



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 10:54 am BST

PDB ID : 3T52
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 : 2.00 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	:	2.11
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

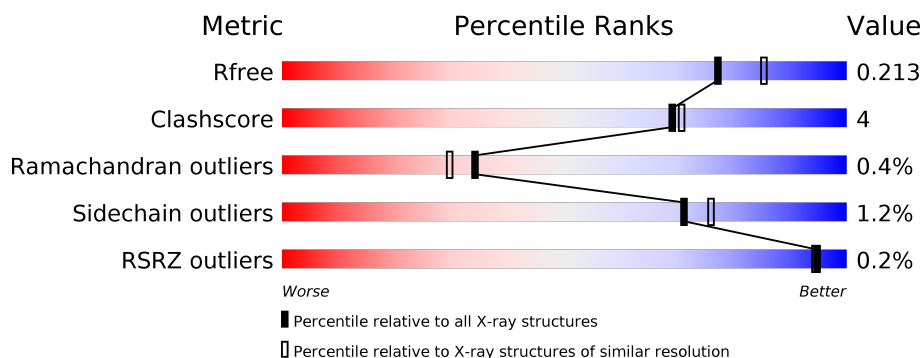
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 ≥ 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>95%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	B	271	<div> <div>93%</div> <div>6%</div> <div></div> </div>
1	C	271	<div> <div>94%</div> <div>6%</div> <div></div> </div>
1	D	271	<div> <div>95%</div> <div></div> <div></div> </div>
1	E	271	<div> <div>96%</div> <div></div> <div></div> </div>
1	F	271	<div> <div>93%</div> <div>7%</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
2	GOL	A	278	-	-	X	-
2	GOL	F	284	-	-	X	-
6	ACT	B	283	-	-	X	-
6	ACT	C	281	-	-	X	-
6	ACT	D	276	-	-	X	-
6	ACT	E	283	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14698 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	362	409	5			
1	B	271	Total	C	N	O	S	0	12	0
			2197	1418	368	406	5			
1	C	271	Total	C	N	O	S	0	8	0
			2173	1401	362	405	5			
1	D	271	Total	C	N	O	S	0	5	0
			2159	1390	363	401	5			
1	E	271	Total	C	N	O	S	0	13	0
			2197	1418	365	409	5			
1	F	271	Total	C	N	O	S	0	11	0
			2194	1413	365	411	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: C₃H₈O₃).



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	B	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	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		

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

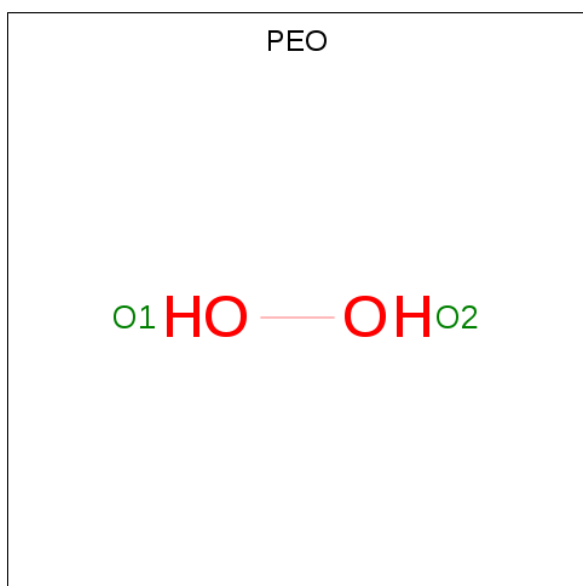


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	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 1 1	0	0
4	A	2	Total Cl 2 2	0	0
4	D	1	Total Cl 1 1	0	0
4	C	2	Total Cl 2 2	0	0
4	E	1	Total Cl 1 1	0	0

- Molecule 5 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H₂O₂).



