



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 11:51 AM EDT

PDB ID : 3HI4
Title : Switching catalysis from hydrolysis to perhydrolysis in *P. fluorescens* esterase
Authors : Purpero, V.M.
Deposited on : 2009-05-18
Resolution : 2.25 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

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 : 2.23.2
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) : 2.23.2

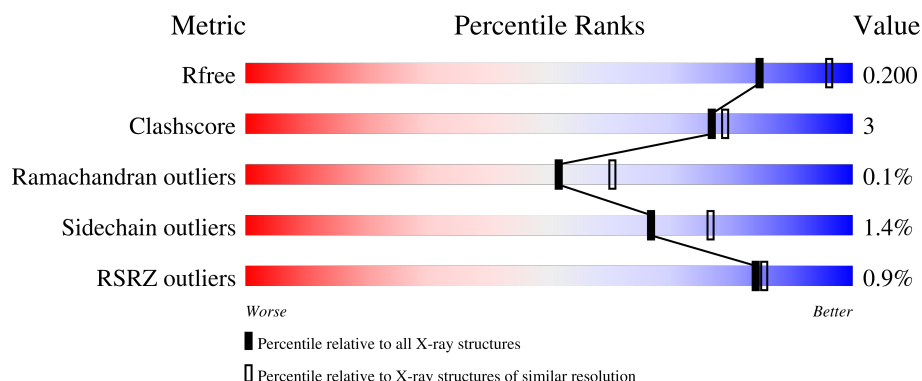
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 ≥ 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>%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	B	271	<div> <div></div> <div> <div>91%</div> <div>8%</div> </div> </div>
1	C	271	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
1	D	271	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	E	271	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	271	 89% 11% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14023 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 2132	C 1371	N 358	O 398	S 5	0	2	0
1	B	271	Total 2132	C 1371	N 358	O 398	S 5	0	2	0
1	C	271	Total 2137	C 1374	N 358	O 400	S 5	0	3	0
1	D	271	Total 2132	C 1371	N 358	O 398	S 5	0	2	0
1	E	271	Total 2137	C 1374	N 358	O 400	S 5	0	3	0
1	F	271	Total 2132	C 1371	N 358	O 398	S 5	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	PRO	LEU	engineered mutation	UNP P22862
B	29	PRO	LEU	engineered mutation	UNP P22862
C	29	PRO	LEU	engineered mutation	UNP P22862
D	29	PRO	LEU	engineered mutation	UNP P22862
E	29	PRO	LEU	engineered mutation	UNP P22862
F	29	PRO	LEU	engineered mutation	UNP P22862

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



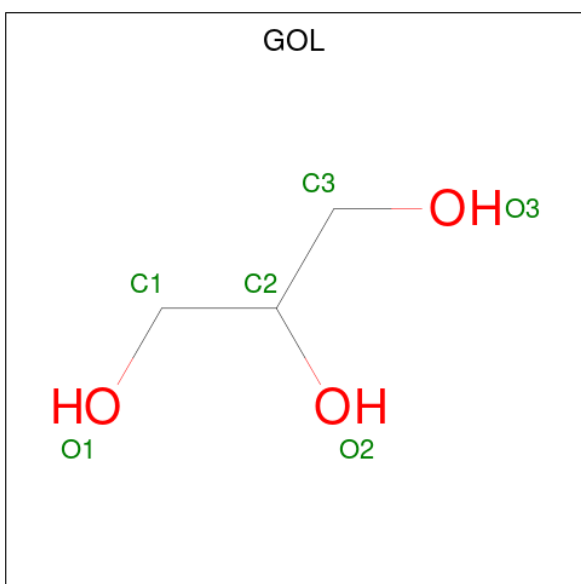
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total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

- 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	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		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

