

# wwPDB X-ray Structure Validation Summary Report (i)

#### 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

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Deposited on : 2016-08-22

Resolution : 1.16 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

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) 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)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

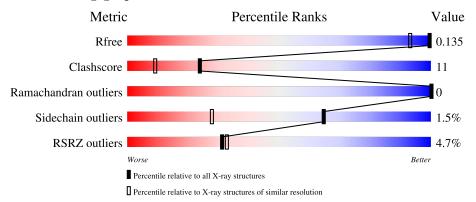
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	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 <=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	В	137	9%		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	В	202	-	X	-	-
8	CO2	В	205	-	-	X	-
8	CO2	В	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			
1	A	25	Total 211	C 134	N 40	O 34	S 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	
2	В	128	Total 1094	C 689	N 207	O 191	S 7	0	12	0

There are 10 discrepancies between the modelled and reference sequences:

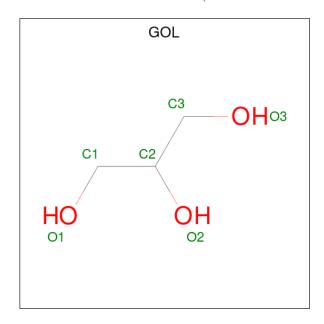


Chain	Residue	Modelled	Actual	Comment	Reference
В	128	SER	-	expression tag	UNP P37613
В	129	GLY	-	expression tag	UNP P37613
В	130	LEU	-	expression tag	UNP P37613
В	131	GLU	-	expression tag	UNP P37613
В	132	HIS	-	expression tag	UNP P37613
В	133	HIS	-	expression tag	UNP P37613
В	134	HIS	-	expression tag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

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	D	102	Total	С	N	О	S	0	7	0
		102	815	510	140	160	5		·	

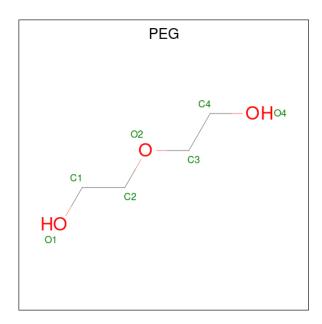
• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

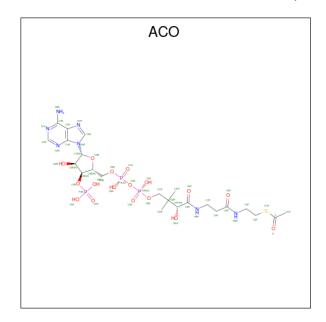
 $\bullet \ \ Molecule \ 5 \ is \ DI(HYDROXYETHYL)ETHER \ (three-letter \ code: \ PEG) \ (formula: \ C_4H_{10}O_3).$ 





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

 $\bullet \ \ \mathrm{Molecule} \ 6 \ \mathrm{is} \ \mathrm{ACETYL} \ \mathrm{COENZYME} \ ^*\mathrm{A} \ (\mathrm{three-letter} \ \mathrm{code} \colon \ \mathrm{ACO}) \ (\mathrm{formula} \colon \ \mathrm{C}_{23}\mathrm{H}_{38}\mathrm{N}_7\mathrm{O}_{17}\mathrm{P}_3\mathrm{S}).$ 



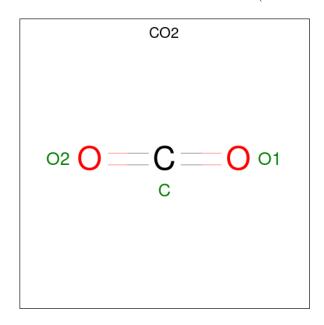
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	В	1	Total 51			O 17	P 3	S 1	0	0

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



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

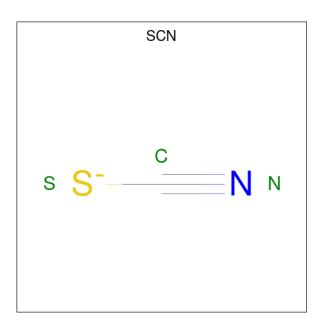
 $\bullet$  Molecule 8 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO2).



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

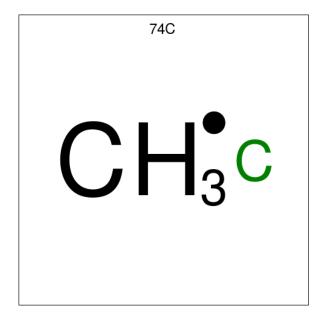
• Molecule 9 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).





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

• Molecule 10 is methyl radical (three-letter code: 74C) (formula: CH<sub>3</sub>).



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

• Molecule 11 is water.



