



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:52 AM GMT

PDB ID : 2J2F
Title : THE T199D MUTANT OF STEAROYL ACYL CARRIER PROTEIN DESATURASE FROM RICINUS COMMUNIS (CASTOR BEAN)
Authors : Guy, J.E.; Abreu, I.A.; Moche, M.; Lindqvist, Y.; Whittle, E.; Shanklin, J.
Deposited on : 2006-08-16
Resolution : 2.65 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

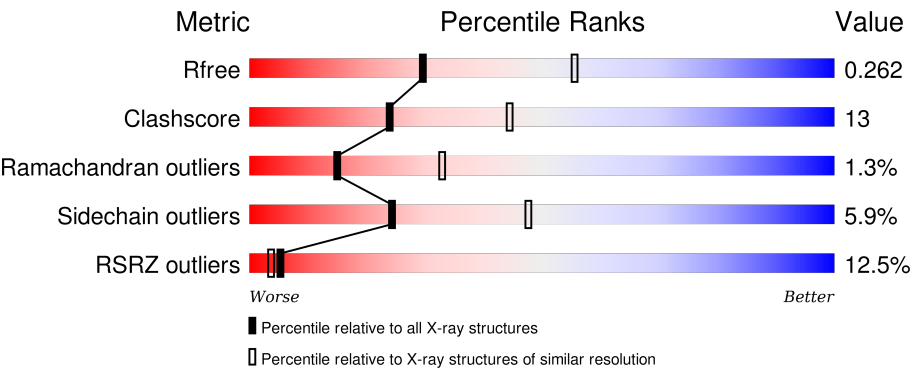
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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. 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	363	<div><div>17%</div><div><div></div><div>68%</div><div>25%</div><div>• •</div></div></div>
1	B	363	<div><div>7%</div><div><div></div><div>73%</div><div>20%</div><div>• •</div></div></div>
1	C	363	<div><div>7%</div><div><div></div><div>68%</div><div>24%</div><div>• 5%</div></div></div>
1	D	363	<div><div>6%</div><div><div></div><div>70%</div><div>22%</div><div>• •</div></div></div>
1	E	363	<div><div>15%</div><div><div></div><div>70%</div><div>23%</div><div>• •</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	363	<div> <div>20%</div> <div>72%</div> <div>20%</div> <div>5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17055 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2824	1791	490	529	14			
1	B	347	Total	C	N	O	S	0	0	0
			2815	1785	488	528	14			
1	C	346	Total	C	N	O	S	0	0	0
			2808	1780	487	527	14			
1	D	347	Total	C	N	O	S	0	0	0
			2815	1785	488	528	14			
1	E	347	Total	C	N	O	S	0	0	0
			2815	1785	488	528	14			
1	F	346	Total	C	N	O	S	0	0	0
			2808	1780	487	527	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ASP	THR	ENGINEERED MUTATION	UNP P22337
B	199	ASP	THR	ENGINEERED MUTATION	UNP P22337
C	199	ASP	THR	ENGINEERED MUTATION	UNP P22337
D	199	ASP	THR	ENGINEERED MUTATION	UNP P22337
E	199	ASP	THR	ENGINEERED MUTATION	UNP P22337
F	199	ASP	THR	ENGINEERED MUTATION	UNP P22337

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

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

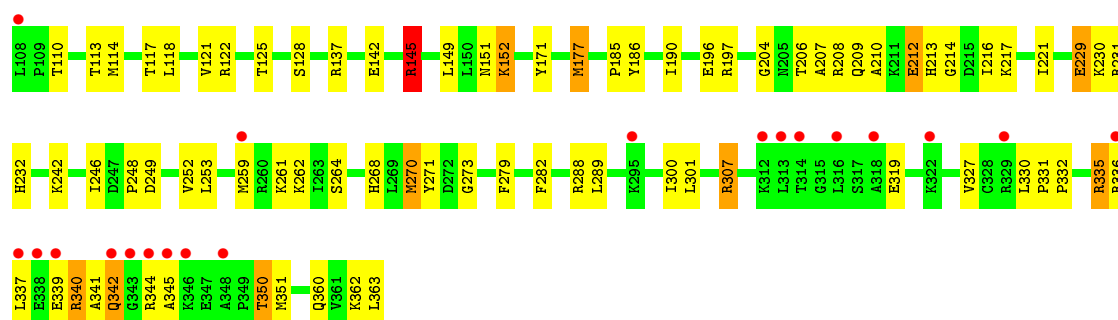
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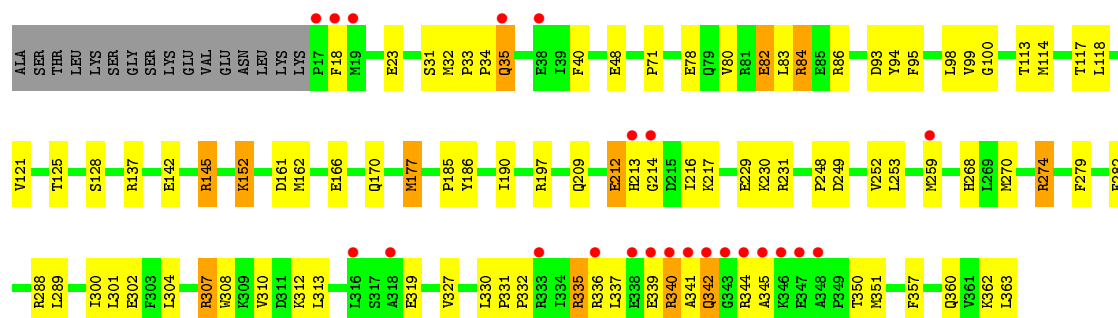
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total 2	Fe 2	0	0
2	A	2	Total 2	Fe 2	0	0
2	F	2	Total 2	Fe 2	0	0

