



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:18 pm BST

PDB ID : 3T4U  
Title : L29I Mutation in an Aryl Esterase from *Pseudomonas fluorescens* Leads to Unique Peptide Flip and Increased Activity  
Authors : Kazlauskas, R.J.; Yin, T.; Purpero, V.M.  
Deposited on : 2011-07-26  
Resolution : 2.02 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](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

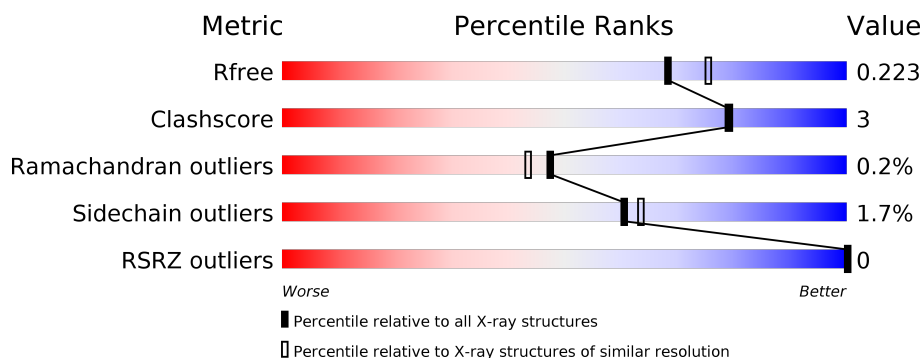
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	271	<div> <div>94%</div> <div>5% •</div> </div>
1	B	271	<div> <div>93%</div> <div>6% •</div> </div>
1	C	271	<div> <div>94%</div> <div>6%</div> </div>
1	D	271	<div> <div>93%</div> <div>6%</div> </div>
1	E	271	<div> <div>94%</div> <div>5% •</div> </div>
1	F	271	<div> <div>92%</div> <div>7% •</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14595 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 Arylesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	10	0
			2180	1404	361	410	5			
1	B	271	Total	C	N	O	S	0	13	0
			2202	1422	365	410	5			
1	C	271	Total	C	N	O	S	0	11	0
			2196	1415	368	408	5			
1	D	271	Total	C	N	O	S	0	5	0
			2155	1389	360	401	5			
1	E	271	Total	C	N	O	S	0	13	0
			2196	1418	362	411	5			
1	F	271	Total	C	N	O	S	0	9	0
			2175	1401	362	407	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ILE	LEU	ENGINEERED MUTATION	UNP P22862
B	29	ILE	LEU	ENGINEERED MUTATION	UNP P22862
C	29	ILE	LEU	ENGINEERED MUTATION	UNP P22862
D	29	ILE	LEU	ENGINEERED MUTATION	UNP P22862
E	29	ILE	LEU	ENGINEERED MUTATION	UNP P22862
F	29	ILE	LEU	ENGINEERED MUTATION	UNP P22862

- Molecule 2 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
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	E	1	Total C O 12 6 6	0	1
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	F	1	Total C O 12 6 6	0	1
2	F	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Na	0	0
			1	1		
5	E	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		
5	A	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	197	Total	O	0	0
			197	197		
6	B	238	Total	O	0	2
			240	240		
6	C	215	Total	O	0	0
			215	215		
6	D	224	Total	O	0	4
			228	228		
6	E	208	Total	O	0	2
			210	210		
6	F	191	Total	O	0	3
			194	194		

### 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: Arylesterase

Chain A:  94% 5%



- Molecule 1: Arylesterase

Chain B:  93% 6%



- Molecule 1: Arylesterase

Chain C:  94% 6%



- Molecule 1: Arylesterase

Chain D:  93% 6%



- Molecule 1: Arylesterase

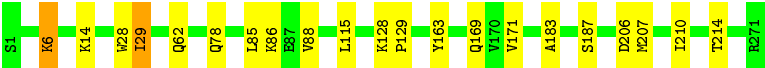
Chain E:  94% 5%



- Molecule 1: Arylesterase

Chain F:  92% 7%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.88Å 145.88Å 128.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.23 – 2.02 48.23 – 2.02	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.23-2.02) 98.6 (48.23-2.02)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.192 , 0.221 0.195 , 0.223	Depositor DCC
$R_{free}$ test set	9963 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 28.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,l 0.019 for h,-h-k,-l 0.046 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14595	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2368e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GOL, CL, SO4, NA

