



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:24 PM UTC

PDB ID : 3HI4 / pdb_00003hi4
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 types of validation reports are described at

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

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

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

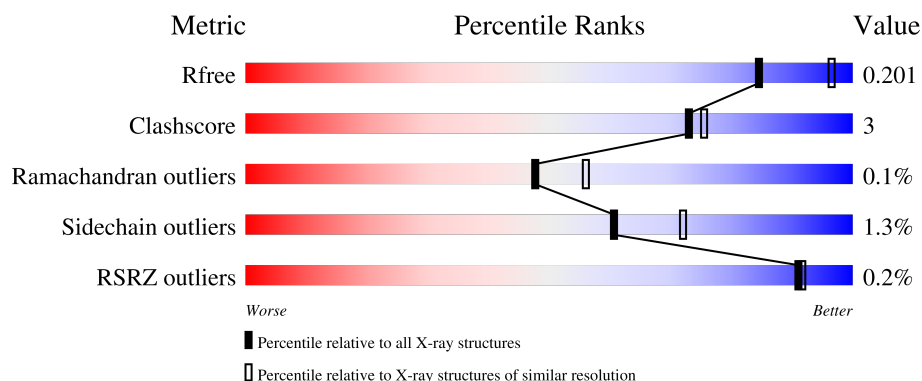
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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	87% 12%
1	B	271	90% 8% .
1	C	271	87% 12% .
1	D	271	87% 11% .
1	E	271	89% 11%

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Mol	Chain	Length	Quality of chain
1	F	271	 87% 12% •

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	C	N	O	S	0	2	0
			2132	1371	358	398	5			
1	B	271	Total	C	N	O	S	0	2	0
			2132	1371	358	398	5			
1	C	271	Total	C	N	O	S	0	3	0
			2137	1374	358	400	5			
1	D	271	Total	C	N	O	S	0	2	0
			2132	1371	358	398	5			
1	E	271	Total	C	N	O	S	0	3	0
			2137	1374	358	400	5			
1	F	271	Total	C	N	O	S	0	2	0
			2132	1371	358	398	5			

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 (CCD ID: ACT) (formula: C₂H₃O₂).



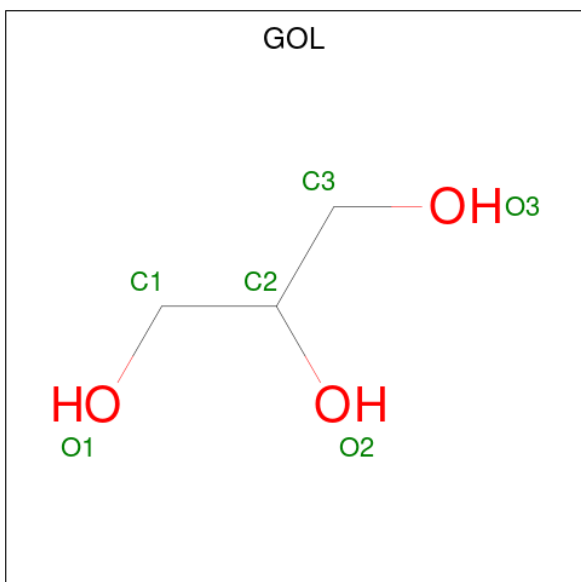
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total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

- Molecule 3 is SULFATE ION (CCD ID: 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 (CCD ID: 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

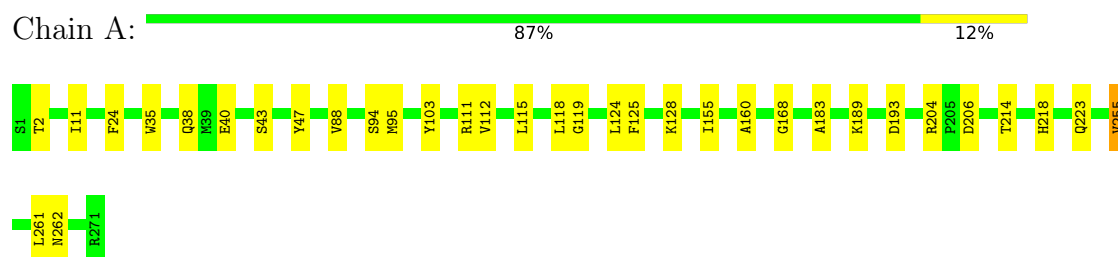
- Molecule 5 is water.

