



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:51 PM GMT

PDB ID : 4YSX
Title : Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from *Ascaris suum* with the specific inhibitor NN23
Authors : Harada, S.; Shiba, T.; Sato, D.; Yamamoto, A.; Nagahama, M.; Yone, A.; Inaoka, D.K.; Sakamoto, K.; Inoue, M.; Honma, T.; Kita, K.
Deposited on : 2015-03-17
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
<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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

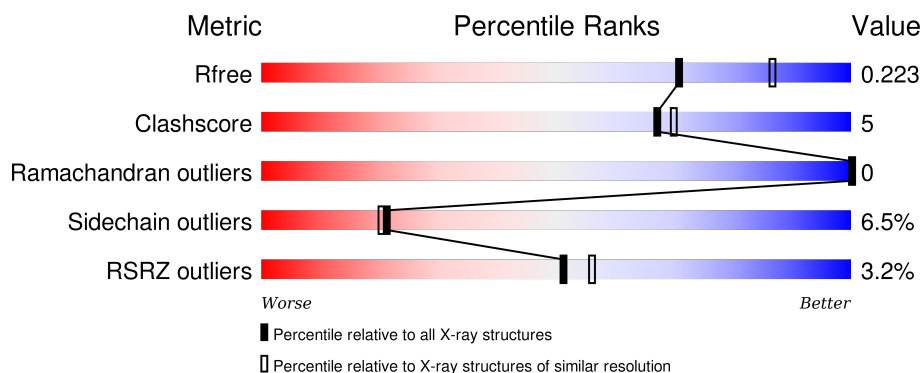
1 Overall quality at a glance

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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	645	<div> <div>2%</div> <div>79%</div> <div>15%</div> <div>• •</div> </div>
1	E	645	<div> <div>2%</div> <div>81%</div> <div>13%</div> <div>• •</div> </div>
2	B	282	<div> <div>2%</div> <div>77%</div> <div>10%</div> <div>• 11%</div> </div>
2	F	282	<div> <div>2%</div> <div>79%</div> <div>9%</div> <div>• 11%</div> </div>
3	C	188	<div> <div>5%</div> <div>73%</div> <div>7%</div> <div>• 19%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	188	
4	D	156	
4	H	156	

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
12	EPH	D	201	-	-	-	X
12	EPH	H	201	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 19103 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 Succinate dehydrogenase flavoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	616	Total	C	N	O	S	0	0	0
			4787	3004	855	900	28			
1	E	616	Total	C	N	O	S	0	0	0
			4787	3004	855	900	28			

- Molecule 2 is a protein called Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	250	Total	C	N	O	S	0	0	0
			1985	1263	338	361	23			
2	F	252	Total	C	N	O	S	0	0	0
			1994	1268	340	363	23			

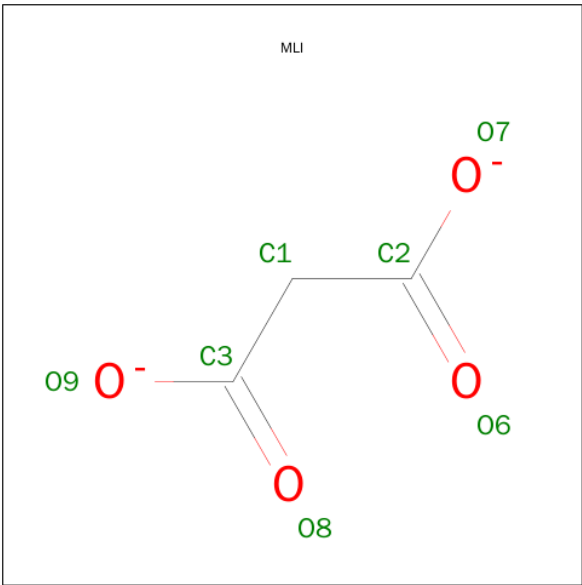
- Molecule 3 is a protein called Cytochrome b-large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	153	Total	C	N	O	S	0	0	0
			1217	813	204	194	6			
3	G	155	Total	C	N	O	S	0	0	0
			1236	823	209	198	6			

- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

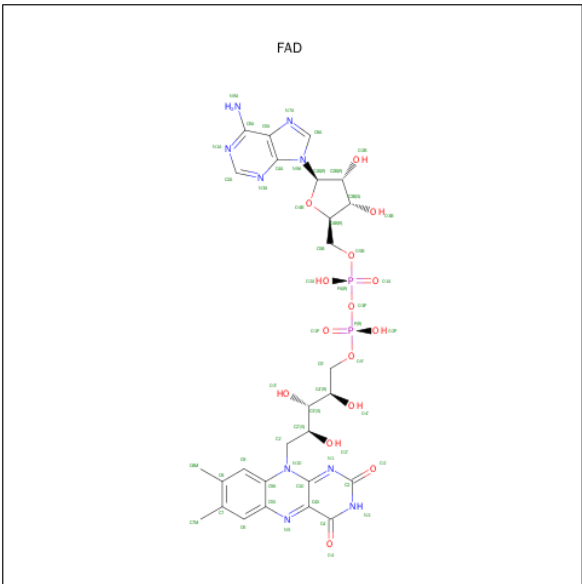
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			
4	H	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		
5	E	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



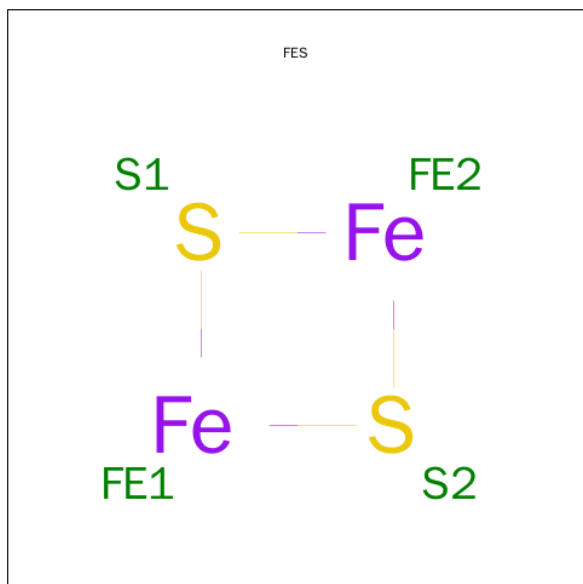
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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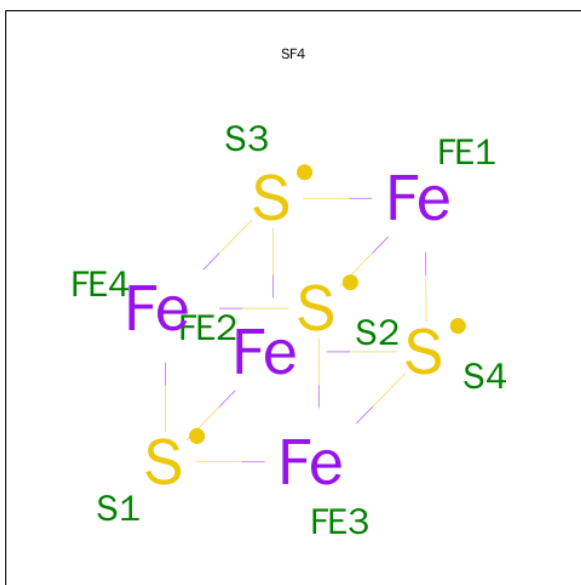
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