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	0.74	0/2257	0.70	0/3060
1	B	0.80	0/2282	0.74	0/3092
1	C	0.75	0/2273	0.70	1/3077 (0.0%)
1	D	0.78	0/2217	0.70	1/3007 (0.0%)
1	E	0.75	0/2282	0.70	0/3094
1	F	0.77	0/2249	0.68	0/3049
All	All	0.77	0/13560	0.70	2/18379 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	31	ASP	CB-CG-OD1	5.48	123.23	118.30
1	D	45	ARG	NE-CZ-NH1	5.09	122.85	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	2180	0	2147	7	0
1	B	2202	0	2185	15	0
1	C	2196	0	2174	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2155	0	2122	15	0
1	E	2196	0	2177	13	0
1	F	2175	0	2145	12	0
2	A	24	0	32	1	0
2	B	12	0	16	0	0
2	C	30	0	40	0	0
2	D	18	0	24	1	0
2	E	36	0	48	1	0
2	F	30	0	40	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
3	F	10	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	197	0	0	2	0
6	B	240	0	0	5	0
6	C	215	0	0	1	0
6	D	228	0	0	3	0
6	E	210	0	0	6	0
6	F	194	0	0	2	0
All	All	14595	0	13150	73	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 3.

All (73) 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:B:124[B]:LEU:HD11	6:B:1032:HOH:O	1.38	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247[A]:LYS:NZ	1:B:248[A]:ASP:OD1	1.98	0.96
1:B:28[A]:TRP:O	6:B:1124:HOH:O	1.84	0.94
1:E:28[A]:TRP:O	6:E:1130:HOH:O	1.87	0.91
1:D:28[B]:TRP:O	1:D:29[B]:ILE:HB	1.70	0.90
1:C:28[B]:TRP:O	6:C:1118:HOH:O	1.88	0.89
1:B:124[B]:LEU:CD1	6:B:1032:HOH:O	2.05	0.87
1:A:28[A]:TRP:O	6:A:1119:HOH:O	1.92	0.86
1:F:169[B]:GLN:OE1	6:F:924[B]:HOH:O	1.95	0.85
1:E:87[A]:GLU:OE2	6:E:956:HOH:O	1.93	0.84
1:A:173[A]:GLN:HG2	6:A:1184:HOH:O	1.79	0.81
1:D:29[B]:ILE:CG2	1:D:29[B]:ILE:O	2.29	0.80
1:D:28[B]:TRP:O	6:D:1131:HOH:O	2.01	0.77
1:D:29[B]:ILE:HG22	6:D:1122:HOH:O	1.86	0.75
1:D:28[B]:TRP:O	1:D:29[B]:ILE:CB	2.36	0.72
1:B:244:LYS:HE2	6:B:1256:HOH:O	1.91	0.70
1:F:28[B]:TRP:O	6:F:1121:HOH:O	2.08	0.70
1:D:29[B]:ILE:CG2	6:D:1122:HOH:O	2.40	0.68
1:D:175:VAL:HG13	2:D:276:GOL:H12	1.79	0.64
1:D:20:LYS:HE2	1:D:87[B]:GLU:OE1	2.00	0.62
1:E:89:THR:CG2	6:E:498:HOH:O	2.47	0.62
1:D:29[B]:ILE:HG23	1:D:29[B]:ILE:O	1.99	0.61
1:B:6:LYS:H	1:B:78[B]:GLN:HE22	1.47	0.61
1:D:29[B]:ILE:HG22	1:D:29[B]:ILE:O	2.03	0.58
1:E:165[A]:ILE:HD11	1:E:171:VAL:HB	1.86	0.58
1:E:29[B]:ILE:HD12	1:E:155:ILE:HG12	1.86	0.56
1:D:144:LYS:HG2	1:D:192:VAL:HG13	1.88	0.55
1:C:88:VAL:HG12	1:C:111:ARG:O	2.06	0.54
1:F:62:GLN:HB3	1:F:187:SER:HB2	1.89	0.54
