



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 12:14 AM BST

PDB ID : 5O80
Title : Crystal Structure of R67A Mutant of alpha-L-arabinofuranosidase Ara51 from Clostridium thermocellum in complex with L-Arabinofuranose
Authors : Lafite, P.; Daniellou, R.
Deposited on : 2017-06-12
Resolution : 2.92 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 ⓘ symbol.

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	:	2.13.1
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)	:	2.13.1

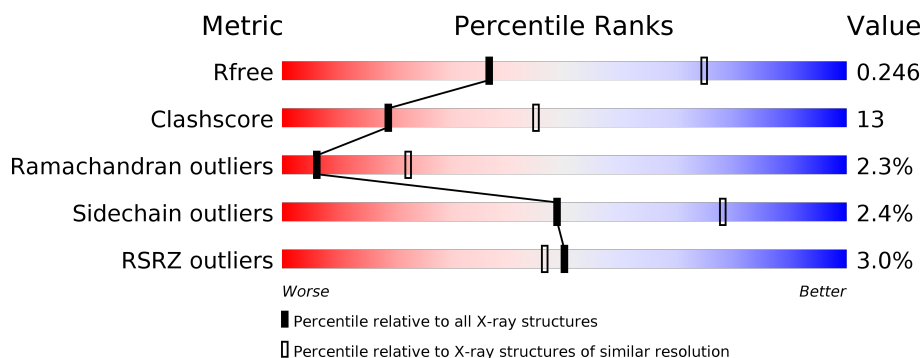
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 ≥ 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	501	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>..</div> </div> </div>
1	B	501	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>..</div> </div> </div>
1	C	501	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>..</div> </div> </div>
1	D	501	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>..</div> </div> </div>
1	E	501	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>..</div> </div> </div>
1	F	501	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>..</div> </div> </div>

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
3	DIO	A	601	-	-	X	-
3	DIO	B	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23944 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.

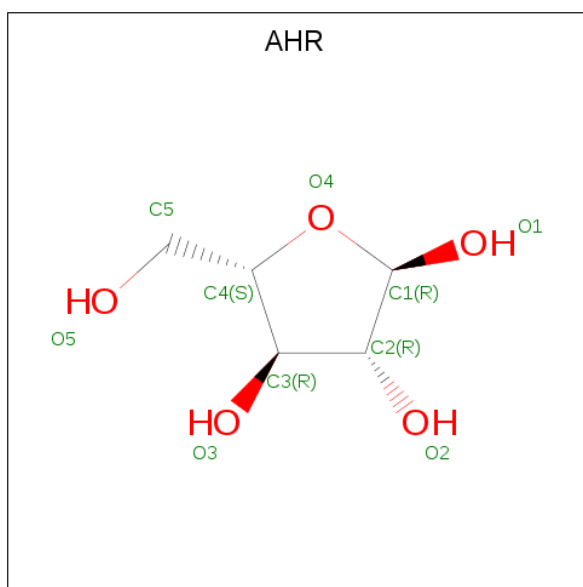
- Molecule 1 is a protein called Intracellular exo-alpha-(1->5)-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	1	0
			3978	2527	675	754	22			
1	B	496	Total	C	N	O	S	0	1	0
			3978	2527	674	755	22			
1	C	496	Total	C	N	O	S	0	1	0
			3962	2518	669	752	23			
1	D	496	Total	C	N	O	S	0	1	0
			3978	2527	674	755	22			
1	E	496	Total	C	N	O	S	0	0	0
			3963	2519	670	752	22			
1	F	496	Total	C	N	O	S	0	1	0
			3977	2527	674	754	22			

There are 6 discrepancies between the modelled and reference sequences:

