Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:21 AM GMT

PDB ID	:	2WP9
Title	:	CRYSTAL STRUCTURE OF THE E. COLI SUCCINATE:QUINONE OXIDOREDUCTASE (SQR) SDHB HIS207THR MUTANT
Authors	:	Ruprecht, J.; Yankovskaya, V.; Maklashina, E.; Iwata, S.; Cecchini, G.
Deposited on	:	2009-08-03
Resolution	:	2.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

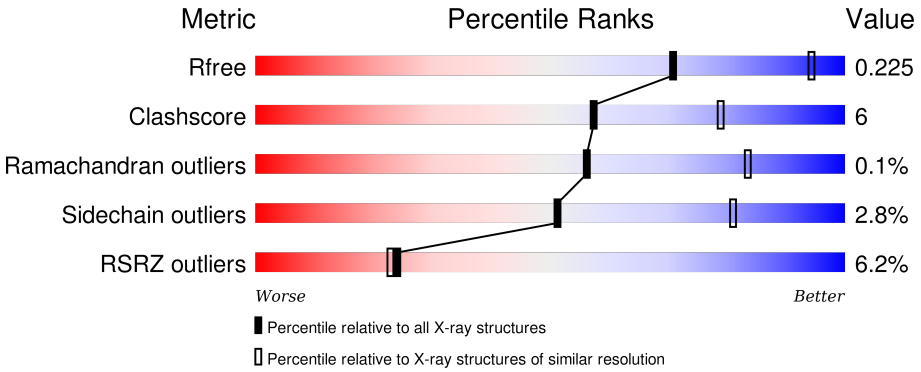
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 <=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	588	86% 13%
1	E	588	4% 87% 13%
1	I	588	11% 87% 12%
2	B	238	4% 86% 13%
2	F	238	5% 86% 12%

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Mol	Chain	Length	Quality of chain
2	J	238	7% 87% 11%
3	C	129	7% 86% 9% 5%
3	G	129	12% 81% 13% 5%
3	K	129	14% 81% 14% 5%
4	D	115	6% 77% 12% 9%
4	H	115	8% 77% 12% 9%
4	L	115	5% 77% 14% 9%

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
6	TEO	A	1589	-	-	-	X
7	NA	A	1590	-	-	-	X
7	NA	E	1590	-	-	-	X
7	NA	I	1590	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 25058 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 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4522	2812	821	861	28			
1	E	588	Total	C	N	O	S	0	0	0
			4522	2812	821	861	28			
1	I	588	Total	C	N	O	S	0	0	0
			4522	2812	821	861	28			

- Molecule 2 is a protein called SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1865	1170	327	348	20			
2	F	238	Total	C	N	O	S	0	0	0
			1865	1170	327	348	20			
2	J	238	Total	C	N	O	S	0	0	0
			1865	1170	327	348	20			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	207	THR	HIS	ENGINEERED MUTATION	UNP P07014
F	207	THR	HIS	ENGINEERED MUTATION	UNP P07014
J	207	THR	HIS	ENGINEERED MUTATION	UNP P07014

- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	122	Total	C	N	O	S	0	0	0
			947	630	153	159	5			

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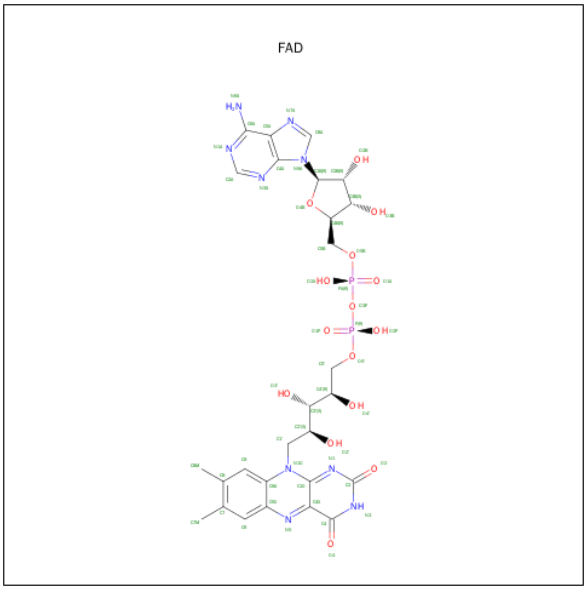
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	122	Total	C	N	O	S	0	0	0
			947	630	153	159	5			
3	K	122	Total	C	N	O	S	0	0	0
			947	630	153	159	5			

- Molecule 4 is a protein called SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT.

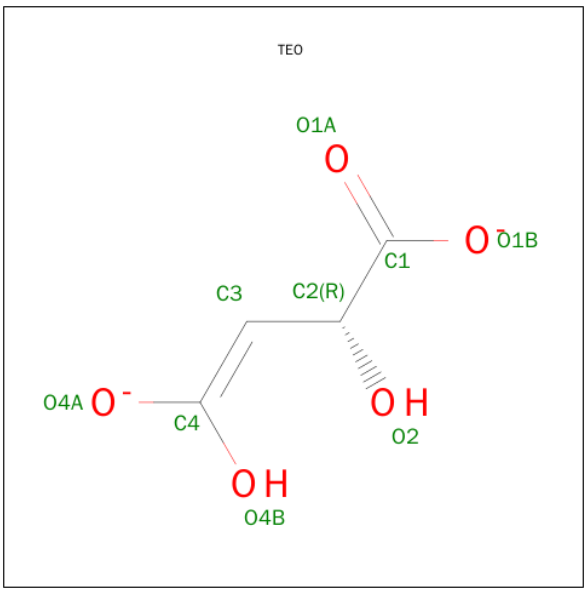
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	105	Total	C	N	O	S	0	0	0
			835	577	123	132	3			
4	H	105	Total	C	N	O	S	0	0	0
			835	577	123	132	3			
4	L	105	Total	C	N	O	S	0	0	0
			835	577	123	132	3			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 6 is MALATE LIKE INTERMEDIATE (three-letter code: TEO) (formula: $C_4H_4O_5$).