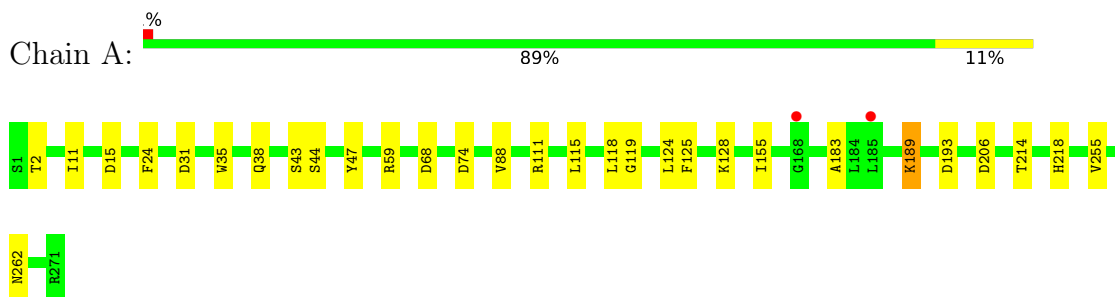
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	157	Total 157	O 157	0	0
5	B	189	Total 189	O 189	0	0
5	C	173	Total 173	O 173	0	0
5	D	178	Total 178	O 178	0	0
5	E	166	Total 166	O 166	0	0
5	F	173	Total 173	O 173	0	0

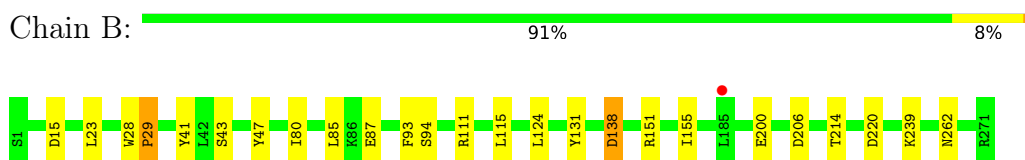
3 Residue-property plots [i](#)

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.