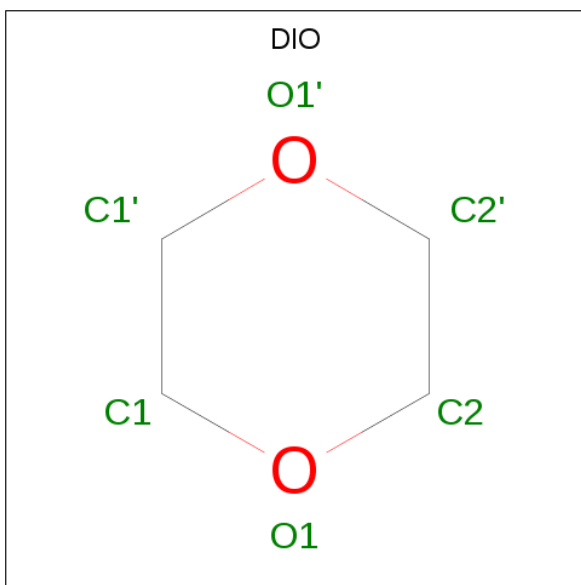
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ALA	ARG	engineered mutation	UNP A3DIH0
B	67	ALA	ARG	engineered mutation	UNP A3DIH0
C	67	ALA	ARG	engineered mutation	UNP A3DIH0
D	67	ALA	ARG	engineered mutation	UNP A3DIH0
E	67	ALA	ARG	engineered mutation	UNP A3DIH0
F	67	ALA	ARG	engineered mutation	UNP A3DIH0

- Molecule 2 is alpha-L-arabinofuranose (three-letter code: AHR) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	1	Total	C	O	0	0
			10	5	5		
2	E	1	Total	C	O	0	0
			10	5	5		
2	F	1	Total	C	O	0	0
			10	5	5		

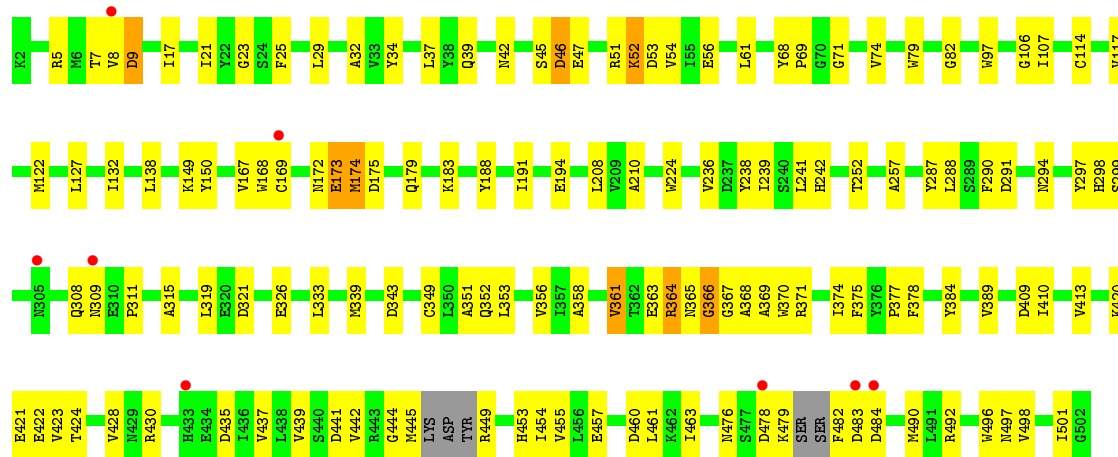
- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



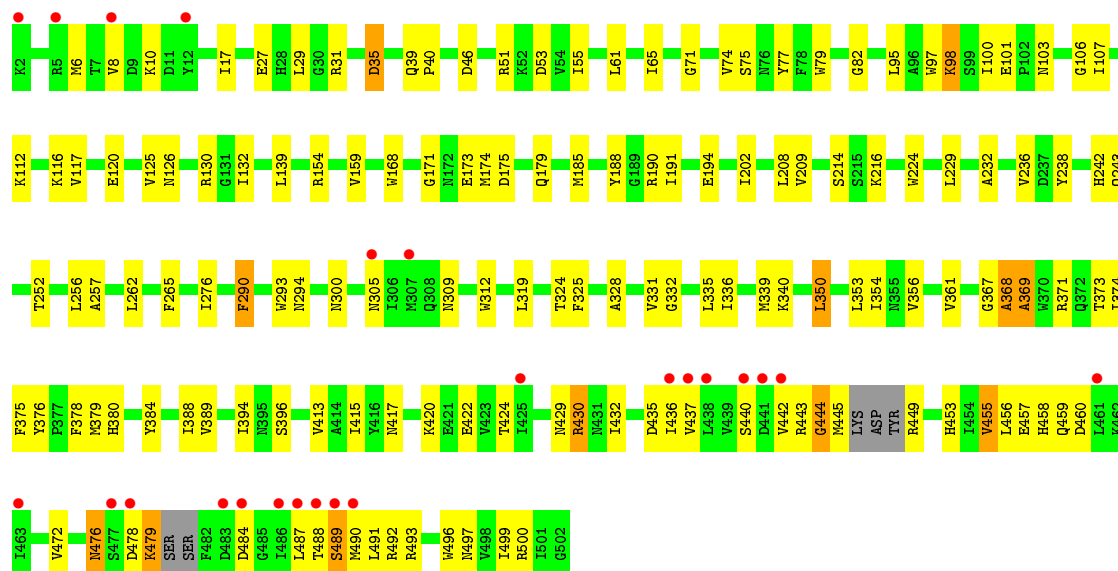
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	B	1	Total	C	O	0	0
			6	4	2		
3	C	1	Total	C	O	0	0
			6	4	2		
3	D	1	Total	C	O	0	0
			6	4	2		
3	E	1	Total	C	O	0	0
			6	4	2		
3	F	1	Total	C	O	0	0
			6	4	2		

