

Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 02:30 am GMT

PDB ID : 4CRY

Title : Direct visualisation of strain-induced protein post-translational modification Authors : Monteiro, D.C.F.; Patel, V.; Bartlett, C.P.; Grant, T.D.; Nozaki, S.; Gowdy,

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Deposited on : 2014-03-02

Resolution : 1.61 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 (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)

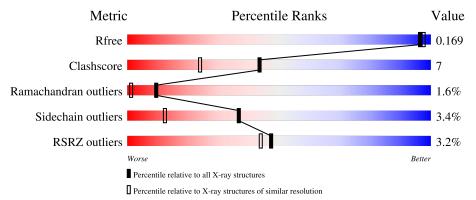
Validation Pipeline (wwPDB-VP) : 2.36

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 1.61 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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%	10%	7%	39%	
2	В	137	6%			20%	5% • 7%
3	G	102		84%			14% •



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 2271 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 209	C 129	N 41	O 37	S 2	0	1	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	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 PANZ.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	127	Total 1079	C 678	N 204	O 190	S 7	0	9	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

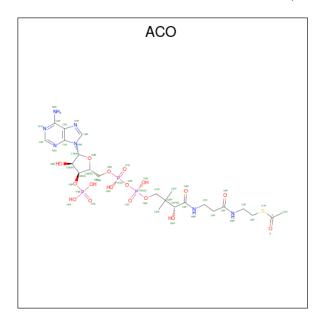
• Molecule 3 is a protein called ASPARTATE 1-DECARBOXYLASE.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	G	102	Total 806	C 504	N 142	O 156	S 4	0	5	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	G 57 VAL THR		THR	engineered mutation	UNP P0A790

• Molecule 4 is ACETYL COENZYME *A (three-letter code: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



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



• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

• Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total Cl 1 1	0	0

• Molecule 7 is water.

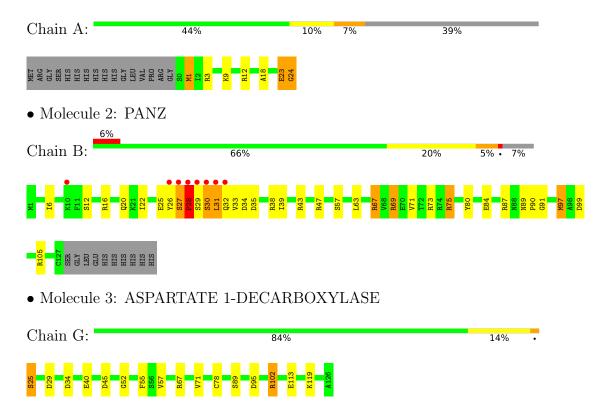
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	19	Total O 19 19	0	0
7	В	56	Total O 56 56	0	0
7	G	49	Total O 49 49	0	0



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	86.40Å 86.40Å 81.00Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.19 - 1.61	Depositor
rtesolution (A)	43.20 - 1.61	EDS
% Data completeness	97.3 (43.19-1.61)	Depositor
(in resolution range)	98.8 (43.20-1.61)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.40 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
D D.	0.129 , 0.150	Depositor
R, R_{free}	0.151 , 0.169	DCC
R_{free} test set	1944 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 50.1	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
Reported twinning fraction	0.841 for H, K, L	Depositor
Reported twinning fraction	0.159 for K, H, -L	Depositor
Outliers	0 of 38084 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2271	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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, MG, CL, ACO

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).

