



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:37 AM UTC

PDB ID : 6JP4 / pdb\_00006jp4  
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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

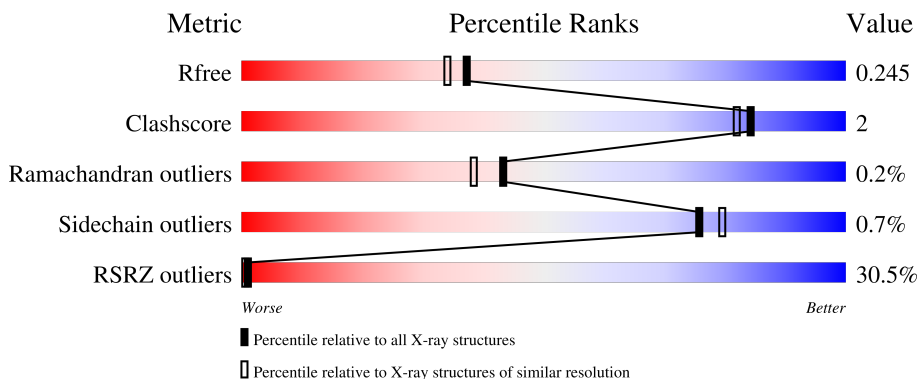
# 1 Overall quality at a glance

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))
$R_{free}$	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (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 of 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	 2% 92% 8%
1	B	770	 5% 92% 8%
1	C	770	 20% 93% 7%
1	D	770	 94% 99% 7%

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
7	CAC	A	812	-	X	-	-

## 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 (CCD ID: MN) (formula: Mn).

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

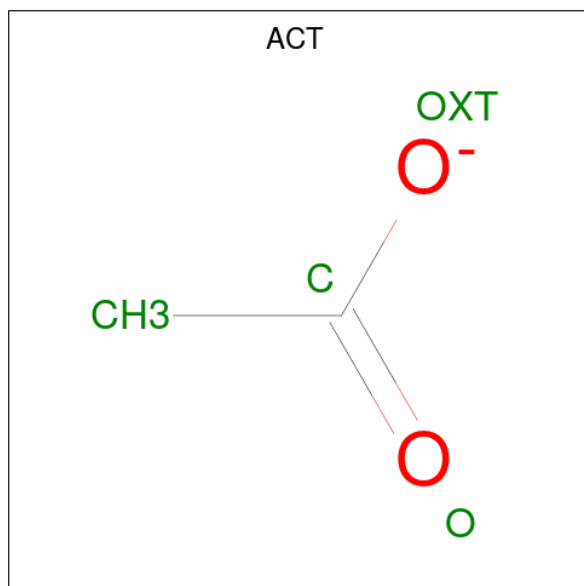
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



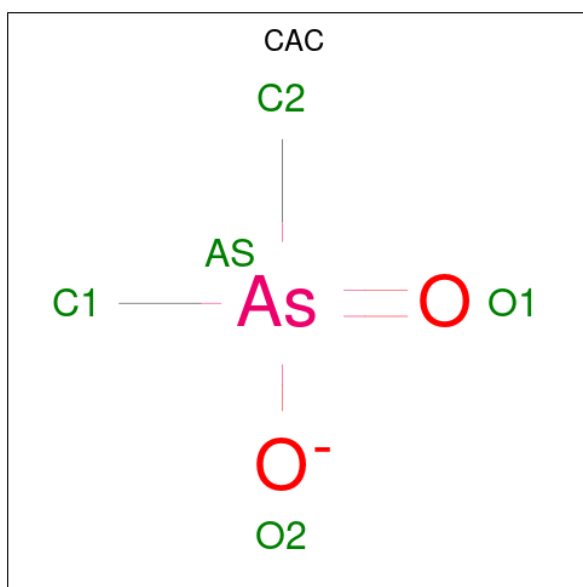
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 7 is CACODYLATE ION (CCD ID: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



