



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 06:00 am BST

PDB ID : 6JP4  
Title : Crystal structure of the catalytic domain of a multi-domain alginate lyase  
Dp0100 from thermophilic bacterium Defluviitalea phaphyphila  
Authors : Ji, S.Q.; Dix, S.R.; Aziz, A.; Sedelnikova, S.E.; Li, F.L.; Rice, D.W.  
Deposited on : 2019-03-25  
Resolution : 2.07 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

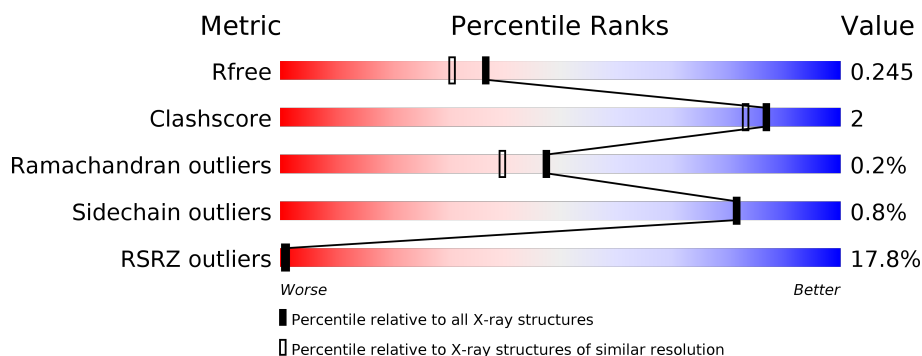
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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  $\geq 3$ , 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	770	
1	B	770	
1	C	770	
1	D	770	

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 22705 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 Alginate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	770	Total	C	N	O	S	0	0	0
			6240	3961	1017	1246	16			
1	B	770	Total	C	N	O	S	0	0	0
			6240	3961	1017	1246	16			
1	C	770	Total	C	N	O	S	0	0	0
			6240	3961	1017	1246	16			
1	D	770	Total	C	N	O		0	0	0
			3080	1540	770	770				

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

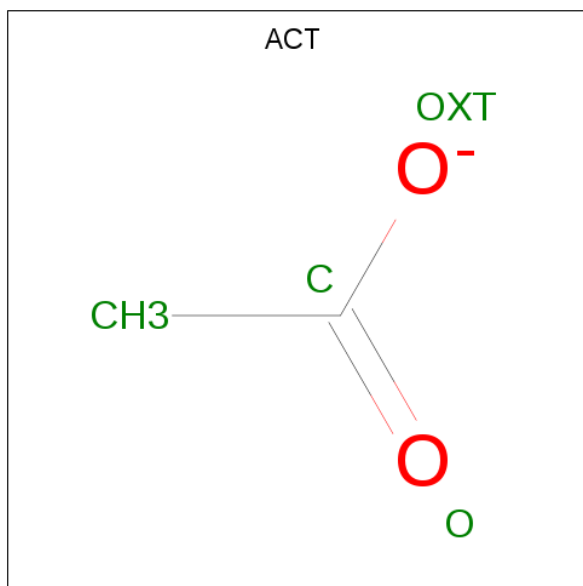
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Ca 2 2	0	0
4	A	2	Total Ca 2 2	0	0
4	C	2	Total Ca 2 2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



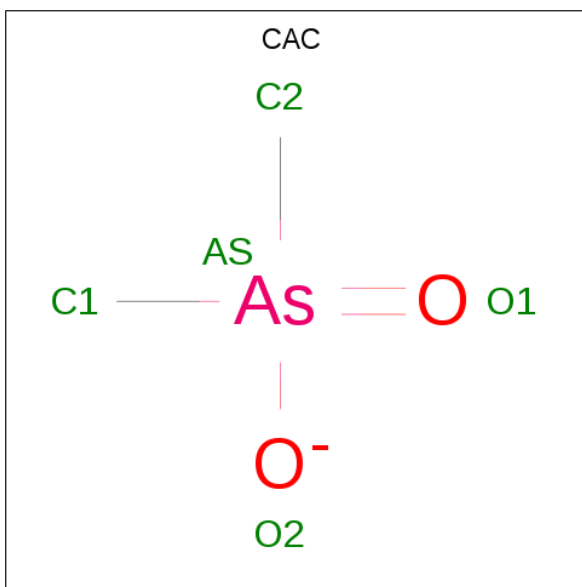
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 7 is CACODYLATE ION (three-letter code: CAC) (formula:  $C_2H_6AsO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	As	C	O	0	0
			5	1	2	2		