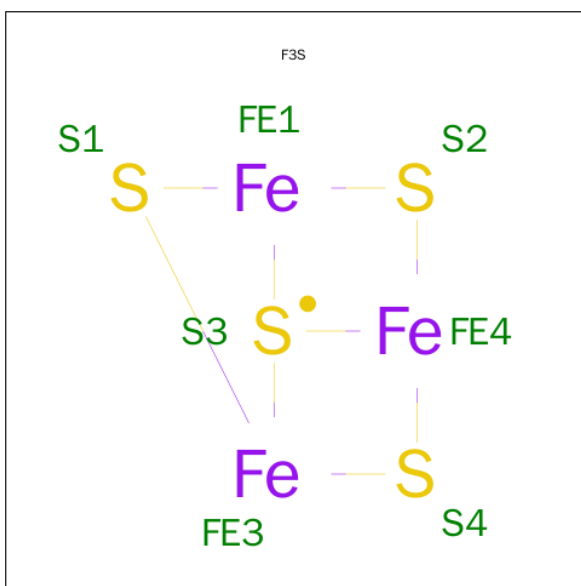
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



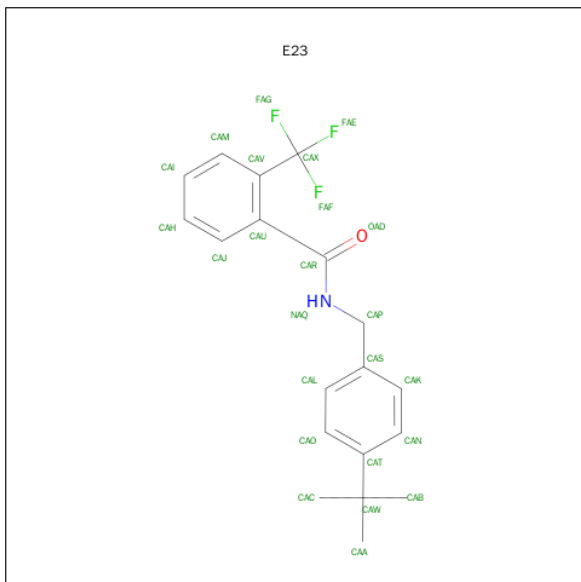
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



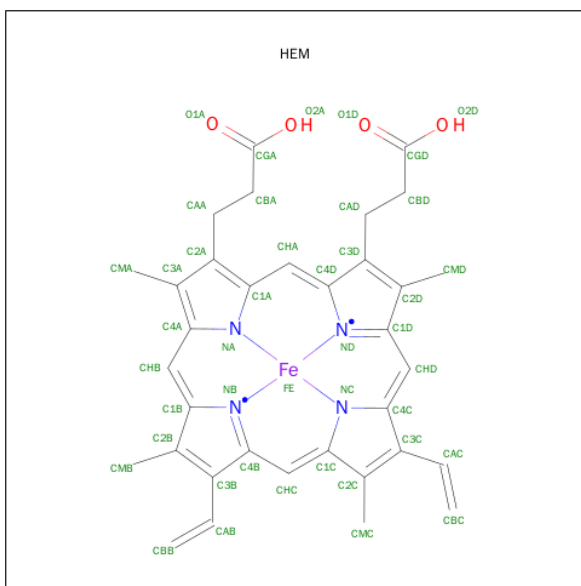
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 10 is N-(4-tert-butylbenzyl)-2-(trifluoromethyl)benzamide (three-letter code: E23) (formula: $C_{19}H_{20}F_3NO$).



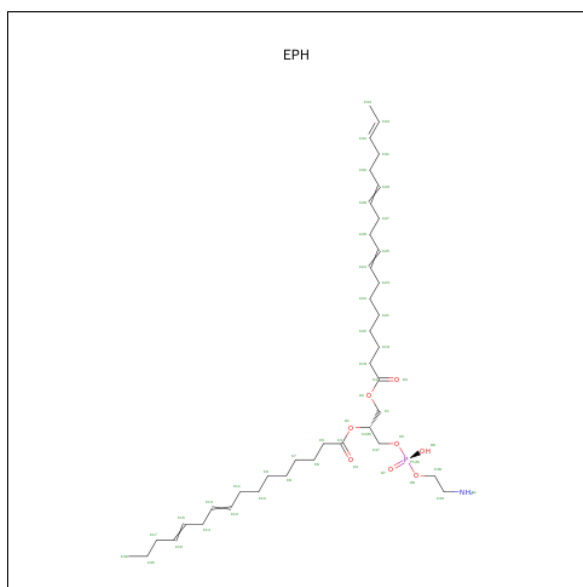
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	F	N	O	0	0
			24	19	3	1	1		
10	G	1	Total	C	F	N	O	0	0
			24	19	3	1	1		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
11	G	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: $C_{39}H_{68}NO_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	
			44	34	1	8	1	
12	H	1	Total	C	N	O	P	
			44	34	1	8	1	

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	186	Total	O		
			186	186	0	0
13	B	104	Total	O		
			104	104	0	0
13	C	33	Total	O		
			33	33	0	0
13	D	27	Total	O		
			27	27	0	0
13	E	207	Total	O		
			207	207	0	0

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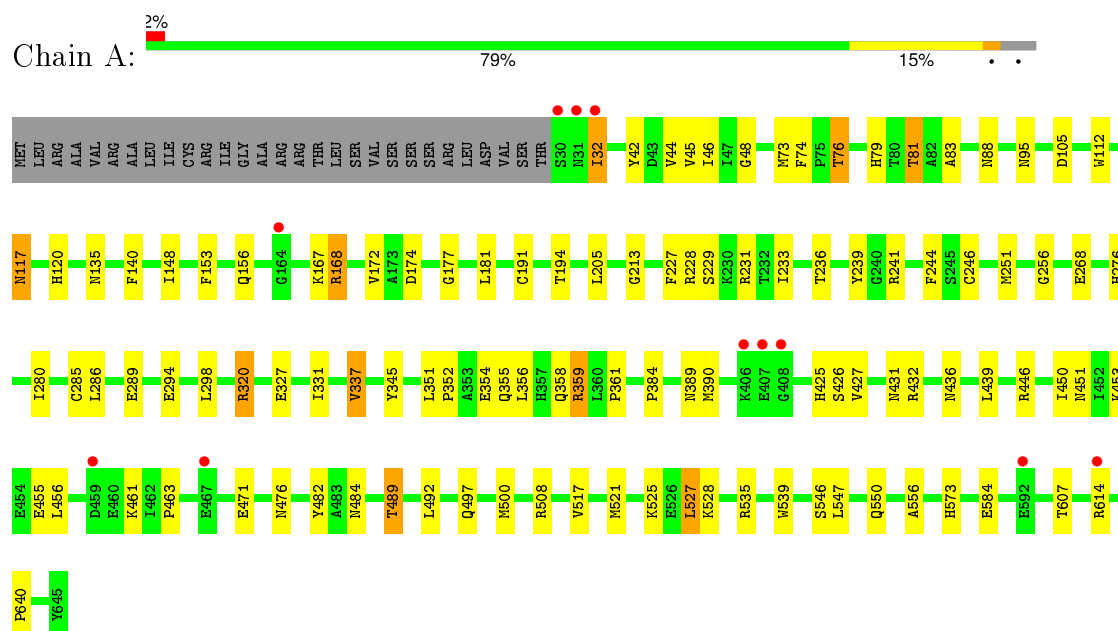
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	F	111	Total 111	O 111	0	0
13	G	36	Total 36	O 36	0	0
13	H	17	Total 17	O 17	0	0