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

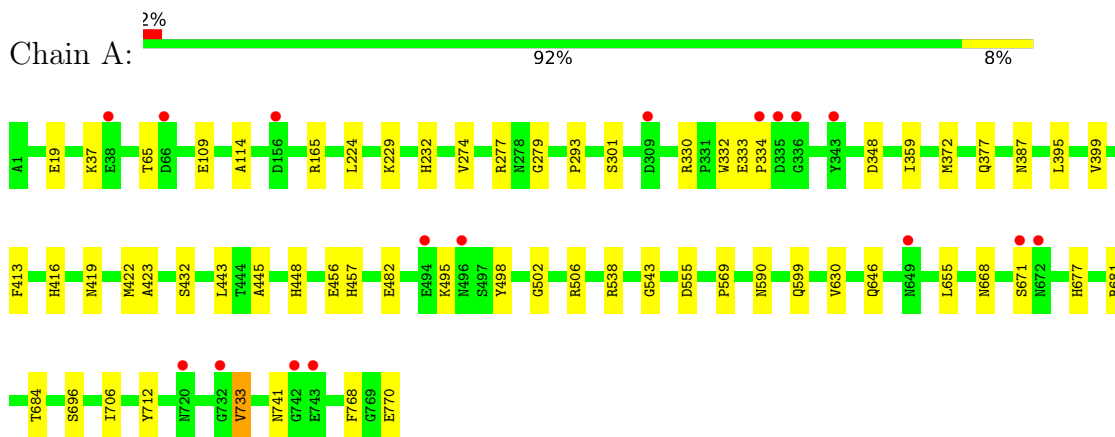
- Molecule 8 is water.

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		

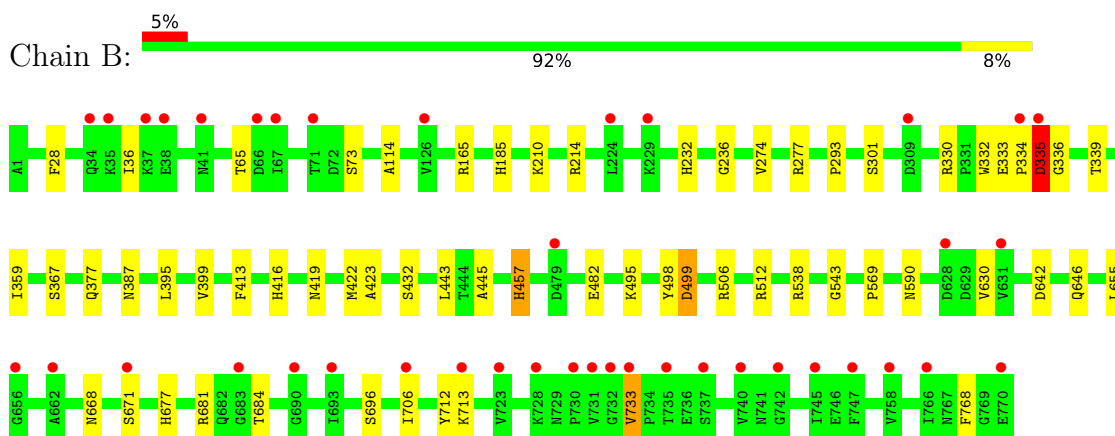
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