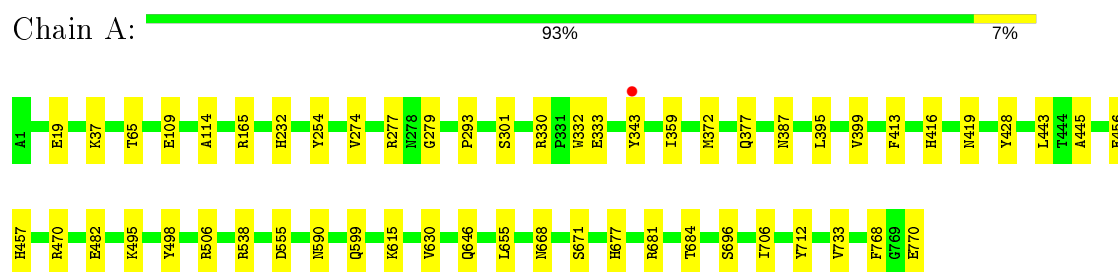
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	490	Total	O	0	0
			490	490		
8	B	267	Total	O	0	0
			267	267		
8	C	74	Total	O	0	0
			74	74		
8	D	1	Total	O	0	0
			1	1		

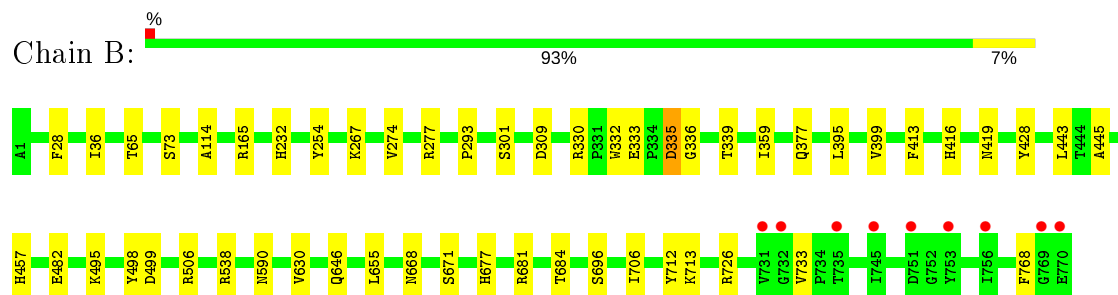
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

