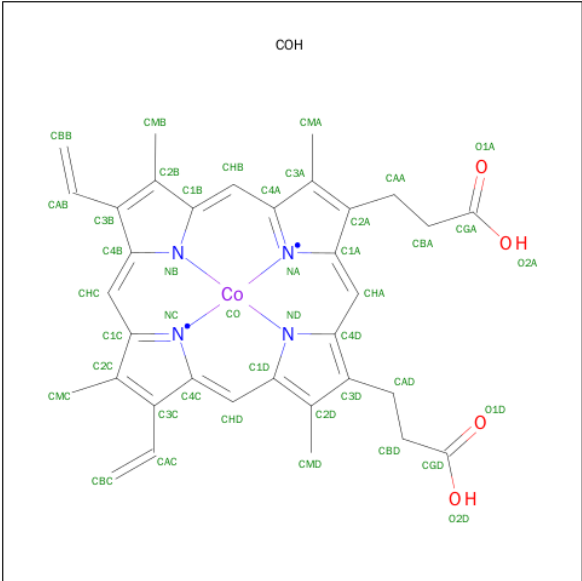
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	HIS	-	EXPRESSION TAG	UNP Q05769
A	30	HIS	-	EXPRESSION TAG	UNP Q05769
A	31	HIS	-	EXPRESSION TAG	UNP Q05769
A	32	HIS	-	EXPRESSION TAG	UNP Q05769
A	33	HIS	-	EXPRESSION TAG	UNP Q05769
A	34	HIS	-	EXPRESSION TAG	UNP Q05769
A	594	ALA	ASN	ENGINEERED MUTATION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

- Molecule 2 is ALPHA-LINOLENIC ACID (three-letter code: LNL) (formula: C₁₈H₃₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	18	2		
2	B	1	Total	C	O	0	0
			20	18	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	C	Co	N	O	0	0
			43	34	1	4	4		

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

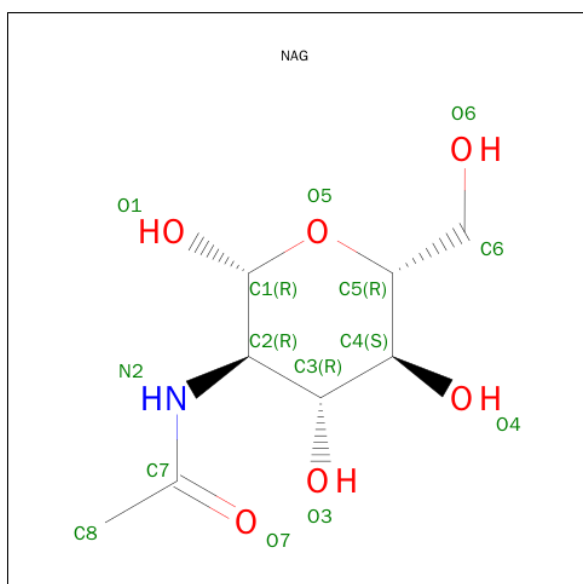
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- 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		
			39	22	2	15		
							0	0

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



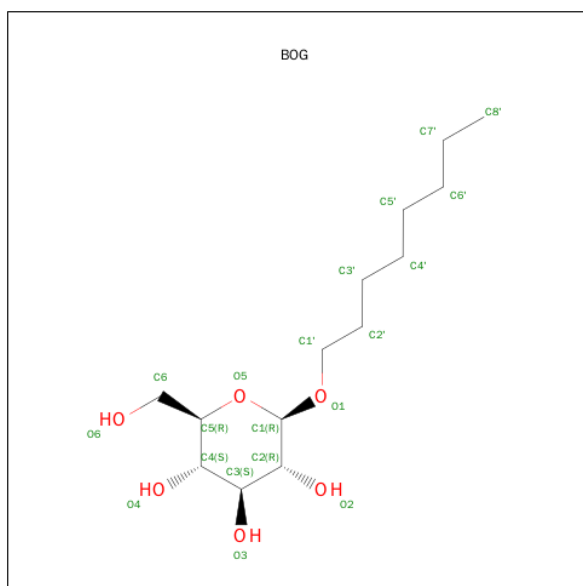
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O		
			14	8	1	5		
							0	0