Mal	Mol Chain		nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	1.83	6/211 (2.8%)	1.80	6/276~(2.2%)	
2	В	1.30	2/1124~(0.2%)	1.47	15/1512 (1.0%)	
3	G	1.41	1/826 (0.1%)	1.53	10/1118 (0.9%)	
All	All	1.40	$9/2161 \ (0.4\%)$	1.53	31/2906 (1.1%)	

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	Ideal(Å)
1	A	24[A]	GLY	N-CA	9.64	1.60	1.46
1	A	24[B]	GLY	N-CA	9.64	1.60	1.46
2	В	57	SER	CB-OG	-7.25	1.32	1.42
1	A	9	LYS	CB-CG	-6.17	1.35	1.52
1	A	3	ARG	NE-CZ	-5.96	1.25	1.33
1	A	23	GLU	CD-OE1	5.79	1.32	1.25
3	G	52	GLY	N-CA	-5.28	1.38	1.46
1	A	23	GLU	C-O	5.22	1.33	1.23
2	В	91	GLY	N-CA	5.06	1.53	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	В	38	ARG	NE-CZ-NH1	16.47	128.54	120.30

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	G	34	ASP	CB-CG-OD2	-13.98	105.72	118.30
2	В	38	ARG	NE-CZ-NH2	-11.60	114.50	120.30
1	A	12	ARG	NE-CZ-NH2	-11.59	114.50	120.30
2	В	47	ARG	NE-CZ-NH2	-10.59	115.01	120.30
3	G	29	ASP	CB-CG-OD2	-9.33	109.91	118.30
2	В	69[A]	ARG	NE-CZ-NH2	-8.51	116.04	120.30
2	В	69[B]	ARG	NE-CZ-NH2	-8.51	116.04	120.30
3	G	25[A]	SER	N-CA-CB	7.51	121.76	110.50
3	G	25[B]	SER	N-CA-CB	7.51	121.76	110.50
1	A	3	ARG	NE-CZ-NH2	-7.47	116.57	120.30
3	G	102[A]	ARG	NE-CZ-NH1	-6.96	116.82	120.30
3	G	102[B]	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	A	12	ARG	NE-CZ-NH1	6.94	123.77	120.30
2	В	97[A]	MET	CG-SD-CE	-6.82	89.29	100.20
2	В	97[B]	MET	CG-SD-CE	-6.82	89.29	100.20
3	G	55	PHE	CB-CG-CD1	6.72	125.51	120.80
1	A	24[A]	GLY	N-CA-C	6.60	129.59	113.10
1	A	24[B]	GLY	N-CA-C	6.60	129.59	113.10
2	В	34	ASP	CB-CG-OD1	6.16	123.84	118.30
2	В	47	ARG	NE-CZ-NH1	6.15	123.37	120.30
2	В	67	ARG	NE-CZ-NH2	-5.93	117.33	120.30
2	В	73	ARG	NE-CZ-NH1	-5.87	117.36	120.30
2	В	75[A]	ARG	NE-CZ-NH1	-5.79	117.41	120.30
2	В	75[B]	ARG	NE-CZ-NH1	-5.79	117.41	120.30
3	G	34	ASP	CB-CG-OD1	5.67	123.40	118.30
2	В	80	TYR	CB-CG-CD1	5.57	124.34	121.00
1	A	1	MET	CG-SD-CE	-5.32	91.68	100.20
2	В	43	ARG	NE-CZ-NH2	-5.29	117.65	120.30
3	G	45	ASP	CB-CG-OD2	5.19	122.97	118.30
3	G	95	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	GLU	Peptide

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	209	0	215	2	0
2	В	1079	0	1108	24	1
3	G	806	0	796	5	1
4	В	51	0	34	0	0
5	В	1	0	0	0	0
6	В	1	0	0	0	0
7	A	19	0	0	0	0
7	В	56	0	0	2	0
7	G	49	0	0	0	0
All	All	2271	0	2153	29	1

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 7.