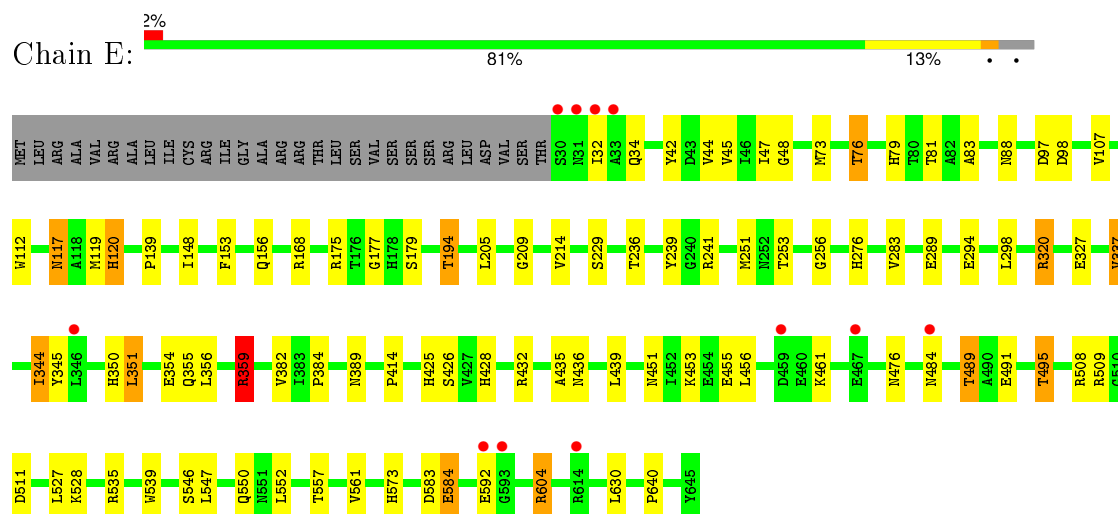
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

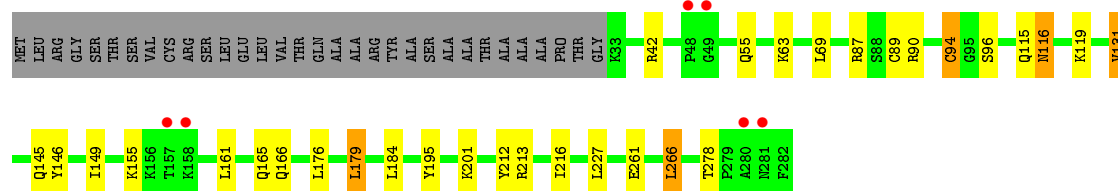
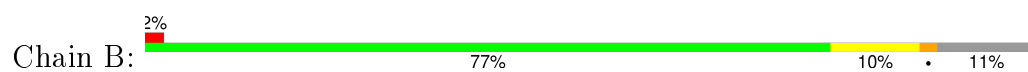
• Molecule 1: Succinate dehydrogenase flavoprotein



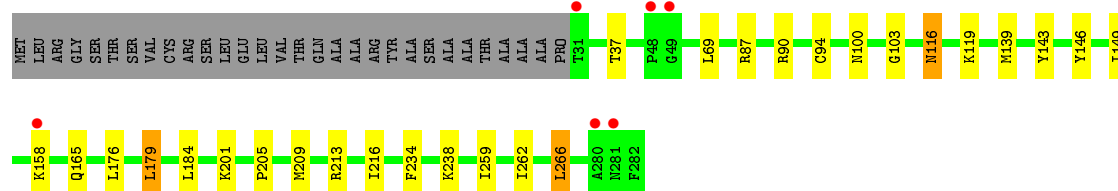
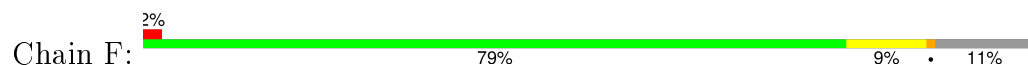
• Molecule 1: Succinate dehydrogenase flavoprotein



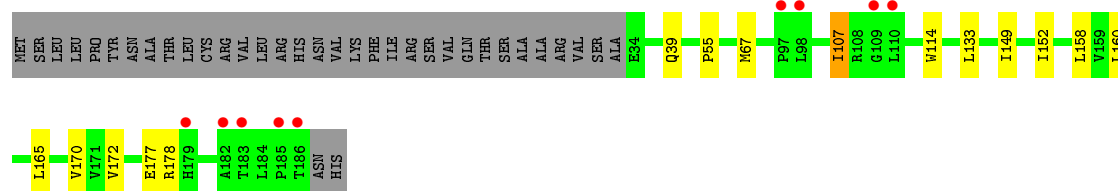
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



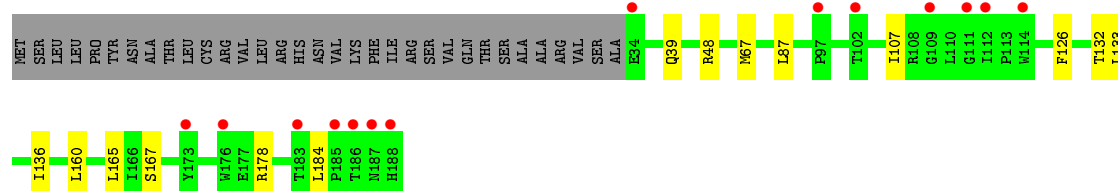
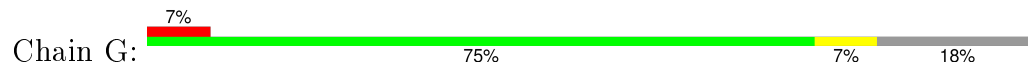
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



- Molecule 3: Cytochrome b-large subunit

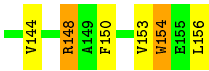


- Molecule 3: Cytochrome b-large subunit

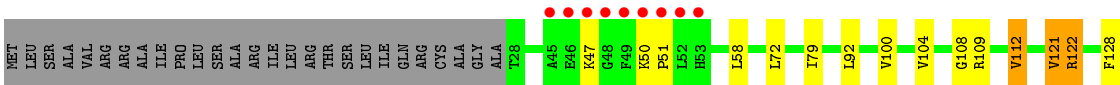


- Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial





- Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.20Å 127.91Å 220.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 20.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.00-2.25) 96.4 (20.00-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.181 , 0.221 0.185 , 0.223	Depositor DCC
R_{free} test set	8058 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.1	EDS
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 160280 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19103	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: E23, SF4, MLI, F3S, FES, EPH, HEM, FAD

