Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 11:42 pm GMT

PDB ID	:	4V0J
Title	:	The channel-block Ser202Glu, Thr104Lys double mutant of Stearoyl-ACP-Desaturase from Castor bean (Ricinus communis)
Authors	:	Moche, M.; Guy, J.; Whittle, E.; Lindqvist, Y.; Shanklin, J.
Deposited on	:	2014-09-17
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

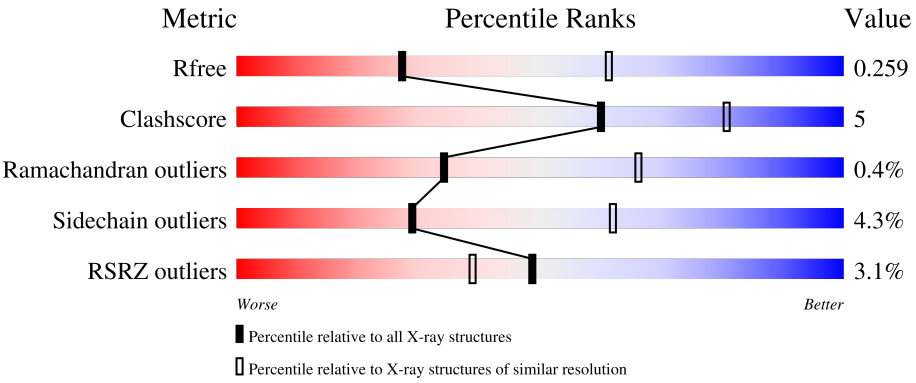
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	331	4% 86% 10%
1	B	331	3% 85% 12%
1	C	331	2% 85% 12%
1	D	331	3% 82% 14%
1	E	331	86% 12%

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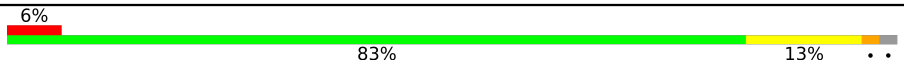
Mol	Chain	Length	Quality of chain
1	F	331	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	1364	-	-	X	-
3	GOL	F	1364	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15959 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 ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2629	1672	450	495	12			
1	B	331	Total	C	N	O	S	0	0	0
			2681	1702	462	505	12			
1	C	329	Total	C	N	O	S	0	0	0
			2667	1692	460	503	12			
1	D	323	Total	C	N	O	S	0	0	0
			2622	1668	450	492	12			
1	E	330	Total	C	N	O	S	0	0	0
			2674	1697	461	504	12			
1	F	324	Total	C	N	O	S	0	0	0
			2637	1675	453	497	12			

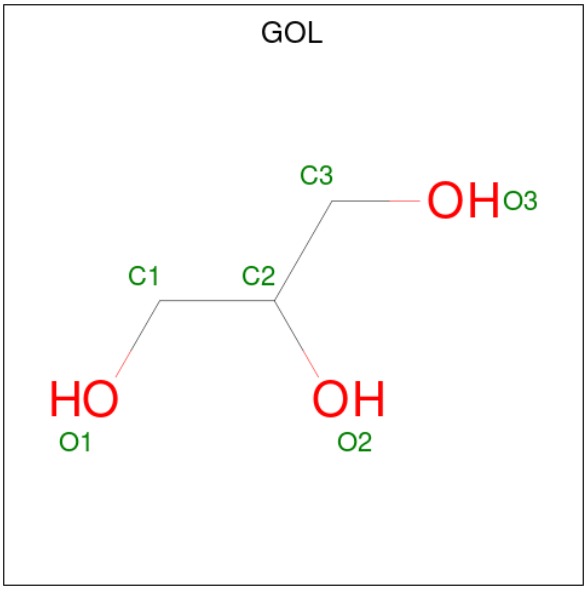
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	LYS	THR	engineered mutation	UNP P22337
A	202	GLU	SER	engineered mutation	UNP P22337
B	104	LYS	THR	engineered mutation	UNP P22337
B	202	GLU	SER	engineered mutation	UNP P22337
C	104	LYS	THR	engineered mutation	UNP P22337
C	202	GLU	SER	engineered mutation	UNP P22337
D	104	LYS	THR	engineered mutation	UNP P22337
D	202	GLU	SER	engineered mutation	UNP P22337
E	104	LYS	THR	engineered mutation	UNP P22337
E	202	GLU	SER	engineered mutation	UNP P22337
F	104	LYS	THR	engineered mutation	UNP P22337
F	202	GLU	SER	engineered mutation	UNP P22337