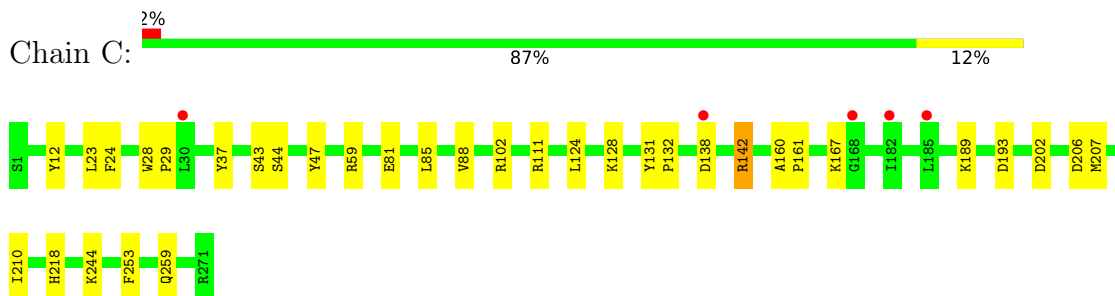
- Molecule 1: Arylesterase



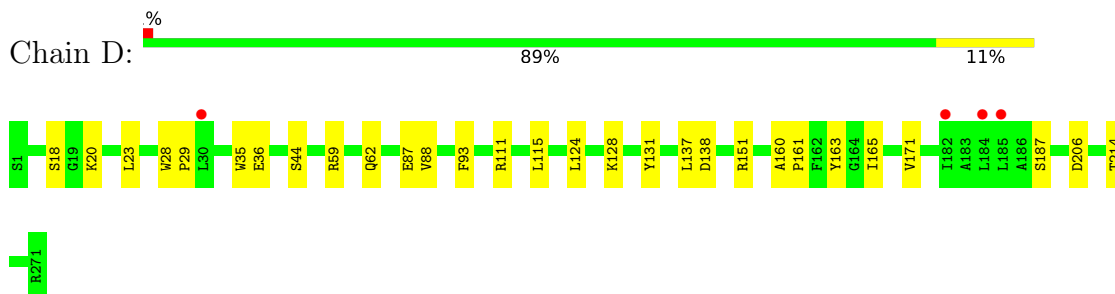
- Molecule 1: Arylesterase



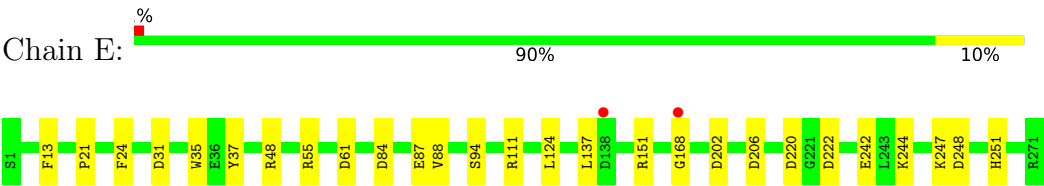
- Molecule 1: Arylesterase



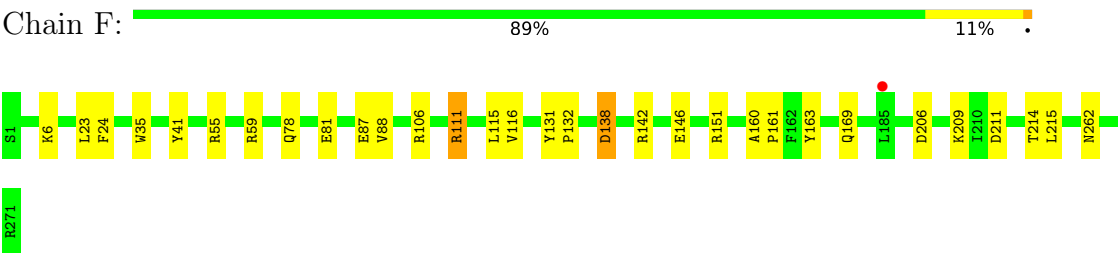
- Molecule 1: Arylesterase



● Molecule 1: Arylesterase



● Molecule 1: Arylesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	145.49Å 145.49Å 129.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.97 – 2.25 39.97 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.97-2.25) 99.6 (39.97-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.24Å)	Xtriage
Refinement program	REFMAC 6.1.1	Depositor
R, R_{free}	0.165 , 0.202 0.166 , 0.200	Depositor DCC
R_{free} test set	7330 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.073 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14023	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 24.42 % 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 3.8486e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, GOL, ACT

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	1.20	2/2187 (0.1%)	0.99	9/2967 (0.3%)
1	B	1.27	6/2187 (0.3%)	1.00	7/2967 (0.2%)
1	C	1.22	8/2195 (0.4%)	0.96	4/2978 (0.1%)
1	D	1.25	4/2187 (0.2%)	0.96	2/2967 (0.1%)
1	E	1.23	5/2195 (0.2%)	0.98	7/2978 (0.2%)
1	F	1.19	2/2187 (0.1%)	0.99	7/2967 (0.2%)
All	All	1.23	27/13138 (0.2%)	0.98	36/17824 (0.2%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	44	SER	CB-OG	-8.87	1.30	1.42
1	C	44	SER	CB-OG	-7.18	1.32	1.42
1	D	87[A]	GLU	CD-OE1	6.23	1.32	1.25
1	D	87[B]	GLU	CD-OE1	6.23	1.32	1.25
1	A	44	SER	CB-OG	-6.21	1.34	1.42
1	C	12	TYR	CD1-CE1	5.98	1.48	1.39
1	B	87[A]	GLU	CB-CG	5.79	1.63	1.52
1	B	87[B]	GLU	CB-CG	5.79	1.63	1.52
1	E	37	TYR	CG-CD2	5.78	1.46	1.39
1	C	81	GLU	CB-CG	5.71	1.62	1.52
1	B	200	GLU	CD-OE1	5.69	1.31	1.25
1	A	189	LYS	CD-CE	5.69	1.65	1.51
1	E	242	GLU	CD-OE1	5.55	1.31	1.25
1	B	138	ASP	CB-CG	-5.54	1.40	1.51
1	C	81	GLU	CG-CD	5.49	1.60	1.51
1	C	253	PHE	CD2-CE2	5.42	1.50	1.39
1	C	59	ARG	CZ-NH2	5.33	1.40	1.33
1	B	239	LYS	CD-CE	5.30	1.64	1.51
1	E	87[A]	GLU	CD-OE2	5.24	1.31	1.25
