



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2023 – 08:21 am GMT

PDB ID : 5LS7
Title : Complex of wild type E. coli alpha aspartate decarboxylase with its processing factor PanZ
Authors : Monteiro, D.C.F.; Webb, M.E.; Pearson, A.R.
Deposited on : 2016-08-22
Resolution : 1.16 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

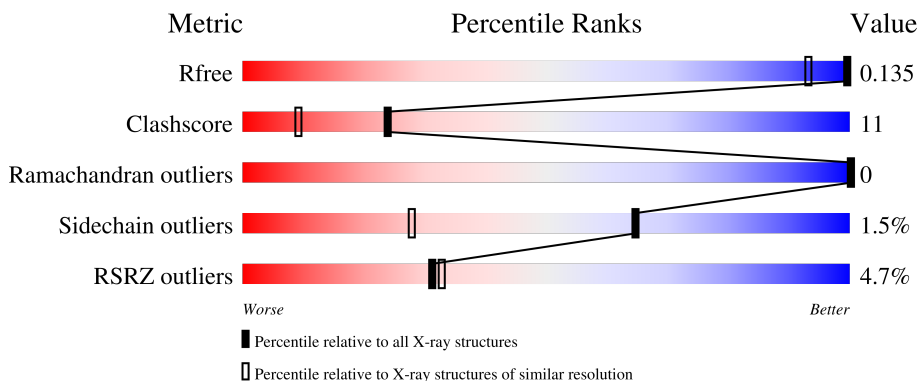
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.16 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}	130704	1758 (1.20-1.12)
Clashscore	141614	1832 (1.20-1.12)
Ramachandran outliers	138981	1768 (1.20-1.12)
Sidechain outliers	138945	1768 (1.20-1.12)
RSRZ outliers	127900	1724 (1.20-1.12)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	41	 44% 17% 39%
2	B	137	 9% 69% 21% .. 7%
3	D	102	 77% 17% 6%

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
10	74C	D	205	-	-	X	-
4	GOL	D	201	-	X	-	-
5	PEG	B	202	-	X	-	-
8	CO2	B	205	-	-	X	-
8	CO2	B	206	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 2506 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 Aspartate 1-decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	25	211	134	40	34	3	0	2	1

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP P0A790
A	-15	ARG	-	expression tag	UNP P0A790
A	-14	GLY	-	expression tag	UNP P0A790
A	-13	SER	-	expression tag	UNP P0A790
A	-12	HIS	-	expression tag	UNP P0A790
A	-11	HIS	-	expression tag	UNP P0A790
A	-10	HIS	-	expression tag	UNP P0A790
A	-9	HIS	-	expression tag	UNP P0A790
A	-8	HIS	-	expression tag	UNP P0A790
A	-7	HIS	-	expression tag	UNP P0A790
A	-6	GLY	-	expression tag	UNP P0A790
A	-5	LEU	-	expression tag	UNP P0A790
A	-4	VAL	-	expression tag	UNP P0A790
A	-3	PRO	-	expression tag	UNP P0A790
A	-2	ARG	-	expression tag	UNP P0A790
A	-1	GLY	-	expression tag	UNP P0A790
A	0	SER	-	expression tag	UNP P0A790

- Molecule 2 is a protein called PanD maturation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	128	1094	689	207	191	7	0	12	0

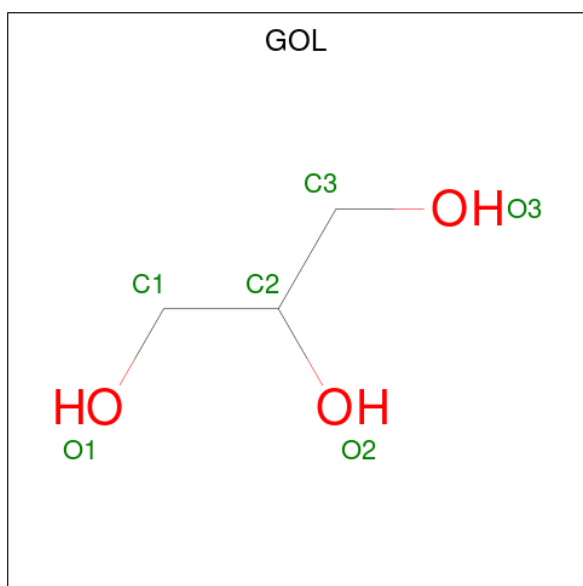
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	128	SER	-	expression tag	UNP P37613
B	129	GLY	-	expression tag	UNP P37613
B	130	LEU	-	expression tag	UNP P37613
B	131	GLU	-	expression tag	UNP P37613
B	132	HIS	-	expression tag	UNP P37613
B	133	HIS	-	expression tag	UNP P37613
B	134	HIS	-	expression tag	UNP P37613
B	135	HIS	-	expression tag	UNP P37613
B	136	HIS	-	expression tag	UNP P37613
B	137	HIS	-	expression tag	UNP P37613