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

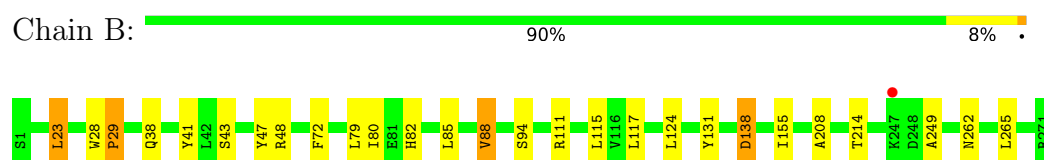
3 Residue-property plots

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.

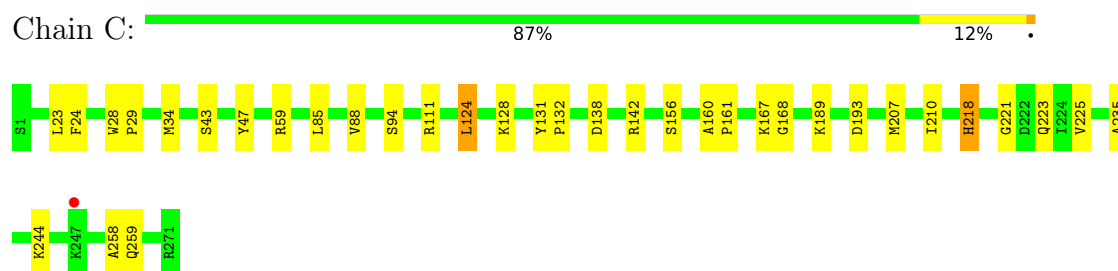
• Molecule 1: Arylesterase



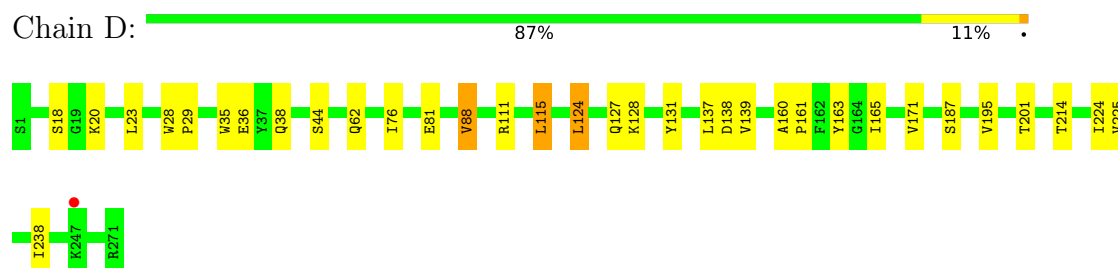
• Molecule 1: Arylesterase



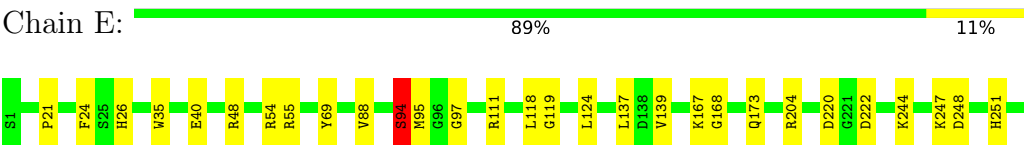
• Molecule 1: Arylesterase



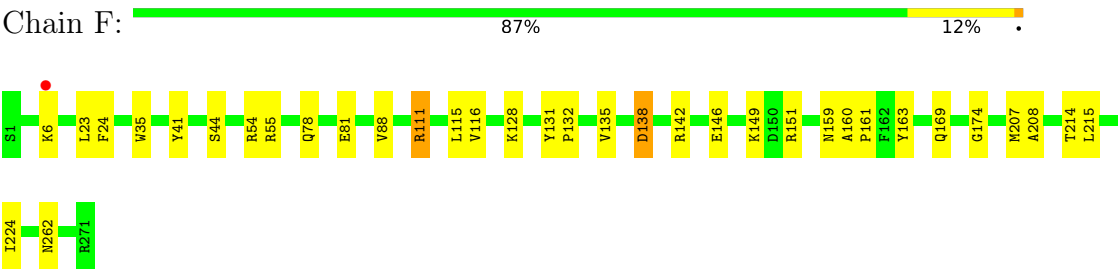
• Molecule 1: Arylesterase



● 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) 99.7 (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 , 0.201	Depositor DCC
R_{free} test set	7330 reflections (5.00%)	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)	0.37 , 40.5	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	0.96	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, ACT, GOL