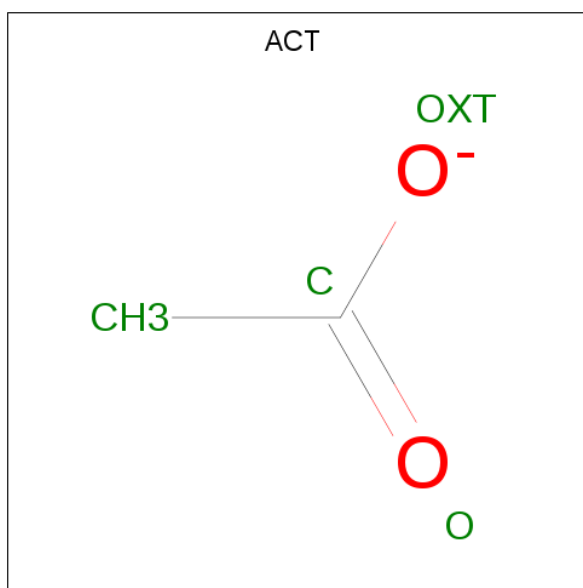
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 2 2	0	0
5	A	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	C	1	Total O 2 2	0	0

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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 8	C 4	O 4	0	1
6	B	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 8	C 4	O 4	0	1

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	163	Total 164	O 164	0	1
7	B	223	Total 223	O 223	0	0
7	C	210	Total 210	O 210	0	0
7	D	209	Total 210	O 210	0	1
7	E	183	Total 184	O 184	0	1
7	F	178	Total 178	O 178	0	0

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:  95%



• Molecule 1: Arylesterase

Chain B:  93% 6%



• Molecule 1: Arylesterase

Chain C:  94% 6%



• Molecule 1: Arylesterase

Chain D:  95%



• Molecule 1: Arylesterase

Chain E:  96%



• Molecule 1: Arylesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	146.02Å 146.02Å 128.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.80 – 2.00 47.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.80-2.00) 99.9 (47.80-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.184 , 0.211 0.187 , 0.213	Depositor DCC
R_{free} test set	10433 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14698	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 23.76 % 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 4.3750e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: ACT, GOL, PEO, SO4, CL

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	0.73	0/2257	0.67	0/3060
1	B	0.83	0/2279	0.72	0/3090
1	C	0.74	0/2244	0.71	0/3043
1	D	0.76	0/2221	0.70	0/3011
1	E	0.75	0/2283	0.67	0/3095
1	F	0.71	0/2274	0.69	0/3082
All	All	0.75	0/13558	0.69	0/18381

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	2180	0	2149	18	0
1	B	2197	0	2183	17	0
1	C	2173	0	2144	19	0
1	D	2159	0	2126	9	0
1	E	2197	0	2182	10	0
1	F	2194	0	2164	18	0
2	A	18	0	24	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	36	0	48	4	0
2	C	30	0	40	4	0
2	D	48	0	63	1	0
2	E	30	0	40	1	0
2	F	42	0	56	8	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	15	0	0	0	0
3	D	5	0	0	0	0
3	E	10	0	0	0	0
3	F	15	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	4	0	0	0	0
5	B	8	0	0	0	0
5	C	4	0	0	0	0
5	D	6	0	0	0	0
5	E	10	0	0	0	0
5	F	6	0	0	0	0
6	A	16	0	12	1	0
6	B	24	0	18	3	0
6	C	24	0	18	5	0
6	D	12	0	9	2	0
6	E	28	0	21	3	0
6	F	16	0	12	1	0
7	A	164	0	0	0	0
7	B	223	0	0	5	0
7	C	210	0	0	5	0
7	D	210	0	0	1	0
7	E	184	0	0	0	0
7	F	178	0	0	1	0
All	All	14698	0	13309	99	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 4.

The worst 5 of 99 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:F:142[B]:ARG:NH1	1:F:142[B]:ARG:HG2	1.65	1.00
1:D:28[B]:TRP:O	1:D:29[B]:ILE:HG12	1.59	1.00
1:F:142[B]:ARG:HG2	1:F:142[B]:ARG:HH11	0.85	0.99
1:F:142[B]:ARG:CG	1:F:142[B]:ARG:HH11	1.76	0.97
1:F:37:TYR:HB3	2:F:284:GOL:H32	1.48	0.95

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%)	269 (96%)	8 (3%)	2 (1%)	22	16
1	B	280/271 (103%)	268 (96%)	8 (3%)	4 (1%)	11	5
1	C	277/271 (102%)	268 (97%)	9 (3%)	0	100	100
1	D	274/271 (101%)	266 (97%)	6 (2%)	2 (1%)	22	16
1	E	282/271 (104%)	273 (97%)	7 (2%)	2 (1%)	22	16
1	F	280/271 (103%)	271 (97%)	7 (2%)	2 (1%)	22	16
All	All	1672/1626 (103%)	1615 (97%)	45 (3%)	12 (1%)	34	16