- Molecule 3 is a protein called Aspartate 1-decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	102	815	510	140	160	5	0	7	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



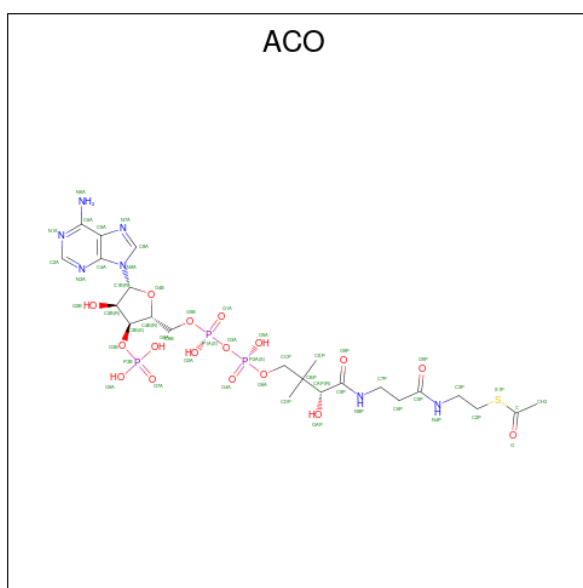
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	6	3	3	0	0
4	D	1	6	3	3	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			5	3	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).

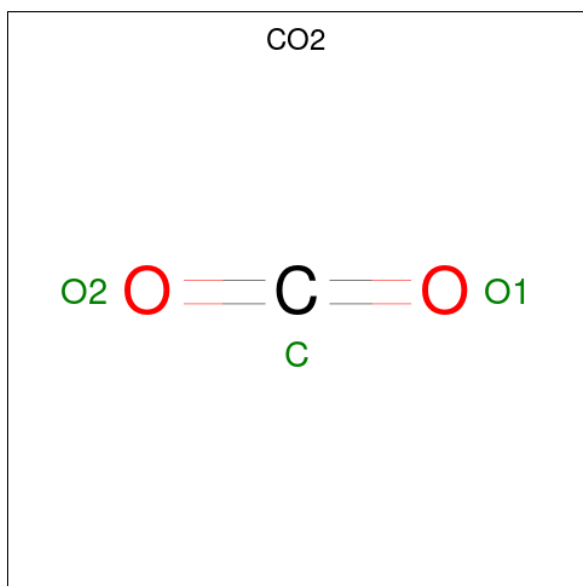


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

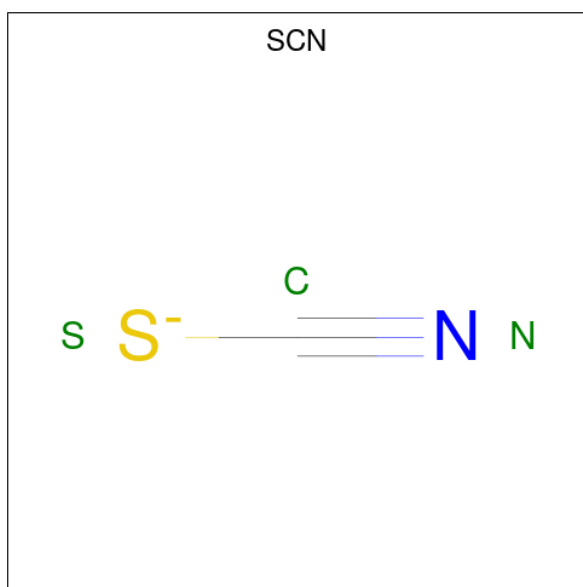
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Mg 1 1	0	0

- Molecule 8 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO₂).