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Fe 2 2	0	0
2	B	2	Total Fe 2 2	0	0
2	C	2	Total Fe 2 2	0	0
2	D	2	Total Fe 2 2	0	0
2	E	2	Total Fe 2 2	0	0
2	F	2	Total Fe 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O 1 1	0	0

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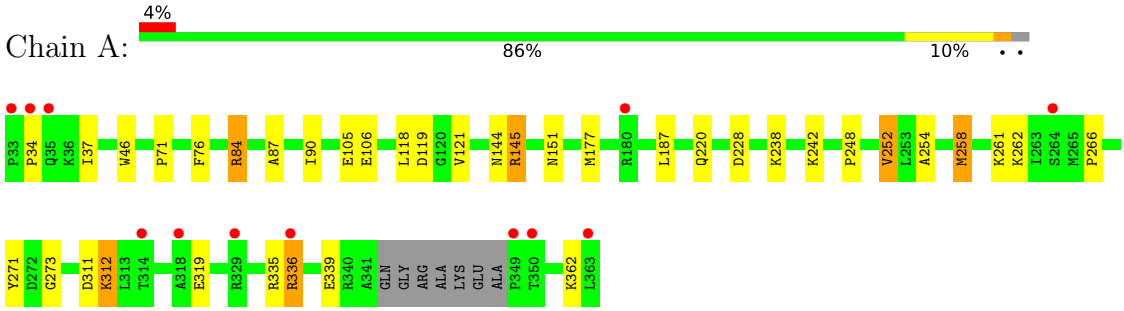
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	2	Total O 2 2	0	0
4	D	8	Total O 8 8	0	0
4	E	7	Total O 7 7	0	0
4	F	1	Total O 1 1	0	0

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.

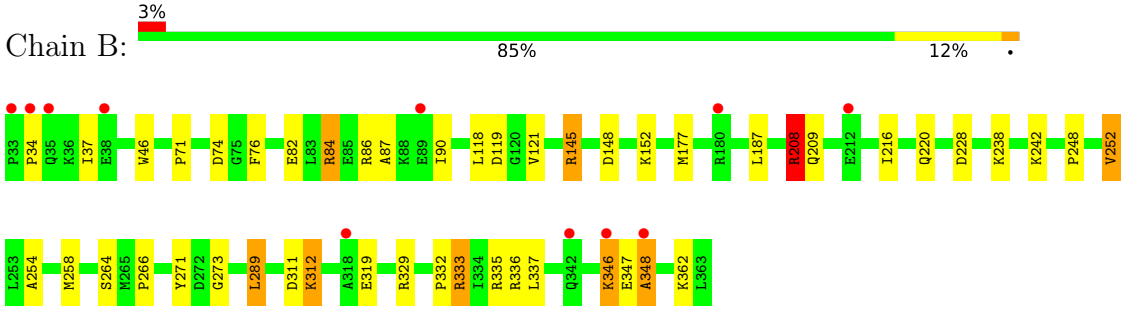
• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE, CHLOROPLASTIC

Chain A:



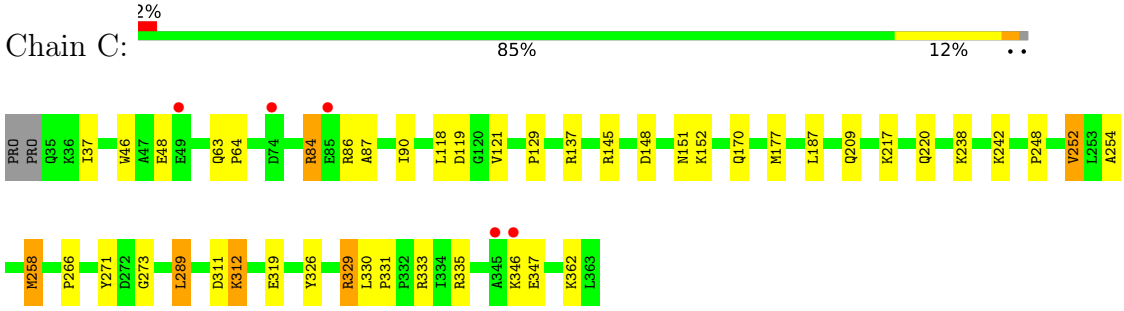
• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE, CHLOROPLASTIC

Chain B:



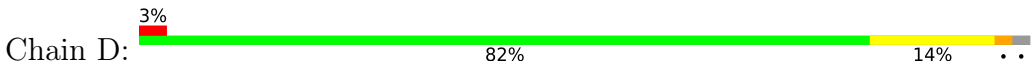
• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE, CHLOROPLASTIC

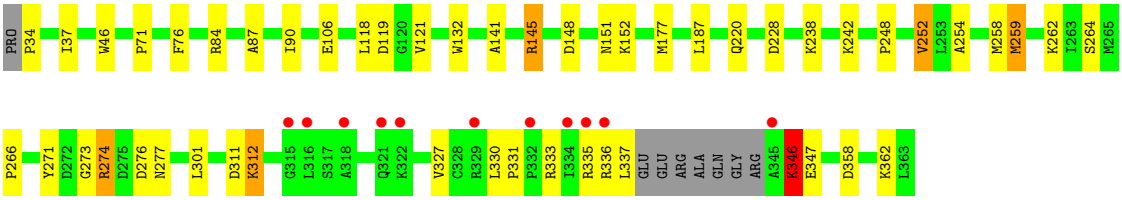
Chain C:



• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE, CHLOROPLASTIC

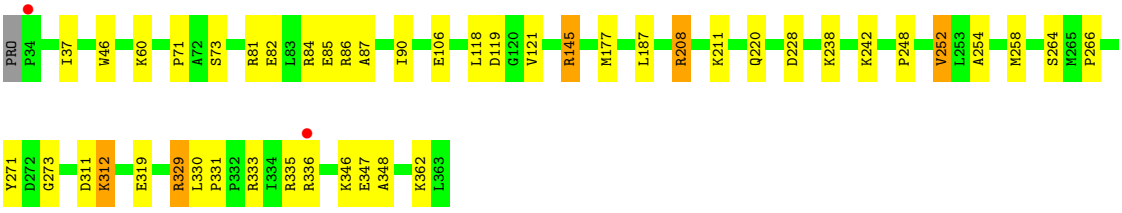
Chain D:





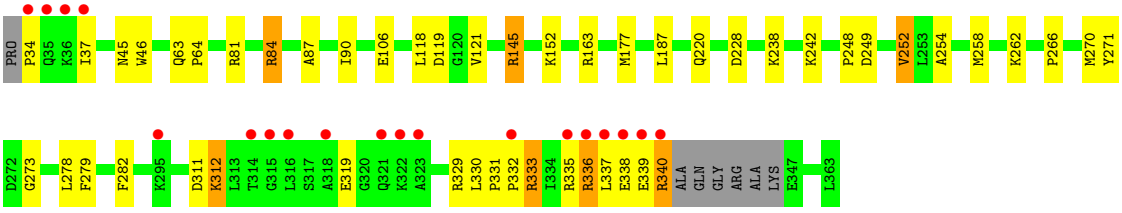
• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE, CHLOROPLASTIC

Chain E:



• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE, CHLOROPLASTIC

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	139.72Å 139.72Å 86.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.80 24.82 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.7 (119.52-2.80) 93.8 (24.82-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.212 , 0.264 0.213 , 0.259	Depositor DCC
R_{free} test set	1772 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.029 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15959	wwPDB-VP
Average B, all atoms (Å^2)	62.0	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 35.94 % 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 5.3972e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, FE2