1	E	87[B]	GLU	CD-OE2	5.24	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	12	TYR	CE2-CZ	5.19	1.45	1.38
1	F	87[A]	GLU	CB-CG	5.15	1.61	1.52
1	F	87[B]	GLU	CB-CG	5.15	1.61	1.52
1	B	93	PHE	CE2-CZ	5.14	1.47	1.37
1	C	37	TYR	CG-CD2	5.13	1.45	1.39
1	E	13	PHE	CE2-CZ	5.08	1.47	1.37
1	D	93	PHE	CE2-CZ	5.04	1.47	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	111	ARG	NE-CZ-NH2	9.87	125.23	120.30
1	B	220	ASP	CB-CG-OD2	-7.74	111.33	118.30
1	F	111	ARG	NE-CZ-NH1	-7.40	116.60	120.30
1	A	15	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	F	211	ASP	CB-CG-OD1	6.77	124.39	118.30
1	E	202	ASP	CB-CG-OD1	6.48	124.14	118.30
1	A	59	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	15	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	138	ASP	CB-CG-OD1	-6.33	112.60	118.30
1	B	220	ASP	CB-CG-OD1	6.29	123.97	118.30
1	A	189	LYS	CD-CE-NZ	-6.29	97.23	111.70
1	A	74	ASP	CB-CG-OD1	6.28	123.95	118.30
1	C	102	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	E	151	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	D	59	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	151	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	A	31	ASP	CB-CG-OD1	5.74	123.46	118.30
1	F	59	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	A	59	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	C	202	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	15	ASP	CB-CG-OD1	5.64	123.38	118.30
1	E	55	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	A	255	VAL	CA-CB-CG1	5.55	119.23	110.90
1	D	151	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	E	61	ASP	CB-CG-OD1	5.49	123.24	118.30
1	F	55	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	68	ASP	CB-CG-OD1	5.44	123.20	118.30
1	F	106	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	C	142	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	138	ASP	CB-CA-C	-5.26	99.88	110.40
1	E	31	ASP	CB-CG-OD1	5.23	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	E	168	GLY	N-CA-C	5.17	126.02	113.10
1	E	84	ASP	CB-CG-OD1	5.16	122.95	118.30
1	B	239	LYS	CD-CE-NZ	5.16	123.56	111.70
1	F	138	ASP	CB-CA-C	5.04	120.47	110.40