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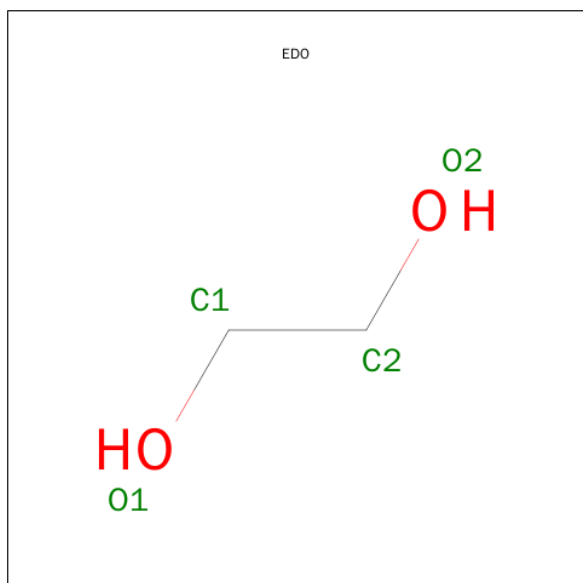
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



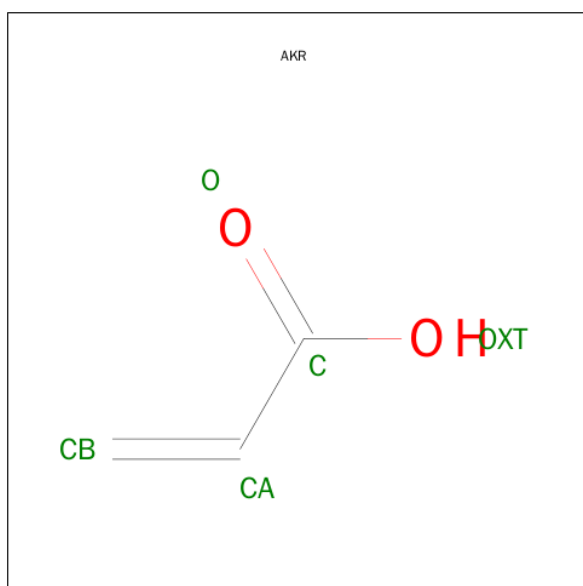
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is ACRYLIC ACID (three-letter code: AKR) (formula: $C_3H_4O_2$).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	395	Total O 395 395	0	0

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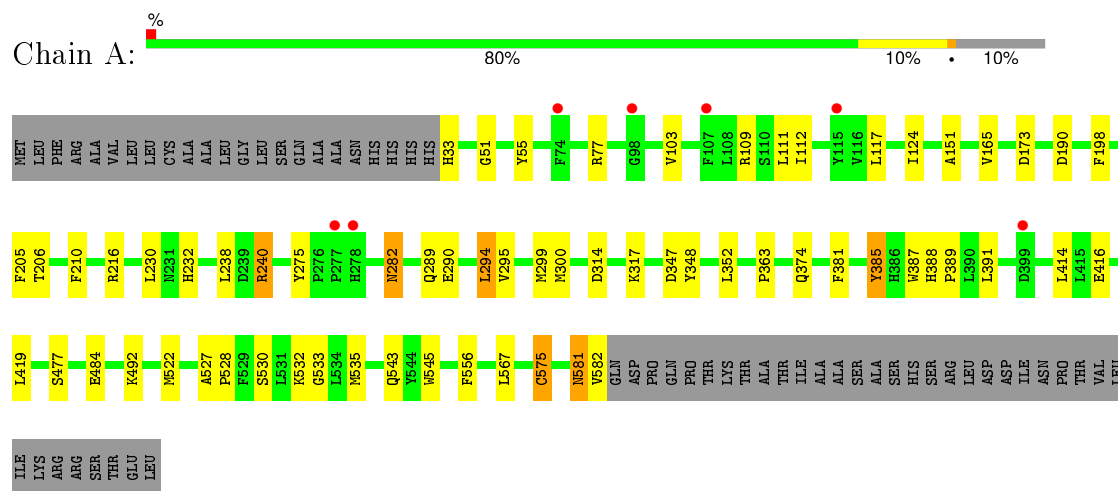
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	351	Total	O	0	0
			351	351		