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	0.53	1/2691 (0.0%)	0.76	5/3641 (0.1%)
1	B	0.49	0/2744	0.74	5/3713 (0.1%)
1	C	0.58	0/2728	0.79	6/3690 (0.2%)
1	D	0.62	0/2683	0.81	7/3629 (0.2%)
1	E	0.57	0/2736	0.77	6/3701 (0.2%)
1	F	0.59	0/2698	0.77	4/3649 (0.1%)
All	All	0.56	1/16280 (0.0%)	0.77	33/22023 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	GLU	CG-CD	5.67	1.60	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	274	ARG	NE-CZ-NH1	11.93	126.26	120.30
1	A	105	GLU	OE1-CD-OE2	-10.51	110.69	123.30
1	C	145	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	A	258	MET	CG-SD-CE	8.46	113.73	100.20
1	C	258	MET	CG-SD-CE	7.97	112.95	100.20
1	C	145	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	C	86	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	E	145	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	D	145	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	F	238	LYS	CD-CE-NZ	7.12	128.08	111.70
1	F	145	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	A	145	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	E	145	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	D	145	ARG	NE-CZ-NH2	-6.39	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	84	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	D	274	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	C	289	LEU	CA-CB-CG	5.92	128.91	115.30
1	E	333	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	F	145	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	289	LEU	CA-CB-CG	5.64	128.28	115.30
1	D	274	ARG	CB-CG-CD	5.63	126.24	111.60
1	D	84	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	145	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	E	329	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	F	81	ARG	CG-CD-NE	5.38	123.11	111.80
1	B	145	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	D	84	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	208	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	E	84	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	145	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	208	ARG	CG-CD-NE	5.08	122.47	111.80
1	A	105	GLU	CG-CD-OE2	5.07	128.43	118.30
1	C	137	ARG	NE-CZ-NH1	5.03	122.82	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	2629	0	2571	21	0
1	B	2681	0	2624	28	0
1	C	2667	0	2609	25	0
1	D	2622	0	2573	37	0
1	E	2674	0	2617	24	0
1	F	2637	0	2580	30	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	6	0	8	3	0
3	C	6	0	8	6	0
3	F	6	0	8	4	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	8	0	0	0	0
4	E	7	0	0	1	0
4	F	1	0	0	0	0
All	All	15959	0	15598	145	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 5.