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	2132	0	2094	12	0
1	B	2132	0	2094	8	0
1	C	2137	0	2098	17	0
1	D	2132	0	2094	15	0
1	E	2137	0	2098	8	0
1	F	2132	0	2094	16	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	8	0	6	0	0
2	D	4	0	3	0	0
2	E	8	0	6	0	0
2	F	12	0	9	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
4	A	18	0	24	0	0
4	B	18	0	24	0	0
4	C	24	0	32	0	0
4	D	18	0	24	1	0
4	E	18	0	24	1	0
4	F	24	0	32	0	0
5	A	157	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	189	0	0	0	0
5	C	173	0	0	4	0
5	D	178	0	0	1	0
5	E	166	0	0	1	0
5	F	173	0	0	1	0
All	All	14023	0	12762	77	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 (77) 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:6:LYS:HG2	1:F:78:GLN:NE2	1.95	0.82
2:F:273:ACT:H2	5:F:590:HOH:O	1.83	0.77
1:C:138[B]:ASP:OD2	5:C:380:HOH:O	2.03	0.75
1:D:124[A]:LEU:HD21	1:D:128:LYS:HG3	1.71	0.72
1:F:23:LEU:C	1:F:23:LEU:HD23	2.18	0.64
1:D:165:ILE:HD11	1:D:171:VAL:HB	1.80	0.63
1:B:124[B]:LEU:HD21	1:B:131:TYR:CE2	2.35	0.61
1:B:85:LEU:O	1:B:111:ARG:HD3	2.01	0.60
1:F:163:TYR:O	1:F:169:GLN:HG3	2.01	0.60
1:E:124[B]:LEU:HD12	1:E:124[B]:LEU:N	2.18	0.59
1:F:6:LYS:HG2	1:F:78:GLN:CD	2.23	0.58
1:F:6:LYS:N	1:F:78:GLN:HE22	2.02	0.58
1:E:137:LEU:HB3	4:E:276:GOL:H12	1.86	0.58
1:C:124[A]:LEU:HD21	1:C:128:LYS:HG3	1.87	0.57
1:F:160:ALA:HB3	1:F:161:PRO:CD	2.35	0.56
1:D:115:LEU:O	1:D:214:THR:HA	2.06	0.55
1:D:137:LEU:HB3	4:D:274:GOL:H12	1.90	0.54
1:D:20:LYS:NZ	5:D:703:HOH:O	2.41	0.52
1:A:88:VAL:HG12	1:A:111:ARG:O	2.10	0.52
1:C:160:ALA:HB3	1:C:161:PRO:CD	2.40	0.52
1:C:124[A]:LEU:HD21	1:C:128:LYS:CG	2.40	0.51
1:F:115:LEU:O	1:F:214:THR:HA	2.11	0.51
1:D:124[B]:LEU:HD21	1:D:131:TYR:CG	2.46	0.50
1:F:131:TYR:N	1:F:132:PRO:CD	2.74	0.50
1:C:88:VAL:HG12	1:C:111:ARG:O	2.12	0.50
1:E:24:PHE:HB3	1:E:35:TRP:CE2	2.47	0.50
1:C:43:SER:HA	1:C:47:TYR:O	2.13	0.49
1:B:115:LEU:O	1:B:214:THR:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:TYR:HB3	1:D:171:VAL:HG21	1.96	0.48
1:E:88:VAL:HG12	1:E:111:ARG:O	2.14	0.48
1:A:119:GLY:HA2	1:A:218:HIS:CE1	2.49	0.47
1:A:43:SER:HA	1:A:47:TYR:O	2.14	0.47
1:D:88:VAL:HG12	1:D:111:ARG:O	2.15	0.47
1:A:2:THR:HA	1:A:11:ILE:O	2.14	0.46
1:C:85:LEU:O	1:C:111:ARG:NH1	2.47	0.46
1:C:142:ARG:HD3	5:C:527:HOH:O	2.15	0.46
1:A:124[A]:LEU:HD21	1:A:128:LYS:CG	2.46	0.46
1:C:244:LYS:HE3	5:C:336:HOH:O	2.15	0.46
1:B:41:TYR:CD2	1:B:262:ASN:HB3	2.51	0.45
1:A:155:ILE:HG21	1:A:183:ALA:CB	2.47	0.45
1:B:80:ILE:CG2	1:B:111:ARG:HD2	2.46	0.45
1:F:88:VAL:HG12	1:F:111:ARG:O	2.17	0.45
1:A:24:PHE:HB3	1:A:35:TRP:CE2	2.52	0.45
1:E:220:ASP:OD1	1:E:248:ASP:N	2.45	0.44
1:B:28:TRP:HA	1:B:29:PRO:HA	1.86	0.44
1:B:23:LEU:C	1:B:23:LEU:HD23	2.38	0.44
1:F:41:TYR:CD2	1:F:262:ASN:HB3	2.52	0.44
1:A:38:GLN:HG3	1:A:262:ASN:OD1	2.17	0.44
1:C:189:LYS:HE3	1:C:193:ASP:OD2	2.18	0.44
1:D:124[B]:LEU:O	1:D:124[B]:LEU:HD13	2.18	0.44
1:C:23:LEU:HD23	1:C:24:PHE:N	2.32	0.44
1:C:124[B]:LEU:HD21	1:C:131:TYR:CG	2.53	0.44
1:F:116:VAL:HA	1:F:215:LEU:O	2.18	0.44
1:A:189:LYS:HE2	1:A:193:ASP:OD1	2.18	0.43
1:C:259:GLN:HG3	5:C:690:HOH:O	2.18	0.43
1:F:23:LEU:HD23	1:F:24:PHE:N	2.34	0.43
1:F:142:ARG:O	1:F:146:GLU:HG3	2.18	0.42
1:F:160:ALA:HB3	1:F:161:PRO:HD2	2.01	0.42
1:C:207:MET:HA	1:C:210:ILE:HD12	2.00	0.42
1:E:222:ASP:OD1	1:E:251:HIS:HB2	2.18	0.42
1:B:43:SER:HA	1:B:47:TYR:O	2.19	0.42
1:C:160:ALA:HB3	1:C:161:PRO:HD3	2.01	0.42
1:D:23:LEU:C	1:D:23:LEU:HD23	2.40	0.41
1:D:35:TRP:O	1:D:36:GLU:C	2.57	0.41
1:D:160:ALA:HB3	1:D:161:PRO:CD	2.50	0.41
1:A:124[A]:LEU:HD21	1:A:128:LYS:HG3	2.03	0.41
1:C:131:TYR:N	1:C:132:PRO:CD	2.83	0.41
1:D:124[B]:LEU:HD21	1:D:131:TYR:CD2	2.55	0.41
1:A:115:LEU:O	1:A:214:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:PHE:HB3	1:F:35:TRP:CE2	2.55	0.41
1:D:28:TRP:HA	1:D:29:PRO:HA	1.90	0.41
1:E:21:PRO:HA	1:E:48:ARG:O	2.21	0.41
1:A:118:LEU:O	1:A:119:GLY:C	2.60	0.41
1:D:62:GLN:HB3	1:D:187:SER:HB2	2.03	0.41
1:E:244:LYS:HE3	5:E:310:HOH:O	2.22	0.40
1:C:28:TRP:HA	1:C:29:PRO:HA	1.81	0.40
1:F:151:ARG:HH21	1:F:151:ARG:HD2	1.73	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	271/271 (100%)	263 (97%)	8 (3%)	0	100	100
1	B	271/271 (100%)	264 (97%)	6 (2%)	1 (0%)	34	37
1	C	272/271 (100%)	264 (97%)	8 (3%)	0	100	100
1	D	271/271 (100%)	262 (97%)	9 (3%)	0	100	100
1	E	272/271 (100%)	259 (95%)	13 (5%)	0	100	100
1	F	271/271 (100%)	263 (97%)	8 (3%)	0	100	100
All	All	1628/1626 (100%)	1575 (97%)	52 (3%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	PRO