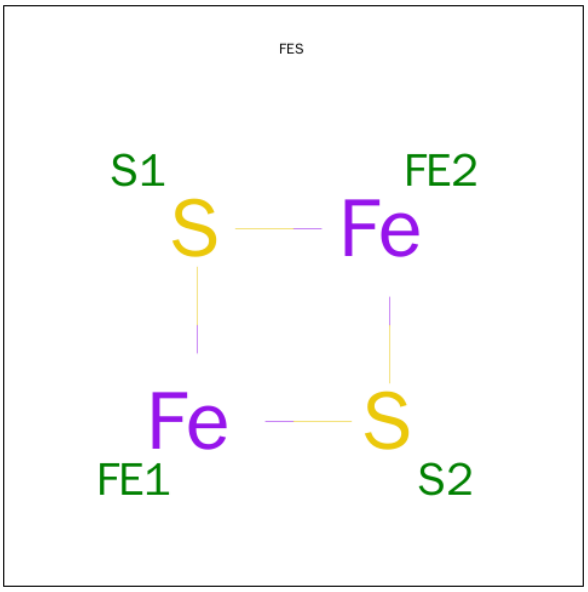


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 4 5	0	0
6	E	1	Total C O 9 4 5	0	0
6	I	1	Total C O 9 4 5	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

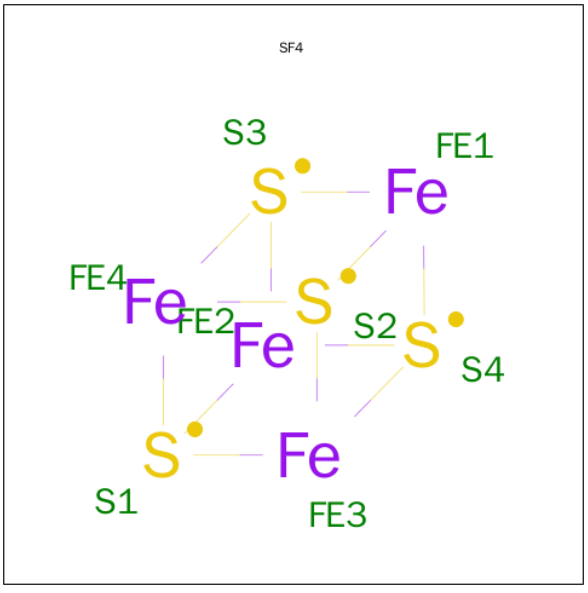
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total Na 1 1	0	0
7	A	1	Total Na 1 1	0	0
7	E	1	Total Na 1 1	0	0

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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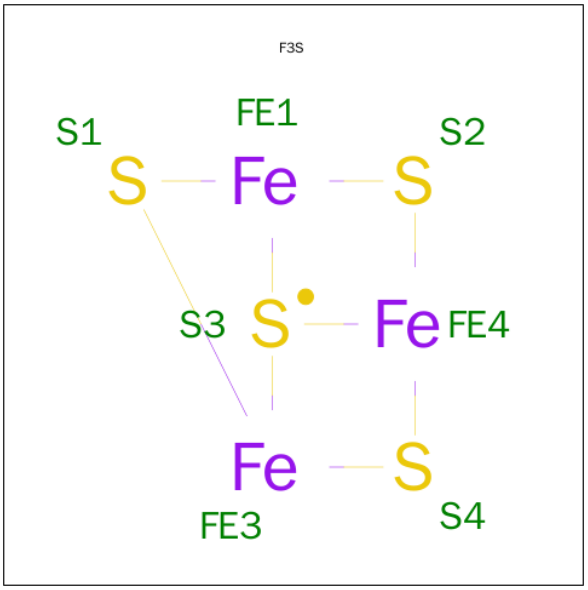
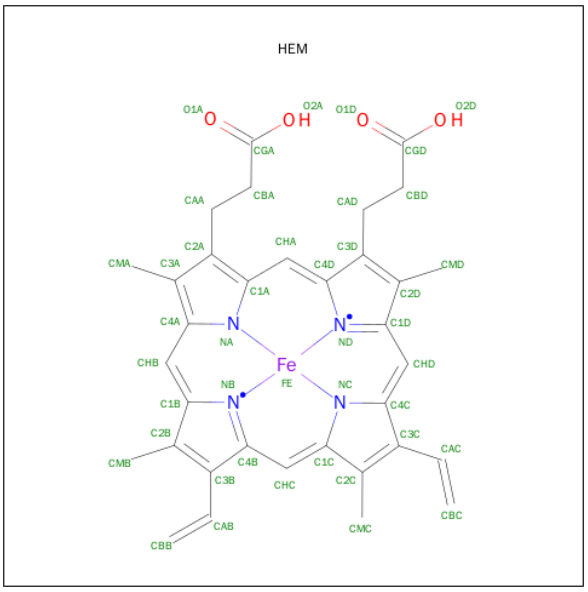
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total Fe S 8 4 4	0	0
9	J	1	Total Fe S 8 4 4	0	0