All (145) 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:D:346:LYS:HD3	1:D:347:GLU:OE1	1.73	0.88
1:E:82:GLU:HG3	1:E:86:ARG:NH1	1.93	0.82
1:D:259:MET:HE3	1:D:301:LEU:HD21	1.62	0.81
1:E:81:ARG:NH1	1:E:85:GLU:OE1	2.21	0.73
1:F:106:GLU:OE1	3:F:1364:GOL:C1	2.42	0.67
1:C:129:PRO:HB2	1:E:211:LYS:HD3	1.78	0.65
1:D:333:ARG:O	1:D:337:LEU:HD13	1.96	0.65
1:D:274:ARG:NH2	1:D:358:ASP:OD2	2.31	0.63
1:A:336:ARG:NH1	1:A:339:GLU:OE1	2.33	0.60
1:C:148:ASP:OD1	3:C:1364:GOL:H11	2.02	0.60
3:C:1364:GOL:O3	1:D:106:GLU:OE1	2.17	0.60
1:D:46:TRP:CZ2	1:D:242:LYS:HG3	2.37	0.59
1:A:46:TRP:CZ2	1:A:242:LYS:HG3	2.38	0.58
1:D:277:ASN:OD1	1:F:163:ARG:NH2	2.36	0.58
3:C:1364:GOL:H31	1:D:148:ASP:OD1	2.02	0.58
1:B:46:TRP:CZ2	1:B:242:LYS:HG3	2.39	0.57
1:A:84:ARG:NH2	1:B:71:PRO:O	2.38	0.56
1:E:46:TRP:CZ2	1:E:242:LYS:HG3	2.40	0.56
1:C:129:PRO:HB2	1:E:211:LYS:CD	2.35	0.56
1:F:46:TRP:CZ2	1:F:242:LYS:HG3	2.40	0.56
1:E:82:GLU:HG3	1:E:86:ARG:HH12	1.69	0.56
1:F:106:GLU:OE1	3:F:1364:GOL:H12	2.05	0.56
1:E:311:ASP:HB3	1:E:312:LYS:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:GLU:OE1	3:F:1364:GOL:O3	2.23	0.56
3:C:1364:GOL:H32	1:D:106:GLU:OE1	2.06	0.55
1:D:259:MET:HE3	1:D:330:LEU:HD23	1.89	0.55
1:D:262:LYS:NZ	1:E:73:SER:HB2	2.21	0.55
1:C:46:TRP:CZ2	1:C:242:LYS:HG3	2.41	0.55
1:F:270:MET:HE1	1:F:282:PHE:HB3	1.87	0.55
3:C:1364:GOL:C3	1:D:106:GLU:OE1	2.55	0.55
1:A:144:ASN:OD1	3:A:1364:GOL:H32	2.07	0.54
1:C:311:ASP:HB3	1:C:312:LYS:HD2	1.89	0.54
1:E:271:TYR:CZ	1:E:273:GLY:HA2	2.43	0.54
1:D:311:ASP:HB3	1:D:312:LYS:HD2	1.90	0.54
1:E:82:GLU:CG	1:E:86:ARG:HH12	2.21	0.54
1:A:71:PRO:O	1:B:84:ARG:NH2	2.41	0.54
1:F:311:ASP:HB3	1:F:312:LYS:HD2	1.90	0.54
1:A:311:ASP:HB3	1:A:312:LYS:HD2	1.90	0.53
1:E:145:ARG:NH2	1:E:228:ASP:OD2	2.42	0.53
1:D:259:MET:CE	1:D:301:LEU:HD21	2.36	0.53
1:A:37:ILE:HG12	1:A:119:ASP:HB3	1.91	0.53
1:B:271:TYR:CZ	1:B:273:GLY:HA2	2.44	0.53
1:F:34:PRO:HA	1:F:37:ILE:HD12	1.90	0.53
1:D:34:PRO:HA	1:D:37:ILE:HD12	1.91	0.52
1:D:37:ILE:HG12	1:D:119:ASP:HB3	1.91	0.52
1:C:118:LEU:HB2	1:C:121:VAL:HG22	1.91	0.52
1:D:118:LEU:HB2	1:D:121:VAL:HG22	1.92	0.52
1:B:37:ILE:HG12	1:B:119:ASP:HB3	1.92	0.52
1:A:118:LEU:HB2	1:A:121:VAL:HG22	1.92	0.52
1:B:311:ASP:HB3	1:B:312:LYS:HD2	1.91	0.51
1:F:37:ILE:HG12	1:F:119:ASP:HB3	1.93	0.51
1:B:118:LEU:HB2	1:B:121:VAL:HG22	1.93	0.51
1:D:346:LYS:CD	1:D:347:GLU:OE1	2.52	0.51
1:B:34:PRO:HA	1:B:37:ILE:HD12	1.92	0.51
1:E:37:ILE:HG12	1:E:119:ASP:HB3	1.93	0.51
1:D:259:MET:SD	1:D:327:VAL:HG22	2.50	0.50
1:F:271:TYR:CZ	1:F:273:GLY:HA2	2.47	0.50
1:B:46:TRP:CE2	1:B:242:LYS:HG3	2.46	0.50
1:C:326:TYR:HA	1:C:329:ARG:HH21	1.77	0.50
1:F:270:MET:CE	1:F:278:LEU:HG	2.42	0.50
1:A:248:PRO:O	1:A:252:VAL:HG22	2.12	0.49
1:C:37:ILE:HG12	1:C:119:ASP:HB3	1.92	0.49
1:C:271:TYR:CZ	1:C:273:GLY:HA2	2.46	0.49
1:C:248:PRO:O	1:C:252:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:PRO:HA	1:A:37:ILE:HD12	1.93	0.49
1:D:145:ARG:NH2	1:D:228:ASP:OD2	2.45	0.49
1:E:118:LEU:HB2	1:E:121:VAL:HG22	1.93	0.49
1:B:145:ARG:NH2	1:B:228:ASP:OD2	2.45	0.49
1:B:248:PRO:O	1:B:252:VAL:HG22	2.12	0.49
1:D:276:ASP:HB2	1:E:60:LYS:O	2.13	0.49
1:A:145:ARG:NH2	1:A:228:ASP:OD2	2.46	0.49
1:C:148:ASP:OD1	3:C:1364:GOL:C1	2.60	0.49
1:B:216:ILE:HD11	1:F:262:LYS:CE	2.42	0.48
1:D:46:TRP:CE2	1:D:242:LYS:HG3	2.49	0.48
1:B:74:ASP:HB2	1:F:336:ARG:HD2	1.95	0.48
1:E:248:PRO:O	1:E:252:VAL:HG22	2.14	0.48
1:C:46:TRP:CE2	1:C:242:LYS:HG3	2.49	0.48