1:E:89:THR:HG22	6:E:498:HOH:O	2.09	0.53
1:E:89:THR:HG23	6:E:498:HOH:O	2.08	0.52
1:D:62:GLN:HB3	1:D:187:SER:HB2	1.92	0.52
1:F:163:TYR:HB3	1:F:171:VAL:HG21	1.93	0.51
1:B:5:ALA:HA	1:B:78[B]:GLN:OE1	2.11	0.51
1:C:77:ALA:O	1:C:81[A]:GLU:HG2	2.10	0.51
1:C:62:GLN:HB3	1:C:187:SER:HB2	1.93	0.51
1:C:271[A]:ARG:HH21	1:C:271[A]:ARG:HG2	1.77	0.49
1:C:28[B]:TRP:CD2	1:C:29[B]:ILE:HG13	2.47	0.49
1:C:29[B]:ILE:HG22	1:C:183:ALA:HB1	1.94	0.49
1:B:228[B]:GLU:CD	1:B:228[B]:GLU:H	2.16	0.48
1:F:115:LEU:O	1:F:214:THR:HA	2.13	0.48
1:D:207:MET:HA	1:D:210:ILE:HD12	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:PHE:O	1:C:271[A]:ARG:HG2	2.15	0.46
1:B:29[A]:ILE:HG22	1:B:183:ALA:HB1	1.98	0.46
1:A:2:THR:HA	1:A:11:ILE:O	2.17	0.45
1:F:207:MET:HA	1:F:210:ILE:HD12	1.97	0.45
1:E:214:THR:O	1:E:242[B]:GLU:HG2	2.16	0.45
1:A:88:VAL:HG12	1:A:111:ARG:O	2.17	0.44
1:F:29[B]:ILE:HG22	1:F:183:ALA:HB1	2.00	0.43
1:F:85:LEU:HB3	1:F:88:VAL:HG22	2.00	0.43
1:C:43:SER:HA	1:C:47:TYR:O	2.19	0.43
1:E:173[A]:GLN:HG3	6:E:1236[A]:HOH:O	2.17	0.43
1:B:209:LYS:NZ	6:B:1282:HOH:O	2.51	0.43
1:E:29[A]:ILE:HD13	1:E:29[A]:ILE:HG21	1.77	0.43
1:D:9:THR:HG23	1:D:61:ASP:HB2	2.01	0.42
1:E:163:TYR:OH	2:E:277[B]:GOL:H32	2.18	0.42
1:E:43:SER:HA	1:E:47:TYR:O	2.20	0.42
1:F:14:LYS:HA	2:F:272:GOL:H11	2.02	0.41
1:B:115:LEU:O	1:B:214:THR:HA	2.21	0.41
1:F:128:LYS:HB3	1:F:129:PRO:HD2	2.03	0.41
1:B:29[A]:ILE:HD13	1:B:29[A]:ILE:HG21	1.78	0.41
1:F:6:LYS:N	1:F:78:GLN:OE1	2.53	0.41
2:A:278:GOL:O3	2:A:278:GOL:O1	2.37	0.41
1:A:29[A]:ILE:HG22	1:A:183:ALA:HB1	2.03	0.41
1:A:24:PHE:HB3	1:A:35:TRP:CE2	2.57	0.40
1:C:163:TYR:HB3	1:C:171:VAL:HG21	2.02	0.40
1:A:207:MET:HA	1:A:210:ILE:HD12	2.02	0.40
1:D:43:SER:HA	1:D:47:TYR:O	2.21	0.40
1:F:29[B]:ILE:HG21	1:F:29[B]:ILE:HD13	1.75	0.40
1:E:29[A]:ILE:HG22	1:E:183:ALA:HB1	2.03	0.40
1:B:88[A]:VAL:HG12	1:B:111:ARG:O	2.21	0.40

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	279/271 (103%)	271 (97%)	6 (2%)	2 (1%)	22	15
1	B	282/271 (104%)	271 (96%)	9 (3%)	2 (1%)	22	15
1	C	279/271 (103%)	270 (97%)	9 (3%)	0	100	100
1	D	274/271 (101%)	266 (97%)	6 (2%)	2 (1%)	22	15
1	E	282/271 (104%)	273 (97%)	7 (2%)	2 (1%)	22	15
1	F	278/271 (103%)	273 (98%)	5 (2%)	0	100	100
All	All	1674/1626 (103%)	1624 (97%)	42 (2%)	8 (0%)	47	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28[A]	TRP
1	B	28[B]	TRP
1	E	28[A]	TRP
1	E	28[B]	TRP
1	A	28[A]	TRP
1	A	28[B]	TRP
1	D	29[A]	ILE
1	D	29[B]	ILE