All (29) 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:G:67[A]:ARG:HH22	3:G:113[A]:GLU:HG2	1.19	1.00
2:B:28:PRO:HA	2:B:29:SER:C	1.88	0.94
3:G:67[A]:ARG:NH2	3:G:113[A]:GLU:HG2	1.83	0.93
2:B:28:PRO:HG2	2:B:31:LEU:HD22	1.65	0.79
2:B:27:SER:N	2:B:28:PRO:HD2	2.01	0.76
2:B:12:SER:O	2:B:16[A]:ARG:HG3	1.92	0.70
2:B:28:PRO:HG3	2:B:31:LEU:HD13	1.75	0.68
2:B:27:SER:N	2:B:28:PRO:CD	2.57	0.66
2:B:28:PRO:HA	2:B:29:SER:O	1.97	0.64
2:B:71:VAL:HG13	7:B:2033:HOH:O	1.98	0.63
2:B:99:ASP:OD2	2:B:105[A]:ARG:NH1	2.31	0.63
2:B:28:PRO:HB3	2:B:31:LEU:HB2	1.88	0.56
1:A:24[A]:GLY:HA2	3:G:25[A]:SER:HA	1.88	0.55
2:B:28:PRO:CG	2:B:31:LEU:HD22	2.35	0.53
2:B:75[B]:ARG:HH11	2:B:75[B]:ARG:HG3	1.75	0.51
2:B:22:ILE:O	2:B:67:ARG:HD2	2.11	0.50
2:B:31:LEU:HG	2:B:39:ILE:HD11	1.95	0.48
2:B:33:VAL:HG13	7:B:2011:HOH:O	2.13	0.48
2:B:28:PRO:CG	2:B:31:LEU:HD13	2.44	0.48
2:B:84:GLU:OE2	2:B:87[A]:ARG:NH2	2.48	0.46
2:B:26:TYR:C	2:B:28:PRO:HD2	2.36	0.46
2:B:69[B]:ARG:HH11	2:B:69[B]:ARG:HD3	1.63	0.45

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Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{array}$	Clash overlap (Å)
2:B:63:LEU:O	2:B:97[B]:MET:HG3	2.17	0.44
3:G:102[A]:ARG:HB3	3:G:119:LYS:O	2.18	0.43
2:B:6:ILE:HG21	2:B:6:ILE:HD13	1.81	0.42
2:B:89:ASN:N	2:B:90:PRO:CD	2.82	0.42
2:B:29:SER:O	2:B:30:SER:CB	2.68	0.41
1:A:18:ALA:HA	3:G:71:VAL:O	2.21	0.41

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

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
2:B:75[A]:ARG:NH1	3:G:40:GLU:OE2[4_555]	1.85	0.35

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	23/41 (56%)	22 (96%)	1 (4%)	0	100 100		
2	В	134/137 (98%)	128 (96%)	3 (2%)	3 (2%)	6 0		
3	G	103/102 (101%)	102 (99%)	0	1 (1%)	15 3		
All	All	260/280 (93%)	252 (97%)	4 (2%)	4 (2%)	9 1		

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	28	PRO
2	В	30	SER
2	В	27	SER
3	G	57	VAL



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	Rotameric Outliers		Percentiles		
1	A	22/35~(63%)	21 (96%)	1 (4%)	27	7		
2	В	116/116 (100%)	111 (96%)	5 (4%)	29	8		
3	G	83/78 (106%)	82 (99%)	1 (1%)	71	52		
All	All	221/229 (96%)	214 (97%)	7 (3%)	37	14		

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
2	В	25	GLU
2	В	28	PRO
2	В	31	LEU
2	В	32	GLN
2	В	35	ASP
3	G	89	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	120	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)

1 non-standard protein/DNA/RNA residue is 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		
IVIOI					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	CSO	G	78	3	3,6,7	1.57	1 (33%)	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	CSO	G	78	3	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
3	G	78	CSO	CB-CA	-2.58	1.47	1.53

There are no bond angle outliers.