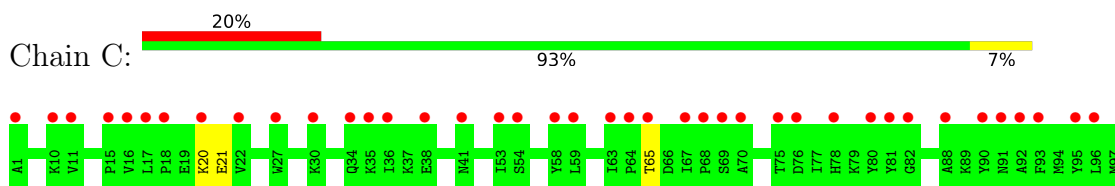
- Molecule 1: Alginate lyase

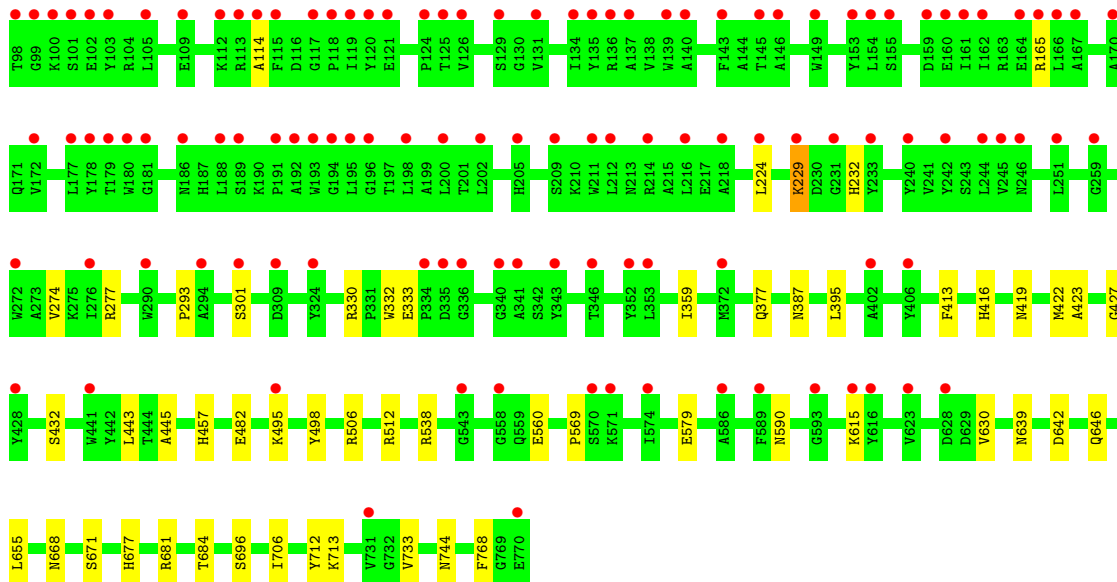


- Molecule 1: Alginate lyase

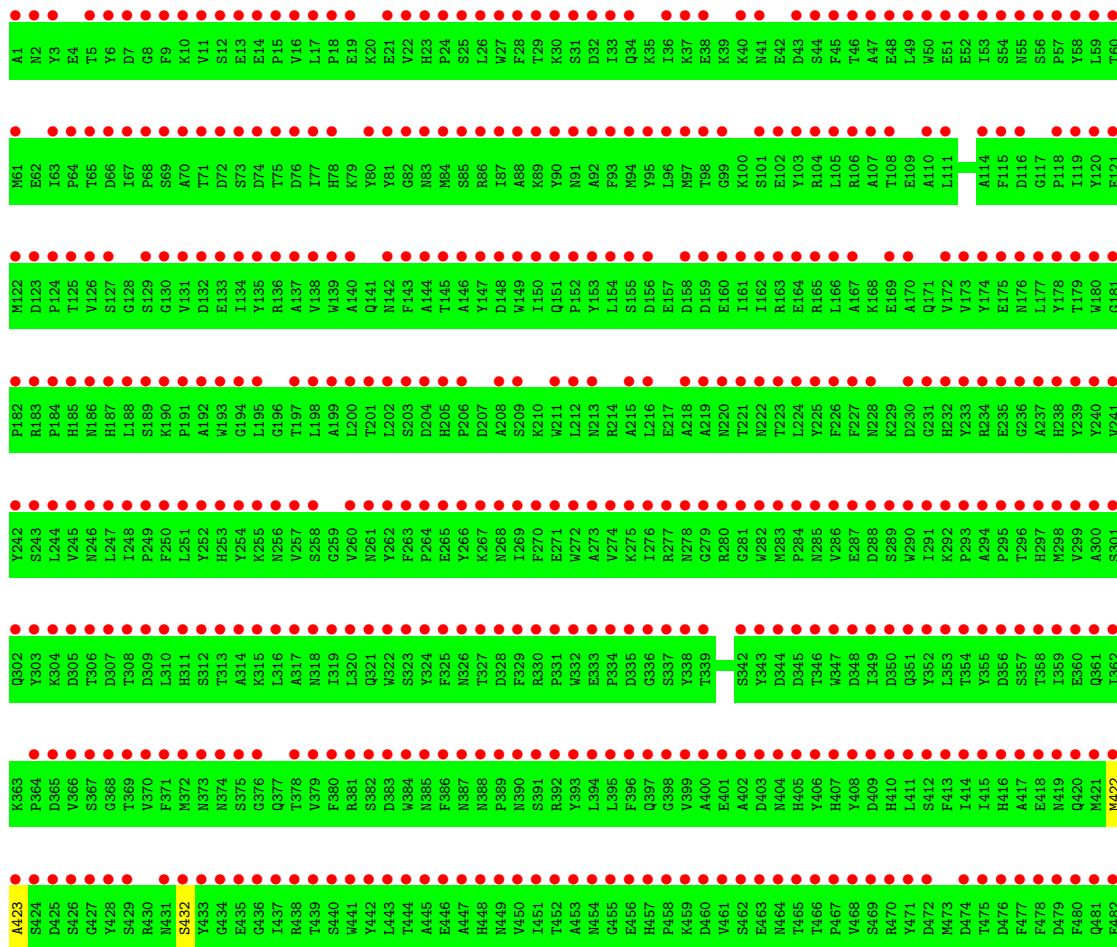


- Molecule 1: Alginate lyase





● Molecule 1: Alginate lyase



K483	G543	D603	T663	V723
E484	E544	T604	F664	E724
A485	G545	M605	A665	L725
V486	M546	F606	Y666	R726
Y487	M547	M607	T667	V727
D488	B548	Q608	N668	K728
G489	L549	I609	E669	N729
F490	M550	I610	M670	F730
T491	T551	V611	S671	V731
F492	Y552	P612	N672	G732
P493	E553	L613	M673	V733
E494	D554	S614	E674	P734
K495	D555	K615	L675	T735
M496	A556	Y616	Q676	E736
S497	Y557	A617	H677	S737
Y498	G558	D618	F678	V738
D499	O559	I619	S679	V739
F500	E560	P620	V680	V740
S501	A561	E621	R681	N741
G502	K562	V622	Q682	G742
A503	M563	V623	G683	E743
Q504	A564	D624	T684	N744
I505	A565	L625	S685	I745
R506	W566	S626	L686	E746