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	0.43	0/4889	0.67	2/6605 (0.0%)
1	E	0.45	0/4889	0.70	7/6605 (0.1%)
2	B	0.46	0/2029	0.67	0/2739
2	F	0.46	1/2038 (0.0%)	0.63	0/2751
3	C	0.40	0/1255	0.59	0/1709
3	G	0.39	0/1275	0.60	0/1735
4	D	0.40	0/1030	0.58	0/1406
4	H	0.40	0/1030	0.60	0/1406
All	All	0.44	1/18435 (0.0%)	0.66	9/24956 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	94	CYS	C-N	-5.26	1.23	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	604	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	E	320	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	E	241	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	A	168	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	359	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	320	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	E	320	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	E	175	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	E	604	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	4787	0	4722	61	0
1	E	4787	0	4720	54	0
2	B	1985	0	2001	16	0
2	F	1994	0	2006	12	0
3	C	1217	0	1265	7	0
3	G	1236	0	1278	8	0
4	D	998	0	985	11	0
4	H	998	0	985	11	0
5	A	7	0	2	0	0
5	E	7	0	2	1	0
6	A	53	0	31	7	0
6	E	53	0	31	7	0
7	B	4	0	0	0	0
7	F	4	0	0	0	0
8	B	8	0	0	0	0
8	F	8	0	0	0	0
9	B	7	0	0	0	0
9	F	7	0	0	0	0
10	B	24	0	20	0	0
10	G	24	0	20	0	0
11	C	43	0	30	5	0
11	G	43	0	30	5	0
12	D	44	0	53	2	0
12	H	44	0	53	1	0
13	A	186	0	0	4	0
13	B	104	0	0	2	0
13	C	33	0	0	0	0
13	D	27	0	0	1	0
13	E	207	0	0	3	0
13	F	111	0	0	3	0
13	G	36	0	0	1	0
13	H	17	0	0	1	0
All	All	19103	0	18234	175	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 (175) 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:79:HIS:NE2	6:A:702:FAD:HM82	1.25	1.48
1:E:79:HIS:NE2	6:E:702:FAD:HM82	1.33	1.36
1:E:79:HIS:NE2	6:E:702:FAD:C8M	2.07	1.16
1:A:79:HIS:NE2	6:A:702:FAD:C8M	2.12	1.13
1:E:476:ASN:HD21	1:E:550:GLN:HE22	1.19	0.91
1:A:476:ASN:HD21	1:A:550:GLN:HE22	1.23	0.86
1:E:79:HIS:CE1	6:E:702:FAD:HM82	2.12	0.85
3:G:107:ILE:HD11	4:H:156:LEU:HD13	1.58	0.85
1:A:76:THR:HG23	13:B:415:HOH:O	1.84	0.77
4:D:144:VAL:HB	4:D:148:ARG:HG2	1.67	0.77
3:G:107:ILE:HD11	4:H:156:LEU:CD1	2.24	0.68
11:G:201:HEM:HBD1	11:G:201:HEM:HHA	1.78	0.66
1:E:289:GLU:OE2	1:E:320:ARG:HD2	1.95	0.65
1:E:76:THR:HG23	13:F:409:HOH:O	1.96	0.64
2:B:89:CYS:HB3	2:B:94:CYS:HB3	1.77	0.64
1:A:135:ASN:ND2	2:B:161:LEU:O	2.31	0.64
1:A:289:GLU:OE2	1:A:320:ARG:HD2	1.98	0.64
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.78	0.63
4:D:108:GLY:O	4:D:122:ARG:NH2	2.32	0.63
1:E:489:THR:HG21	1:E:546:SER:OG	1.99	0.63
1:E:337:VAL:HG21	1:E:345:TYR:CE2	2.35	0.61
2:F:179:LEU:HD23	2:F:216:ILE:HD11	1.83	0.61
11:C:201:HEM:HBD1	11:C:201:HEM:HHA	1.83	0.61
1:A:294:GLU:CD	1:A:359:ARG:HG2	2.22	0.60
11:G:201:HEM:HHC	11:G:201:HEM:HBB2	1.83	0.60
5:E:701:MLI:H12	6:E:702:FAD:N5	2.17	0.59
2:F:262:ILE:HG22	2:F:266:LEU:HD22	1.83	0.59
4:H:108:GLY:O	4:H:122:ARG:NH2	2.35	0.59
1:E:508:ARG:HH11	1:E:573:HIS:HD2	1.50	0.59
1:A:425:HIS:N	1:A:426:SER:HA	2.17	0.57
1:E:79:HIS:NE2	6:E:702:FAD:HM81	2.14	0.57
1:E:97:ASP:OD1	1:E:168:ARG:CG	2.53	0.57
1:E:425:HIS:N	1:E:426:SER:HA	2.20	0.57
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.86	0.57
1:E:76:THR:CG2	13:F:409:HOH:O	2.53	0.56
3:G:87:LEU:HD22	4:H:128:PHE:CE1	2.40	0.56
1:A:79:HIS:CD2	6:A:702:FAD:C8M	2.88	0.56
1:E:327:GLU:OE2	1:E:344:ILE:HD11	2.06	0.56
1:E:107:VAL:HG22	1:E:119:MET:HE3	1.88	0.56
11:G:201:HEM:HBD2	13:H:303:HOH:O	2.05	0.55
1:E:491:GLU:O	1:E:495:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PHE:HA	1:A:172:VAL:HG22	1.89	0.54
1:E:83:ALA:HA	6:E:702:FAD:C6	2.38	0.54
1:E:327:GLU:OE2	1:E:344:ILE:CD1	2.56	0.53
1:E:476:ASN:HD21	1:E:550:GLN:NE2	1.98	0.53
11:C:201:HEM:HBB2	11:C:201:HEM:HHC	1.90	0.53
3:G:132:THR:HG23	11:G:201:HEM:CAB	2.39	0.53
4:H:104:VAL:HG13	4:H:121:VAL:CG1	2.38	0.53
1:E:239:TYR:H	1:E:389:ASN:ND2	2.07	0.53
1:A:79:HIS:CE1	6:A:702:FAD:HM82	2.27	0.52
2:F:209:MET:HE2	13:F:479:HOH:O	2.09	0.52
1:A:42:TYR:O	1:A:229:SER:HA	2.09	0.52
1:A:489:THR:HG21	1:A:546:SER:OG	2.10	0.52
3:G:178:ARG:NH2	4:H:156:LEU:OXT	2.44	0.51
1:A:45:VAL:HG23	1:A:229:SER:HB3	1.93	0.51
1:E:42:TYR:O	1:E:229:SER:HA	2.11	0.51
1:E:350:HIS:CD2	1:E:351:LEU:HD13	2.46	0.50
1:A:112:TRP:CE2	1:A:640:PRO:HA	2.46	0.50
1:A:191:CYS:HB3	13:A:907:HOH:O	2.12	0.50
1:A:88:ASN:ND2	1:A:156:GLN:HE22	2.08	0.50
11:C:201:HEM:HBD2	13:D:310:HOH:O	2.11	0.50
3:C:107:ILE:HD11	4:D:156:LEU:HD13	1.93	0.50
2:B:155:LYS:HD2	2:B:166:GLN:NE2	2.27	0.50
1:E:194:THR:HG23	13:E:954:HOH:O	2.11	0.50
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.93	0.49
11:G:201:HEM:HBC2	11:G:201:HEM:HHD	1.94	0.49
2:B:42:ARG:HG3	2:B:55:GLN:HE21	1.77	0.49
1:E:209:GLY:O	1:E:414:PRO:HD2	2.13	0.48
1:A:492:LEU:HD21	1:A:527:LEU:HD12	1.94	0.48
4:D:109:ARG:HB2	4:D:112:VAL:HG12	1.94	0.48
2:B:179:LEU:HD23	2:B:216:ILE:HD11	1.95	0.48
1:A:117:ASN:HD22	1:A:117:ASN:N	2.11	0.48
3:C:170:VAL:HG22	4:D:77:TYR:CE1	2.49	0.47
1:A:500:MET:HE1	1:A:556:ALA:O	2.14	0.47
11:C:201:HEM:HBC2	11:C:201:HEM:HHD	1.96	0.47
1:E:32:ILE:HG13	1:E:32:ILE:O	2.14	0.47
1:A:241:ARG:HD2	1:A:246:CYS:SG	2.53	0.47