- Molecule 10 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



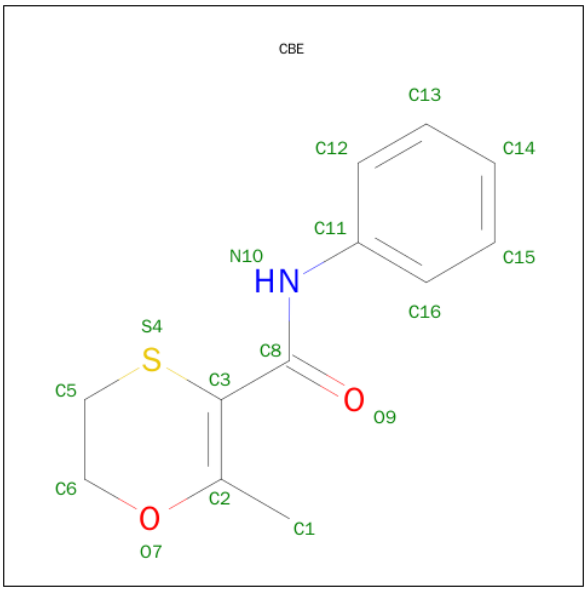
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Fe S 7 3 4	0	0
10	F	1	Total Fe S 7 3 4	0	0
10	J	1	Total Fe S 7 3 4	0	0

- 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	0	0
			43	34	1	4	4		
11	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 12 is 2-METHYL-N-PHENYL-5,6-DIHYDRO-1,4-OXATHIINE-3-CARBOXAMIDE (three-letter code: CBE) (formula: $C_{12}H_{13}NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
12	G	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
12	K	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

- Molecule 13 is water.

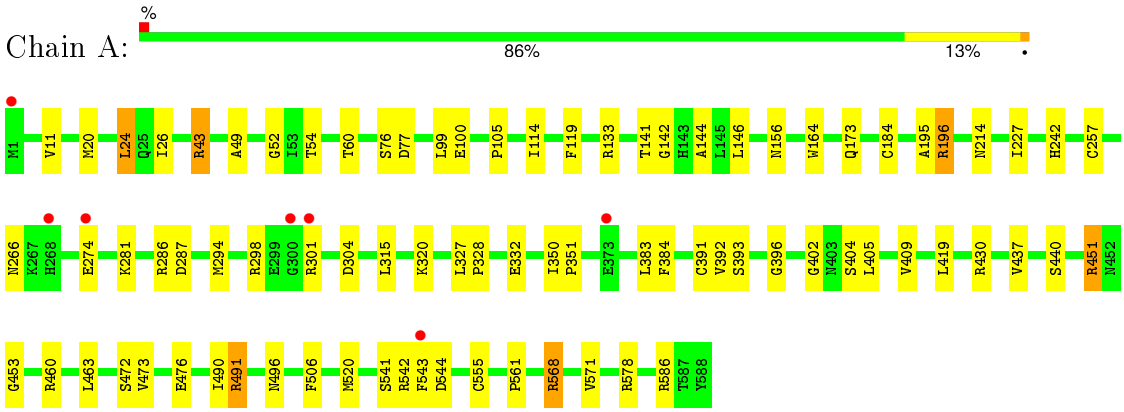
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	53	Total	O	0	0
			53	53		
13	B	17	Total	O	0	0
			17	17		
13	C	1	Total	O	0	0
			1	1		
13	D	1	Total	O	0	0
			1	1		
13	E	23	Total	O	0	0
			23	23		
13	F	7	Total	O	0	0
			7	7		
13	H	1	Total	O	0	0
			1	1		
13	I	13	Total	O	0	0
			13	13		
13	J	12	Total	O	0	0
			12	12		

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.

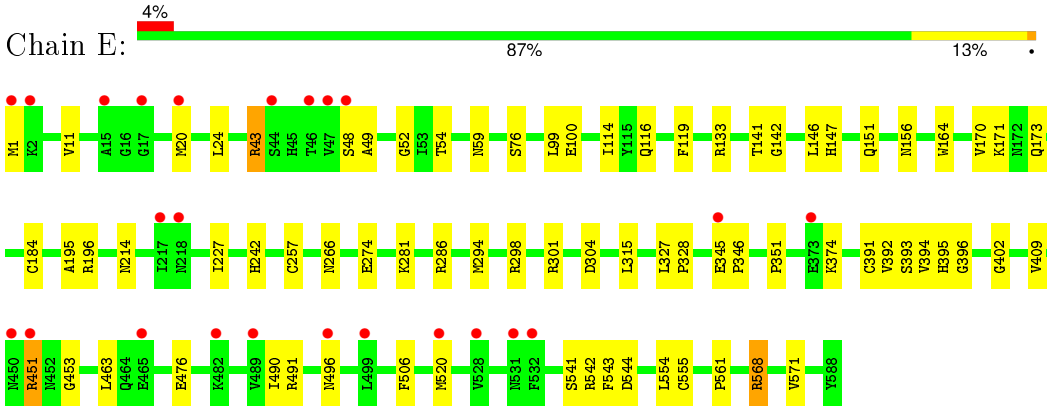
- Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

Chain A:



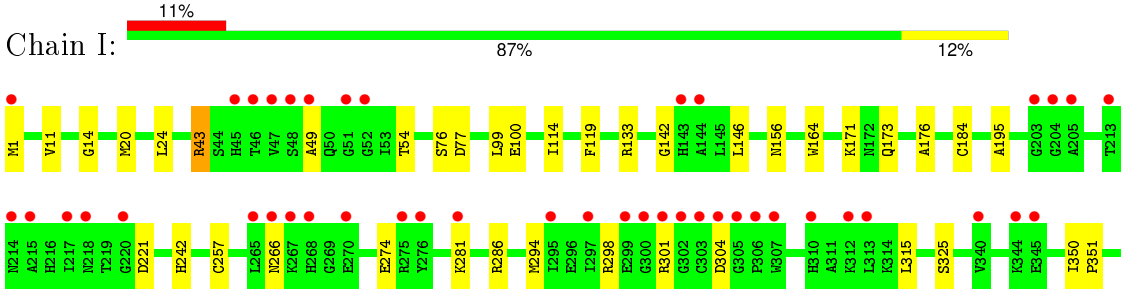
- Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

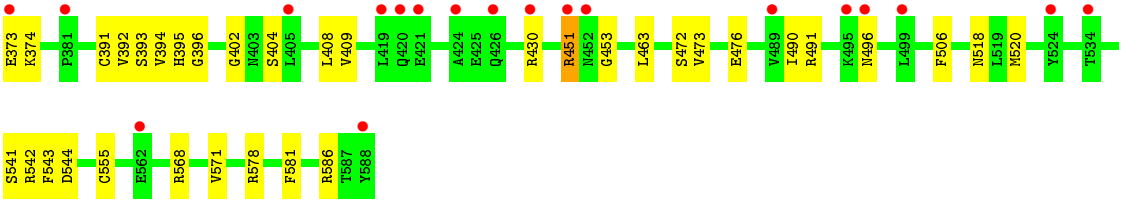
Chain E:



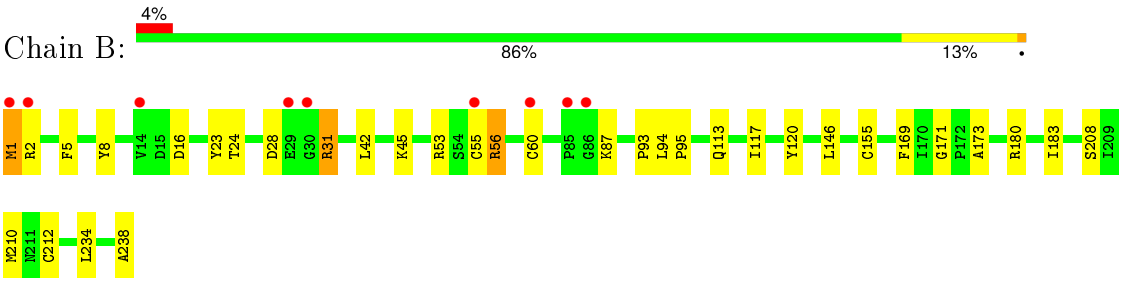
- Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

Chain I:

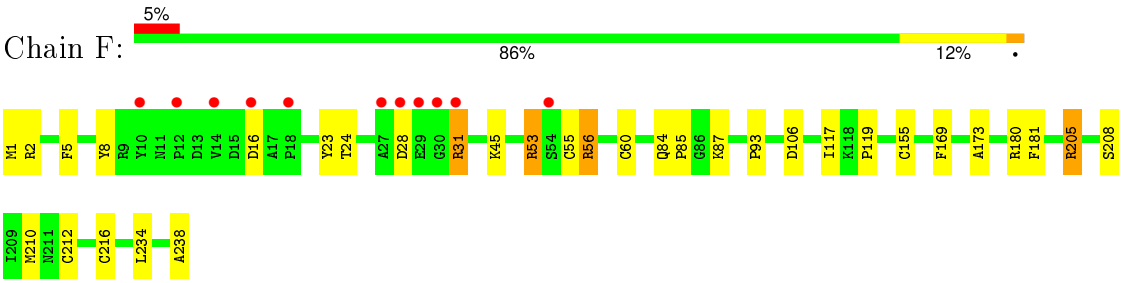




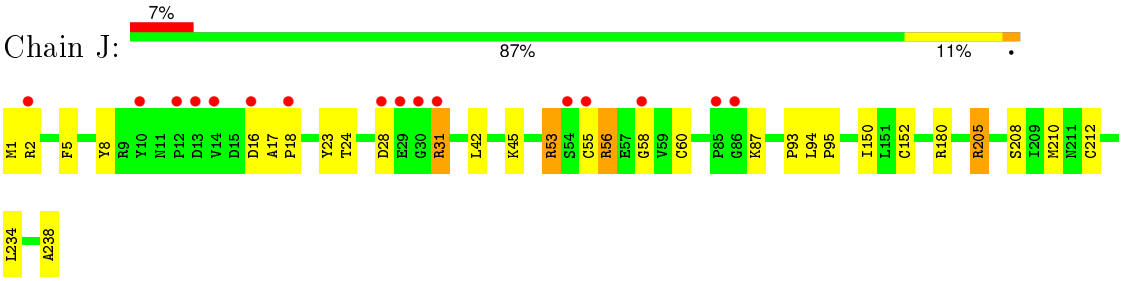
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