### 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	230/220 (104%)	225 (98%)	5 (2%)	52	53
1	B	232/220 (106%)	226 (97%)	6 (3%)	46	46
1	C	231/220 (105%)	228 (99%)	3 (1%)	69	72
1	D	225/220 (102%)	221 (98%)	4 (2%)	59	61
1	E	233/220 (106%)	228 (98%)	5 (2%)	53	55
1	F	229/220 (104%)	224 (98%)	5 (2%)	52	53
All	All	1380/1320 (104%)	1352 (98%)	28 (2%)	60	57

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29[A]	ILE
1	A	29[B]	ILE
1	A	81	GLU
1	A	137	LEU
1	A	206	ASP
1	B	6	LYS
1	B	29[A]	ILE
1	B	29[B]	ILE
1	B	142	ARG
1	B	206	ASP
1	B	218	HIS
1	C	29[A]	ILE
1	C	29[B]	ILE
1	C	206	ASP
1	D	29[A]	ILE
1	D	29[B]	ILE
1	D	149	LYS
1	D	206	ASP
1	E	29[A]	ILE
1	E	29[B]	ILE
1	E	89	THR
1	E	206	ASP
1	E	218	HIS
1	F	6	LYS
1	F	29[A]	ILE
1	F	29[B]	ILE
1	F	86	LYS
1	F	206	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 46 ligands modelled in this entry, 12 are monoatomic - leaving 34 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	$\# Z  > 2$
2	GOL	C	279	-	5,5,5	0.35	0	5,5,5	0.46	0
3	SO4	F	273	-	4,4,4	0.24	0	6,6,6	0.29	0
2	GOL	C	273	-	5,5,5	0.37	0	5,5,5	0.60	0
2	GOL	F	276	-	5,5,5	0.40	0	5,5,5	0.92	0
2	GOL	D	276	-	5,5,5	0.47	0	5,5,5	0.52	0
2	GOL	F	272	-	5,5,5	0.48	0	5,5,5	0.43	0
2	GOL	E	276	-	5,5,5	0.43	0	5,5,5	0.56	0
3	SO4	D	274	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	C	274	-	4,4,4	0.18	0	6,6,6	0.14	0
3	SO4	D	275	-	4,4,4	0.13	0	6,6,6	0.39	0
2	GOL	D	273	-	5,5,5	0.40	0	5,5,5	0.61	0
3	SO4	F	274	-	4,4,4	0.16	0	6,6,6	0.08	0
2	GOL	A	278	-	5,5,5	0.41	0	5,5,5	0.36	0
2	GOL	C	277	-	5,5,5	0.41	0	5,5,5	0.60	0
2	GOL	F	275[B]	-	5,5,5	0.32	0	5,5,5	0.29	0
3	SO4	E	274	-	4,4,4	0.15	0	6,6,6	0.22	0
2	GOL	A	276	-	5,5,5	0.49	0	5,5,5	1.03	0
2	GOL	B	273	-	5,5,5	0.53	0	5,5,5	0.56	0
3	SO4	C	275	-	4,4,4	0.11	0	6,6,6	0.10	0
2	GOL	C	278	-	5,5,5	0.46	0	5,5,5	0.22	0
2	GOL	F	275[A]	-	5,5,5	0.35	0	5,5,5	0.26	0
2	GOL	E	277[A]	-	5,5,5	0.37	0	5,5,5	0.64	0
2	GOL	E	277[B]	-	5,5,5	0.31	0	5,5,5	0.64	0
2	GOL	E	272	-	5,5,5	0.44	0	5,5,5	0.56	0
2	GOL	F	277	-	5,5,5	0.44	0	5,5,5	1.15	1 (20%)
2	GOL	A	275	-	5,5,5	0.39	0	5,5,5	1.07	0
3	SO4	A	273	-	4,4,4	0.13	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	D	272	-	5,5,5	0.31	0	5,5,5	0.35	0
2	GOL	E	273	-	5,5,5	0.41	0	5,5,5	0.31	0
2	GOL	E	278	-	5,5,5	0.37	0	5,5,5	0.54	0
2	GOL	B	272	-	5,5,5	0.32	0	5,5,5	0.46	0
3	SO4	B	274	-	4,4,4	0.19	0	6,6,6	0.26	0
2	GOL	C	272	-	5,5,5	0.32	0	5,5,5	0.69	0
2	GOL	A	272	-	5,5,5	0.40	0	5,5,5	0.48	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
2	GOL	C	279	-	-	4/4/4/4	-
2	GOL	C	273	-	-	2/4/4/4	-
2	GOL	F	276	-	-	4/4/4/4	-
2	GOL	D	276	-	-	2/4/4/4	-
2	GOL	F	272	-	-	0/4/4/4	-
2	GOL	E	276	-	-	2/4/4/4	-
2	GOL	D	273	-	-	0/4/4/4	-
2	GOL	D	272	-	-	1/4/4/4	-
2	GOL	A	278	-	-	1/4/4/4	-
2	GOL	C	277	-	-	0/4/4/4	-
2	GOL	F	275[B]	-	-	4/4/4/4	-
2	GOL	A	276	-	-	0/4/4/4	-
2	GOL	B	273	-	-	0/4/4/4	-
2	GOL	C	278	-	-	2/4/4/4	-
2	GOL	F	275[A]	-	-	4/4/4/4	-
2	GOL	E	277[A]	-	-	2/4/4/4	-
2	GOL	E	277[B]	-	-	2/4/4/4	-
2	GOL	E	272	-	-	0/4/4/4	-
2	GOL	F	277	-	-	4/4/4/4	-
2	GOL	A	275	-	-	2/4/4/4	-
2	GOL	E	273	-	-	2/4/4/4	-
2	GOL	E	278	-	-	3/4/4/4	-
2	GOL	B	272	-	-	0/4/4/4	-
2	GOL	C	272	-	-	0/4/4/4	-
2	GOL	A	272	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	F	277	GOL	O3-C3-C2	-2.25	99.42	110.20