A507	W567	T627	D687	F747
I508	F568	D628	Y688	S748
G509	F569	D629	K689	V749
F510	S570	V630	G690	E750
P511	K571	V631	E691	D751
R512	E572	G632	M692	G752
O513	S573	G633	I693	V753
D514	L574	T634	F694	T754
Y515	F575	V635	V695	V755
F516	D576	V636	S696	I756
V517	D577	K637	N697	Q757
V518	K578	D638	K698	V758
A519	E579	M639	P699	A759
D520	G580	E640	I700	E760
Q521	E581	K641	T701	G761
F523	V582	D642	F702	G762
S524	M583	T643	A703	D763
D525	Y584	F644	L704	I764
K526	E585	M645	D705	M765
E527	A586	Q646	I706	I766
V528	G587	Q647	S707	M767
Q529	A588	L648	D708	F768
Y530	F589	M649	E709	G769
D531	M590	M650	T710	E770
L532	S591	A651	Q711	
Y533	Y592	E652	Y712	
L534	G593	M653	K713	
H535	Y594	S654	G714	
G536	L595	L655	T715	
O537	M596	G656	I716	
R538	A597	D657	A717	
G539	R598	I658	A718	
E540	Q599	T659	L719	
M541	L600	T660	N720	
S542	K602	A662	E721	
			T722	