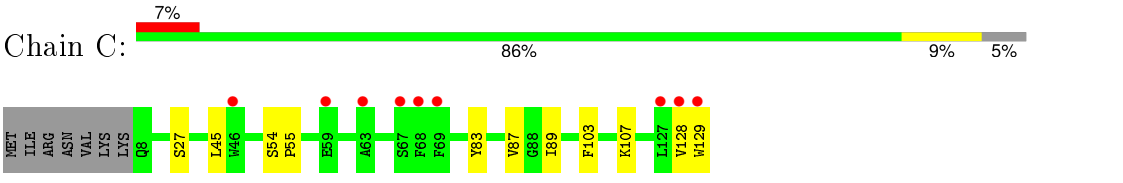
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



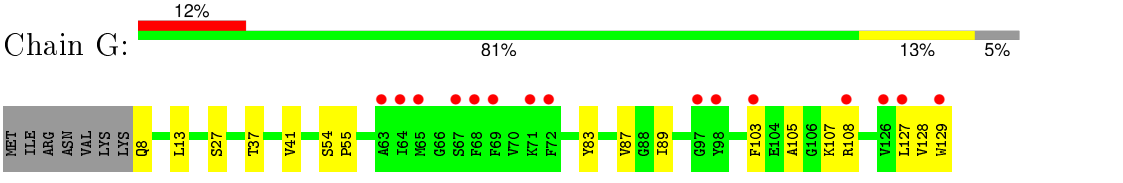
• Molecule 2: SUCCINATE DEHYDROGENASE IRON-SULFUR SUBUNIT



• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

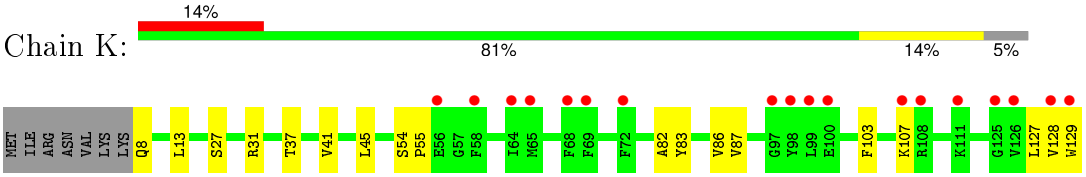


• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT



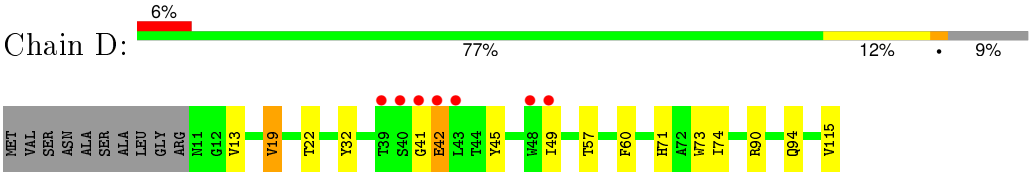
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B556 SUBUNIT

Chain K:



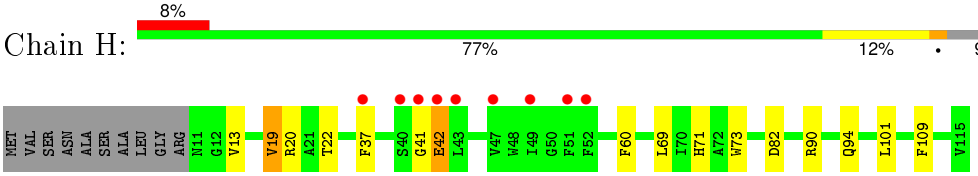
• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT

Chain D:



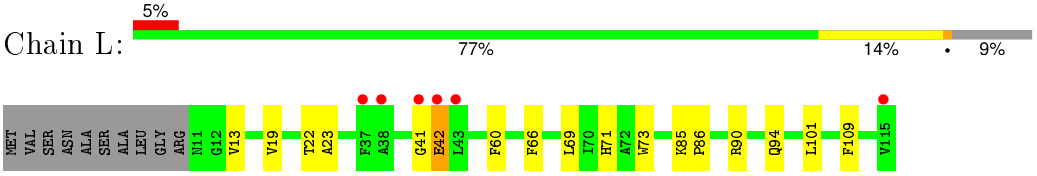
• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT

Chain H:



• Molecule 4: SUCCINATE DEHYDROGENASE HYDROPHOBIC MEMBRANE ANCHOR SUBUNIT

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.85Å 183.80Å 202.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 2.70 48.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.85-2.70) 99.6 (48.87-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.190 , 0.222 0.193 , 0.225	Depositor DCC
R_{free} test set	6188 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	2 of 122766 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25058	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CBE, NA, SF4, TEO, F3S, FES, 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	0.67	1/4611 (0.0%)	0.69	2/6237 (0.0%)
1	E	0.57	0/4611	0.64	0/6237
1	I	0.52	0/4611	0.62	0/6237
2	B	0.66	0/1903	0.72	0/2573
2	F	0.61	0/1903	0.68	1/2573 (0.0%)
2	J	0.56	0/1903	0.65	0/2573
3	C	0.60	0/969	0.59	0/1316
3	G	0.54	0/969	0.58	0/1316
3	K	0.52	0/969	0.54	0/1316
4	D	0.64	0/858	0.63	0/1175
4	H	0.60	0/858	0.58	0/1175
4	L	0.56	0/858	0.58	0/1175
All	All	0.59	1/25023 (0.0%)	0.64	3/33903 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	GLU	CG-CD	5.63	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	491	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	24	LEU	CB-CG-CD2	-5.77	101.19	111.00
2	F	106	ASP	CB-CG-OD1	5.47	123.23	118.30