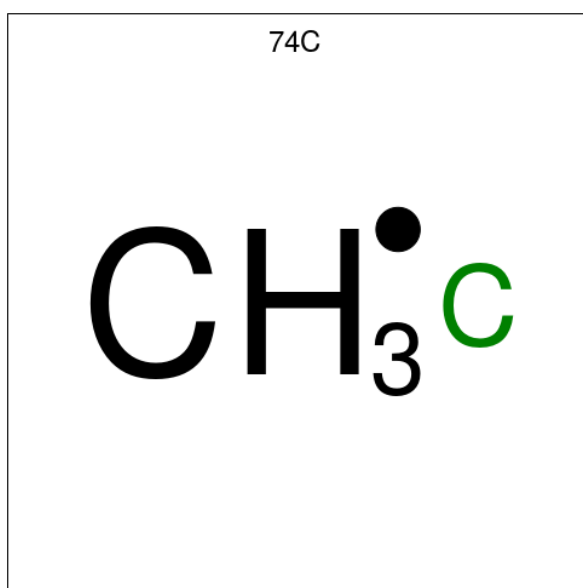
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 3 1 2	0	0
8	B	1	Total C O 3 1 2	0	0
8	D	1	Total C O 3 1 2	0	0

- Molecule 9 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	1	Total	C	N	S	0	0
			3	1	1	1		
9	D	1	Total	C	N	S	0	1
			6	2	2	2		

- Molecule 10 is methyl radical (three-letter code: 74C) (formula: CH₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total	C	0	0
			1	1		

- Molecule 11 is water.

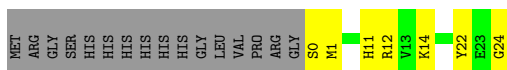
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	28	Total 29	O 29	0	1
11	B	153	Total 154	O 154	0	2
11	D	111	Total 111	O 111	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Aspartate 1-decarboxylase

Chain A: 



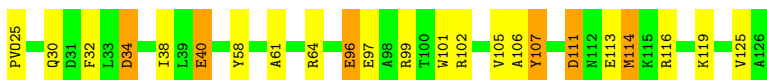
- Molecule 2: PanD maturation factor

Chain B: 



- Molecule 3: Aspartate 1-decarboxylase

Chain D: 



4 Data and refinement statistics i

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	85.86Å 85.86Å 80.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.28 – 1.16 29.28 – 1.16	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.28-1.16) 99.6 (29.28-1.16)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.16Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.113 , 0.137 0.111 , 0.135	Depositor DCC
R_{free} test set	4966 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtrriage
Anisotropy	1.023	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.032 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2506	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CSO, GOL, PVO, 74C, PEG, ACO, SCN, MG, CO2