- Molecule 4 is water.

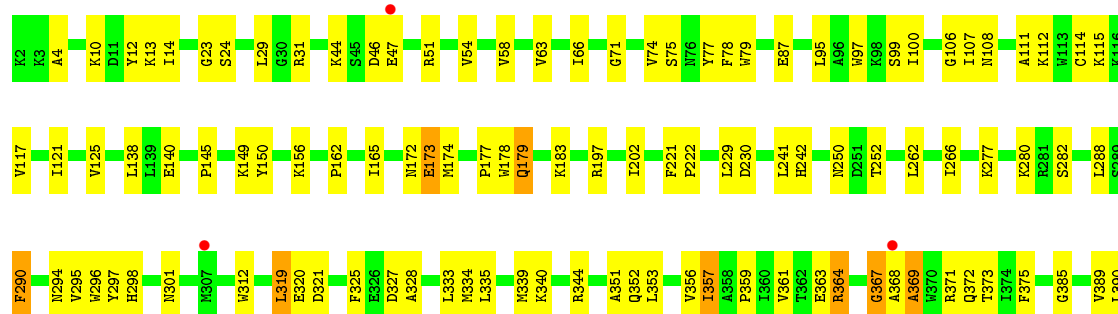
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	2	Total	O	0	0
			2	2		
4	C	2	Total	O	0	0
			2	2		
4	D	2	Total	O	0	0
			2	2		
4	E	3	Total	O	0	0
			3	3		
4	F	2	Total	O	0	0
			2	2		