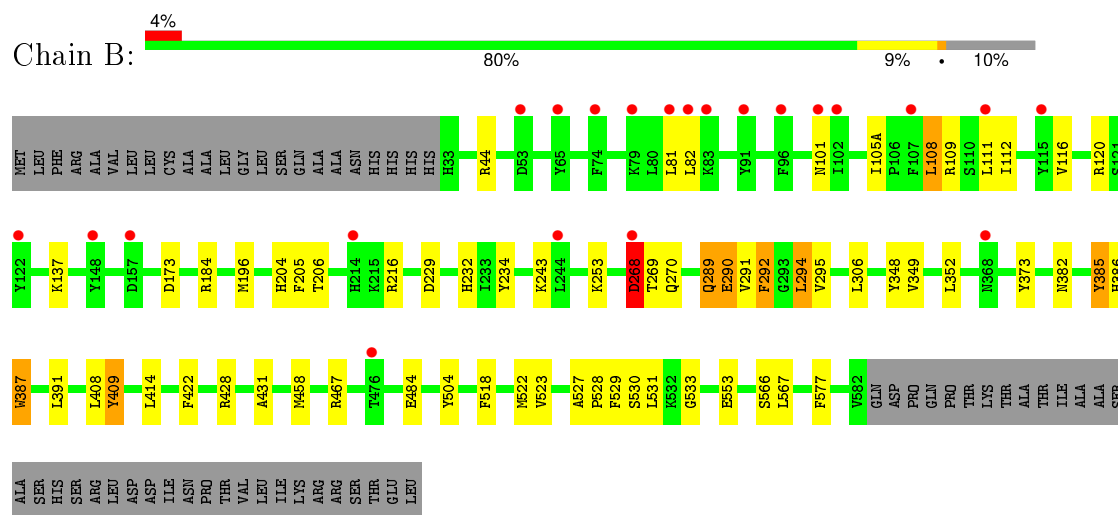
3 Residue-property plots

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



• Molecule 1: Prostaglandin G/H synthase 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.38Å 132.13Å 180.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.10) 99.4 (19.95-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.159 , 0.203 0.175 , 0.215	Depositor DCC
R_{free} test set	4187 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 83234 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9967	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 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, AKR, EDO, LNL, 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	1.13	6/4582 (0.1%)	0.92	12/6227 (0.2%)
1	B	1.11	11/4592 (0.2%)	0.94	10/6236 (0.2%)
All	All	1.12	17/9174 (0.2%)	0.93	22/12463 (0.2%)

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	1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	575	CYS	CB-SG	6.72	1.93	1.82
1	A	275	TYR	CD2-CE2	6.17	1.48	1.39
1	B	566	SER	CB-OG	5.97	1.50	1.42
1	B	290	GLU	CG-CD	-5.85	1.43	1.51
1	B	529	PHE	CE2-CZ	5.77	1.48	1.37

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	B	467	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	299	MET	CG-SD-CE	-7.62	88.00	100.20
1	B	294	LEU	CA-CB-CG	6.80	130.94	115.30
1	B	173	ASP	CB-CG-OD2	6.68	124.32	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	581	ASN	Peptide

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	4436	0	4250	68	0
1	B	4450	0	4297	64	0
2	A	20	0	29	18	0
2	B	20	0	29	19	0
3	A	43	0	30	3	0
3	B	43	0	30	3	0
4	A	28	0	25	1	0
4	B	56	0	50	12	0
5	A	39	0	34	9	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
7	A	20	0	28	1	0
8	A	8	0	12	2	0
8	B	20	0	30	6	0
9	A	10	0	6	6	0
10	A	395	0	0	12	0
10	B	351	0	0	3	0
All	All	9967	0	8876	145	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 8.

The worst 5 of 145 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ASN:HB2	10:A:1184:HOH:O	1.39	1.19
1:A:205:PHE:HE2	2:A:701:LNL:H13	1.04	1.18
1:A:216:ARG:NH1	5:A:706:NAG:H83	1.54	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:LNL:C5	2:B:701:LNL:H9	1.62	1.16
2:B:701:LNL:H51	2:B:701:LNL:H9	1.23	1.15

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	554/610 (91%)	535 (97%)	19 (3%)	0	100	100
1	B	553/610 (91%)	539 (98%)	14 (2%)	0	100	100
All	All	1107/1220 (91%)	1074 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	475/542 (88%)	469 (99%)	6 (1%)	76	82
1	B	480/542 (89%)	471 (98%)	9 (2%)	65	70
All	All	955/1084 (88%)	940 (98%)	15 (2%)	70	76