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	222/220 (101%)	220 (99%)	2 (1%)	78	86
1	B	222/220 (101%)	218 (98%)	4 (2%)	59	68
1	C	223/220 (101%)	220 (99%)	3 (1%)	69	79
1	D	222/220 (101%)	219 (99%)	3 (1%)	67	76
1	E	223/220 (101%)	220 (99%)	3 (1%)	69	79
1	F	222/220 (101%)	218 (98%)	4 (2%)	59	68
All	All	1334/1320 (101%)	1315 (99%)	19 (1%)	67	76

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	PHE
1	A	206	ASP
1	B	94	SER
1	B	138	ASP
1	B	155	ILE
1	B	206	ASP
1	C	167	LYS
1	C	206	ASP
1	C	218	HIS
1	D	18	SER
1	D	138	ASP
1	D	206	ASP
1	E	94	SER
1	E	206	ASP
1	E	247	LYS
1	F	81	GLU
1	F	138	ASP
1	F	206	ASP
1	F	209	LYS

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

35 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	$\# Z > 2$
4	GOL	A	274	-	5,5,5	0.67	0	5,5,5	0.51	0
2	ACT	F	273	-	1,3,3	2.31	1 (100%)	0,3,3	-	-
3	SO4	C	273	-	4,4,4	0.21	0	6,6,6	0.84	0
4	GOL	F	278	-	5,5,5	0.61	0	5,5,5	1.40	1 (20%)
2	ACT	F	274	-	1,3,3	2.79	1 (100%)	0,3,3	-	-
2	ACT	C	274	-	1,3,3	3.76	1 (100%)	0,3,3	-	-
3	SO4	E	273	-	4,4,4	0.22	0	6,6,6	0.68	0
2	ACT	E	274	-	1,3,3	2.72	1 (100%)	0,3,3	-	-
4	GOL	F	275	-	5,5,5	0.45	0	5,5,5	0.56	0
4	GOL	B	275	-	5,5,5	0.67	0	5,5,5	0.24	0
4	GOL	F	276	-	5,5,5	0.41	0	5,5,5	0.51	0
4	GOL	B	276	-	5,5,5	0.48	0	5,5,5	1.23	1 (20%)
3	SO4	A	273	-	4,4,4	0.33	0	6,6,6	0.89	0
4	GOL	F	277	-	5,5,5	0.70	0	5,5,5	0.47	0
4	GOL	C	278	-	5,5,5	0.53	0	5,5,5	0.78	0
4	GOL	C	276	-	5,5,5	0.41	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	F	272	-	1,3,3	2.65	1 (100%)	0,3,3	-	-
3	SO4	D	273	-	4,4,4	0.13	0	6,6,6	0.64	0
2	ACT	C	272	-	1,3,3	3.09	1 (100%)	0,3,3	-	-
2	ACT	D	272	-	1,3,3	2.31	1 (100%)	0,3,3	-	-
4	GOL	D	274	-	5,5,5	0.77	0	5,5,5	0.66	0
4	GOL	C	277	-	5,5,5	0.39	0	5,5,5	1.36	0
4	GOL	A	276	-	5,5,5	0.57	0	5,5,5	0.97	0
2	ACT	E	272	-	1,3,3	2.22	1 (100%)	0,3,3	-	-
4	GOL	D	275	-	5,5,5	1.08	0	5,5,5	0.44	0
4	GOL	A	275	-	5,5,5	0.39	0	5,5,5	0.69	0
4	GOL	E	277	-	5,5,5	0.32	0	5,5,5	0.97	1 (20%)
2	ACT	B	272	-	1,3,3	2.61	1 (100%)	0,3,3	-	-
4	GOL	E	275	-	5,5,5	0.65	0	5,5,5	0.72	0
3	SO4	B	273	-	4,4,4	0.21	0	6,6,6	1.52	2 (33%)
4	GOL	C	275	-	5,5,5	0.60	0	5,5,5	0.68	0
4	GOL	B	274	-	5,5,5	0.36	0	5,5,5	0.74	0
4	GOL	E	276	-	5,5,5	0.29	0	5,5,5	0.58	0
2	ACT	A	272	-	1,3,3	2.31	1 (100%)	0,3,3	-	-
4	GOL	D	276	-	5,5,5	0.96	0	5,5,5	1.56	2 (40%)