5 of 12 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

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%)	228 (99%)	2 (1%)	78	83
1	B	232/220 (106%)	229 (99%)	3 (1%)	69	74
1	C	228/220 (104%)	223 (98%)	5 (2%)	52	55
1	D	225/220 (102%)	223 (99%)	2 (1%)	78	83
1	E	233/220 (106%)	231 (99%)	2 (1%)	78	83
1	F	231/220 (105%)	228 (99%)	3 (1%)	69	74
All	All	1379/1320 (104%)	1362 (99%)	17 (1%)	71	76

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	206	ASP
1	C	218	HIS
1	E	206	ASP
1	C	29[B]	ILE
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 102 ligands modelled in this entry, 7 are monoatomic - leaving 95 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	0.45	0	5,5,5	0.48	0
2	GOL	F	272	-	5,5,5	0.54	0	5,5,5	0.52	0
6	ACT	E	284	-	1,3,3	0.46	0	0,3,3	0.00	-
3	SO4	C	274	-	4,4,4	0.23	0	6,6,6	0.17	0
2	GOL	C	289	-	5,5,5	0.47	0	5,5,5	0.74	0
6	ACT	B	285	-	1,3,3	1.66	0	0,3,3	0.00	-
6	ACT	C	283	-	1,3,3	0.65	0	0,3,3	0.00	-
3	SO4	B	274	-	4,4,4	0.16	0	6,6,6	0.48	0
6	ACT	A	280	-	1,3,3	1.20	0	0,3,3	0.00	-
6	ACT	E	287	-	1,3,3	1.36	0	0,3,3	0.00	-
5	PEO	D	278	-	1,1,1	0.68	0	-		
2	GOL	B	272	-	5,5,5	0.32	0	5,5,5	0.54	0
3	SO4	A	273	-	4,4,4	0.14	0	6,6,6	0.30	0
2	GOL	D	286	-	5,5,5	0.39	0	5,5,5	0.24	0
6	ACT	F	281	-	1,3,3	0.82	0	0,3,3	0.00	-
5	PEO	E	280	-	1,1,1	0.52	0	-		
5	PEO	B	281	-	1,1,1	0.58	0	-		
6	ACT	D	283	-	1,3,3	0.72	0	0,3,3	0.00	-
2	GOL	D	273	-	5,5,5	0.53	0	5,5,5	0.56	0
6	ACT	C	282	-	1,3,3	1.79	0	0,3,3	0.00	-
2	GOL	B	288	-	5,5,5	0.39	0	5,5,5	0.37	0
2	GOL	A	272	-	5,5,5	0.50	0	5,5,5	0.19	0
5	PEO	B	280	-	1,1,1	0.52	0	-		
5	PEO	F	277	-	1,1,1	0.56	0	-		
2	GOL	B	277	-	5,5,5	0.38	0	5,5,5	0.26	0
2	GOL	F	285[A]	-	5,5,5	0.45	0	5,5,5	0.33	0
2	GOL	F	285[B]	-	5,5,5	0.57	0	5,5,5	0.44	0
2	GOL	D	280[A]	-	5,5,5	0.80	0	5,5,5	0.90	0
6	ACT	B	284	-	1,3,3	0.66	0	0,3,3	0.00	-
5	PEO	B	282	-	1,1,1	0.61	0	-		
2	GOL	C	273	-	5,5,5	0.37	0	5,5,5	0.42	0
3	SO4	C	275	-	4,4,4	0.16	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	B	286[A]	-	1,3,3	0.18	0	0,3,3	0.00	-
6	ACT	D	276	-	1,3,3	1.44	0	0,3,3	0.00	-
6	ACT	B	286[B]	-	1,3,3	0.04	0	0,3,3	0.00	-
2	GOL	B	273	-	5,5,5	0.57	0	5,5,5	0.63	0
3	SO4	C	276	-	4,4,4	0.14	0	6,6,6	0.26	0
6	ACT	F	286	-	1,3,3	0.65	0	0,3,3	0.00	-
6	ACT	F	283	-	1,3,3	1.44	0	0,3,3	0.00	-
5	PEO	F	279	-	1,1,1	0.66	0	-		
5	PEO	B	279	-	1,1,1	0.77	0	-		
2	GOL	C	272	-	5,5,5	0.44	0	5,5,5	0.56	0
6	ACT	E	283	-	1,3,3	1.81	0	0,3,3	0.00	-
2	GOL	E	272	-	5,5,5	0.47	0	5,5,5	0.64	0
5	PEO	E	288	-	1,1,1	0.64	0	-		
6	ACT	F	282	-	1,3,3	1.83	0	0,3,3	0.00	-
3	SO4	F	273	-	4,4,4	0.19	0	6,6,6	0.21	0
6	ACT	D	282	-	1,3,3	2.23	1 (100%)	0,3,3	0.00	-
2	GOL	F	284	-	5,5,5	0.45	0	5,5,5	0.75	0
6	ACT	A	279	-	1,3,3	1.69	0	0,3,3	0.00	-
2	GOL	C	288	-	5,5,5	0.48	0	5,5,5	0.44	0
5	PEO	A	276	-	1,1,1	0.58	0	-		
6	ACT	E	285	-	1,3,3	1.20	0	0,3,3	0.00	-
2	GOL	E	281	-	5,5,5	0.33	0	5,5,5	0.56	0
2	GOL	D	272	-	5,5,5	0.39	0	5,5,5	0.29	0
2	GOL	F	287	-	5,5,5	0.38	0	5,5,5	0.22	0