3:G:126:PHE:HA	3:G:167:SER:OG	2.14	0.47
1:A:228:ARG:HD2	1:A:463:PRO:O	2.15	0.47
1:A:76:THR:CG2	13:B:415:HOH:O	2.53	0.47
1:A:148:ILE:H	2:B:165:GLN:HE22	1.63	0.47
1:E:489:THR:HG23	13:E:875:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:THR:OG1	1:E:256:GLY:HA3	2.14	0.47
1:E:584:GLU:OE2	1:E:604:ARG:HD3	2.15	0.47
1:A:294:GLU:OE1	1:A:359:ARG:HG2	2.15	0.46
4:H:150:PHE:HB3	12:H:201:EPH:H2	1.95	0.46
2:F:201:LYS:HA	3:G:39:GLN:HG2	1.98	0.46
4:D:77:TYR:CD1	12:D:201:EPH:H11	2.49	0.46
4:D:150:PHE:HB3	12:D:201:EPH:H2	1.98	0.46
1:E:451:ASN:O	1:E:455:GLU:HG3	2.15	0.46
1:A:32:ILE:HD11	1:A:482:TYR:CZ	2.50	0.46
1:E:344:ILE:CD1	1:E:382:VAL:HG23	2.45	0.46
2:F:116:ASN:HD22	2:F:116:ASN:C	2.18	0.45
2:F:179:LEU:CD2	2:F:216:ILE:HD11	2.47	0.45
1:E:120:HIS:HD2	1:E:630:LEU:H	1.65	0.45
1:A:239:TYR:H	1:A:389:ASN:ND2	2.13	0.45
2:B:227:LEU:HD22	2:B:266:LEU:HD13	1.98	0.45
1:E:509:ARG:HD2	1:E:511:ASP:OD2	2.16	0.45
1:E:294:GLU:CD	1:E:359:ARG:HG2	2.37	0.45
2:B:146:TYR:O	2:B:149:ILE:HG12	2.16	0.45
4:D:153:VAL:HG23	4:D:154:TRP:HE3	1.82	0.44
1:E:557:THR:O	1:E:561:VAL:HG13	2.17	0.44
3:G:48:ARG:NH2	13:G:301:HOH:O	2.35	0.44
1:A:425:HIS:HB2	1:A:427:VAL:HG13	1.99	0.44
1:A:81:THR:HB	1:A:181:LEU:HD23	1.99	0.44
1:A:337:VAL:HG21	1:A:345:TYR:CE2	2.52	0.44
4:H:50:LYS:N	4:H:51:PRO:CD	2.80	0.44
1:A:73:MET:SD	1:A:251:MET:HG3	2.58	0.44
4:H:104:VAL:HG13	4:H:121:VAL:HG12	1.99	0.44
1:A:117:ASN:HD22	1:A:117:ASN:H	1.65	0.44
1:A:517:VAL:O	1:A:521:MET:HG2	2.18	0.44
1:A:451:ASN:O	1:A:455:GLU:HG3	2.17	0.44
2:B:116:ASN:C	2:B:116:ASN:HD22	2.20	0.44
1:A:48:GLY:HA2	6:A:702:FAD:H1B	2.00	0.43
1:A:88:ASN:HD21	1:A:156:GLN:HE22	1.66	0.43
1:A:508:ARG:HH11	1:A:573:HIS:HD2	1.64	0.43
1:E:47:ILE:HD11	1:E:214:VAL:HG21	2.00	0.43
2:F:205:PRO:HA	2:F:259:ILE:HD11	2.00	0.43
1:E:48:GLY:HA2	6:E:702:FAD:H1B	2.00	0.43
1:A:148:ILE:H	2:B:165:GLN:NE2	2.17	0.43
1:E:112:TRP:CE2	1:E:640:PRO:HA	2.54	0.43
2:F:100:ASN:HD21	2:F:103:GLY:CA	2.30	0.43
1:A:105:ASP:OD2	1:A:168:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:109:ARG:HB2	4:H:112:VAL:HG13	2.00	0.43
1:E:253:THR:HA	1:E:552:LEU:HD21	2.01	0.43
1:A:174:ASP:HB2	1:A:361:PRO:HD2	2.01	0.43
1:E:432:ARG:HH21	1:E:435:ALA:H	1.66	0.43
1:A:276:HIS:O	1:A:384:PRO:HA	2.19	0.43
2:F:234:PHE:CD1	2:F:238:LYS:HG3	2.54	0.43
1:E:117:ASN:N	1:E:117:ASN:HD22	2.17	0.42
1:A:280:ILE:HD12	1:A:285:CYS:HB2	2.01	0.42
3:C:178:ARG:NH2	4:D:156:LEU:OXT	2.48	0.42
1:A:268:GLU:HA	1:A:607:THR:O	2.20	0.42
1:A:359:ARG:NH2	13:A:810:HOH:O	2.52	0.42
2:B:155:LYS:HD2	2:B:166:GLN:HE21	1.85	0.42
1:A:431:ASN:ND2	13:A:812:HOH:O	2.53	0.42
1:A:471:GLU:OE2	4:D:28:THR:HA	2.20	0.42
1:A:236:THR:OG1	1:A:256:GLY:HA3	2.20	0.42
1:A:231:ARG:NH2	13:A:809:HOH:O	2.52	0.42
2:F:139:MET:HB3	2:F:143:TYR:CE2	2.55	0.42
1:A:83:ALA:HA	6:A:702:FAD:C6	2.50	0.42
1:A:337:VAL:HG21	1:A:345:TYR:CD2	2.55	0.41
1:E:88:ASN:ND2	1:E:156:GLN:HE22	2.18	0.41
1:E:476:ASN:ND2	1:E:550:GLN:HE22	2.00	0.41
2:F:146:TYR:O	2:F:149:ILE:HG12	2.19	0.41
1:A:213:GLY:HA3	1:A:227:PHE:O	2.20	0.41
1:A:286:LEU:HD22	6:A:702:FAD:C6	2.51	0.41
1:E:45:VAL:HG23	1:E:229:SER:HB3	2.01	0.41
2:B:145:GLN:NE2	2:B:195:TYR:OH	2.53	0.41
1:E:148:ILE:H	2:F:165:GLN:HE22	1.68	0.41
1:A:244:PHE:HA	1:A:497:GLN:HB3	2.02	0.41
1:A:352:PRO:HD2	1:A:355:GLN:HE21	1.85	0.41
1:E:583:ASP:OD1	1:E:604:ARG:HG3	2.20	0.41
1:E:355:GLN:O	1:E:359:ARG:HB2	2.21	0.41
2:B:131:VAL:HG22	3:C:55:PRO:HG2	2.02	0.41
1:A:74:PHE:CE2	1:A:76:THR:HB	2.56	0.41
4:H:144:VAL:HB	4:H:148:ARG:HG2	2.03	0.41
1:E:337:VAL:HG21	1:E:345:TYR:CD2	2.55	0.41
11:C:201:HEM:CBD	11:C:201:HEM:HHA	2.48	0.41
1:A:327:GLU:O	1:A:331:ILE:HG12	2.21	0.41
2:B:212:TYR:OH	2:B:261:GLU:HG2	2.20	0.41
1:E:97:ASP:OD2	1:E:98:ASP:N	2.50	0.41
4:D:57:THR:O	4:D:61:ILE:HG23	2.20	0.41
1:E:428:HIS:CE1	1:E:432:ARG:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:MET:SD	1:E:251:MET:HG3	2.61	0.40
1:A:446:ARG:HD3	1:A:450:ILE:HD11	2.02	0.40
2:B:94:CYS:SG	2:B:96:SER:HB2	2.61	0.40
1:A:95:ASN:HD21	1:A:167:LYS:HB2	1.85	0.40
1:E:139:PRO:HD2	1:E:179:SER:OG	2.21	0.40
1:E:276:HIS:O	1:E:384:PRO:HA	2.20	0.40
3:C:149:ILE:HA	3:C:152:ILE:HD12	2.03	0.40
3:C:158:LEU:HD23	3:C:158:LEU:C	2.42	0.40
1:A:354:GLU:O	1:A:358:GLN:HB2	2.20	0.40
1:E:359:ARG:NH2	13:E:814:HOH:O	2.55	0.40
1:A:46:ILE:HG12	1:A:233: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	614/645 (95%)	594 (97%)	20 (3%)	0	100	100
1	E	614/645 (95%)	599 (98%)	15 (2%)	0	100	100
2	B	248/282 (88%)	239 (96%)	9 (4%)	0	100	100
2	F	250/282 (89%)	243 (97%)	7 (3%)	0	100	100
3	C	151/188 (80%)	147 (97%)	4 (3%)	0	100	100
3	G	153/188 (81%)	151 (99%)	2 (1%)	0	100	100
4	D	127/156 (81%)	125 (98%)	2 (2%)	0	100	100
4	H	127/156 (81%)	122 (96%)	5 (4%)	0	100	100
All	All	2284/2542 (90%)	2220 (97%)	64 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	502/527 (95%)	471 (94%)	31 (6%)	23	22
1	E	502/527 (95%)	470 (94%)	32 (6%)	22	21
2	B	220/242 (91%)	205 (93%)	15 (7%)	20	18
2	F	220/242 (91%)	208 (94%)	12 (6%)	27	27
3	C	127/158 (80%)	119 (94%)	8 (6%)	22	21
3	G	129/158 (82%)	123 (95%)	6 (5%)	32	36
4	D	98/119 (82%)	89 (91%)	9 (9%)	11	9
4	H	98/119 (82%)	87 (89%)	11 (11%)	7	5
All	All	1896/2092 (91%)	1772 (94%)	124 (6%)	21	20