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
4	GOL	A	274	-	-	0/4/4/4	-
4	GOL	F	278	-	-	1/4/4/4	-
4	GOL	F	275	-	-	0/4/4/4	-
4	GOL	B	275	-	-	0/4/4/4	-
4	GOL	F	276	-	-	1/4/4/4	-
4	GOL	B	276	-	-	0/4/4/4	-
4	GOL	F	277	-	-	2/4/4/4	-
4	GOL	C	278	-	-	3/4/4/4	-
4	GOL	D	274	-	-	4/4/4/4	-
4	GOL	C	277	-	-	1/4/4/4	-
4	GOL	A	276	-	-	0/4/4/4	-
4	GOL	D	275	-	-	0/4/4/4	-
4	GOL	A	275	-	-	0/4/4/4	-
4	GOL	E	277	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	E	275	-	-	0/4/4/4	-
4	GOL	C	275	-	-	0/4/4/4	-
4	GOL	B	274	-	-	2/4/4/4	-
4	GOL	E	276	-	-	2/4/4/4	-
4	GOL	C	276	-	-	2/4/4/4	-
4	GOL	D	276	-	-	0/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	274	ACT	CH3-C	3.76	1.53	1.48
2	C	272	ACT	CH3-C	3.09	1.52	1.48
2	F	274	ACT	CH3-C	2.79	1.52	1.48
2	E	274	ACT	CH3-C	2.72	1.52	1.48
2	F	272	ACT	CH3-C	2.65	1.52	1.48
2	B	272	ACT	CH3-C	2.61	1.52	1.48
2	A	272	ACT	CH3-C	2.31	1.51	1.48
2	D	272	ACT	CH3-C	2.31	1.51	1.48
2	F	273	ACT	CH3-C	2.31	1.51	1.48
2	E	272	ACT	CH3-C	2.22	1.51	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	273	SO4	O4-S-O3	-2.60	97.95	109.06
4	D	276	GOL	O2-C2-C1	-2.37	98.68	109.12
4	D	276	GOL	O3-C3-C2	2.31	121.30	110.20
4	F	278	GOL	O2-C2-C1	-2.18	99.51	109.12
4	B	276	GOL	O2-C2-C1	-2.17	99.56	109.12
3	B	273	SO4	O3-S-O1	2.09	120.20	109.31
4	E	277	GOL	C3-C2-C1	-2.03	103.82	111.70

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	274	GOL	O1-C1-C2-C3
4	C	276	GOL	O1-C1-C2-C3
4	C	278	GOL	O1-C1-C2-C3
4	D	274	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	F	277	GOL	C1-C2-C3-O3
4	D	274	GOL	C1-C2-C3-O3
4	E	277	GOL	C1-C2-C3-O3
4	F	278	GOL	C1-C2-C3-O3
4	B	274	GOL	O1-C1-C2-O2
4	C	276	GOL	O1-C1-C2-O2
4	F	277	GOL	O2-C2-C3-O3
4	D	274	GOL	O1-C1-C2-O2
4	E	276	GOL	O1-C1-C2-O2
4	D	274	GOL	O2-C2-C3-O3
4	F	276	GOL	O1-C1-C2-O2
4	C	278	GOL	O1-C1-C2-O2
4	C	278	GOL	O2-C2-C3-O3
4	C	277	GOL	C1-C2-C3-O3
4	E	276	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	273	ACT	1	0
4	D	274	GOL	1	0
4	E	276	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