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	4522	0	4426	57	0
1	E	4522	0	4426	57	0
1	I	4522	0	4426	51	0
2	B	1865	0	1850	19	0
2	F	1865	0	1850	24	0
2	J	1865	0	1850	20	0
3	C	947	0	989	8	0
3	G	947	0	989	12	0
3	K	947	0	989	10	0
4	D	835	0	875	10	0
4	H	835	0	875	11	0
4	L	835	0	875	10	0
5	A	53	0	30	7	0
5	E	53	0	29	5	0
5	I	53	0	29	7	0
6	A	9	0	3	2	0
6	E	9	0	3	2	0
6	I	9	0	3	2	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
8	B	4	0	0	0	0
8	F	4	0	0	0	0
8	J	4	0	0	1	0
9	B	8	0	0	0	0
9	F	8	0	0	1	0
9	J	8	0	0	0	0
10	B	7	0	0	0	0
10	F	7	0	0	0	0
10	J	7	0	0	0	0
11	C	43	0	30	2	0
11	G	43	0	30	7	0
11	K	43	0	30	7	0
12	C	16	0	13	2	0
12	G	16	0	13	2	0
12	K	16	0	13	2	0
13	A	53	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	B	17	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	E	23	0	0	0	0
13	F	7	0	0	0	0
13	H	1	0	0	1	0
13	I	13	0	0	0	0
13	J	12	0	0	0	0
All	All	25058	0	24646	298	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 6.