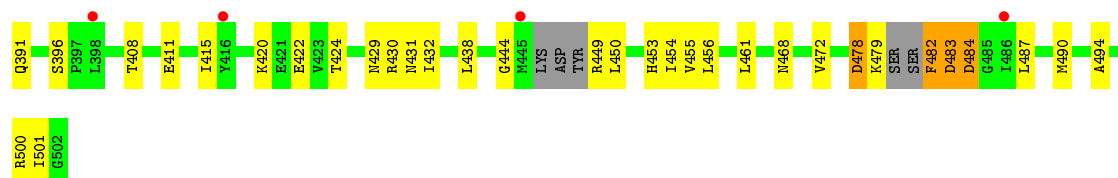


• Molecule 1: Intracellular exo- α -(1 \rightarrow 5)-L-arabinofuranosidase

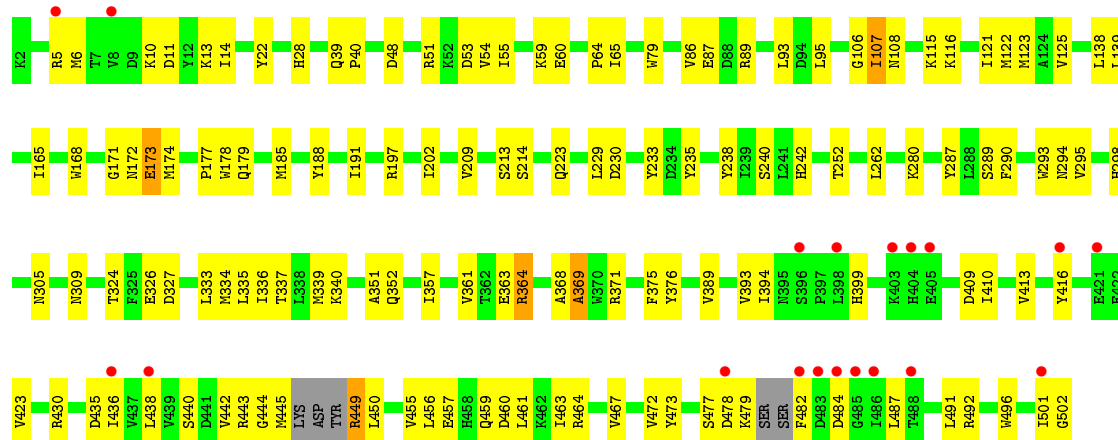


• Molecule 1: Intracellular exo- α -(1 \rightarrow 5)-L-arabinofuranosidase





- Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.74Å 173.74Å 271.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 2.92 48.76 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.76-2.92) 99.9 (48.76-2.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.179 , 0.246 0.179 , 0.246	Depositor DCC
R_{free} test set	4538 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23944	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AHR, DIO

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	0.55	0/4068	0.69	0/5509
1	B	0.49	0/4068	0.66	0/5509
1	C	0.54	0/4055	0.67	0/5494
1	D	0.49	0/4068	0.68	0/5509
1	E	0.48	0/4053	0.64	0/5490
1	F	0.50	0/4067	0.64	0/5508
All	All	0.51	0/24379	0.66	0/33019

There are no bond length outliers.

There are no bond angle outliers.

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	3978	0	3869	128	0
1	B	3978	0	3867	102	0
1	C	3962	0	3845	102	0
1	D	3978	0	3867	124	0
1	E	3963	0	3851	93	0
1	F	3977	0	3864	86	0
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
3	A	6	0	8	4	0
3	B	6	0	8	4	0
3	C	6	0	8	2	0
3	D	6	0	8	2	0
3	E	6	0	8	1	0
3	F	6	0	8	3	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
All	All	23944	0	23211	619	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 13.

The worst 5 of 619 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:240:SER:C	1:A:241:LEU:HD23	1.66	1.15
1:A:240:SER:C	1:A:241:LEU:CD2	2.16	1.14
1:D:256:LEU:O	1:D:430:ARG:NH2	1.83	1.11
1:A:240:SER:O	1:A:241:LEU:HD22	1.51	1.10
1:A:241:LEU:HD11	1:A:269:VAL:HG11	1.13	1.09

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	491/501 (98%)	447 (91%)	36 (7%)	8 (2%)	9	31
1	B	491/501 (98%)	436 (89%)	42 (9%)	13 (3%)	5	19
1	C	491/501 (98%)	438 (89%)	40 (8%)	13 (3%)	5	19
1	D	491/501 (98%)	427 (87%)	55 (11%)	9 (2%)	8	28
1	E	490/501 (98%)	438 (89%)	39 (8%)	13 (3%)	5	18
1	F	491/501 (98%)	441 (90%)	38 (8%)	12 (2%)	6	21
All	All	2945/3006 (98%)	2627 (89%)	250 (8%)	68 (2%)	6	22

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	GLU
1	A	364	ARG
1	A	444	GLY
1	A	484	ASP
1	B	250	ASN

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	429/439 (98%)	416 (97%)	13 (3%)	41	73
1	B	429/439 (98%)	416 (97%)	13 (3%)	41	73
1	C	427/439 (97%)	422 (99%)	5 (1%)	71	90
1	D	429/439 (98%)	417 (97%)	12 (3%)	43	75
1	E	427/439 (97%)	417 (98%)	10 (2%)	50	79
1	F	428/439 (98%)	418 (98%)	10 (2%)	50	79
All	All	2569/2634 (98%)	2506 (98%)	63 (2%)	49	77

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	290	PHE
1	D	396	SER
1	F	416	TYR
1	C	361	VAL
1	D	290	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	309	ASN
1	D	172	ASN
1	E	250	ASN
1	C	497	ASN
1	D	72	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DIO	E	601	-	6,6,6	0.54	0	6,6,6	0.72	0
3	DIO	D	601	-	6,6,6	0.54	0	6,6,6	0.61	0
3	DIO	A	601	-	6,6,6	0.52	0	6,6,6	0.36	0
3	DIO	B	601	-	6,6,6	0.44	0	6,6,6	0.57	0
2	AHR	A	600	-	10,10,10	1.66	2 (20%)	13,14,14	1.11	1 (7%)
2	AHR	B	600	-	10,10,10	1.95	2 (20%)	13,14,14	1.60	3 (23%)
2	AHR	C	600	-	10,10,10	1.71	2 (20%)	13,14,14	1.74	3 (23%)
3	DIO	F	601	-	6,6,6	0.48	0	6,6,6	0.71	0
2	AHR	E	600	-	10,10,10	1.94	4 (40%)	13,14,14	1.60	3 (23%)
2	AHR	D	600	-	10,10,10	1.63	2 (20%)	13,14,14	1.35	1 (7%)
3	DIO	C	601	-	6,6,6	0.41	0	6,6,6	0.40	0
2	AHR	F	600	-	10,10,10	1.64	3 (30%)	13,14,14	1.39	2 (15%)