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	271/271 (100%)	-0.46	2 (0%) 87 88	20, 29, 41, 53	3 (1%)
1	B	271/271 (100%)	-0.65	1 (0%) 92 93	18, 26, 37, 49	4 (1%)
1	C	271/271 (100%)	-0.44	5 (1%) 68 71	19, 28, 41, 55	1 (0%)
1	D	271/271 (100%)	-0.42	4 (1%) 73 75	18, 27, 39, 52	3 (1%)
1	E	271/271 (100%)	-0.51	2 (0%) 87 88	20, 29, 41, 58	2 (0%)
1	F	271/271 (100%)	-0.56	1 (0%) 92 93	19, 27, 38, 56	6 (2%)
All	All	1626/1626 (100%)	-0.51	15 (0%) 84 85	18, 27, 40, 58	19 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	168	GLY	3.1
1	C	185	LEU	3.0
1	D	185	LEU	3.0
1	D	182	ILE	2.9
1	D	30	LEU	2.6
1	D	184	LEU	2.5
1	A	168	GLY	2.5
1	C	30	LEU	2.4
1	A	185	LEU	2.3
1	E	138[A]	ASP	2.3
1	F	185	LEU	2.3
1	C	138[A]	ASP	2.2
1	C	182	ILE	2.1
1	B	185	LEU	2.1
1	C	168	GLY	2.1

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 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(\AA^2)	Q<0.9
4	GOL	F	277	6/6	0.66	0.37	59,66,69,70	2
2	ACT	E	274	4/4	0.86	0.11	61,62,62,62	0
2	ACT	C	274	4/4	0.86	0.13	47,48,48,49	0
2	ACT	F	274	4/4	0.89	0.11	50,51,51,52	0
4	GOL	C	278	6/6	0.90	0.21	64,68,69,69	0
4	GOL	D	276	6/6	0.91	0.28	41,43,44,45	0
3	SO4	A	273	5/5	0.92	0.21	39,39,45,47	5
3	SO4	E	273	5/5	0.92	0.19	41,42,49,49	5
4	GOL	A	276	6/6	0.92	0.20	44,45,47,51	0
4	GOL	F	278	6/6	0.92	0.36	43,43,46,47	0
3	SO4	C	273	5/5	0.93	0.26	32,32,38,40	5
4	GOL	C	277	6/6	0.93	0.28	39,48,50,51	0
3	SO4	B	273	5/5	0.93	0.17	34,38,41,44	5
4	GOL	B	276	6/6	0.94	0.20	40,45,45,46	0
4	GOL	A	275	6/6	0.94	0.16	41,48,53,55	0
3	SO4	D	273	5/5	0.94	0.15	33,35,36,42	5
4	GOL	E	277	6/6	0.95	0.19	41,45,47,49	0
4	GOL	B	274	6/6	0.95	0.20	32,49,55,60	0
4	GOL	E	276	6/6	0.95	0.19	43,46,50,52	0
4	GOL	F	276	6/6	0.96	0.24	40,46,50,53	0
4	GOL	C	276	6/6	0.96	0.20	44,51,54,58	0
2	ACT	C	272	4/4	0.96	0.20	29,32,33,33	0
2	ACT	A	272	4/4	0.97	0.13	28,30,31,32	0
4	GOL	D	274	6/6	0.97	0.21	32,34,40,47	0
4	GOL	D	275	6/6	0.97	0.11	28,30,31,33	0
2	ACT	F	272	4/4	0.98	0.12	28,29,30,31	0
4	GOL	B	275	6/6	0.98	0.07	26,27,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	E	275	6/6	0.98	0.09	25,27,29,30	0
2	ACT	F	273	4/4	0.98	0.11	48,49,49,50	0
2	ACT	D	272	4/4	0.98	0.15	25,25,27,27	0
4	GOL	A	274	6/6	0.98	0.12	24,26,29,32	0
2	ACT	E	272	4/4	0.98	0.14	31,33,34,34	0
2	ACT	B	272	4/4	0.98	0.13	26,27,27,28	0
4	GOL	F	275	6/6	0.99	0.09	26,27,29,34	0
4	GOL	C	275	6/6	0.99	0.09	23,25,26,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.