1:D:248:PRO:O	1:D:252:VAL:HG22	2.13	0.48
1:F:248:PRO:O	1:F:252:VAL:HG22	2.13	0.48
1:F:106:GLU:OE1	3:F:1364:GOL:O1	2.30	0.48
1:F:118:LEU:HB2	1:F:121:VAL:HG22	1.94	0.48
1:A:271:TYR:CZ	1:A:273:GLY:HA2	2.49	0.47
1:F:270:MET:HE3	1:F:278:LEU:HG	1.95	0.47
1:E:46:TRP:CE2	1:E:242:LYS:HG3	2.49	0.47
1:C:84:ARG:NH2	1:D:71:PRO:O	2.48	0.47
1:D:271:TYR:CZ	1:D:273:GLY:HA2	2.49	0.47
1:F:145:ARG:NH2	1:F:228:ASP:OD2	2.47	0.47
1:A:46:TRP:CE2	1:A:242:LYS:HG3	2.50	0.47
1:D:177:MET:HG3	1:D:266:PRO:HA	1.96	0.46
1:F:177:MET:HG3	1:F:266:PRO:HA	1.98	0.46
1:D:259:MET:HE2	1:D:327:VAL:HA	1.98	0.46
1:E:71:PRO:O	1:F:84:ARG:NH2	2.48	0.46
1:B:333:ARG:O	1:B:337:LEU:HD13	2.16	0.46
1:F:46:TRP:CE2	1:F:242:LYS:HG3	2.51	0.45
1:B:177:MET:HG3	1:B:266:PRO:HA	1.98	0.45
1:E:82:GLU:CG	1:E:86:ARG:NH1	2.71	0.45
1:B:216:ILE:HD11	1:F:262:LYS:HE3	1.99	0.45
1:F:63:GLN:O	1:F:64:PRO:C	2.54	0.45
1:A:106:GLU:OE1	3:A:1364:GOL:O3	2.24	0.45
1:F:333:ARG:O	1:F:337:LEU:HD13	2.16	0.44
1:B:346:LYS:O	1:B:348:ALA:N	2.51	0.44
1:C:152:LYS:HE3	1:D:151:ASN:OD1	2.18	0.44
1:A:151:ASN:OD1	1:B:152:LYS:HE3	2.19	0.43
1:C:151:ASN:OD1	1:D:152:LYS:HE3	2.18	0.43
1:B:209:GLN:OE1	1:B:289:LEU:HD12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MET:HG3	1:A:266:PRO:HA	2.01	0.43
1:F:330:LEU:HB3	1:F:331:PRO:HD3	2.00	0.43
1:E:177:MET:HG3	1:E:266:PRO:HA	2.00	0.43
1:D:187:LEU:HD12	1:D:254:ALA:HB1	2.01	0.43
1:E:330:LEU:HB3	1:E:331:PRO:HD3	1.99	0.43
1:F:338:GLU:O	1:F:340:ARG:N	2.52	0.43
1:A:187:LEU:HD12	1:A:254:ALA:HB1	2.01	0.43
1:C:170:GLN:HG3	1:D:141:ALA:HB1	2.00	0.43
1:D:71:PRO:HA	1:D:76:PHE:CD1	2.54	0.43
1:C:177:MET:HG3	1:C:266:PRO:HA	2.00	0.43
1:A:261:LYS:O	1:A:262:LYS:HB2	2.19	0.42
1:B:208:ARG:HH11	1:B:208:ARG:HG3	1.85	0.42
1:C:48:GLU:OE1	1:E:208:ARG:NH1	2.53	0.42
1:C:151:ASN:OD1	1:D:152:LYS:CE	2.67	0.42
1:C:152:LYS:CE	1:D:151:ASN:OD1	2.68	0.42
1:C:187:LEU:HD12	1:C:254:ALA:HB1	2.01	0.42
1:A:71:PRO:HA	1:A:76:PHE:CD1	2.55	0.42
1:C:330:LEU:HB3	1:C:331:PRO:HD3	2.01	0.42
1:F:87:ALA:HA	1:F:90:ILE:HD12	2.02	0.41
4:E:2003:HOH:O	1:F:152:LYS:NZ	2.40	0.41
1:F:187:LEU:HD12	1:F:254:ALA:HB1	2.02	0.41
1:B:82:GLU:HG3	1:B:86:ARG:NH1	2.35	0.41
1:C:63:GLN:O	1:C:64:PRO:C	2.58	0.41
1:E:187:LEU:HD12	1:E:254:ALA:HB1	2.01	0.41
1:B:329:ARG:O	1:B:332:PRO:HD2	2.21	0.41
3:A:1364:GOL:H11	1:B:148:ASP:OD1	2.20	0.41
1:B:71:PRO:HA	1:B:76:PHE:CD1	2.56	0.41
1:B:187:LEU:HD12	1:B:254:ALA:HB1	2.02	0.41
1:C:87:ALA:HA	1:C:90:ILE:HD12	2.02	0.41
1:C:209:GLN:OE1	1:C:289:LEU:HD12	2.20	0.41
1:F:270:MET:CE	1:F:279:PHE:HA	2.51	0.41
1:F:329:ARG:O	1:F:332:PRO:HD2	2.21	0.41
1:A:87:ALA:HA	1:A:90:ILE:HD12	2.03	0.40
1:A:151:ASN:OD1	1:B:152:LYS:CE	2.68	0.40
1:B:87:ALA:HA	1:B:90:ILE:HD12	2.04	0.40
1:D:87:ALA:HA	1:D:90:ILE:HD12	2.02	0.40
1:D:330:LEU:HB3	1:D:331:PRO:HD3	2.03	0.40
1:B:333:ARG:HA	1:B:333:ARG:HD2	1.76	0.40
1:D:121:VAL:HB	1:D:132:TRP:HB3	2.03	0.40
1:E:87:ALA:HA	1:E:90:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/331 (97%)	311 (97%)	9 (3%)	0	100	100
1	B	329/331 (99%)	319 (97%)	8 (2%)	2 (1%)	25	56
1	C	327/331 (99%)	316 (97%)	10 (3%)	1 (0%)	41	72
1	D	319/331 (96%)	309 (97%)	9 (3%)	1 (0%)	41	72
1	E	328/331 (99%)	318 (97%)	8 (2%)	2 (1%)	25	56
1	F	320/331 (97%)	311 (97%)	8 (2%)	1 (0%)	41	72
All	All	1943/1986 (98%)	1884 (97%)	52 (3%)	7 (0%)	34	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	346	LYS
1	B	347	GLU
1	E	347	GLU
1	F	339	GLU
1	C	347	GLU
1	B	348	ALA
1	E	348	ALA