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	1.42	5/2187 (0.2%)	1.18	10/2967 (0.3%)
1	B	1.43	10/2187 (0.5%)	1.20	3/2967 (0.1%)
1	C	1.42	8/2195 (0.4%)	1.19	6/2978 (0.2%)
1	D	1.46	9/2187 (0.4%)	1.20	4/2967 (0.1%)
1	E	1.43	5/2195 (0.2%)	1.20	6/2978 (0.2%)
1	F	1.38	4/2187 (0.2%)	1.17	6/2967 (0.2%)
All	All	1.42	41/13138 (0.3%)	1.19	35/17824 (0.2%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	SER	CA-C	7.48	1.59	1.52
1	D	139	VAL	CA-C	7.11	1.61	1.52
1	F	128	LYS	C-O	6.77	1.29	1.24
1	A	103	TYR	C-O	-6.45	1.16	1.24
1	D	225	VAL	N-CA	6.42	1.51	1.46
1	B	79	LEU	CA-C	6.40	1.60	1.52
1	A	125	PHE	CA-C	6.23	1.58	1.52
1	C	235	ALA	CA-CB	6.14	1.62	1.53
1	B	72	PHE	N-CA	6.10	1.53	1.46
1	B	88	VAL	CA-CB	6.03	1.62	1.54
1	E	139	VAL	CA-C	6.01	1.60	1.52
1	A	112	VAL	CA-CB	5.74	1.61	1.54
1	D	44	SER	CB-OG	-5.71	1.30	1.42
1	A	160	ALA	CA-CB	5.54	1.60	1.53
1	B	117	LEU	C-O	5.44	1.30	1.24
1	D	88	VAL	CA-CB	5.40	1.60	1.54
1	C	218	HIS	ND1-CE1	5.39	1.38	1.32
1	E	40	GLU	C-O	-5.37	1.17	1.24
1	B	249	ALA	CA-CB	-5.34	1.42	1.53
1	F	159	ASN	CA-C	5.33	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	HIS	C-O	-5.27	1.17	1.24
1	C	94	SER	CA-C	5.25	1.57	1.52
1	F	208	ALA	CA-CB	5.24	1.62	1.53
1	D	76	ILE	CA-C	5.23	1.59	1.52
1	B	208	ALA	CA-CB	5.22	1.62	1.53
1	D	115	LEU	C-O	5.21	1.30	1.23
1	D	127	GLN	CD-OE1	5.18	1.33	1.23
1	B	48	ARG	CA-C	5.17	1.59	1.52
1	C	221	GLY	CA-C	5.15	1.59	1.51
1	F	135	VAL	CA-CB	5.14	1.61	1.53
1	E	173	GLN	CD-NE2	5.14	1.44	1.33
1	C	258	ALA	C-O	5.12	1.29	1.24
1	B	23	LEU	C-O	5.11	1.29	1.24
1	E	94	SER	CA-C	5.11	1.57	1.53
1	C	34	MET	N-CA	5.09	1.52	1.46
1	B	94	SER	CA-C	5.08	1.57	1.53
1	C	156	SER	N-CA	-5.08	1.40	1.46
1	D	201	THR	CA-CB	5.08	1.60	1.53
1	D	238	ILE	C-O	5.07	1.30	1.24
1	E	258	ALA	CA-CB	5.05	1.61	1.53
1	C	59	ARG	CZ-NH2	5.03	1.40	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	111	ARG	NE-CZ-NH2	6.71	125.23	119.20
1	A	204	ARG	CA-C-N	-6.55	112.07	119.28
1	A	204	ARG	C-N-CA	-6.55	112.07	119.28
1	B	138	ASP	CB-CA-C	-6.36	99.88	110.68
1	E	97	GLY	N-CA-C	-6.30	104.99	113.24
1	E	204	ARG	CA-C-N	-6.27	112.38	119.28
1	E	204	ARG	C-N-CA	-6.27	112.38	119.28
1	A	255	VAL	N-CA-CB	6.00	119.92	110.31
1	C	168	GLY	N-CA-C	5.99	123.33	115.36
1	E	69	TYR	N-CA-C	5.89	118.45	111.33
1	C	218	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	D	38	GLN	N-CA-C	-5.75	104.62	111.69
1	A	223	GLN	CA-C-N	-5.73	117.29	123.08
1	A	223	GLN	C-N-CA	-5.73	117.29	123.08
1	D	195	VAL	CB-CA-C	-5.67	104.71	111.97
1	A	168	GLY	N-CA-C	5.58	123.34	115.30