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	1.79	4/220 (1.8%)	1.44	4/289 (1.4%)
2	B	1.61	20/1145 (1.7%)	1.50	21/1540 (1.4%)
3	D	1.62	11/832 (1.3%)	1.49	18/1126 (1.6%)
All	All	1.63	35/2197 (1.6%)	1.49	43/2955 (1.5%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	96	GLU	CD-OE2	14.83	1.42	1.25
1	A	0	SER	C-O	13.72	1.49	1.23
3	D	96	GLU	CD-OE1	11.24	1.38	1.25
2	B	103	GLU	CD-OE2	11.22	1.38	1.25
3	D	40[A]	GLU	CD-OE2	10.76	1.37	1.25
3	D	40[B]	GLU	CD-OE2	10.76	1.37	1.25
2	B	93	SER	CB-OG	-10.35	1.28	1.42
2	B	83	GLU	CD-OE1	9.25	1.35	1.25
2	B	88	ASN	CB-CG	8.90	1.71	1.51
3	D	96	GLU	CG-CD	8.80	1.65	1.51
2	B	102	VAL	CB-CG1	-7.07	1.38	1.52
2	B	24	PRO	C-O	7.06	1.37	1.23
1	A	24	GLY	CA-C	7.01	1.63	1.51
2	B	105	ARG	CZ-NH2	6.98	1.42	1.33
3	D	40[A]	GLU	CB-CG	6.95	1.65	1.52
3	D	40[B]	GLU	CB-CG	6.95	1.65	1.52
2	B	23	TRP	CE3-CZ3	6.64	1.49	1.38
2	B	88	ASN	CG-OD1	6.51	1.38	1.24
3	D	101	TRP	C-O	-6.26	1.11	1.23
2	B	24	PRO	N-CA	6.10	1.57	1.47
2	B	11	PHE	CG-CD2	-5.70	1.30	1.38
2	B	97	MET	SD-CE	-5.69	1.46	1.77
1	A	24	GLY	C-O	-5.51	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	113	GLU	CB-CG	-5.48	1.41	1.52
2	B	125	GLU	CB-CG	-5.36	1.42	1.52
3	D	64	ARG	CZ-NH1	5.35	1.40	1.33
2	B	23	TRP	CZ3-CH2	-5.32	1.31	1.40
3	D	58	TYR	CE2-CZ	-5.31	1.31	1.38
2	B	121	GLN	CD-OE1	5.30	1.35	1.24
2	B	69[A]	ARG	CZ-NH1	-5.27	1.26	1.33
2	B	69[B]	ARG	CZ-NH1	-5.27	1.26	1.33
1	A	22	TYR	CE1-CZ	-5.23	1.31	1.38
2	B	103	GLU	CD-OE1	5.07	1.31	1.25
2	B	69[A]	ARG	CG-CD	5.03	1.64	1.51
2	B	69[B]	ARG	CG-CD	5.03	1.64	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	111[A]	ASP	CB-CG-OD2	-12.31	107.22	118.30
3	D	111[B]	ASP	CB-CG-OD2	-12.31	107.22	118.30
2	B	43[A]	ARG	NE-CZ-NH2	-9.90	115.35	120.30
2	B	43[B]	ARG	NE-CZ-NH2	-9.90	115.35	120.30
2	B	104	ASP	CB-CG-OD1	8.83	126.25	118.30
3	D	32	PHE	CB-CG-CD1	8.78	126.95	120.80
2	B	69[A]	ARG	NE-CZ-NH2	8.19	124.40	120.30
2	B	69[B]	ARG	NE-CZ-NH2	8.19	124.40	120.30
2	B	16[A]	ARG	NE-CZ-NH1	-8.07	116.26	120.30
2	B	16[B]	ARG	NE-CZ-NH1	-8.07	116.26	120.30
3	D	96	GLU	CG-CD-OE1	-7.84	102.61	118.30
2	B	102	VAL	CA-CB-CG1	7.83	122.64	110.90
1	A	1[A]	MET	CG-SD-CE	-7.75	87.80	100.20
1	A	1[B]	MET	CG-SD-CE	-7.75	87.80	100.20
2	B	47	ARG	NE-CZ-NH2	-7.62	116.49	120.30
3	D	116	ARG	NE-CZ-NH2	-7.57	116.51	120.30
2	B	11	PHE	CB-CG-CD2	7.31	125.92	120.80
3	D	96	GLU	OE1-CD-OE2	7.31	132.07	123.30
3	D	64	ARG	NE-CZ-NH1	7.21	123.91	120.30
3	D	34	ASP	CB-CG-OD1	6.86	124.47	118.30
2	B	35	ASP	CB-CG-OD2	-6.82	112.16	118.30
3	D	111[A]	ASP	CB-CG-OD1	6.75	124.37	118.30
3	D	111[B]	ASP	CB-CG-OD1	6.75	124.37	118.30
2	B	47	ARG	NE-CZ-NH1	6.73	123.66	120.30
2	B	34	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	12	ARG	NE-CZ-NH1	6.16	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	99	ARG	NE-CZ-NH2	-6.03	117.29	120.30
2	B	13	ASP	CB-CG-OD2	-5.95	112.94	118.30
2	B	75[A]	ARG	NE-CZ-NH2	-5.83	117.38	120.30
2	B	75[B]	ARG	NE-CZ-NH2	-5.83	117.38	120.30
2	B	104	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	0	SER	O-C-N	5.44	131.40	122.70
2	B	40	TYR	CB-CG-CD2	5.41	124.25	121.00
3	D	107	TYR	CB-CG-CD1	-5.34	117.79	121.00
3	D	107	TYR	CB-CG-CD2	5.33	124.20	121.00
3	D	32	PHE	CB-CG-CD2	-5.27	117.11	120.80
3	D	114[A]	MET	CG-SD-CE	5.24	108.58	100.20
3	D	114[B]	MET	CG-SD-CE	5.24	108.58	100.20
2	B	7	ARG	NE-CZ-NH1	-5.22	117.69	120.30
2	B	11	PHE	CB-CG-CD1	-5.22	117.15	120.80
3	D	64	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
2	B	103	GLU	OE1-CD-OE2	5.06	129.37	123.30
3	D	116	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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	211	0	227	2	0
2	B	1094	0	1133	27	1
3	D	815	0	798	19	0
4	B	6	0	8	0	0
4	D	6	0	7	2	0
5	B	5	0	5	1	0
5	D	4	0	5	0	0
6	B	51	0	34	0	0
7	B	1	0	0	0	0
8	B	6	0	0	11	0
8	D	3	0	0	0	0
9	D	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	1	0	0	5	0
11	A	29	0	0	1	0
11	B	154	0	0	4	0
11	D	111	0	0	9	2
All	All	2506	0	2217	49	2

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 11.