All (298) 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:451:ARG:HG2	1:A:451:ARG:HH11	1.02	1.17
1:I:490:ILE:HG22	1:I:520:MET:HE3	1.43	0.97
1:E:490:ILE:HG22	1:E:520:MET:HE3	1.50	0.94
11:G:1129:HEM:HHD	11:G:1129:HEM:HBC2	1.55	0.88
11:K:1129:HEM:HBB2	11:K:1129:HEM:HHC	1.55	0.88
3:G:103:PHE:CE2	3:G:107:LYS:HE2	2.11	0.85
1:A:490:ILE:HG22	1:A:520:MET:HE3	1.59	0.84
1:E:490:ILE:HG22	1:E:520:MET:CE	2.08	0.82
1:A:451:ARG:CG	1:A:451:ARG:HH11	1.89	0.82
1:I:555:CYS:SG	1:I:568:ARG:HD2	2.20	0.81
1:I:286:ARG:HH22	6:I:1589:TEO:C3	1.92	0.81
1:E:555:CYS:SG	1:E:568:ARG:HD2	2.20	0.81
11:K:1129:HEM:HBA2	11:K:1129:HEM:HHA	1.60	0.81
1:I:490:ILE:HG22	1:I:520:MET:CE	2.10	0.80
1:A:451:ARG:NH1	1:A:451:ARG:HG2	1.74	0.80
3:K:103:PHE:CE2	3:K:107:LYS:HE2	2.17	0.80
1:E:392:VAL:N	1:E:393:SER:HA	1.99	0.77
3:C:54:SER:HB2	3:C:55:PRO:HD2	1.67	0.77
1:A:24:LEU:HD11	1:A:156:ASN:OD1	1.85	0.77
12:K:1130:CBE:O9	12:K:1130:CBE:H16	1.84	0.76
12:C:1130:CBE:O9	12:C:1130:CBE:H16	1.83	0.76
1:I:257:CYS:HB3	1:I:315:LEU:HD21	1.68	0.76
3:C:103:PHE:CE2	3:C:107:LYS:HE2	2.21	0.76
1:E:49:ALA:HA	5:E:601:FAD:C5X	2.17	0.75
3:G:54:SER:HB2	3:G:55:PRO:HD2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:ARG:HH22	6:E:1589:TEO:C3	2.00	0.74
1:A:555:CYS:HA	1:A:571:VAL:HG23	1.70	0.74
1:E:451:ARG:HH11	1:E:451:ARG:HG2	1.51	0.73
2:F:205:ARG:HD2	13:H:2001:HOH:O	1.88	0.73
1:I:392:VAL:N	1:I:393:SER:HA	2.04	0.71
1:E:49:ALA:HA	5:E:601:FAD:C6	2.20	0.71
1:E:555:CYS:HA	1:E:571:VAL:HG23	1.71	0.71
1:A:555:CYS:SG	1:A:568:ARG:HD2	2.30	0.71
1:E:257:CYS:HB3	1:E:315:LEU:HD21	1.73	0.71
1:A:257:CYS:HB3	1:A:315:LEU:HD21	1.71	0.70
2:F:56:ARG:HG2	2:F:56:ARG:O	1.92	0.70
2:B:238:ALA:O	4:H:90:ARG:NH2	2.26	0.69
3:K:54:SER:HB2	3:K:55:PRO:HD2	1.74	0.69
1:A:54:THR:OG1	1:A:402:GLY:HA3	1.94	0.68
1:A:392:VAL:N	1:A:393:SER:HA	2.06	0.68
1:I:11:VAL:HG23	1:I:195:ALA:HB2	1.76	0.68
1:A:286:ARG:HH22	6:A:1589:TEO:C3	2.08	0.66
1:I:451:ARG:HH11	1:I:451:ARG:HG2	1.59	0.66
1:I:49:ALA:HA	5:I:601:FAD:C5X	2.25	0.66
1:I:555:CYS:HA	1:I:571:VAL:HG23	1.77	0.65
1:I:49:ALA:HA	5:I:601:FAD:C6	2.27	0.65
1:E:49:ALA:HA	5:E:601:FAD:N5	2.12	0.65
11:G:1129:HEM:HBD1	4:H:19:VAL:HG11	1.80	0.64
1:E:24:LEU:HD11	1:E:156:ASN:OD1	1.97	0.64
11:G:1129:HEM:CBC	11:G:1129:HEM:HHD	2.26	0.64
2:F:208:SER:O	2:F:210:MET:HG3	1.98	0.64
1:A:490:ILE:HG22	1:A:520:MET:CE	2.28	0.63
12:C:1130:CBE:O9	12:C:1130:CBE:C16	2.47	0.63
2:J:2:ARG:HH11	2:J:24:THR:HG21	1.64	0.63
1:E:451:ARG:HG2	1:E:451:ARG:NH1	2.12	0.63
2:B:2:ARG:HH11	2:B:24:THR:HG21	1.64	0.62
12:G:1130:CBE:O9	12:G:1130:CBE:H16	2.00	0.61
1:A:49:ALA:HA	5:A:601:FAD:C5X	2.32	0.60
2:F:55:CYS:O	2:F:56:ARG:HD3	2.01	0.59
2:F:234:LEU:HD23	4:H:13:VAL:HG13	1.85	0.59
1:I:453:GLY:HA3	1:I:496:ASN:O	2.01	0.59
1:E:20:MET:CE	1:E:146:LEU:CD1	2.81	0.59
1:E:11:VAL:HG23	1:E:195:ALA:HB2	1.84	0.59
2:F:238:ALA:O	4:L:90:ARG:NH2	2.36	0.58
11:G:1129:HEM:CHD	11:G:1129:HEM:HBC2	2.28	0.58
2:J:208:SER:O	2:J:210:MET:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:HA	5:A:601:FAD:C6	2.35	0.57
2:B:55:CYS:O	2:B:56:ARG:CD	2.53	0.57
4:D:73:TRP:HH2	4:D:94:GLN:HG2	1.71	0.56
2:F:55:CYS:O	2:F:56:ARG:CD	2.53	0.56
2:F:53:ARG:HD3	2:F:53:ARG:O	2.05	0.56
1:I:451:ARG:NH1	1:I:451:ARG:HG2	2.18	0.56
1:E:490:ILE:CG2	1:E:520:MET:CE	2.83	0.56
4:D:90:ARG:NH2	2:J:238:ALA:O	2.39	0.56
1:E:49:ALA:HB3	1:E:142:GLY:HA3	1.87	0.55
3:C:89:ILE:HG13	11:C:1129:HEM:HBC1	1.88	0.55
1:E:463:LEU:C	1:E:463:LEU:HD23	2.26	0.55
1:A:77:ASP:OD1	1:A:586:ARG:HD2	2.06	0.55
11:G:1129:HEM:HHA	11:G:1129:HEM:HBA2	1.88	0.55
2:B:208:SER:O	2:B:210:MET:HG3	2.06	0.55
1:A:404:SER:HB3	5:A:601:FAD:N1	2.22	0.55
1:E:54:THR:OG1	1:E:402:GLY:HA3	2.06	0.54
1:A:196:ARG:HD3	13:A:2001:HOH:O	2.08	0.54
1:I:490:ILE:CG2	1:I:520:MET:CE	2.85	0.54
1:E:453:GLY:HA3	1:E:496:ASN:O	2.08	0.54
1:E:20:MET:HE2	1:E:146:LEU:HD11	1.89	0.54