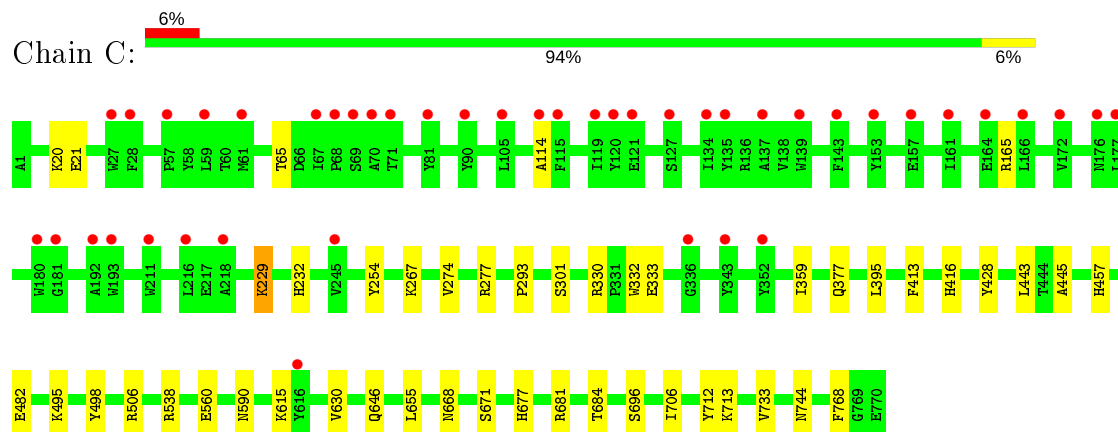
#### • Molecule 1: Alginate lyase



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A1	Y103	H205	H511	D383	A445	V518	N583	F644	L704	I764
T5	R104	L212	S312	W384	E446	A519	N584	M645	D705	I765
Y6	L105	N213	T313	F386	H447	D520	G587	Q646	I706	I766
A107	R106	A219	A314	N387	N448	Q521	A588	L648	S707	I767
F9	T108	L223	K315	N388	N449	F522	F589	M649	D708	F768
S25	L111	Y223	L316	P389	V450	S524	N590	M650	E709	F769
L26	A114	Y233	A317	N390	I451	D525	S591	A651	T710	E770
W27	F115	Y233	N318	N391	A452	R526	Y592	E652	Y712	
F28	D116	F115	L319	R392	A453	K527	G593	N653	K713	
T29	G117	V241	Q321	R393	N454	V528	Y594	S654	G714	
K30	F118	V245	W322	L394	E456	Y529	L595	L655	T715	
S31	I119	F245	F325	L395	H457	Y530	N596	G656	T716	
D32	Y120	L248	N526	F396	V461	D531	A597	D657	A717	
I33	E121	P249	F329	Q397	S462	L532	R598	T659	L718	
Q34	Y125	F250	F329	R397	A466	Y533	Q599	T660	L719	
K35	T126	Y254	E332	A401	T466	G536	I600	D661	N720	
I36	V126	V257	E333	A402	P467	G537	A601	A662	E721	
M41	S127	V260	P334	H405	V468	R538	K602	T663	T722	
T46	G128	N261	D335	Y406	S469	G539	D603	F664	T723	
E48	I129	Y138	G336	H407	R470	E540	T604	A665	E724	
L49	G130		S337	Y408	D474	S542	M605	Y666	L725	
W50	Y139		Y443	D409	D475	G543	F606	T667	R726	
E51	N142		T346	H410	D476	T544	I609	E669	T727	
T60	A144		T349	S412	F477	N546	V611	M670	F730	
M61	A147		D350	F413	F478	Y547	G612	N672	G732	
E62	D148		Q351	S414	D479	R548	L613	N673	T733	
T65	Y149		T352	I414	Q481	L549	S614	E674	P734	
D66	Y153		S357	H415	Q482	H550	K615	L675	T735	
I67	L154		T358	H416	K483	T551	G616	Q676	E736	
P68	S155		I359	E418	E484	Y552	A617	H677	S737	
S69	D158		E360	N419	V486	G558	D618	F678	V738	
A70	D159		Q361	Q420	M496	A561	I619	S679	V739	
D72	E160		K363	M421	N496	R562	P620	E681	W740	
S73	I161		P364	M422	S497	M563	E621	Q682	N741	
D74	I182		D365	A423	Y498	A564	V622	G683	G742	
I77	A167		V366	S426	D499	A565	D624	T684	E743	
I87	Y172		S367	S427	F500	V566	L625	L686	I745	
A88	G181		T368	Y428	S501	V567	S626	D887	E746	
K89	G194		T369	R430	G502	F568	T627	Y688	F747	
N91	G194		V370	N431	K503	P569	D628	K689	V749	
A92	L200		F371	Y433	Q504	S570	V630	G690	E750	
F93	T201		N372	Y434	I505	K571	V631	E691	D751	
N94	I202		N373	E435	R506	E572	G632	N692	G752	
Y95	S203		N374	E436	A507	S573	G633	I693	Y753	
L96	T202		S301	G436	I508	L574	T634	F694	T754	
N97	I203		Q302	I437	G509	F575	V635	V695	V755	
T98	S204		D307	R438	F510	V576	V636	S696	I756	
G99			T308	T439	P511	D577	K637	N697	Q757	
			D309	W441	R512	K578	D638	K698	V758	
			T310	Y442	Q513	E579	N639	P699	A759	
				L443	F516	G580	E640	I700	E760	
				S382	V517	V582	K641	T701	G761	
							D642	F702	E762	
							T643	A703	D763	