All (49) 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)
3:D:114[A]:MET:HE3	10:D:205:74C:C	1.22	1.59
3:D:114[B]:MET:HE3	10:D:205:74C:C	1.38	1.47
3:D:114[B]:MET:HE1	10:D:205:74C:C	1.55	1.21
3:D:114[A]:MET:HE2	10:D:205:74C:C	1.73	1.17
2:B:70[B]:GLU:CG	8:B:206:CO2:C	2.26	1.13
3:D:30[A]:GLN:NE2	11:D:303:HOH:O	1.79	1.12
2:B:70[A]:GLU:CG	8:B:206:CO2:C	2.41	0.97
2:B:70[A]:GLU:CG	8:B:206:CO2:O2	2.19	0.91
2:B:70[B]:GLU:CG	8:B:206:CO2:O1	2.19	0.90
2:B:67[B]:ARG:NH2	8:B:205:CO2:O1	2.07	0.87
1:A:14[B]:LYS:NZ	11:A:101:HOH:O	2.09	0.85
3:D:30[B]:GLN:NE2	11:D:304:HOH:O	2.10	0.83
3:D:102:ARG:NH2	11:D:305:HOH:O	2.14	0.79
2:B:109[A]:THR:CG2	2:B:113:GLN:HE21	1.95	0.79
2:B:103:GLU:HG3	11:B:304:HOH:O	1.85	0.75
3:D:30[A]:GLN:OE1	11:D:301:HOH:O	2.12	0.66
2:B:109[A]:THR:HG23	2:B:113:GLN:HE21	1.61	0.66
2:B:22:ILE:O	2:B:67[A]:ARG:HD2	2.01	0.59
2:B:109[A]:THR:HG21	11:B:314:HOH:O	2.04	0.58
3:D:30[A]:GLN:CD	11:D:303:HOH:O	2.22	0.58
2:B:109[A]:THR:CG2	2:B:113:GLN:NE2	2.68	0.56
2:B:70[B]:GLU:CB	8:B:206:CO2:C	2.86	0.53
2:B:109[A]:THR:HG22	2:B:113:GLN:HE21	1.71	0.52
3:D:34:ASP:OD1	4:D:201:GOL:H31	2.10	0.51
2:B:118[B]:THR:HG23	11:B:332:HOH:O	2.10	0.50
3:D:111[B]:ASP:OD1	11:D:306:HOH:O	2.20	0.50
3:D:125:VAL:O	9:D:203[A]:SCN:S	2.70	0.50
3:D:105[B]:VAL:HG11	3:D:107:TYR:CZ	2.47	0.49
2:B:84:GLU:OE1	5:B:202:PEG:C2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109[A]:THR:HG22	2:B:113:GLN:NE2	2.29	0.47
2:B:109[A]:THR:HG1	2:B:124:TRP:HZ2	1.58	0.47
3:D:38:ILE:O	4:D:201:GOL:H32	2.13	0.47
2:B:70[A]:GLU:CB	8:B:206:CO2:C	2.91	0.46
2:B:20:GLN:OE1	2:B:24:PRO:HA	2.15	0.45
2:B:70[A]:GLU:H	8:B:205:CO2:C	2.29	0.45
1:A:11:HIS:HD2	11:D:333:HOH:O	1.99	0.44
2:B:35:ASP:CG	11:B:305:HOH:O	2.55	0.44
2:B:70[B]:GLU:H	8:B:205:CO2:C	2.29	0.44
3:D:30[A]:GLN:CG	11:D:303:HOH:O	2.65	0.44
2:B:109[A]:THR:HG1	2:B:124:TRP:HE1	1.64	0.44
3:D:105[B]:VAL:HG12	3:D:106:ALA:N	2.32	0.44
3:D:40[B]:GLU:HG2	3:D:61:ALA:HB2	2.01	0.43
2:B:67[B]:ARG:HH22	8:B:205:CO2:C	2.28	0.42
2:B:75[B]:ARG:HH11	2:B:75[B]:ARG:HD3	1.63	0.41
2:B:70[A]:GLU:HB3	8:B:206:CO2:C	2.51	0.41
3:D:119:LYS:NZ	11:D:310:HOH:O	2.53	0.41
2:B:11:PHE:CD1	2:B:11:PHE:N	2.88	0.41
3:D:96:GLU:HG2	3:D:97[B]:GLU:OE2	2.20	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
11:D:394:HOH:O	11:D:394:HOH:O[3_555]	1.97	0.23
2:B:71[B]:VAL:CG2	11:D:304:HOH:O[4_555]	2.11	0.09