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	279	GOL	O1-C1-C2-C3
2	C	273	GOL	O1-C1-C2-C3
2	D	276	GOL	C1-C2-C3-O3
2	D	276	GOL	O2-C2-C3-O3
2	E	276	GOL	O1-C1-C2-C3
2	C	278	GOL	O1-C1-C2-C3
2	E	277[B]	GOL	C1-C2-C3-O3
2	F	277	GOL	C1-C2-C3-O3
2	F	277	GOL	O2-C2-C3-O3
2	A	275	GOL	C1-C2-C3-O3
2	E	273	GOL	O1-C1-C2-C3
2	E	278	GOL	O1-C1-C2-C3
2	C	279	GOL	O1-C1-C2-O2
2	E	277[B]	GOL	O2-C2-C3-O3
2	A	275	GOL	O2-C2-C3-O3
2	C	279	GOL	C1-C2-C3-O3
2	F	276	GOL	O1-C1-C2-C3
2	F	276	GOL	C1-C2-C3-O3
2	D	272	GOL	C1-C2-C3-O3
2	F	275[B]	GOL	O1-C1-C2-C3
2	F	275[B]	GOL	C1-C2-C3-O3
2	F	275[A]	GOL	O1-C1-C2-C3
2	F	275[A]	GOL	C1-C2-C3-O3
2	E	277[A]	GOL	O1-C1-C2-C3
2	E	278	GOL	C1-C2-C3-O3
2	F	276	GOL	O2-C2-C3-O3
2	E	276	GOL	O1-C1-C2-O2
2	E	278	GOL	O1-C1-C2-O2
2	C	279	GOL	O2-C2-C3-O3
2	C	273	GOL	O1-C1-C2-O2
2	F	275[B]	GOL	O2-C2-C3-O3
2	E	273	GOL	O1-C1-C2-O2
2	F	275[B]	GOL	O1-C1-C2-O2
2	E	277[A]	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	F	277	GOL	O1-C1-C2-O2
2	F	275[A]	GOL	O1-C1-C2-O2
2	F	275[A]	GOL	O2-C2-C3-O3
2	A	278	GOL	O1-C1-C2-C3
2	F	276	GOL	O1-C1-C2-O2
2	F	277	GOL	O1-C1-C2-C3
2	C	278	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	276	GOL	1	0
2	F	272	GOL	1	0
2	A	278	GOL	1	0
2	E	277[B]	GOL	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	271/271 (100%)	-0.52	0 100 100	12, 20, 30, 40	1 (0%)
1	B	271/271 (100%)	-0.53	0 100 100	11, 17, 26, 36	0
1	C	271/271 (100%)	-0.54	0 100 100	12, 19, 28, 35	0
1	D	271/271 (100%)	-0.58	0 100 100	13, 19, 28, 38	2 (0%)
1	E	271/271 (100%)	-0.47	0 100 100	13, 20, 30, 42	1 (0%)
1	F	271/271 (100%)	-0.50	0 100 100	13, 20, 31, 42	1 (0%)
All	All	1626/1626 (100%)	-0.52	0 100 100	11, 19, 29, 42	5 (0%)

There are no RSRZ outliers to report.