5.3.2 Protein sidechains (i)

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	280/285 (98%)	270 (96%)	10 (4%)	35	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	284/285 (100%)	270 (95%)	14 (5%)	25 57
1	C	282/285 (99%)	269 (95%)	13 (5%)	27 60
1	D	279/285 (98%)	268 (96%)	11 (4%)	32 66
1	E	283/285 (99%)	270 (95%)	13 (5%)	27 60
1	F	281/285 (99%)	269 (96%)	12 (4%)	29 62
All	All	1689/1710 (99%)	1616 (96%)	73 (4%)	29 62

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	220	GLN
1	A	238	LYS
1	A	252	VAL
1	A	258	MET
1	A	312	LYS
1	A	319	GLU
1	A	335	ARG
1	A	336	ARG
1	A	362	LYS
1	B	84	ARG
1	B	208	ARG
1	B	220	GLN
1	B	238	LYS
1	B	252	VAL
1	B	258	MET
1	B	264	SER
1	B	312	LYS
1	B	319	GLU
1	B	333	ARG
1	B	335	ARG
1	B	336	ARG
1	B	346	LYS
1	B	362	LYS
1	C	84	ARG
1	C	217	LYS
1	C	220	GLN
1	C	238	LYS
1	C	252	VAL
1	C	258	MET

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Mol	Chain	Res	Type
1	C	312	LYS
1	C	319	GLU
1	C	329	ARG
1	C	333	ARG
1	C	335	ARG
1	C	346	LYS
1	C	362	LYS
1	D	220	GLN
1	D	238	LYS
1	D	252	VAL
1	D	258	MET
1	D	259	MET
1	D	264	SER
1	D	312	LYS
1	D	335	ARG
1	D	336	ARG
1	D	346	LYS
1	D	362	LYS
1	E	208	ARG
1	E	220	GLN
1	E	238	LYS
1	E	252	VAL
1	E	258	MET
1	E	264	SER
1	E	312	LYS
1	E	319	GLU
1	E	329	ARG
1	E	335	ARG
1	E	336	ARG
1	E	346	LYS
1	E	362	LYS
1	F	45	ASN
1	F	84	ARG
1	F	220	GLN
1	F	249	ASP
1	F	252	VAL
1	F	258	MET
1	F	312	LYS
1	F	319	GLU
1	F	333	ARG
1	F	335	ARG
1	F	336	ARG