- Molecule 3 is water.

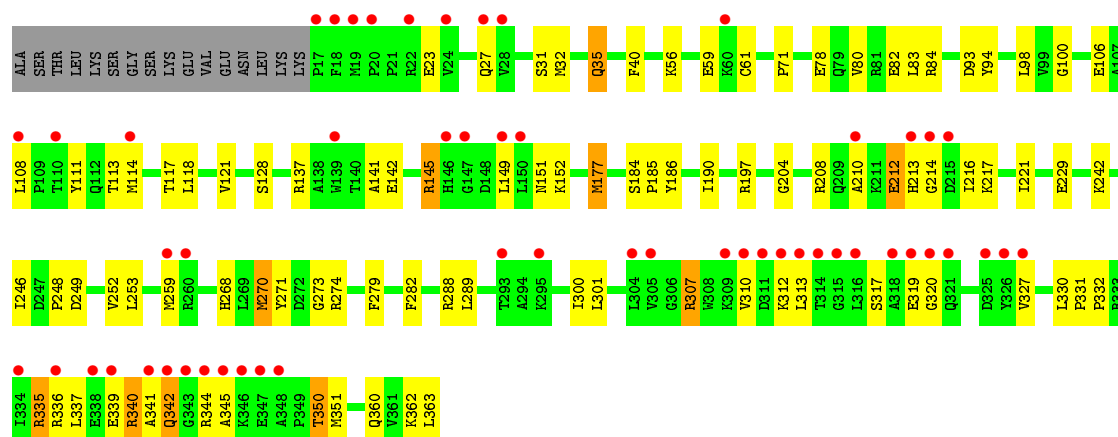
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total 20	O 20	0	0
3	B	38	Total 38	O 38	0	0
3	C	27	Total 27	O 27	0	0
3	D	33	Total 33	O 33	0	0
3	E	20	Total 20	O 20	0	0
3	F	20	Total 20	O 20	0	0



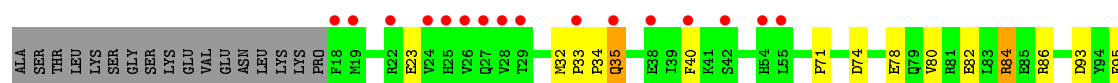
• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE

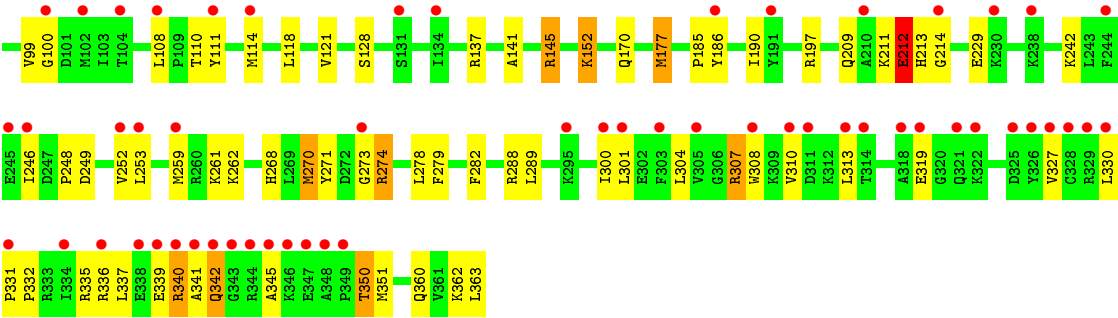


• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.05Å 145.77Å 193.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.65 33.67 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.00-2.65) 97.9 (33.67-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.272 0.232 , 0.262	Depositor DCC
R_{free} test set	3388 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 66623 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17055	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FE

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	0.65	0/2893	0.69	4/3916 (0.1%)
1	B	0.80	0/2884	0.78	4/3904 (0.1%)
1	C	0.75	0/2876	0.75	5/3893 (0.1%)
1	D	0.79	1/2884 (0.0%)	0.77	2/3904 (0.1%)
1	E	0.71	0/2884	0.71	0/3904
1	F	0.69	0/2876	0.72	5/3893 (0.1%)
All	All	0.73	1/17297 (0.0%)	0.74	20/23414 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	82	GLU	CG-CD	5.80	1.60	1.51

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	C	86	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	B	86	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	C	84	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	F	274	ARG	NE-CZ-NH1	7.90	124.25	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	2824	0	2765	83	2
1	B	2815	0	2753	70	1
1	C	2808	0	2745	80	0
1	D	2815	0	2753	74	0
1	E	2815	0	2753	79	0
1	F	2808	0	2745	71	1
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
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	20	0	0	1	0
3	B	38	0	0	2	0
3	C	27	0	0	3	0
3	D	33	0	0	2	0
3	E	20	0	0	5	0
3	F	20	0	0	9	0
All	All	17055	0	16514	439	3

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 13.