6	ACT	A	281	-	1,3,3	1.79	0	0,3,3	0.00	-
6	ACT	A	282	-	1,3,3	0.43	0	0,3,3	0.00	-
3	SO4	B	275	-	4,4,4	0.12	0	6,6,6	0.24	0
2	GOL	E	289	-	5,5,5	0.36	0	5,5,5	0.53	0
2	GOL	B	278	-	5,5,5	0.37	0	5,5,5	0.42	0
3	SO4	E	275	-	4,4,4	0.57	0	6,6,6	0.35	0
3	SO4	F	274	-	4,4,4	0.20	0	6,6,6	0.25	0
3	SO4	E	274	-	4,4,4	0.12	0	6,6,6	0.21	0
2	GOL	F	280	-	5,5,5	0.32	0	5,5,5	0.40	0
6	ACT	C	281	-	1,3,3	0.79	0	0,3,3	0.00	-
2	GOL	D	277	-	5,5,5	0.45	0	5,5,5	0.76	0
6	ACT	C	286	-	1,3,3	1.80	0	0,3,3	0.00	-
2	GOL	D	285	-	5,5,5	1.10	1 (20%)	5,5,5	0.63	0
5	PEO	F	278	-	1,1,1	0.56	0	-		
5	PEO	C	284	-	1,1,1	0.58	0	-		
3	SO4	F	275	-	4,4,4	0.16	0	6,6,6	0.17	0
6	ACT	B	287	-	1,3,3	0.78	0	0,3,3	0.00	-
5	PEO	E	278	-	1,1,1	0.73	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	B	283	-	1,3,3	2.42	1 (100%)	0,3,3	0.00	-
2	GOL	A	283	-	5,5,5	0.42	0	5,5,5	0.51	0
2	GOL	E	273	-	5,5,5	0.44	0	5,5,5	0.32	0
2	GOL	D	280[B]	-	5,5,5	0.91	0	5,5,5	0.51	0
2	GOL	A	278	-	5,5,5	0.58	0	5,5,5	0.89	0
6	ACT	E	286[B]	-	1,3,3	1.55	0	0,3,3	0.00	-
5	PEO	E	282	-	1,1,1	0.51	0	-		
5	PEO	D	279	-	1,1,1	0.66	0	-		
6	ACT	E	286[A]	-	1,3,3	0.92	0	0,3,3	0.00	-
5	PEO	A	277	-	1,1,1	0.52	0	-		
5	PEO	D	281	-	1,1,1	0.68	0	-		
2	GOL	F	276	-	5,5,5	0.54	0	5,5,5	0.58	0
2	GOL	D	284	-	5,5,5	0.51	0	5,5,5	0.91	0
3	SO4	D	274	-	4,4,4	0.14	0	6,6,6	0.31	0
5	PEO	E	279	-	1,1,1	0.41	0	-		
2	GOL	B	289	-	5,5,5	0.41	0	5,5,5	0.51	0
6	ACT	C	285	-	1,3,3	1.05	0	0,3,3	0.00	-
6	ACT	C	287	-	1,3,3	1.01	0	0,3,3	0.00	-
2	GOL	E	277	-	5,5,5	0.44	0	5,5,5	0.47	0
6	ACT	E	290	-	1,3,3	0.90	0	0,3,3	0.00	-
5	PEO	C	280	-	1,1,1	0.68	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	-	-	0/4/4/4	-
2	GOL	F	272	-	-	0/4/4/4	-
2	GOL	F	280	-	-	2/4/4/4	-
2	GOL	D	277	-	-	2/4/4/4	-
2	GOL	D	273	-	-	0/4/4/4	-
2	GOL	C	289	-	-	4/4/4/4	-
2	GOL	D	285	-	-	3/4/4/4	-
2	GOL	B	288	-	-	0/4/4/4	-
2	GOL	C	272	-	-	0/4/4/4	-
2	GOL	A	272	-	-	0/4/4/4	-
2	GOL	E	272	-	-	0/4/4/4	-
2	GOL	B	277	-	-	2/4/4/4	-
2	GOL	F	285[A]	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	F	285[B]	-	-	2/4/4/4	-
2	GOL	A	283	-	-	2/4/4/4	-
2	GOL	E	273	-	-	2/4/4/4	-
2	GOL	B	272	-	-	0/4/4/4	-
2	GOL	D	280[B]	-	-	2/4/4/4	-
2	GOL	F	284	-	-	0/4/4/4	-
2	GOL	D	280[A]	-	-	0/4/4/4	-
2	GOL	C	288	-	-	2/4/4/4	-
2	GOL	A	278	-	-	2/4/4/4	-
2	GOL	E	281	-	-	0/4/4/4	-
2	GOL	B	278	-	-	2/4/4/4	-
2	GOL	C	273	-	-	2/4/4/4	-
2	GOL	F	276	-	-	3/4/4/4	-
2	GOL	D	284	-	-	4/4/4/4	-
2	GOL	D	272	-	-	0/4/4/4	-
2	GOL	F	287	-	-	2/4/4/4	-
2	GOL	B	273	-	-	0/4/4/4	-
2	GOL	B	289	-	-	4/4/4/4	-
2	GOL	D	286	-	-	2/4/4/4	-
2	GOL	E	289	-	-	2/4/4/4	-
2	GOL	E	277	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	283	ACT	CH3-C	2.42	1.51	1.48
2	D	285	GOL	O2-C2	-2.27	1.36	1.43
6	D	282	ACT	CH3-C	2.23	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	277	GOL	C1-C2-C3-O3
2	F	285[A]	GOL	O1-C1-C2-O2
2	F	285[A]	GOL	O1-C1-C2-C3
2	F	285[B]	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	F	285[B]	GOL	O1-C1-C2-C3