1	D	224	ILE	N-CA-C	-5.42	106.52	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	168	GLY	N-CA-C	5.42	126.02	113.18
1	A	95	MET	N-CA-C	-5.39	105.97	112.54
1	F	149	LYS	N-CA-C	-5.32	106.84	113.55
1	F	174	GLY	N-CA-C	-5.30	105.99	112.77
1	F	224	ILE	N-CA-C	-5.29	106.64	111.67
1	A	40	GLU	N-CA-C	-5.27	105.61	111.36
1	C	223	GLN	CA-C-N	-5.25	117.78	123.08
1	C	223	GLN	C-N-CA	-5.25	117.78	123.08
1	A	255	VAL	CA-CB-CG1	5.20	119.23	110.40
1	C	225	VAL	N-CA-C	-5.16	103.04	108.15
1	D	225	VAL	N-CA-C	-5.14	103.06	108.15
1	B	38	GLN	N-CA-C	-5.12	105.78	111.36
1	E	26	HIS	N-CA-C	5.12	116.70	110.41
1	F	138	ASP	CB-CA-C	5.10	120.47	110.67
1	F	44	SER	CB-CA-C	5.08	119.15	110.01
1	C	218	HIS	CB-CG-ND1	5.07	130.31	122.70
1	A	261	LEU	N-CA-C	-5.04	105.86	111.36
1	B	265	LEU	N-CA-C	-5.01	105.90	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2132	0	2094	12	0
1	B	2132	0	2094	8	0
1	C	2137	0	2098	18	0
1	D	2132	0	2094	15	0
1	E	2137	0	2098	11	0
1	F	2132	0	2094	17	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	82	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 (82) 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)
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	0.68
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:23:LEU:C	1:B:23:LEU:HD23	2.38	0.49
1:B:115:LEU:O	1:B:214:THR:HA	2.13	0.48
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:23:LEU:C	1:D:23:LEU:HD23	2.40	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:D:35:TRP:O	1:D:36:GLU:C	2.57	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:118:LEU:O	1:A:119:GLY:C	2.60	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: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:F:54:ARG:O	1:F:55:ARG:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:GLN:HG3	5:C:690:HOH:O	2.18	0.43
1:E:54:ARG:O	1:E:55:ARG:C	2.62	0.43
1:F:23:LEU:HD23	1:F:24:PHE:N	2.34	0.43
1:C:23:LEU:HD23	1:C:23:LEU:C	2.43	0.43
1:F:23:LEU:C	1:F:23:LEU:CD2	2.90	0.42
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:F:207:MET:HA	1:F:207:MET:HE2	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: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:E:118:LEU:O	1:E:119:GLY:C	2.63	0.41
1:A:115:LEU:O	1:A:214:THR:HA	2.20	0.41
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:D:62:GLN:HB3	1:D:187:SER:HB2	2.03	0.41
1:E:94:SER:O	1:E:95:MET:C	2.62	0.40
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%)	30	31
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%)	48	56