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	DIO	E	601	-	-	-	0/1/1/1
3	DIO	D	601	-	-	-	0/1/1/1
3	DIO	A	601	-	-	-	0/1/1/1
3	DIO	F	601	-	-	-	0/1/1/1
3	DIO	B	601	-	-	-	0/1/1/1
2	AHR	A	600	-	-	0/2/18/18	0/1/1/1
2	AHR	C	600	-	-	0/2/18/18	0/1/1/1
2	AHR	B	600	-	-	2/2/18/18	0/1/1/1
2	AHR	E	600	-	-	1/2/18/18	0/1/1/1
2	AHR	D	600	-	-	0/2/18/18	0/1/1/1
3	DIO	C	601	-	-	-	0/1/1/1
2	AHR	F	600	-	-	0/2/18/18	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	AHR	C2-C3	-3.70	1.43	1.53
2	B	600	AHR	C1-C2	-3.69	1.48	1.52
2	A	600	AHR	C2-C3	-3.62	1.43	1.53
2	C	600	AHR	C2-C3	-3.56	1.43	1.53
2	E	600	AHR	C2-C3	-3.37	1.44	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	AHR	C1-C2-C3	4.28	107.66	102.30
2	C	600	AHR	C5-C4-C3	-4.10	105.20	115.09
2	E	600	AHR	C1-C2-C3	3.84	107.10	102.30
2	F	600	AHR	C1-C2-C3	3.52	106.70	102.30
2	B	600	AHR	C1-C2-C3	3.39	106.54	102.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	AHR	O4-C4-C5-O5
2	B	600	AHR	C3-C4-C5-O5
2	E	600	AHR	O4-C4-C5-O5

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	DIO	1	0
3	D	601	DIO	2	0
3	A	601	DIO	4	0
3	B	601	DIO	4	0
3	F	601	DIO	3	0
3	C	601	DIO	2	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	496/501 (99%)	-0.11	12 (2%) 59 57	31, 51, 83, 116	0
1	B	496/501 (99%)	0.05	18 (3%) 42 39	31, 54, 89, 117	0
1	C	496/501 (99%)	0.01	8 (1%) 72 71	32, 54, 96, 120	0
1	D	496/501 (99%)	0.06	24 (4%) 30 27	34, 56, 100, 130	0
1	E	496/501 (99%)	0.01	7 (1%) 75 76	29, 56, 99, 125	0
1	F	496/501 (99%)	-0.10	19 (3%) 40 37	31, 53, 92, 118	0
All	All	2976/3006 (99%)	-0.01	88 (2%) 50 46	29, 54, 94, 130	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	169[A]	CYS	4.8
1	F	501	ILE	4.3
1	E	368	ALA	4.2
1	A	483	ASP	4.0
1	A	484	ASP	3.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DIO	D	601	6/6	0.85	0.32	67,71,71,74	0
3	DIO	C	601	6/6	0.85	0.32	71,74,75,87	0
3	DIO	B	601	6/6	0.87	0.27	67,69,71,75	0
2	AHR	C	600	10/10	0.89	0.28	49,54,63,66	0
2	AHR	D	600	10/10	0.90	0.24	47,56,61,66	0
3	DIO	E	601	6/6	0.90	0.24	64,67,69,73	0
3	DIO	A	601	6/6	0.91	0.25	65,67,74,77	0
3	DIO	F	601	6/6	0.91	0.29	64,70,74,76	0
2	AHR	A	600	10/10	0.92	0.20	38,49,58,59	0
2	AHR	E	600	10/10	0.92	0.20	43,56,61,62	0
2	AHR	B	600	10/10	0.95	0.20	46,57,67,70	0
2	AHR	F	600	10/10	0.96	0.21	46,54,61,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.