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	25/41 (61%)	25 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	138/137 (101%)	133 (96%)	5 (4%)	0	100	100
3	D	106/102 (104%)	103 (97%)	3 (3%)	0	100	100
All	All	269/280 (96%)	261 (97%)	8 (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	23/35 (66%)	23 (100%)	0	100	100
2	B	118/116 (102%)	115 (98%)	3 (2%)	47	9
3	D	83/77 (108%)	83 (100%)	0	100	100
All	All	224/228 (98%)	221 (99%)	3 (1%)	65	32

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	24	PRO
2	B	32	GLN
2	B	35	ASP

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

Mol	Chain	Res	Type
1	A	11	HIS
2	B	113	GLN
2	B	121	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
3	PVO	D	25	3	4,5,6	4.72	3 (75%)	3,7,9	3.25	2 (66%)
3	CSO	D	78	3	3,6,7	0.78	0	0,6,8	-	-

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
3	PVO	D	25	3	-	0/0/3/6	-
3	CSO	D	78	3	-	0/1/5/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	25	PVO	OAG-CA	6.73	1.50	1.40
3	D	25	PVO	CAE-CA	-6.22	1.43	1.51
3	D	25	PVO	OAF-CA	2.23	1.43	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	25	PVO	OAG-CA-CAE	3.99	117.47	108.76
3	D	25	PVO	OAF-CA-CAE	3.95	117.38	108.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates i

There are no monosaccharides in this entry.

5.6 Ligand geometry i

Of 13 ligands modelled in this entry, 1 is monoatomic and 1 is modelled with single atom - leaving 11 for Mogul analysis.

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	GOL	D	201	-	5,5,5	2.38	3 (60%)	5,5,5	3.14	3 (60%)
5	PEG	D	204	-	3,3,6	1.17	0	2,2,5	1.98	1 (50%)
4	GOL	B	201	-	5,5,5	0.82	0	5,5,5	0.47	0
6	ACO	B	203	7	45,53,53	1.07	3 (6%)	56,79,79	1.48	10 (17%)
9	SCN	D	202	-	1,2,2	0.64	0	0,1,1	-	-
5	PEG	B	202	-	4,4,6	2.53	2 (50%)	3,3,5	4.41	1 (33%)
9	SCN	D	203[A]	-	1,2,2	0.38	0	0,1,1	-	-
9	SCN	D	203[B]	-	1,2,2	1.60	0	0,1,1	-	-
8	CO2	B	205	-	2,2,2	3.21	1 (50%)	1,1,1	0.32	0
8	CO2	D	206	-	2,2,2	0.38	0	1,1,1	0.52	0
8	CO2	B	206	-	2,2,2	0.42	0	1,1,1	0.49	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. ^{1,2} means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	201	-	-	4/4/4/4	-
5	PEG	D	204	-	-	0/1/1/4	-
4	GOL	B	201	-	-	0/4/4/4	-
6	ACO	B	203	7	-	3/47/67/67	0/3/3/3
5	PEG	B	202	-	-	1/2/2/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	205	CO2	O2-C	-4.53	0.89	1.16
5	B	202	PEG	O2-C2	3.77	1.61	1.42
4	D	201	GOL	O1-C1	3.60	1.57	1.42
4	D	201	GOL	C3-C2	-3.29	1.38	1.51
5	B	202	PEG	O2-C3	3.06	1.57	1.40
6	B	203	ACO	O4B-C1B	2.33	1.44	1.41
6	B	203	ACO	C8A-N7A	-2.21	1.30	1.34
4	D	201	GOL	O2-C2	2.03	1.49	1.43
6	B	203	ACO	C7P-C6P	2.02	1.57	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	202	PEG	C2-O2-C3	7.52	159.74	112.96
4	D	201	GOL	O2-C2-C3	-4.79	88.03	109.12
4	D	201	GOL	C3-C2-C1	4.32	128.49	111.70
6	B	203	ACO	C4A-C5A-N7A	4.14	113.72	109.40
6	B	203	ACO	O-C-CH3	3.74	138.43	123.07
6	B	203	ACO	O-C-S1P	-3.46	107.22	122.60
6	B	203	ACO	N3A-C2A-N1A	-3.21	123.66	128.68
5	D	204	PEG	O4-C4-C3	2.79	132.02	111.91
6	B	203	ACO	C5A-C6A-N6A	2.74	124.51	120.35
6	B	203	ACO	C2A-N1A-C6A	2.47	122.97	118.75
6	B	203	ACO	CDP-CBP-CAP	2.44	113.05	108.82
6	B	203	ACO	C2P-C3P-N4P	-2.41	107.35	112.42
6	B	203	ACO	C5A-C6A-N1A	-2.36	115.00	120.35
6	B	203	ACO	C3P-N4P-C5P	-2.18	118.79	122.84
4	D	201	GOL	O2-C2-C1	2.00	117.94	109.12

There are no chirality outliers.