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%)	70	79
1	B	222/220 (101%)	219 (99%)	3 (1%)	59	70
1	C	223/220 (101%)	219 (98%)	4 (2%)	51	63
1	D	222/220 (101%)	217 (98%)	5 (2%)	44	55
1	E	223/220 (101%)	220 (99%)	3 (1%)	61	72
1	F	222/220 (101%)	220 (99%)	2 (1%)	70	79
All	All	1334/1320 (101%)	1315 (99%)	19 (1%)	61	70

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

Mol	Chain	Res	Type
1	A	206	ASP
1	A	255	VAL
1	B	88	VAL
1	B	138	ASP

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Mol	Chain	Res	Type
1	B	155	ILE
1	C	124[A]	LEU
1	C	124[B]	LEU
1	C	167	LYS
1	C	218	HIS
1	D	18	SER
1	D	81	GLU
1	D	124[A]	LEU
1	D	124[B]	LEU
1	D	138	ASP
1	E	94	SER
1	E	167	LYS
1	E	247	LYS
1	F	81	GLU
1	F	138	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	38	GLN
1	B	127	GLN
1	B	166	ASN
1	B	173	GLN
1	B	223	GLN
1	C	38	GLN
1	C	176	GLN
1	D	38	GLN
1	E	38	GLN
1	E	176	GLN
1	F	38	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	ACT	A	272	-	3,3,3	0.61	0	3,3,3	2.14	1 (33%)
4	GOL	E	276	-	5,5,5	0.30	0	5,5,5	0.62	0
4	GOL	A	275	-	5,5,5	0.40	0	5,5,5	0.74	0
2	ACT	C	272	-	3,3,3	1.02	0	3,3,3	2.07	2 (66%)
4	GOL	F	276	-	5,5,5	0.42	0	5,5,5	0.55	0
2	ACT	F	273	-	3,3,3	0.82	0	3,3,3	1.30	0
4	GOL	C	277	-	5,5,5	0.40	0	5,5,5	1.44	0
4	GOL	C	278	-	5,5,5	0.56	0	5,5,5	0.82	0
2	ACT	D	272	-	3,3,3	0.99	0	3,3,3	1.63	1 (33%)
4	GOL	A	276	-	5,5,5	0.58	0	5,5,5	1.04	1 (20%)
4	GOL	E	275	-	5,5,5	0.67	0	5,5,5	0.77	0
3	SO4	D	273	-	4,4,4	0.23	0	6,6,6	0.60	0
3	SO4	E	273	-	4,4,4	0.33	0	6,6,6	0.70	0
2	ACT	F	274	-	3,3,3	1.47	1 (33%)	3,3,3	0.55	0
2	ACT	E	272	-	3,3,3	0.68	0	3,3,3	2.03	1 (33%)
4	GOL	C	276	-	5,5,5	0.43	0	5,5,5	0.38	0
2	ACT	E	274	-	3,3,3	1.15	0	3,3,3	0.70	0
4	GOL	A	274	-	5,5,5	0.71	0	5,5,5	0.56	0
4	GOL	F	278	-	5,5,5	0.63	0	5,5,5	1.48	1 (20%)
3	SO4	A	273	-	4,4,4	0.44	0	6,6,6	0.84	0
4	GOL	E	277	-	5,5,5	0.32	0	5,5,5	1.04	1 (20%)
4	GOL	B	274	-	5,5,5	0.38	0	5,5,5	0.80	0
3	SO4	B	273	-	4,4,4	0.33	0	6,6,6	1.32	1 (16%)
4	GOL	F	277	-	5,5,5	0.74	0	5,5,5	0.49	0
2	ACT	F	272	-	3,3,3	0.70	0	3,3,3	2.25	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	275	-	5,5,5	0.71	0	5,5,5	0.26	0
2	ACT	C	274	-	3,3,3	1.12	0	3,3,3	1.65	1 (33%)
2	ACT	B	272	-	3,3,3	0.57	0	3,3,3	1.79	1 (33%)
4	GOL	D	276	-	5,5,5	0.99	0	5,5,5	1.65	2 (40%)
4	GOL	D	274	-	5,5,5	0.82	0	5,5,5	0.69	0
4	GOL	F	275	-	5,5,5	0.46	0	5,5,5	0.61	0
4	GOL	C	275	-	5,5,5	0.61	0	5,5,5	0.73	0
4	GOL	D	275	-	5,5,5	1.13	0	5,5,5	0.46	0
4	GOL	B	276	-	5,5,5	0.49	0	5,5,5	1.30	1 (20%)
3	SO4	C	273	-	4,4,4	0.26	0	6,6,6	0.75	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
4	GOL	E	276	-	-	1/4/4/4	-
4	GOL	A	275	-	-	0/4/4/4	-
4	GOL	F	276	-	-	1/4/4/4	-
4	GOL	C	277	-	-	1/4/4/4	-
4	GOL	C	278	-	-	3/4/4/4	-
4	GOL	A	276	-	-	0/4/4/4	-
4	GOL	E	275	-	-	0/4/4/4	-
4	GOL	C	276	-	-	2/4/4/4	-
4	GOL	A	274	-	-	0/4/4/4	-
4	GOL	F	278	-	-	1/4/4/4	-
4	GOL	E	277	-	-	1/4/4/4	-
4	GOL	B	274	-	-	2/4/4/4	-
4	GOL	F	277	-	-	2/4/4/4	-
4	GOL	B	275	-	-	0/4/4/4	-
4	GOL	D	276	-	-	0/4/4/4	-
4	GOL	D	274	-	-	4/4/4/4	-
4	GOL	F	275	-	-	0/4/4/4	-
4	GOL	C	275	-	-	0/4/4/4	-
4	GOL	D	275	-	-	0/4/4/4	-
4	GOL	B	276	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	274	ACT	O-C	2.42	1.32	1.22