### 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(Å <sup>2</sup> )	Q<0.9
2	GOL	E	278	6/6	0.79	0.16	52,53,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	A	277	1/1	0.81	0.08	68,68,68,68	0
2	GOL	A	278	6/6	0.85	0.21	51,51,52,52	0
2	GOL	D	276	6/6	0.86	0.14	38,47,49,51	0
2	GOL	F	275[A]	6/6	0.87	0.24	33,36,36,37	6
2	GOL	F	275[B]	6/6	0.87	0.24	48,49,50,51	6
2	GOL	A	276	6/6	0.87	0.17	38,44,47,47	0
2	GOL	C	278	6/6	0.89	0.14	51,53,54,55	0
3	SO4	F	274	5/5	0.90	0.20	100,100,100,100	0
2	GOL	E	277[A]	6/6	0.91	0.24	25,30,30,30	6
2	GOL	E	277[B]	6/6	0.91	0.24	37,39,39,40	6
4	CL	C	276	1/1	0.91	0.08	64,64,64,64	0
3	SO4	E	274	5/5	0.91	0.17	72,73,73,74	0
2	GOL	C	279	6/6	0.91	0.20	57,58,58,58	0
2	GOL	A	275	6/6	0.92	0.18	35,37,39,42	0
2	GOL	F	276	6/6	0.92	0.13	38,41,42,44	0
2	GOL	E	273	6/6	0.92	0.17	36,39,42,44	0
2	GOL	C	277	6/6	0.92	0.18	31,36,38,39	0
3	SO4	B	274	5/5	0.92	0.15	71,71,71,72	0
2	GOL	C	273	6/6	0.92	0.18	29,37,38,41	0
2	GOL	D	273	6/6	0.93	0.14	15,21,22,23	6
2	GOL	F	277	6/6	0.93	0.16	30,36,39,42	0
3	SO4	F	273	5/5	0.94	0.18	50,53,54,54	0
3	SO4	D	274	5/5	0.94	0.14	75,76,76,76	0
3	SO4	A	273	5/5	0.94	0.08	71,71,72,72	0
2	GOL	E	272	6/6	0.94	0.13	21,26,26,28	0
3	SO4	D	275	5/5	0.95	0.17	34,35,37,37	5
2	GOL	C	272	6/6	0.95	0.16	18,23,26,27	0
2	GOL	E	276	6/6	0.95	0.13	33,36,37,37	0
2	GOL	B	273	6/6	0.96	0.11	18,20,21,21	0
2	GOL	B	272	6/6	0.96	0.12	28,31,34,36	0
3	SO4	C	275	5/5	0.96	0.11	51,51,52,52	5
2	GOL	D	272	6/6	0.96	0.20	25,32,35,39	0
2	GOL	A	272	6/6	0.96	0.10	20,22,24,26	0
4	CL	D	277	1/1	0.96	0.06	61,61,61,61	0
4	CL	B	275	1/1	0.98	0.05	38,38,38,38	0
4	CL	E	275	1/1	0.98	0.09	52,52,52,52	0
3	SO4	C	274	5/5	0.98	0.20	64,64,65,65	0
2	GOL	F	272	6/6	0.98	0.09	18,24,25,26	0
5	NA	F	278	1/1	0.99	0.08	14,14,14,14	0
4	CL	A	274	1/1	0.99	0.06	43,43,43,43	0
5	NA	E	279	1/1	0.99	0.09	19,19,19,19	0
5	NA	C	280	1/1	0.99	0.12	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NA	A	279	1/1	0.99	0.09	16,16,16,16	0
5	NA	B	276	1/1	0.99	0.11	16,16,16,16	0
5	NA	D	278	1/1	1.00	0.08	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.