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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 Re		Res	Link	Bond lengths			Bond angles			
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACO	В	1128	5	45,53,53	1.27	2 (4%)	56,79,79	1.83	16 (28%)

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACO	В	1128	5	-	4/47/67/67	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
4	В	1128	ACO	P3B-O3B	4.19	1.67	1.59
4	В	1128	ACO	C4A-N3A	2.43	1.39	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^{o})$
4	В	1128	ACO	N3A-C2A-N1A	-4.71	121.32	128.68
4	В	1128	ACO	O9A-P3B-O8A	3.91	122.59	107.64
4	В	1128	ACO	O9A-P3B-O7A	3.63	124.91	110.68
4	В	1128	ACO	O6A-CCP-CBP	-3.59	104.78	110.55
4	В	1128	ACO	O5P-C5P-N4P	-3.04	117.28	123.01
4	В	1128	ACO	O9P-C9P-N8P	-3.04	116.47	122.99
4	В	1128	ACO	O8A-P3B-O7A	-2.87	99.46	110.68
4	В	1128	ACO	O5P-C5P-C6P	2.72	127.00	122.02
4	В	1128	ACO	C2P-C3P-N4P	-2.72	106.70	112.42
4	В	1128	ACO	O9P-C9P-CAP	2.68	129.24	121.06
4	В	1128	ACO	C4A-C5A-N7A	-2.66	106.63	109.40
4	В	1128	ACO	O4B-C1B-C2B	-2.59	103.14	106.93
4	В	1128	ACO	C1B-N9A-C4A	-2.54	122.18	126.64
4	В	1128	ACO	O3B-C3B-C2B	2.25	119.83	111.68
4	В	1128	ACO	O2B-C2B-C3B	-2.24	104.79	111.17
4	В	1128	ACO	C2A-N1A-C6A	2.13	122.40	118.75

There are no chirality outliers.

All (4) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
4	В	1128	ACO	C5B-O5B-P1A-O1A
4	В	1128	ACO	C5B-O5B-P1A-O2A
4	В	1128	ACO	C5B-O5B-P1A-O3A
4	В	1128	ACO	CCP-O6A-P2A-O4A

There are no ring outliers.

No monomer is involved in short contacts.

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>	$\# \mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	A	25/41 (60%)	-0.07	0 100 100	14, 17, 32, 52	0
2	В	127/137 (92%)	0.02	8 (6%) 20 17	16, 29, 51, 100	0
3	G	101/102 (99%)	-0.20	0 100 100	13, 17, 33, 36	0
All	All	253/280 (90%)	-0.08	8 (3%) 47 44	13, 22, 45, 100	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	29	SER	5.7
2	В	28	PRO	5.4
2	В	27	SER	5.0
2	В	32	GLN	4.9
2	В	31	LEU	3.0
2	В	30	SER	2.7
2	В	26	TYR	2.4
2	В	10	LYS	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, 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
3	CSO	G	78	7/8	0.99	0.08	15,17,24,33	0



6.3 Carbohydrates (i)

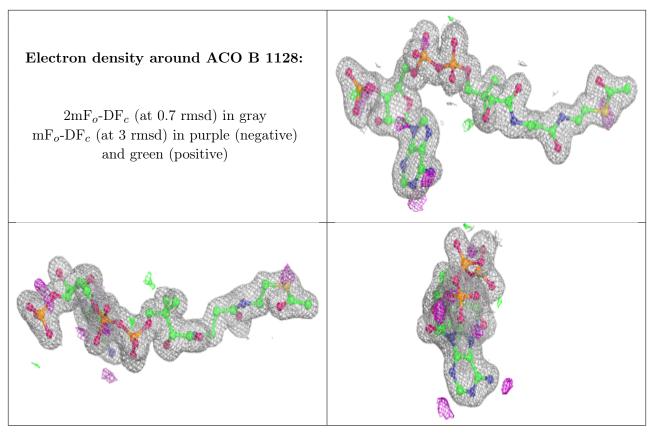
There are no monosaccharides in this entry.

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	${f B-factors}({f \AA}^2)$	Q<0.9
6	CL	В	1130	1/1	0.92	0.48	30,30,30,30	1
4	ACO	В	1128	51/51	0.98	0.06	18,28,36,37	0
5	MG	В	1129	1/1	1.00	0.07	26,26,26,26	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.