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	272	ACT	OXT-C-CH3	2.97	127.52	115.05
2	F	272	ACT	OXT-C-CH3	2.95	127.42	115.05
2	E	272	ACT	OXT-C-CH3	2.83	126.91	115.05
2	C	272	ACT	OXT-C-CH3	2.80	126.78	115.05
4	D	276	GOL	O2-C2-C1	-2.53	98.68	109.18
2	B	272	ACT	OXT-C-CH3	2.49	125.51	115.05
2	F	272	ACT	OXT-C-O	-2.44	112.97	122.03
4	D	276	GOL	O3-C3-C2	2.43	121.30	110.38
4	F	278	GOL	O2-C2-C1	-2.33	99.51	109.18
4	B	276	GOL	O2-C2-C1	-2.32	99.56	109.18
2	C	274	ACT	OXT-C-CH3	2.28	124.63	115.05
2	D	272	ACT	OXT-C-CH3	2.23	124.40	115.05
4	E	277	GOL	C3-C2-C1	-2.17	103.82	111.80
2	C	272	ACT	O-C-CH3	-2.12	113.82	122.53
4	A	276	GOL	O2-C2-C1	-2.10	100.48	109.18
3	B	273	SO4	O3-S-O1	2.04	120.20	109.56

There are no chirality outliers.