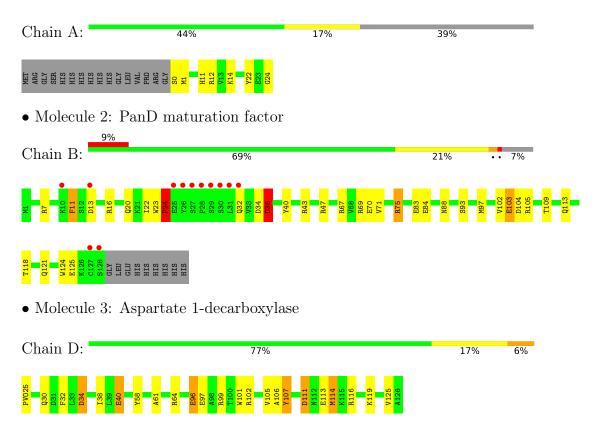
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	28	Total O 29 29	0	1
11	В	153	Total O 154 154	0	2
11	D	111	Total O 111 111	0	0



# 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





# 4 Data and refinement statistics (i)

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

Xtriage'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.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	1.79	4/220~(1.8%)	1.44	4/289 (1.4%)	
2	В	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%)	

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
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	В	103	GLU	CD-OE2	11.22	1.38	1.25
3	D	40[A]	GLU	CD-OE2	10.76	1.37	1.25

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
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	В	43[A]	ARG	NE-CZ-NH2	-9.90	115.35	120.30
2	В	43[B]	ARG	NE-CZ-NH2	-9.90	115.35	120.30
2	В	104	ASP	CB-CG-OD1	8.83	126.25	118.30

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	В	1094	0	1133	27	1
3	D	815	0	798	19	0
4	В	6	0	8	0	0
4	D	6	0	7	2	0
5	В	5	0	5	1	0
5	D	4	0	5	0	0
6	В	51	0	34	0	0
7	В	1	0	0	0	0
8	В	6	0	0	11	0
8	D	3	0	0	0	0
9	D	9	0	0	1	0
10	D	1	0	0	5	0
11	A	29	0	0	1	0
11	В	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.

The worst 5 of 49 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
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

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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	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	Perce	ntiles
1	A	25/41~(61%)	25 (100%)	0	0	100	100
2	В	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	Percentile	$\mathbf{s}$
1	A	23/35~(66%)	23 (100%)	0	100 100	
2	В	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	В	24	PRO
2	В	32	GLN
2	В	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	В	113	GLN
2	В	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 (i)

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).

Mo	ol Type Chain Res Link		$\mathbf{B}$	Bond lengths			Sond ang	gles		
1010	Type	Chain	nes	Lilik	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	$\operatorname{Res}$	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	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
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	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
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	Trino	Chain	Dec	Res Link		Bond lengths			Bond angles		
MIOI	Type	Chain	nes	LIIIK	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	В	201	-	5,5,5	0.82	0	5,5,5	0.47	0	
6	ACO	В	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	В	202	-	4,4,6	2.53	2 (50%)	3,3,5	4.41	1 (33%)	



Mol	Tuno	Chain	Res	Link	Во	ond leng	${ m ths}$	Е	ond ang	gles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	В	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	В	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. '-' 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	В	201	-	-	0/4/4/4	-
6	ACO	В	203	7	-	3/47/67/67	0/3/3/3
5	PEG	В	202	-	-	1/2/2/4	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	Ideal(A)
8	В	205	CO2	О2-С	-4.53	0.89	1.16
5	В	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	В	202	PEG	O2-C3	3.06	1.57	1.40

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^{o})$
5	В	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	В	203	ACO	C4A-C5A-N7A	4.14	113.72	109.40
6	В	203	ACO	O-C-CH3	3.74	138.43	123.07

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	201	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	В	203	ACO	C5B-O5B-P1A-O1A
6	В	203	ACO	C5B-O5B-P1A-O2A
4	D	201	GOL	O1-C1-C2-C3
4	D	201	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mo	ol	Chain	Res	Type	Clashes	Symm-Clashes
4		D	201	GOL	2	0
5		В	202	PEG	1	0
9		D	203[A]	SCN	1	0
8		В	205	CO2	4	0
8		В	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 then 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 (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,  $95^{th}$  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	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	A	25/41~(60%)	0.01	0 100 100	9, 11, 22, 38	0
2	В	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

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	29	SER	10.8
2	В	28	PRO	9.6
2	В	31	LEU	6.3
2	В	27	SER	5.5
2	В	128	SER	5.2

#### 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,  $95^{th}$  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.

Mo	l Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
3	PVO	D	25	6/7	0.96	0.09	11,14,15,16	0
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.



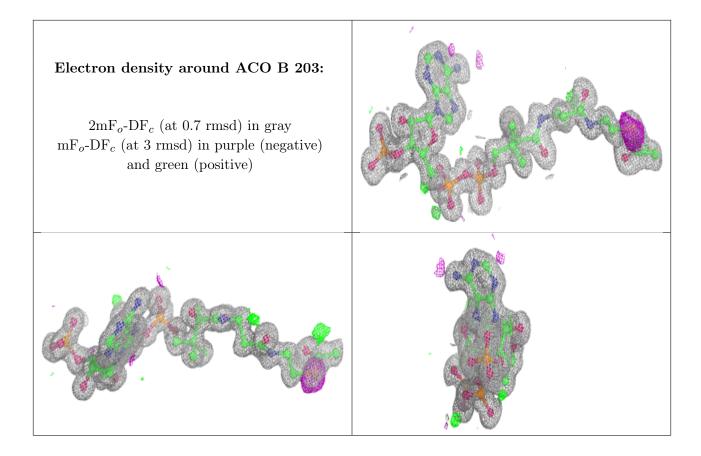
## 6.4 Ligands (i)

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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
8	CO2	В	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	В	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	В	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	В	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	В	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	В	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.