All (8) torsion outliers are listed below:

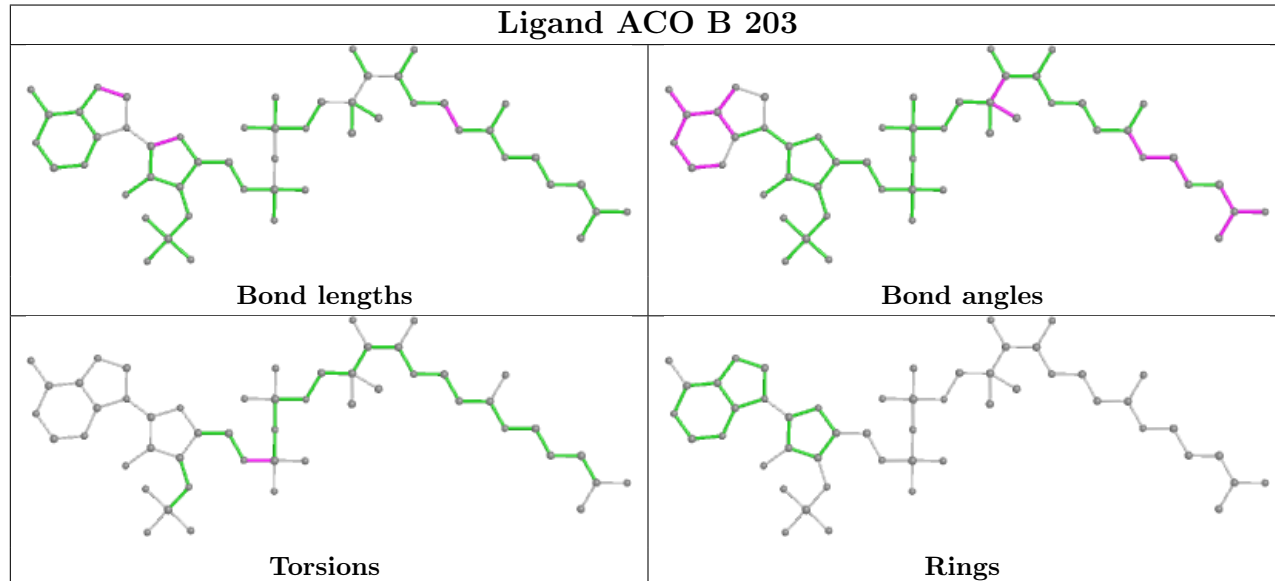
Mol	Chain	Res	Type	Atoms
4	D	201	GOL	C1-C2-C3-O3
6	B	203	ACO	C5B-O5B-P1A-O1A
6	B	203	ACO	C5B-O5B-P1A-O2A
4	D	201	GOL	O1-C1-C2-C3
4	D	201	GOL	O2-C2-C3-O3
5	B	202	PEG	O2-C3-C4-O4
6	B	203	ACO	C5B-O5B-P1A-O3A
4	D	201	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	201	GOL	2	0
5	B	202	PEG	1	0
9	D	203[A]	SCN	1	0
8	B	205	CO2	4	0
8	B	206	CO2	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

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 [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	25/41 (60%)	0.01	0 100 100	9, 11, 22, 38	0
2	B	128/137 (93%)	0.47	12 (9%) 8 9	10, 16, 44, 87	0
3	D	100/102 (98%)	0.05	0 100 100	8, 11, 24, 28	0
All	All	253/280 (90%)	0.26	12 (4%) 31 33	8, 14, 35, 87	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	29	SER	10.8
2	B	28	PRO	9.6
2	B	31	LEU	6.3
2	B	27	SER	5.5
2	B	128	SER	5.2
2	B	32	GLN	4.2
2	B	127	CYS	4.2
2	B	26	TYR	3.9
2	B	10	LYS	3.3
2	B	30	SER	2.7
2	B	25	GLU	2.4
2	B	13	ASP	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å ²)	Q<0.9
3	PVO	D	25	6/7	0.96	0.09	11,14,15,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CSO	D	78	7/8	0.99	0.06	9,10,19,29	0