All (18) 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
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

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Mol	Chain	Res	Type	Atoms
4	C	278	GOL	O2-C2-C3-O3
4	C	277	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	276	GOL	1	0
2	F	273	ACT	1	0
4	D	274	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, 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%)	-0.68	0 100 100	13, 29, 41, 53	5 (1%)
1	B	271/271 (100%)	-0.79	1 (0%) 88 89	12, 26, 37, 49	6 (2%)
1	C	271/271 (100%)	-0.72	1 (0%) 88 89	12, 28, 41, 55	4 (1%)
1	D	271/271 (100%)	-0.76	1 (0%) 88 89	12, 27, 39, 52	5 (1%)
1	E	271/271 (100%)	-0.67	0 100 100	14, 28, 40, 58	5 (1%)
1	F	271/271 (100%)	-0.73	1 (0%) 88 89	13, 27, 38, 56	8 (2%)
All	All	1626/1626 (100%)	-0.73	4 (0%) 91 92	12, 27, 40, 58	33 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	6	LYS	3.1
1	B	247	LYS	2.7
1	C	247	LYS	2.2
1	D	247	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
2	ACT	F	274	4/4	0.81	0.20	50,51,51,52	0
2	ACT	C	274	4/4	0.82	0.16	47,48,48,49	0
4	GOL	C	278	6/6	0.84	0.17	64,68,69,69	0
2	ACT	E	274	4/4	0.86	0.22	61,62,62,62	0
4	GOL	F	277	6/6	0.86	0.30	59,66,69,70	2
2	ACT	F	273	4/4	0.89	0.13	48,49,49,50	0
4	GOL	C	276	6/6	0.90	0.12	44,51,54,58	0
3	SO4	A	273	5/5	0.90	0.09	39,39,45,47	5
3	SO4	E	273	5/5	0.90	0.10	41,42,49,49	5
4	GOL	F	278	6/6	0.90	0.13	43,43,46,47	0
4	GOL	C	277	6/6	0.91	0.13	39,48,50,51	0
4	GOL	A	275	6/6	0.92	0.11	41,48,53,55	0
3	SO4	D	273	5/5	0.92	0.11	33,35,36,42	5
3	SO4	B	273	5/5	0.92	0.10	34,38,41,44	5
4	GOL	D	276	6/6	0.93	0.12	41,43,44,45	0
4	GOL	E	277	6/6	0.93	0.10	41,45,47,49	0
4	GOL	B	276	6/6	0.93	0.11	40,45,45,46	0
3	SO4	C	273	5/5	0.93	0.12	32,32,38,40	5
4	GOL	A	276	6/6	0.94	0.11	44,45,47,51	0
4	GOL	B	274	6/6	0.94	0.10	32,49,55,60	0
2	ACT	C	272	4/4	0.95	0.09	29,32,33,33	0
2	ACT	F	272	4/4	0.96	0.08	28,29,30,31	0
4	GOL	F	276	6/6	0.96	0.08	40,46,50,53	0
4	GOL	D	274	6/6	0.96	0.10	32,34,40,47	0
2	ACT	A	272	4/4	0.96	0.08	28,30,31,32	0
4	GOL	E	276	6/6	0.97	0.07	43,46,50,52	0
4	GOL	C	275	6/6	0.97	0.07	23,25,26,29	0
4	GOL	D	275	6/6	0.97	0.06	28,30,31,33	0
2	ACT	E	272	4/4	0.97	0.06	31,33,34,34	0
4	GOL	E	275	6/6	0.97	0.06	25,27,29,30	0
4	GOL	A	274	6/6	0.98	0.06	24,26,29,32	0
4	GOL	F	275	6/6	0.98	0.05	26,27,29,34	0
4	GOL	B	275	6/6	0.98	0.06	26,27,28,28	0
2	ACT	B	272	4/4	0.98	0.05	26,27,27,28	0
2	ACT	D	272	4/4	0.98	0.06	25,25,27,27	0

6.5 Other polymers

There are no such residues in this entry.