## 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 98.90 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.5 (98.90-2.07) 99.5 (98.90-2.07)	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)	Xtrriage
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	Xtrriage
Anisotropy	0.494	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 66.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage'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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, CA, MG, MN, CAC, EDO

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	1.01	2/6413 (0.0%)	1.32	10/8727 (0.1%)
1	B	1.00	3/6413 (0.0%)	1.33	13/8727 (0.1%)
1	C	0.97	0/6413	1.31	6/8727 (0.1%)
1	D	1.42	0/3079	1.80	2/3847 (0.1%)
All	All	1.06	5/22318 (0.0%)	1.39	31/30028 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	448	HIS	CE1-NE2	6.84	1.39	1.32
1	A	502	GLY	C-O	5.45	1.29	1.23
1	B	457	HIS	CE1-NE2	5.40	1.38	1.32
1	B	214	ARG	CD-NE	5.29	1.53	1.46
1	B	185	HIS	CE1-NE2	5.13	1.37	1.32

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	770	GLU	CA-C-O	-7.19	108.58	120.80
1	B	499	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	569	PRO	CA-C-N	6.55	130.64	120.82
1	A	569	PRO	C-N-CA	6.55	130.64	120.82
1	B	335	ASP	CA-CB-CG	6.55	119.15	112.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6240	0	5798	37	0
1	B	6240	0	5798	30	0
1	C	6240	0	5798	29	0
1	D	3080	0	834	1	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	8	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	94	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 94 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	768/770 (100%)	740 (96%)	27 (4%)	1 (0%)	48	44
1	B	768/770 (100%)	738 (96%)	29 (4%)	1 (0%)	48	44
1	C	768/770 (100%)	736 (96%)	31 (4%)	1 (0%)	48	44
1	D	768/770 (100%)	727 (95%)	39 (5%)	2 (0%)	36	30
All	All	3072/3080 (100%)	2941 (96%)	126 (4%)	5 (0%)	43	38

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 [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	671/671 (100%)	668 (100%)	3 (0%)	84	87
1	B	671/671 (100%)	665 (99%)	6 (1%)	70	74
1	C	671/671 (100%)	665 (99%)	6 (1%)	70	74
All	All	2013/2013 (100%)	1998 (99%)	15 (1%)	76	79

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

Mol	Chain	Res	Type
1	B	713	LYS
1	C	639	ASN
1	B	733	VAL
1	C	713	LYS
1	C	229	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	692	ASN
1	C	481	GLN
1	B	744	ASN
1	C	416	HIS
1	C	559	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](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	A	807	-	3,3,3	0.28	0	2,2,2	0.22	0
6	EDO	B	807	-	3,3,3	0.13	0	2,2,2	0.07	0
6	EDO	B	809	-	3,3,3	0.09	0	2,2,2	0.09	0
6	EDO	C	806	-	3,3,3	0.08	0	2,2,2	0.12	0
5	ACT	C	805	-	3,3,3	0.97	0	3,3,3	0.89	0
7	CAC	A	812	-	2,4,4	2.67	2 (100%)	4,6,6	1.88	2 (50%)
6	EDO	A	810	-	3,3,3	0.08	0	2,2,2	0.21	0
6	EDO	B	808	-	3,3,3	0.24	0	2,2,2	0.14	0
5	ACT	A	805	-	3,3,3	1.26	0	3,3,3	0.54	0
5	ACT	A	806	-	3,3,3	0.88	0	3,3,3	0.91	0
5	ACT	B	805	-	3,3,3	0.85	0	3,3,3	1.01	0
6	EDO	A	809	-	3,3,3	0.09	0	2,2,2	0.13	0
6	EDO	A	811	-	3,3,3	0.17	0	2,2,2	0.30	0
5	ACT	B	806	-	3,3,3	1.14	0	3,3,3	0.67	0
6	EDO	A	808	-	3,3,3	0.07	0	2,2,2	0.11	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
6	EDO	A	807	-	-	0/1/1/1	-
6	EDO	B	807	-	-	0/1/1/1	-
6	EDO	B	809	-	-	0/1/1/1	-
6	EDO	C	806	-	-	1/1/1/1	-
6	EDO	A	810	-	-	1/1/1/1	-
6	EDO	B	808	-	-	0/1/1/1	-
6	EDO	A	809	-	-	0/1/1/1	-
6	EDO	A	811	-	-	0/1/1/1	-
6	EDO	A	808	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	812	CAC	AS-C2	2.76	1.96	1.90
7	A	812	CAC	AS-C1	2.58	1.96	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	812	CAC	O1-AS-C1	-2.56	108.31	111.50
7	A	812	CAC	O1-AS-C2	-2.02	108.99	111.50