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ILE
1	A	44	VAL
1	A	76	THR
1	A	81	THR
1	A	117	ASN
1	A	120	HIS
1	A	153	PHE
1	A	194	THR
1	A	205	LEU
1	A	298	LEU
1	A	337	VAL
1	A	351	LEU
1	A	356	LEU
1	A	359	ARG
1	A	390	MET
1	A	432	ARG
1	A	436	ASN
1	A	439	LEU
1	A	453	LYS

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Mol	Chain	Res	Type
1	A	456	LEU
1	A	461	LYS
1	A	484	ASN
1	A	489	THR
1	A	525	LYS
1	A	527	LEU
1	A	528	LYS
1	A	535	ARG
1	A	539	TRP
1	A	547	LEU
1	A	584	GLU
1	A	614	ARG
2	B	63	LYS
2	B	69	LEU
2	B	87	ARG
2	B	90	ARG
2	B	94	CYS
2	B	115	GLN
2	B	116	ASN
2	B	119	LYS
2	B	131	VAL
2	B	176	LEU
2	B	179	LEU
2	B	184	LEU
2	B	213	ARG
2	B	266	LEU
2	B	278	THR
3	C	67	MET
3	C	107	ILE
3	C	114	TRP
3	C	133	LEU
3	C	160	LEU
3	C	165	LEU
3	C	172	VAL
3	C	177	GLU
4	D	58	LEU
4	D	61	ILE
4	D	72	LEU
4	D	79	ILE
4	D	92	LEU
4	D	122	ARG
4	D	136	LEU

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Mol	Chain	Res	Type
4	D	148	ARG
4	D	154	TRP
1	E	34	GLN
1	E	44	VAL
1	E	76	THR
1	E	81	THR
1	E	117	ASN
1	E	120	HIS
1	E	153	PHE
1	E	194	THR
1	E	205	LEU
1	E	283	VAL
1	E	298	LEU
1	E	337	VAL
1	E	344	ILE
1	E	351	LEU
1	E	354	GLU
1	E	356	LEU
1	E	359	ARG
1	E	436	ASN
1	E	439	LEU
1	E	453	LYS
1	E	456	LEU
1	E	461	LYS
1	E	484	ASN
1	E	489	THR
1	E	495	THR
1	E	527	LEU
1	E	528	LYS
1	E	535	ARG
1	E	539	TRP
1	E	547	LEU
1	E	584	GLU
1	E	592	GLU
2	F	37	THR
2	F	69	LEU
2	F	87	ARG
2	F	90	ARG
2	F	116	ASN
2	F	119	LYS
2	F	158	LYS
2	F	176	LEU

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Mol	Chain	Res	Type
2	F	179	LEU
2	F	184	LEU
2	F	213	ARG
2	F	266	LEU
3	G	67	MET
3	G	133	LEU
3	G	136	ILE
3	G	160	LEU
3	G	165	LEU
3	G	184	LEU
4	H	47	LYS
4	H	58	LEU
4	H	72	LEU
4	H	79	ILE
4	H	92	LEU
4	H	100	VAL
4	H	112	VAL
4	H	121	VAL
4	H	122	ARG
4	H	136	LEU
4	H	154	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	95	ASN
1	A	117	ASN
1	A	125	ASN
1	A	252	ASN
1	A	355	GLN
1	A	389	ASN
1	A	436	ASN
1	A	451	ASN
1	A	476	ASN
1	A	497	GLN
1	A	551	ASN
1	A	573	HIS
2	B	55	GLN
2	B	100	ASN
2	B	105	ASN
2	B	116	ASN