6.3 Carbohydrates [i](#)

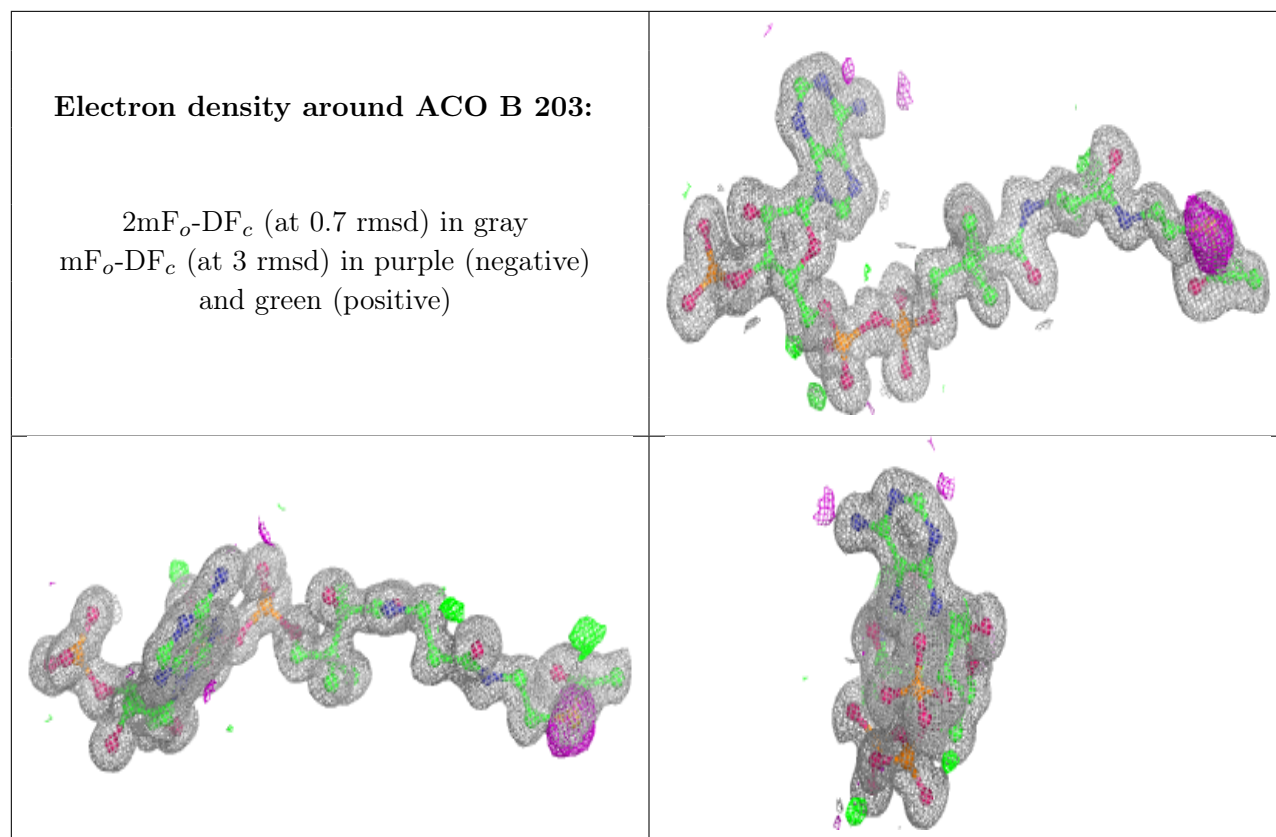
There are no monosaccharides in this entry.

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. 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	B-factors(Å ²)	Q<0.9
8	CO2	B	206	3/3	0.69	0.36	36,36,38,44	0
8	CO2	D	206	3/3	0.87	0.12	26,26,29,35	3
4	GOL	D	201	6/6	0.90	0.20	15,19,28,28	6
5	PEG	B	202	5/7	0.91	0.14	18,23,41,50	0
10	74C	D	205	1/1	0.93	0.18	14,14,14,14	1
8	CO2	B	205	3/3	0.95	0.25	15,15,20,30	0
5	PEG	D	204	4/7	0.96	0.15	21,23,26,29	4
4	GOL	B	201	6/6	0.97	0.09	17,18,20,20	0
9	SCN	D	203[A]	3/3	0.98	0.15	9,9,25,33	3
9	SCN	D	203[B]	3/3	0.98	0.15	10,10,36,40	3
6	ACO	B	203	51/51	0.98	0.06	10,15,22,37	0
9	SCN	D	202	3/3	0.99	0.06	10,10,12,12	0
7	MG	B	204	1/1	1.00	0.03	16,16,16,16	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.