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%)	-0.06	17 (2%) 62 64	22, 33, 56, 87	0
1	B	770/770 (100%)	0.54	40 (5%) 33 32	26, 44, 76, 120	0
1	C	770/770 (100%)	1.26	156 (20%) 3 2	41, 60, 89, 115	0
1	D	770/770 (100%)	3.72	726 (94%) 0 0	60, 90, 129, 146	0
All	All	3080/3080 (100%)	1.36	939 (30%) 1 0	22, 55, 112, 146	0

The worst 5 of 939 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	233	TYR	8.7
1	D	270	PHE	8.0
1	D	272	TRP	7.7
1	D	303	TYR	7.6
1	D	402	ALA	7.0

### 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 oligosaccharides 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	0.73	0.27	63,88,90,104	0
6	EDO	C	806	4/4	0.77	0.25	74,77,86,98	0
7	CAC	A	812	5/5	0.77	0.21	46,62,135,159	0
6	EDO	A	811	4/4	0.82	0.22	47,48,52,86	0
3	MG	C	802	1/1	0.84	0.14	72,72,72,72	0
5	ACT	B	806	4/4	0.86	0.22	48,52,60,77	0
6	EDO	B	809	4/4	0.86	0.22	55,61,62,70	0
5	ACT	A	806	4/4	0.87	0.18	53,56,64,67	0
6	EDO	A	809	4/4	0.88	0.18	72,74,74,77	0
6	EDO	B	807	4/4	0.89	0.17	42,46,49,50	0
5	ACT	C	805	4/4	0.89	0.17	60,67,68,70	0
6	EDO	B	808	4/4	0.91	0.14	31,38,44,57	0
5	ACT	A	805	4/4	0.91	0.16	31,40,50,56	0
5	ACT	B	805	4/4	0.92	0.15	33,44,46,64	0
6	EDO	A	808	4/4	0.94	0.13	66,69,75,79	0
6	EDO	A	807	4/4	0.95	0.09	24,25,31,32	0
3	MG	A	802	1/1	0.95	0.07	50,50,50,50	0
3	MG	B	802	1/1	0.96	0.05	56,56,56,56	0
4	CA	C	803	1/1	0.97	0.06	51,51,51,51	0
4	CA	B	804	1/1	0.98	0.04	46,46,46,46	0
2	MN	C	801	1/1	0.98	0.05	51,51,51,51	0
4	CA	C	804	1/1	0.98	0.05	45,45,45,45	0
4	CA	A	804	1/1	0.99	0.02	29,29,29,29	0
4	CA	B	803	1/1	0.99	0.02	30,30,30,30	0
2	MN	B	801	1/1	0.99	0.02	28,28,28,28	0
4	CA	A	803	1/1	0.99	0.02	26,26,26,26	0
2	MN	A	801	1/1	1.00	0.02	24,24,24,24	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.