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Mol	Chain	Res	Type
1	F	340	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	GLN
1	B	321	GLN
1	B	342	GLN
1	C	321	GLN
1	C	342	GLN
1	D	321	GLN
1	E	321	GLN
1	F	321	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	GOL	F	1364	-	5,5,5	0.45	0	5,5,5	0.67	0
3	GOL	A	1364	-	5,5,5	0.13	0	5,5,5	0.55	0
3	GOL	C	1364	-	5,5,5	0.88	0	5,5,5	1.24	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
3	GOL	F	1364	-	-	2/4/4/4	-
3	GOL	A	1364	-	-	2/4/4/4	-
3	GOL	C	1364	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1364	GOL	C1-C2-C3-O3
3	F	1364	GOL	C1-C2-C3-O3
3	F	1364	GOL	O2-C2-C3-O3
3	A	1364	GOL	O2-C2-C3-O3
3	C	1364	GOL	O1-C1-C2-O2
3	C	1364	GOL	O2-C2-C3-O3
3	C	1364	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1364	GOL	4	0
3	A	1364	GOL	3	0
3	C	1364	GOL	6	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, 95^{th} 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	324/331 (97%)	0.10	12 (3%)	41	31	43, 70, 98, 149	0
1	B	331/331 (100%)	0.04	11 (3%)	46	36	35, 70, 107, 175	0
1	C	329/331 (99%)	-0.11	5 (1%)	73	68	25, 57, 89, 111	0
1	D	323/331 (97%)	-0.14	11 (3%)	45	35	28, 44, 102, 143	0
1	E	330/331 (99%)	-0.25	2 (0%)	89	86	26, 52, 90, 150	0
1	F	324/331 (97%)	0.10	19 (5%)	22	14	27, 56, 132, 174	0
All	All	1961/1986 (98%)	-0.04	60 (3%)	49	39	25, 59, 104, 175	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	314	THR	7.6
1	F	315	GLY	7.3
1	A	33	PRO	6.3
1	B	33	PRO	6.2
1	B	34	PRO	5.4
1	F	338	GLU	5.3
1	F	316	LEU	5.0
1	F	336	ARG	4.8
1	F	34	PRO	4.3
1	F	35	GLN	4.3
1	E	34	PRO	4.0
1	D	334	ILE	3.8
1	F	339	GLU	3.8
1	B	346	LYS	3.7
1	A	363	LEU	3.7
1	A	350	THR	3.7
1	B	318	ALA	3.7
1	D	318	ALA	3.6
1	F	322	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	321	GLN	3.3
1	F	318	ALA	3.3
1	A	34	PRO	3.3
1	B	89	GLU	3.2
1	C	49	GLU	3.2
1	A	318	ALA	3.2
1	D	332	PRO	3.1
1	F	335	ARG	3.1
1	F	37	ILE	3.0
1	A	35	GLN	3.0
1	F	332	PRO	3.0
1	B	212	GLU	2.9
1	D	336	ARG	2.8
1	D	321	GLN	2.8
1	F	340	ARG	2.8
1	C	85	GLU	2.8
1	D	322	LYS	2.7
1	F	337	LEU	2.7
1	B	35	GLN	2.5
1	C	346	LYS	2.5
1	F	323	ALA	2.5
1	A	349	PRO	2.4
1	B	348	ALA	2.4
1	D	315	GLY	2.4
1	E	336	ARG	2.4
1	D	335	ARG	2.3
1	F	36	LYS	2.3
1	D	345	ALA	2.2
1	B	342	GLN	2.2
1	A	180	ARG	2.2
1	A	264	SER	2.2
1	C	345	ALA	2.2
1	B	38	GLU	2.2
1	A	314	THR	2.2
1	A	336	ARG	2.2
1	C	74	ASP	2.1
1	D	329	ARG	2.1
1	B	180	ARG	2.1
1	F	295	LYS	2.1
1	D	316	LEU	2.0
1	A	329	ARG	2.0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	F	1364	6/6	0.86	0.36	57,62,66,68	0
3	GOL	C	1364	6/6	0.88	0.27	40,44,49,50	0
2	FE2	A	364	1/1	0.90	0.09	78,78,78,78	0
2	FE2	E	364	1/1	0.92	0.05	56,56,56,56	0
2	FE2	C	364	1/1	0.92	0.07	61,61,61,61	0
2	FE2	C	365	1/1	0.92	0.09	59,59,59,59	0
3	GOL	A	1364	6/6	0.94	0.24	67,68,70,77	0
2	FE2	B	364	1/1	0.95	0.08	66,66,66,66	0
2	FE2	F	364	1/1	0.97	0.08	63,63,63,63	0
2	FE2	A	365	1/1	0.97	0.08	69,69,69,69	0
2	FE2	B	365	1/1	0.98	0.09	69,69,69,69	0
2	FE2	D	364	1/1	0.98	0.07	50,50,50,50	0
2	FE2	F	365	1/1	0.98	0.07	56,56,56,56	0
2	FE2	E	365	1/1	0.99	0.04	55,55,55,55	0
2	FE2	D	365	1/1	0.99	0.07	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.