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	LEU
1	B	82	LEU
1	B	289	GLN
1	A	556	PHE
1	B	268	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	400	GLN
1	B	289	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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	703	1,4	14,14,15	0.83	0	15,19,21	2.01	4 (26%)
4	NAG	A	704	4	14,14,15	0.60	0	15,19,21	1.69	2 (13%)
5	NAG	A	705	1,5	14,14,15	0.99	0	15,19,21	1.73	4 (26%)
5	NAG	A	706	5	14,14,15	0.80	1 (7%)	15,19,21	2.23	5 (33%)
5	MAN	A	707	5	11,11,12	0.62	0	14,15,17	2.16	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	703	1,4	14,14,15	2.35	1 (7%)	15,19,21	3.27	5 (33%)
4	NAG	B	704	4	14,14,15	0.81	1 (7%)	15,19,21	1.59	2 (13%)
4	NAG	B	705	1,4	14,14,15	0.83	0	15,19,21	1.49	3 (20%)
4	NAG	B	706	4	14,14,15	0.92	0	15,19,21	2.63	5 (33%)

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	703	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	704	4	-	0/6/23/26	0/1/1/1
5	NAG	A	705	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	706	5	-	0/6/23/26	0/1/1/1
5	MAN	A	707	5	-	0/2/19/22	1/1/1/1
4	NAG	B	703	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	704	4	-	0/6/23/26	0/1/1/1
4	NAG	B	705	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	706	4	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	NAG	O5-C1	-8.34	1.29	1.43
4	B	704	NAG	O5-C1	-2.08	1.40	1.43
5	A	706	NAG	C8-C7	-2.05	1.46	1.50

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	NAG	C1-O5-C5	-10.86	98.46	112.25
4	B	706	NAG	C1-O5-C5	-6.89	103.50	112.25
4	A	703	NAG	C3-C4-C5	-4.99	101.50	110.20
5	A	706	NAG	C3-C4-C5	-4.44	102.46	110.20
4	B	704	NAG	C2-N2-C7	-4.35	117.44	123.04

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	707	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	704	NAG	1	0
5	A	706	NAG	7	0
5	A	707	MAN	2	0
4	B	706	NAG	12	0

5.6 Ligand geometry ⓘ

16 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	LNL	A	701	-	16,19,19	1.75	3 (18%)	16,19,19	1.44	3 (18%)
3	COH	A	702	1	28,50,50	2.64	10 (35%)	19,82,82	2.31	8 (42%)
6	NAG	A	708	1	14,14,15	0.78	1 (7%)	15,19,21	1.94	3 (20%)
7	BOG	A	709	-	20,20,20	0.85	1 (5%)	25,25,25	0.96	2 (8%)
8	EDO	A	710	-	3,3,3	1.05	0	2,2,2	1.08	0
8	EDO	A	711	-	3,3,3	0.60	0	2,2,2	0.51	0
9	AKR	A	712	-	1,4,4	1.59	0	0,4,4	0.00	-
9	AKR	A	713	-	1,4,4	1.89	0	0,4,4	0.00	-
2	LNL	B	701	-	16,19,19	1.87	3 (18%)	16,19,19	1.07	1 (6%)
3	COH	B	702	1	28,50,50	2.52	11 (39%)	19,82,82	2.35	6 (31%)
6	NAG	B	707	1	14,14,15	0.65	0	15,19,21	1.21	2 (13%)
8	EDO	B	708	-	3,3,3	0.94	0	2,2,2	1.24	0
8	EDO	B	709	-	3,3,3	0.09	0	2,2,2	1.81	1 (50%)
8	EDO	B	710	-	3,3,3	0.66	0	2,2,2	0.42	0
8	EDO	B	711	-	3,3,3	0.49	0	2,2,2	0.98	0
8	EDO	B	712	-	3,3,3	0.58	0	2,2,2	0.45	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	LNL	A	701	-	-	0/15/17/17	0/0/0/0
3	COH	A	702	1	-	0/6/54/54	0/0/8/8
6	NAG	A	708	1	-	0/6/23/26	0/1/1/1
7	BOG	A	709	-	-	0/11/31/31	0/1/1/1
8	EDO	A	710	-	-	0/1/1/1	0/0/0/0
8	EDO	A	711	-	-	0/1/1/1	0/0/0/0
9	AKR	A	712	-	-	0/0/2/2	0/0/0/0
9	AKR	A	713	-	-	0/0/2/2	0/0/0/0
2	LNL	B	701	-	-	0/15/17/17	0/0/0/0
3	COH	B	702	1	-	0/6/54/54	0/0/8/8
6	NAG	B	707	1	-	0/6/23/26	0/1/1/1
8	EDO	B	708	-	-	0/1/1/1	0/0/0/0
8	EDO	B	709	-	-	0/1/1/1	0/0/0/0
8	EDO	B	710	-	-	0/1/1/1	0/0/0/0
8	EDO	B	711	-	-	0/1/1/1	0/0/0/0
8	EDO	B	712	-	-	0/1/1/1	0/0/0/0