There are no ring outliers.

21 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	289	GOL	3	0
6	C	282	ACT	1	0
2	B	288	GOL	2	0
2	F	285[B]	GOL	3	0
6	B	284	ACT	1	0
6	B	286[A]	ACT	1	0
6	D	276	ACT	2	0
6	E	283	ACT	2	0
6	F	282	ACT	1	0
2	F	284	GOL	4	0
2	C	288	GOL	1	0
2	F	287	GOL	1	0
6	A	282	ACT	1	0
6	C	281	ACT	4	0
6	B	283	ACT	2	0
2	E	273	GOL	1	0
2	A	278	GOL	6	0
6	E	286[A]	ACT	1	0
2	D	284	GOL	1	0
2	B	289	GOL	2	0
6	E	290	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, 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	271/271 (100%)	-0.57	1 (0%) 92 92	17, 25, 36, 51	0
1	B	271/271 (100%)	-0.71	0 100 100	14, 21, 29, 37	1 (0%)
1	C	271/271 (100%)	-0.64	1 (0%) 92 92	15, 23, 34, 51	1 (0%)
1	D	271/271 (100%)	-0.64	0 100 100	15, 22, 33, 45	1 (0%)
1	E	271/271 (100%)	-0.61	1 (0%) 92 92	16, 25, 35, 49	0
1	F	271/271 (100%)	-0.61	1 (0%) 92 92	16, 24, 35, 50	0
All	All	1626/1626 (100%)	-0.63	4 (0%) 95 94	14, 23, 34, 51	3 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	ARG	3.0
1	E	271	ARG	3.0
1	C	271	ARG	2.9
1	F	271	ARG	2.5