The worst 5 of 439 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:A:16:LYS:HG2	1:A:19:MET:HE3	1.39	1.04
1:A:16:LYS:HG2	1:A:19:MET:CE	1.90	1.02
1:E:217:LYS:HE2	3:E:2018:HOH:O	1.67	0.95
1:D:114:MET:CE	1:D:177:MET:HB3	1.96	0.95
1:B:59:GLU:HG3	1:C:18:PHE:CD2	2.03	0.94

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:HIS:CD2	1:A:49:GLU:OE2[4_555]	2.15	0.05
1:A:25:HIS:CD2	1:A:49:GLU:OE1[4_555]	2.18	0.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:GLU:OE1	1:F:35:GLN:OE1[4_555]	2.19	0.01

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	346/363 (95%)	317 (92%)	23 (7%)	6 (2%)	11	25
1	B	345/363 (95%)	324 (94%)	17 (5%)	4 (1%)	16	35
1	C	344/363 (95%)	321 (93%)	19 (6%)	4 (1%)	16	35
1	D	345/363 (95%)	316 (92%)	25 (7%)	4 (1%)	16	35
1	E	345/363 (95%)	317 (92%)	24 (7%)	4 (1%)	16	35
1	F	344/363 (95%)	317 (92%)	22 (6%)	5 (2%)	13	28
All	All	2069/2178 (95%)	1912 (92%)	130 (6%)	27 (1%)	15	33

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	PRO
1	A	213	HIS
1	A	340	ARG
1	B	213	HIS
1	B	340	ARG

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	302/315 (96%)	286 (95%)	16 (5%)	28	54
1	B	301/315 (96%)	284 (94%)	17 (6%)	26	50
1	C	300/315 (95%)	279 (93%)	21 (7%)	19	38
1	D	301/315 (96%)	284 (94%)	17 (6%)	26	50
1	E	301/315 (96%)	281 (93%)	20 (7%)	21	42
1	F	300/315 (95%)	284 (95%)	16 (5%)	28	54
All	All	1805/1890 (96%)	1698 (94%)	107 (6%)	24	48

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	340	ARG
1	D	177	MET
1	F	270	MET
1	C	342	GLN
1	D	31	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	342	GLN
1	D	50	ASN
1	F	268	HIS
1	D	35	GLN
1	D	268	HIS

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 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	348/363 (95%)	0.88	60 (17%) 2 1	31, 33, 34, 50	0
1	B	347/363 (95%)	0.36	25 (7%) 18 16	31, 33, 34, 48	0
1	C	346/363 (95%)	0.40	26 (7%) 17 14	22, 33, 34, 36	0
1	D	347/363 (95%)	0.29	23 (6%) 22 19	31, 33, 34, 44	0
1	E	347/363 (95%)	0.84	54 (15%) 3 2	31, 33, 34, 50	0
1	F	346/363 (95%)	1.13	72 (20%) 1 1	31, 33, 34, 45	0
All	All	2081/2178 (95%)	0.65	260 (12%) 5 4	22, 33, 34, 50	0

The worst 5 of 260 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	345	ALA	11.7
1	E	345	ALA	10.1
1	E	338	GLU	9.0
1	B	345	ALA	9.0
1	E	344	ARG	8.6

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	FE	A	371	1/1	0.93	0.07	-2.46	50,50,50,50	0
2	FE	E	371	1/1	0.99	0.05	-2.54	49,49,49,49	0
2	FE	E	370	1/1	0.96	0.06	-2.74	48,48,48,48	0
2	FE	A	370	1/1	0.94	0.07	-2.83	48,48,48,48	0
2	FE	F	371	1/1	0.90	0.08	-3.28	49,49,49,49	0
2	FE	B	370	1/1	0.92	0.06	-4.00	48,48,48,48	0
2	FE	C	371	1/1	0.97	0.03	-4.42	50,50,50,50	0
2	FE	C	370	1/1	0.95	0.04	-4.50	48,48,48,48	0
2	FE	D	371	1/1	0.97	0.03	-4.86	50,50,50,50	0
2	FE	B	371	1/1	0.98	0.06	-4.93	49,49,49,49	0
2	FE	F	370	1/1	0.96	0.04	-5.34	48,48,48,48	0
2	FE	D	370	1/1	0.94	0.04	-5.44	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.