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Mol	Chain	Res	Type
2	B	145	GLN
2	B	154	GLN
2	B	165	GLN
3	C	66	GLN
4	D	140	ASN
1	E	34	GLN
1	E	88	ASN
1	E	117	ASN
1	E	120	HIS
1	E	135	ASN
1	E	150	GLN
1	E	252	ASN
1	E	355	GLN
1	E	389	ASN
1	E	436	ASN
1	E	451	ASN
1	E	476	ASN
1	E	484	ASN
1	E	497	GLN
1	E	503	HIS
1	E	551	ASN
1	E	573	HIS
2	F	55	GLN
2	F	100	ASN
2	F	105	ASN
2	F	115	GLN
2	F	116	ASN
2	F	145	GLN
2	F	154	GLN
2	F	165	GLN
3	G	66	GLN
3	G	187	ASN
4	H	140	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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$
5	MLI	A	701	-	0,6,6	0.00	-	0,7,7	0.00	-
6	FAD	A	702	-	52,58,58	1.26	8 (15%)	52,89,89	2.44	13 (25%)
7	FES	B	301	2	0,4,4	0.00	-	0,4,4	0.00	-
8	SF4	B	302	2	0,12,12	0.00	-	0,24,24	0.00	-
9	F3S	B	303	2	0,9,9	0.00	-	0,15,15	0.00	-
10	E23	B	304	-	25,25,25	0.48	0	36,37,37	1.08	3 (8%)
11	HEM	C	201	3,4	24,50,50	1.01	1 (4%)	16,82,82	2.21	5 (31%)
12	EPH	D	201	-	42,43,48	1.12	2 (4%)	43,48,53	1.22	4 (9%)
5	MLI	E	701	-	0,6,6	0.00	-	0,7,7	0.00	-
6	FAD	E	702	-	52,58,58	1.30	7 (13%)	52,89,89	2.27	13 (25%)
7	FES	F	301	2	0,4,4	0.00	-	0,4,4	0.00	-
8	SF4	F	302	2	0,12,12	0.00	-	0,24,24	0.00	-
9	F3S	F	303	2	0,9,9	0.00	-	0,15,15	0.00	-
11	HEM	G	201	3,4	24,50,50	1.04	2 (8%)	16,82,82	2.29	5 (31%)
10	E23	G	202	-	25,25,25	0.40	0	36,37,37	0.97	3 (8%)
12	EPH	H	201	-	42,43,48	1.15	2 (4%)	43,48,53	1.26	4 (9%)

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
5	MLI	A	701	-	-	0/0/4/4	0/0/0/0
6	FAD	A	702	-	-	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FES	B	301	2	-	0/0/4/4	0/1/1/1
8	SF4	B	302	2	-	0/0/48/48	0/6/5/5
9	F3S	B	303	2	-	0/0/24/24	0/0/3/3
10	E23	B	304	-	-	0/21/21/21	0/2/2/2
11	HEM	C	201	3,4	-	1/6/54/54	0/0/8/8
12	EPH	D	201	-	-	0/47/47/52	0/0/0/0
5	MLI	E	701	-	-	0/0/4/4	0/0/0/0
6	FAD	E	702	-	-	0/30/50/50	0/6/6/6
7	FES	F	301	2	-	0/0/4/4	0/1/1/1
8	SF4	F	302	2	-	0/0/48/48	0/6/5/5
9	F3S	F	303	2	-	0/0/24/24	0/0/3/3
11	HEM	G	201	3,4	-	2/6/54/54	0/0/8/8
10	E23	G	202	-	-	0/21/21/21	0/2/2/2
12	EPH	H	201	-	-	0/47/47/52	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	201	HEM	C3B-C2B	-3.68	1.35	1.40
11	C	201	HEM	C3B-C2B	-3.54	1.35	1.40
6	A	702	FAD	C1'-N10	-2.71	1.45	1.48
6	A	702	FAD	C6-C5X	-2.68	1.37	1.41
6	E	702	FAD	C1'-N10	-2.23	1.46	1.48
6	A	702	FAD	C2-N3	-2.09	1.33	1.38
11	G	201	HEM	C1B-NB	-2.04	1.34	1.36
6	E	702	FAD	C8-C7	2.21	1.46	1.41
6	A	702	FAD	C8-C7	2.42	1.47	1.41
6	E	702	FAD	C9A-C5X	2.61	1.48	1.42
6	E	702	FAD	C9A-N10	2.61	1.42	1.38
6	A	702	FAD	C5A-C4A	2.63	1.46	1.40
6	A	702	FAD	C4X-C10	2.64	1.45	1.40
6	A	702	FAD	C9A-C5X	2.78	1.48	1.42
6	E	702	FAD	C5A-C4A	2.79	1.46	1.40
6	A	702	FAD	C4-C4X	3.09	1.47	1.41
6	E	702	FAD	C4-C4X	3.51	1.48	1.41
6	E	702	FAD	C4X-C10	3.93	1.48	1.40
12	D	201	EPH	O1-C3	4.42	1.47	1.34
12	H	201	EPH	O1-C3	4.42	1.47	1.34
12	D	201	EPH	O2-C4	4.55	1.46	1.33
12	H	201	EPH	O2-C4	4.91	1.47	1.33

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	702	FAD	N3A-C2A-N1A	-9.02	121.78	128.87
6	E	702	FAD	N3A-C2A-N1A	-7.86	122.70	128.87
6	A	702	FAD	C4-C4X-C10	-5.62	116.34	119.94
6	E	702	FAD	C4X-C4-N3	-4.37	117.81	123.52
6	A	702	FAD	C1B-N9A-C4A	-3.90	122.45	126.81
6	A	702	FAD	C4X-C4-N3	-3.63	118.78	123.52
11	G	201	HEM	CAD-C3D-C2D	-3.53	118.92	129.00
6	E	702	FAD	C1B-N9A-C4A	-3.51	122.88	126.81
6	A	702	FAD	N3-C2-N1	-3.47	121.85	127.69
6	E	702	FAD	C4-C4X-C10	-3.18	117.90	119.94
11	C	201	HEM	CAD-C3D-C2D	-3.17	119.94	129.00
10	B	304	E23	FAE-CAX-CAV	-3.07	107.45	112.67
6	E	702	FAD	N3-C2-N1	-3.06	122.54	127.69
10	B	304	E23	FAF-CAX-CAV	-2.92	107.70	112.67
12	D	201	EPH	O2-C4-O4	-2.75	116.31	123.51
12	H	201	EPH	O2-C4-O4	-2.49	116.97	123.51
10	G	202	E23	FAG-CAX-CAV	-2.32	108.72	112.67
12	D	201	EPH	O1-C3-O3	-2.29	117.43	123.67
11	C	201	HEM	CMA-C3A-C4A	-2.27	124.45	128.31
10	G	202	E23	FAF-CAX-CAV	-2.25	108.83	112.67
6	A	702	FAD	O2'-C2'-C3'	-2.25	103.17	108.96
10	G	202	E23	CAS-CAP-NAQ	-2.23	108.12	112.98
11	G	201	HEM	C3C-C4C-NC	-2.03	107.11	110.94
11	G	201	HEM	C3B-C4B-NB	-2.03	106.59	109.21
11	C	201	HEM	C3B-C4B-NB	-2.01	106.61	109.21
6	A	702	FAD	C2A-N1A-C6A	2.17	122.64	118.77
6	E	702	FAD	C1'-C2'-C3'	2.32	116.44	109.82
10	B	304	E23	CAP-NAQ-CAR	2.33	127.84	121.79
6	A	702	FAD	C1'-C2'-C3'	2.34	116.50	109.82
6	E	702	FAD	C4-C4X-N5	2.35	121.55	118.70
6	E	702	FAD	O4B-C1B-N9A	2.43	112.70	108.11
6	E	702	FAD	C2A-N1A-C6A	2.46	123.16	118.77
6	A	702	FAD	O4B-C1B-N9A	2.57	112.96	108.11
12	H	201	EPH	C1-O2-C4	2.66	124.93	117.00
6	E	702	FAD	C5X-C9A-N10	2.72	119.62	117.58
6	A	702	FAD	C4-C4X-N5	2.74	122.03	118.70
6	A	702	FAD	C4X-N5-C5X	3.42	120.75	116.72
12	D	201	EPH	O2-C4-C18	3.85	123.71	111.85
6	E	702	FAD	C1'-N10-C9A	3.97	123.43	118.83
12	H	201	EPH	O2-C4-C18	4.01	124.19	111.85
6	A	702	FAD	C1'-N10-C9A	4.05	123.53	118.83
6	E	702	FAD	C4X-N5-C5X	4.25	121.73	116.72
12	D	201	EPH	O1-C3-C5	4.26	120.51	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	201	EPH	O1-C3-C5	4.36	120.72	111.53
11	C	201	HEM	CAD-CBD-CGD	4.52	121.58	112.78
11	G	201	HEM	CAD-CBD-CGD	4.97	122.45	112.78
11	G	201	HEM	CBD-CAD-C3D	5.14	121.48	112.47
11	C	201	HEM	CBD-CAD-C3D	5.23	121.65	112.47
6	E	702	FAD	C4-N3-C2	7.89	121.74	115.16
6	A	702	FAD	C4-N3-C2	8.27	122.06	115.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	G	201	HEM	C4D-C3D-CAD-CBD
11	C	201	HEM	C2D-C3D-CAD-CBD
11	G	201	HEM	C2D-C3D-CAD-CBD