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, 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
5	PEO	A	276	2/2	0.44	0.20	49,49,49,51	0
6	ACT	C	281	4/4	0.47	0.28	65,65,65,66	0
5	PEO	C	284	2/2	0.56	0.21	50,50,50,51	0
4	CL	C	278	1/1	0.60	0.18	70,70,70,70	0
2	GOL	B	288	6/6	0.60	0.29	61,62,63,63	0
5	PEO	C	280	2/2	0.60	0.17	42,42,42,42	0
6	ACT	C	286	4/4	0.63	0.18	58,59,59,59	0
5	PEO	F	278	2/2	0.64	0.20	49,49,49,50	0
5	PEO	B	280	2/2	0.65	0.17	49,49,49,51	0
5	PEO	A	277	2/2	0.66	0.23	57,57,57,58	0
2	GOL	C	289	6/6	0.66	0.25	50,56,57,57	0
2	GOL	D	280[A]	6/6	0.68	0.24	58,59,59,59	6
2	GOL	D	280[B]	6/6	0.68	0.24	54,54,55,55	6
5	PEO	D	281	2/2	0.69	0.19	38,38,38,44	0
5	PEO	F	279	2/2	0.69	0.22	50,50,50,52	0
6	ACT	E	286[A]	4/4	0.71	0.27	68,68,68,68	4
6	ACT	E	286[B]	4/4	0.71	0.27	37,38,38,38	4
5	PEO	B	282	2/2	0.72	0.19	46,46,46,48	0
5	PEO	B	281	2/2	0.73	0.35	48,48,48,50	0
3	SO4	E	275	5/5	0.73	0.31	76,76,76,76	5
5	PEO	E	288	2/2	0.73	0.14	44,44,44,47	0
5	PEO	B	279	2/2	0.74	0.16	37,37,37,40	0
2	GOL	A	278	6/6	0.75	0.24	43,49,53,53	0
2	GOL	F	280	6/6	0.76	0.17	63,64,64,65	0
2	GOL	F	285[B]	6/6	0.77	0.27	28,32,33,33	6
2	GOL	D	286	6/6	0.77	0.25	52,56,58,58	0
6	ACT	A	279	4/4	0.77	0.23	61,61,61,61	0
2	GOL	B	289	6/6	0.77	0.29	63,65,65,65	0
2	GOL	F	285[A]	6/6	0.77	0.27	30,36,36,38	6
2	GOL	F	287	6/6	0.78	0.32	58,61,61,61	0
5	PEO	D	278	2/2	0.78	0.10	34,34,34,38	0
3	SO4	F	274	5/5	0.78	0.29	72,72,73,73	5
2	GOL	F	284	6/6	0.80	0.30	44,48,49,51	0
4	CL	D	275	1/1	0.80	0.10	76,76,76,76	0
5	PEO	E	282	2/2	0.81	0.17	47,47,47,50	0
2	GOL	D	285	6/6	0.81	0.28	61,62,63,63	0
2	GOL	B	272	6/6	0.81	0.21	42,50,52,54	0
2	GOL	D	284	6/6	0.82	0.29	37,38,39,44	6
2	GOL	E	273	6/6	0.82	0.21	43,47,51,51	0
6	ACT	A	280	4/4	0.82	0.13	40,40,41,41	0
2	GOL	D	272	6/6	0.83	0.23	37,46,48,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	ACT	E	290	4/4	0.83	0.18	50,51,51,51	4
2	GOL	C	273	6/6	0.83	0.25	44,51,52,53	0
2	GOL	B	278	6/6	0.86	0.19	24,36,38,40	6
6	ACT	B	286[B]	4/4	0.86	0.18	39,39,39,39	4
2	GOL	E	281	6/6	0.86	0.18	38,40,42,43	6
3	SO4	C	276	5/5	0.86	0.21	61,62,63,63	5
6	ACT	B	286[A]	4/4	0.86	0.18	44,44,45,45	4
5	PEO	D	279	2/2	0.87	0.17	35,35,35,42	0
2	GOL	C	288	6/6	0.87	0.14	61,62,63,63	0