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	COH	C3B-C2B	-3.53	1.35	1.40
3	B	702	COH	C3C-C2C	-3.50	1.35	1.40
3	A	702	COH	C3B-C2B	-3.25	1.36	1.40
3	A	702	COH	C3C-C2C	-3.20	1.36	1.40
7	A	709	BOG	O5-C5	-2.24	1.38	1.44

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	COH	C3C-CAC-CBC	-4.60	116.90	126.32
3	B	702	COH	CBD-CAD-C3D	-4.53	104.42	112.53
3	A	702	COH	C3C-CAC-CBC	-4.33	117.46	126.32
3	A	702	COH	CBD-CAD-C3D	-4.28	104.85	112.53
3	B	702	COH	C3D-C4D-ND	-3.91	105.24	108.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	LNL	18	0
3	A	702	COH	3	0
7	A	709	BOG	1	0
8	A	711	EDO	2	0
9	A	712	AKR	3	0
9	A	713	AKR	3	0
2	B	701	LNL	19	0
3	B	702	COH	3	0
8	B	709	EDO	4	0
8	B	711	EDO	1	0
8	B	712	EDO	1	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	551/610 (90%)	-0.35	7 (1%) 79 84	15, 25, 39, 52	0
1	B	551/610 (90%)	-0.07	22 (3%) 42 51	17, 29, 46, 54	0
All	All	1102/1220 (90%)	-0.21	29 (2%) 59 66	15, 27, 44, 54	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	LEU	5.4
1	B	91	TYR	4.7
1	B	102	ILE	4.4
1	B	122	TYR	4.3
1	B	81	LEU	4.3

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](#)

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(Å ²)	Q<0.9
4	NAG	B	703	14/15	0.79	0.29	6.53	46,52,58,66	0
4	NAG	A	703	14/15	0.89	0.21	3.88	42,49,56,61	0
5	NAG	A	705	14/15	0.96	0.08	-0.45	24,29,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	B	705	14/15	0.97	0.08	-0.78	21,27,29,37	0
4	NAG	B	706	14/15	0.81	0.30	-	37,49,56,58	0
4	NAG	B	704	14/15	0.78	0.42	-	72,76,78,80	0
5	MAN	A	707	11/12	0.73	0.38	-	65,70,73,74	0
5	NAG	A	706	14/15	0.91	0.16	-	33,43,49,59	0
4	NAG	A	704	14/15	0.59	0.43	-	69,73,74,76	0

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
6	NAG	B	707	14/15	0.80	0.32	8.36	56,62,65,66	0
2	LNL	A	701	20/20	0.81	0.23	6.17	36,47,55,56	0
6	NAG	A	708	14/15	0.90	0.27	5.59	43,47,52,54	0
2	LNL	B	701	20/20	0.77	0.23	4.74	32,52,63,65	0
3	COH	B	702	43/43	0.70	0.29	3.88	61,75,82,85	0
3	COH	A	702	43/43	0.74	0.25	3.87	61,76,86,88	0
9	AKR	A	713	5/5	0.92	0.24	3.40	42,43,44,45	0
8	EDO	B	710	4/4	0.96	0.12	1.64	23,26,28,32	0
8	EDO	A	711	4/4	0.97	0.10	1.39	26,27,30,30	0
8	EDO	A	710	4/4	0.96	0.12	1.14	29,30,33,39	0
9	AKR	A	712	5/5	0.93	0.17	1.07	42,43,44,45	0
7	BOG	A	709	20/20	0.95	0.10	0.42	28,34,39,40	0
8	EDO	B	709	4/4	0.93	0.16	-0.11	43,44,46,47	0
8	EDO	B	712	4/4	0.97	0.09	-0.21	25,26,30,33	0
8	EDO	B	711	4/4	0.95	0.09	-0.29	43,44,45,46	0
8	EDO	B	708	4/4	0.96	0.10	-0.66	29,31,34,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.