There are no ring outliers.

7 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	702	FAD	7	0
11	C	201	HEM	5	0
12	D	201	EPH	2	0
5	E	701	MLI	1	0
6	E	702	FAD	7	0
11	G	201	HEM	5	0
12	H	201	EPH	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	616/645 (95%)	-0.26	11 (1%) 71 75	32, 46, 70, 100	0
1	E	616/645 (95%)	-0.32	11 (1%) 71 75	31, 43, 64, 123	0
2	B	250/282 (88%)	-0.29	6 (2%) 62 66	32, 41, 64, 87	0
2	F	252/282 (89%)	-0.29	6 (2%) 62 66	33, 41, 68, 98	0
3	C	153/188 (81%)	-0.09	9 (5%) 26 28	35, 50, 88, 127	0
3	G	155/188 (82%)	-0.04	14 (9%) 12 13	38, 51, 88, 129	0
4	D	129/156 (82%)	-0.18	7 (5%) 29 33	40, 51, 91, 116	0
4	H	129/156 (82%)	0.00	9 (6%) 19 21	42, 53, 110, 151	0
All	All	2300/2542 (90%)	-0.24	73 (3%) 51 56	31, 46, 76, 151	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	188	HIS	8.4
4	H	51	PRO	8.3
4	H	49	PHE	8.1
4	H	52	LEU	7.6
3	C	186	THR	7.2
4	H	50	LYS	7.2
1	E	31	ASN	6.7
3	G	186	THR	5.3
1	E	30	SER	5.2
4	D	48	GLY	4.7
1	E	32	ILE	4.7
3	G	185	PRO	4.7
2	F	31	THR	4.6
4	D	49	PHE	4.4
2	F	48	PRO	4.2
4	H	53	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	459	ASP	4.1
4	H	47	LYS	4.0
2	B	48	PRO	4.0
1	E	614	ARG	4.0
3	C	182	ALA	4.0
3	G	109	GLY	3.9
1	A	30	SER	3.8
1	A	592	GLU	3.7
3	G	187	ASN	3.3
4	D	53	HIS	3.3
1	A	614	ARG	3.2
1	E	33	ALA	3.2
3	C	185	PRO	3.1
4	D	50	LYS	3.1
3	G	183	THR	3.0
3	C	179	HIS	3.0
2	F	49	GLY	2.9
2	F	281	ASN	2.9
4	H	45	ALA	2.7
1	E	592	GLU	2.7
2	F	280	ALA	2.7
2	B	280	ALA	2.6
2	B	158	LYS	2.6
4	D	52	LEU	2.6
3	C	183	THR	2.6
3	C	110	LEU	2.6
3	G	102	THR	2.5
1	E	593	GLY	2.5
3	C	97	PRO	2.5
1	A	31	ASN	2.5
4	H	46	GLU	2.5
2	F	158	LYS	2.5
2	B	49	GLY	2.5
3	C	109	GLY	2.5
3	G	111	GLY	2.4
1	E	484	ASN	2.4
1	A	407	GLU	2.4
4	D	47	LYS	2.4
2	B	281	ASN	2.4
4	D	36	ALA	2.4
1	A	408	GLY	2.3
3	G	173	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	467	GLU	2.2
1	E	346	LEU	2.2
3	G	97	PRO	2.2
1	A	32	ILE	2.2
3	G	176	TRP	2.2
1	A	406	LYS	2.2
3	G	114	TRP	2.2
1	E	459	ASP	2.1
3	C	98	LEU	2.1
2	B	157	THR	2.1
4	H	48	GLY	2.1
3	G	34	GLU	2.1
3	G	112	ILE	2.1
1	A	467	GLU	2.0
1	A	164	GLY	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 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
12	EPH	H	201	44/49	0.80	0.26	3.77	61,76,84,97	0
12	EPH	D	201	44/49	0.89	0.18	2.51	57,68,73,87	0
11	HEM	G	201	43/43	0.97	0.12	0.72	43,45,54,59	0
11	HEM	C	201	43/43	0.98	0.12	0.47	43,47,52,56	0
6	FAD	E	702	53/53	0.98	0.10	-0.30	30,34,40,45	0
10	E23	B	304	24/24	0.97	0.09	-0.36	36,40,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	E23	G	202	24/24	0.95	0.10	-0.37	36,42,60,61	0
9	F3S	B	303	7/7	0.99	0.10	-0.67	35,36,38,38	0
6	FAD	A	702	53/53	0.98	0.08	-0.69	31,35,39,40	0
9	F3S	F	303	7/7	0.99	0.09	-0.77	35,35,37,37	0
5	MLI	A	701	7/7	0.98	0.07	-0.95	40,41,45,46	0
8	SF4	F	302	8/8	0.97	0.07	-0.97	35,36,37,37	0
7	FES	B	301	4/4	0.99	0.07	-1.33	33,33,34,34	0
7	FES	F	301	4/4	0.98	0.07	-1.34	32,32,33,34	0
5	MLI	E	701	7/7	0.98	0.07	-1.39	37,39,42,45	0
8	SF4	B	302	8/8	0.98	0.07	-1.62	34,35,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.