2	GOL	D	277	6/6	0.88	0.17	33,43,45,49	0
3	SO4	A	273	5/5	0.88	0.14	55,55,57,57	5
6	ACT	F	283	4/4	0.88	0.14	46,47,47,47	0
4	CL	B	276	1/1	0.89	0.15	60,60,60,60	0
3	SO4	E	274	5/5	0.89	0.15	56,57,58,58	5
4	CL	E	276	1/1	0.89	0.04	64,64,64,64	0
6	ACT	C	285	4/4	0.90	0.13	40,40,40,41	0
3	SO4	C	275	5/5	0.90	0.17	56,56,58,58	5
4	CL	C	277	1/1	0.90	0.12	60,60,60,60	0
6	ACT	F	286	4/4	0.91	0.19	35,36,36,36	4
3	SO4	B	274	5/5	0.91	0.16	54,54,55,56	5
3	SO4	D	274	5/5	0.91	0.17	54,55,56,56	5
5	PEO	E	278	2/2	0.91	0.13	34,34,34,37	0
2	GOL	A	283	6/6	0.91	0.12	45,49,50,54	0
5	PEO	E	280	2/2	0.91	0.27	49,49,49,54	0
6	ACT	B	285	4/4	0.91	0.11	40,41,41,41	0
6	ACT	E	285	4/4	0.92	0.12	34,35,35,36	0
3	SO4	B	275	5/5	0.92	0.25	57,58,58,59	5
2	GOL	E	289	6/6	0.92	0.11	51,52,53,55	0
4	CL	A	275	1/1	0.92	0.13	68,68,68,68	0
6	ACT	C	282	4/4	0.92	0.11	32,32,33,33	0
6	ACT	B	287	4/4	0.93	0.11	35,35,36,36	4
6	ACT	C	287	4/4	0.93	0.10	45,46,46,46	0
3	SO4	F	275	5/5	0.93	0.21	69,69,69,69	5
2	GOL	F	276	6/6	0.93	0.15	35,42,44,46	0
3	SO4	F	273	5/5	0.94	0.24	51,53,53,53	5
2	GOL	C	279	6/6	0.94	0.11	35,40,41,43	0
2	GOL	B	277	6/6	0.94	0.13	36,44,46,48	0
5	PEO	E	279	2/2	0.95	0.11	43,43,43,46	0
2	GOL	E	277	6/6	0.95	0.08	38,44,45,47	0
6	ACT	B	283	4/4	0.95	0.14	28,29,29,30	0
6	ACT	E	284	4/4	0.95	0.09	34,34,34,35	0
6	ACT	E	283	4/4	0.96	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	ACT	C	283	4/4	0.96	0.08	32,32,32,32	0
4	CL	A	274	1/1	0.96	0.06	59,59,59,59	0
6	ACT	D	276	4/4	0.96	0.19	40,40,41,42	0
6	ACT	F	282	4/4	0.96	0.10	32,33,33,33	0
5	PEO	F	277	2/2	0.96	0.08	42,42,42,44	0
6	ACT	A	281	4/4	0.96	0.12	33,33,34,34	0
6	ACT	A	282	4/4	0.96	0.09	33,33,33,33	0
6	ACT	D	282	4/4	0.96	0.07	27,28,28,28	0
6	ACT	E	287	4/4	0.96	0.13	48,49,49,49	0
3	SO4	C	274	5/5	0.96	0.20	47,47,49,49	5
2	GOL	D	273	6/6	0.97	0.09	20,21,22,22	0
2	GOL	A	272	6/6	0.97	0.12	22,23,24,25	0
2	GOL	B	273	6/6	0.98	0.08	18,18,20,21	0
6	ACT	F	281	4/4	0.98	0.09	31,31,31,32	0
6	ACT	B	284	4/4	0.98	0.07	29,29,29,29	0
6	ACT	D	283	4/4	0.98	0.11	31,32,32,32	0
2	GOL	E	272	6/6	0.98	0.09	23,23,23,24	0
2	GOL	C	272	6/6	0.98	0.09	17,19,20,21	0
2	GOL	F	272	6/6	0.98	0.09	18,20,21,23	0

6.5 Other polymers

There are no such residues in this entry.