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	261.32Å 394.81Å 112.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.90 – 2.07 98.70 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.5 (98.90-2.07) 99.5 (98.70-2.07)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.222 , 0.240 0.228 , 0.245	Depositor DCC
$R_{free}$ test set	17175 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, CA, MN, EDO, ACT, CAC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.69	0/6413	0.85	4/8727 (0.0%)
1	B	0.67	0/6413	0.83	3/8727 (0.0%)
1	C	0.65	0/6413	0.81	0/8727
1	D	0.87	0/3079	0.87	0/3847
All	All	0.70	0/22318	0.83	7/30028 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	MET	CA-CB-CG	-6.10	102.93	113.30
1	B	309	ASP	CB-CA-C	-5.49	99.41	110.40
1	A	770	GLU	CA-C-O	-5.49	108.58	120.10
1	A	470	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	B	726	ARG	NE-CZ-NH1	-5.41	117.60	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	6240	0	5798	36	0
1	B	6240	0	5798	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6240	0	5798	27	0
1	D	3080	0	834	0	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	8	0	6	1	0
5	B	8	0	6	0	0
5	C	4	0	3	0	0
6	A	20	0	30	0	0
6	B	12	0	18	0	0
6	C	4	0	6	0	0
7	A	5	0	0	2	0
8	A	490	0	0	7	0
8	B	267	0	0	3	0
8	C	74	0	0	1	0
8	D	1	0	0	0	0
All	All	22705	0	18297	86	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 2.

The worst 5 of 86 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:668:ASN:HD22	1:A:677:HIS:HD2	1.27	0.82
1:A:599:GLN:HE21	7:A:812:CAC:C1	1.96	0.78
1:C:668:ASN:HD22	1:C:677:HIS:HD2	1.32	0.78
1:B:668:ASN:HD22	1:B:677:HIS:HD2	1.32	0.77
1:A:37:LYS:NZ	1:C:744:ASN:HD21	1.93	0.67

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	768/770 (100%)	740 (96%)	27 (4%)	1 (0%)	51	45
1	B	768/770 (100%)	738 (96%)	29 (4%)	1 (0%)	51	45
1	C	768/770 (100%)	736 (96%)	31 (4%)	1 (0%)	51	45
1	D	768/770 (100%)	727 (95%)	39 (5%)	2 (0%)	41	32
All	All	3072/3080 (100%)	2941 (96%)	126 (4%)	5 (0%)	47	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	671	SER
1	B	671	SER
1	C	671	SER
1	D	671	SER
1	D	711	GLN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	671/671 (100%)	668 (100%)	3 (0%)	91	91
1	B	671/671 (100%)	664 (99%)	7 (1%)	76	75
1	C	671/671 (100%)	665 (99%)	6 (1%)	78	78
All	All	2013/2013 (100%)	1997 (99%)	16 (1%)	81	81

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	428	TYR
1	B	499	ASP
1	C	254	TYR
1	B	335	ASP
1	C	267	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	535	HIS
1	B	668	ASN
1	C	677	HIS
1	B	559	GLN
1	B	596	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 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
6	EDO	C	806	-	3,3,3	0.08	0	2,2,2	0.19	0
7	CAC	A	812	-	0,4,4	0.00	-	0,6,6	0.00	-
6	EDO	B	807	-	3,3,3	0.13	0	2,2,2	0.01	0
6	EDO	A	807	-	3,3,3	0.28	0	2,2,2	0.30	0
5	ACT	A	805	-	1,3,3	3.07	1 (100%)	0,3,3	0.00	-
6	EDO	A	810	-	3,3,3	0.08	0	2,2,2	0.29	0
5	ACT	B	805	-	1,3,3	3.39	1 (100%)	0,3,3	0.00	-
5	ACT	A	806	-	1,3,3	2.93	1 (100%)	0,3,3	0.00	-
6	EDO	B	809	-	3,3,3	0.09	0	2,2,2	0.10	0
5	ACT	B	806	-	1,3,3	3.66	1 (100%)	0,3,3	0.00	-
6	EDO	A	811	-	3,3,3	0.17	0	2,2,2	0.36	0
6	EDO	A	809	-	3,3,3	0.09	0	2,2,2	0.19	0
6	EDO	A	808	-	3,3,3	0.07	0	2,2,2	0.18	0
6	EDO	B	808	-	3,3,3	0.24	0	2,2,2	0.20	0
5	ACT	C	805	-	1,3,3	3.70	1 (100%)	0,3,3	0.00	-

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
6	EDO	C	806	-	-	1/1/1/1	-
6	EDO	A	811	-	-	0/1/1/1	-
6	EDO	B	807	-	-	0/1/1/1	-
6	EDO	A	807	-	-	0/1/1/1	-
6	EDO	A	810	-	-	1/1/1/1	-
6	EDO	B	809	-	-	0/1/1/1	-
6	EDO	A	808	-	-	0/1/1/1	-
6	EDO	B	808	-	-	0/1/1/1	-
6	EDO	A	809	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	805	ACT	CH3-C	3.70	1.53	1.48
5	B	806	ACT	CH3-C	3.66	1.53	1.48
5	B	805	ACT	CH3-C	3.39	1.53	1.48
5	A	805	ACT	CH3-C	3.07	1.52	1.48
5	A	806	ACT	CH3-C	2.93	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	806	EDO	O1-C1-C2-O2
6	A	810	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	812	CAC	2	0
5	A	806	ACT	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	770/770 (100%)	0.09	1 (0%) 95 95	22, 33, 56, 87	0
1	B	770/770 (100%)	0.07	9 (1%) 79 80	26, 44, 77, 120	0
1	C	770/770 (100%)	0.33	44 (5%) 23 24	41, 60, 89, 115	0
1	D	770/770 (100%)	3.11	493 (64%) 0 0	60, 90, 129, 146	0
All	All	3080/3080 (100%)	0.90	547 (17%) 1 1	22, 55, 112, 146	0

The worst 5 of 547 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	706	ILE	13.3
1	D	732	GLY	12.9
1	D	731	VAL	12.8
1	D	658	ILE	11.1
1	D	753	TYR	10.5

### 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](#)

There are no carbohydrates 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
6	EDO	A	810	4/4	0.31	0.29	63,88,90,104	0
7	CAC	A	812	5/5	0.74	0.30	46,62,135,159	0
6	EDO	A	809	4/4	0.74	0.18	72,74,74,77	0
6	EDO	C	806	4/4	0.76	0.22	74,77,86,98	0
3	MG	C	802	1/1	0.81	0.08	72,72,72,72	0
6	EDO	B	809	4/4	0.83	0.29	55,61,62,70	0
6	EDO	A	808	4/4	0.83	0.16	66,69,75,79	0
5	ACT	A	806	4/4	0.87	0.12	53,56,64,67	0
5	ACT	C	805	4/4	0.90	0.12	60,67,68,70	0
6	EDO	B	807	4/4	0.91	0.19	42,46,49,50	0
6	EDO	A	811	4/4	0.91	0.14	47,48,52,86	0
6	EDO	A	807	4/4	0.92	0.16	24,25,31,32	0
3	MG	B	802	1/1	0.92	0.07	56,56,56,56	0
5	ACT	B	806	4/4	0.93	0.14	48,52,60,77	0
4	CA	C	803	1/1	0.94	0.11	51,51,51,51	0
6	EDO	B	808	4/4	0.94	0.12	31,38,44,57	0
5	ACT	B	805	4/4	0.95	0.15	33,44,46,64	0
3	MG	A	802	1/1	0.95	0.04	50,50,50,50	0
2	MN	C	801	1/1	0.96	0.14	51,51,51,51	0
5	ACT	A	805	4/4	0.96	0.18	31,40,50,56	0
4	CA	C	804	1/1	0.97	0.14	45,45,45,45	0
4	CA	A	804	1/1	0.98	0.18	29,29,29,29	0
4	CA	B	804	1/1	0.99	0.15	46,46,46,46	0
2	MN	A	801	1/1	0.99	0.20	24,24,24,24	0
4	CA	A	803	1/1	0.99	0.18	26,26,26,26	0
4	CA	B	803	1/1	0.99	0.16	30,30,30,30	0
2	MN	B	801	1/1	0.99	0.19	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.