1:E:20:MET:CE	1:E:146:LEU:HD11	2.38	0.54
11:K:1129:HEM:HBA2	11:K:1129:HEM:CHA	2.31	0.53
1:I:408:LEU:HD11	5:I:601:FAD:H4'	1.91	0.53
1:A:76:SER:HB2	1:A:396:GLY:HA3	1.91	0.53
4:L:73:TRP:HH2	4:L:94:GLN:HG2	1.74	0.53
2:J:234:LEU:HD23	4:L:13:VAL:HG13	1.90	0.53
1:I:476:GLU:HG2	1:I:543:PHE:HD2	1.73	0.53
1:I:274:GLU:HG2	1:I:281:LYS:HE3	1.90	0.53
2:J:55:CYS:O	2:J:56:ARG:CD	2.56	0.53
2:B:55:CYS:O	2:B:56:ARG:HD3	2.08	0.53
4:H:41:GLY:O	4:H:42:GLU:C	2.47	0.53
4:D:73:TRP:CH2	4:D:94:GLN:HG2	2.44	0.52
1:A:11:VAL:HG23	1:A:195:ALA:HB2	1.91	0.52
1:A:460:ARG:HD2	13:A:2040:HOH:O	2.10	0.52
1:A:327:LEU:N	1:A:328:PRO:CD	2.71	0.52
4:L:41:GLY:O	4:L:42:GLU:C	2.47	0.52
3:G:54:SER:HB2	3:G:55:PRO:CD	2.37	0.52
11:C:1129:HEM:HHC	11:C:1129:HEM:HBB2	1.90	0.52
1:I:20:MET:HE3	1:I:146:LEU:CD1	2.40	0.52
4:D:22:THR:OG1	4:D:71:HIS:HB2	2.09	0.52
1:A:453:GLY:HA3	1:A:496:ASN:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:GLU:HG2	1:E:281:LYS:HE3	1.90	0.52
2:F:56:ARG:CG	2:F:56:ARG:O	2.57	0.52
1:A:43:ARG:HD3	2:B:60:CYS:O	2.09	0.52
1:I:24:LEU:HD11	1:I:156:ASN:OD1	2.09	0.52
1:A:54:THR:HG23	1:A:133:ARG:HG3	1.92	0.51
1:E:20:MET:HE2	1:E:146:LEU:CD1	2.40	0.51
1:A:274:GLU:HG2	1:A:281:LYS:HE3	1.93	0.51
1:A:320:LYS:HE3	13:A:2028:HOH:O	2.10	0.51
3:K:83:TYR:CZ	3:K:87:VAL:HG21	2.46	0.51
1:A:49:ALA:HB3	1:A:142:GLY:HA3	1.92	0.51
1:E:327:LEU:N	1:E:328:PRO:CD	2.73	0.51
4:L:22:THR:OG1	4:L:71:HIS:HB2	2.10	0.51
3:G:83:TYR:CZ	3:G:87:VAL:HG21	2.46	0.50
2:J:55:CYS:O	2:J:56:ARG:HD3	2.10	0.50
1:A:463:LEU:C	1:A:463:LEU:HD23	2.31	0.50
4:H:22:THR:OG1	4:H:71:HIS:HB2	2.12	0.50
1:A:242:HIS:O	1:A:351:PRO:HA	2.12	0.50
1:A:24:LEU:CD1	1:A:156:ASN:OD1	2.57	0.50
1:E:490:ILE:CG2	1:E:520:MET:HE1	2.41	0.49
1:I:463:LEU:C	1:I:463:LEU:HD23	2.33	0.49
1:E:48:SER:HB3	5:E:601:FAD:HM72	1.94	0.49
1:A:49:ALA:HA	5:A:601:FAD:N5	2.27	0.49
3:C:54:SER:HB2	3:C:55:PRO:CD	2.40	0.49
1:E:286:ARG:HH22	6:E:1589:TEO:C4	2.26	0.49
1:A:476:GLU:HG2	1:A:543:PHE:HD2	1.78	0.49
1:E:242:HIS:O	1:E:351:PRO:HA	2.12	0.49
4:L:73:TRP:CH2	4:L:94:GLN:HG2	2.46	0.49
3:C:83:TYR:CZ	3:C:87:VAL:HG21	2.48	0.49
1:E:294:MET:O	1:E:298:ARG:HG3	2.13	0.49
2:F:155:CYS:SG	2:F:173:ALA:HB2	2.52	0.49
1:I:394:VAL:HG23	1:I:395:HIS:CE1	2.47	0.49
1:I:99:LEU:HD11	1:I:409:VAL:HG21	1.94	0.49
1:E:391:CYS:SG	1:E:393:SER:HB2	2.53	0.48
1:E:54:THR:HG23	1:E:133:ARG:HG3	1.93	0.48
3:G:89:ILE:HG13	11:G:1129:HEM:HBC1	1.94	0.48
1:I:49:ALA:HA	5:I:601:FAD:N5	2.28	0.48
1:E:266:ASN:HB2	1:E:301:ARG:O	2.13	0.48
1:E:76:SER:HB2	1:E:396:GLY:HA3	1.93	0.48
1:A:391:CYS:SG	1:A:393:SER:HB2	2.53	0.48
1:E:227:ILE:HG23	1:E:561:PRO:HB3	1.95	0.48
1:I:76:SER:HB2	1:I:396:GLY:HA3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:1129:HEM:HHA	11:K:1129:HEM:CBA	2.40	0.48
1:A:173:GLN:CD	1:A:430:ARG:HH11	2.16	0.48
1:A:405:LEU:HG	5:A:601:FAD:C2	2.44	0.48
2:F:205:ARG:HD3	2:F:205:ARG:HA	1.52	0.48
2:B:55:CYS:O	2:B:56:ARG:HD2	2.13	0.48
1:A:350:ILE:HG13	1:A:351:PRO:HD2	1.96	0.48
1:I:242:HIS:O	1:I:351:PRO:HA	2.13	0.48
1:A:542:ARG:HB3	1:A:544:ASP:OD1	2.13	0.47
1:E:451:ARG:HH11	1:E:451:ARG:CG	2.22	0.47
1:A:99:LEU:HD11	1:A:409:VAL:HG21	1.95	0.47
4:D:45:TYR:OH	4:D:49:ILE:HD12	2.14	0.47
1:E:214:ASN:N	1:E:214:ASN:HD22	2.12	0.47
1:I:77:ASP:OD1	1:I:586:ARG:HD2	2.15	0.47
2:F:28:ASP:HB3	2:F:31:ARG:HE	1.80	0.47
1:I:221:ASP:OD1	1:I:518:ASN:ND2	2.46	0.47
1:E:99:LEU:HD11	1:E:409:VAL:HG21	1.97	0.46
2:F:55:CYS:HB3	2:F:60:CYS:HB3	1.97	0.46
1:E:476:GLU:HG2	1:E:543:PHE:HD2	1.80	0.46
1:I:164:TRP:CH2	1:I:184:CYS:HB2	2.50	0.46
1:E:392:VAL:H	1:E:393:SER:HA	1.78	0.46
3:K:31:ARG:HB2	11:K:1129:HEM:O1A	2.15	0.46
1:I:451:ARG:HH11	1:I:451:ARG:CG	2.28	0.46
11:K:1129:HEM:CBA	11:K:1129:HEM:CHA	2.93	0.46
2:J:5:PHE:HB2	2:J:23:TYR:HB2	1.98	0.46
2:F:84:GLN:O	2:F:85:PRO:C	2.54	0.46
1:I:578:ARG:NH1	1:I:581:PHE:CZ	2.83	0.46
1:E:59:ASN:HB2	1:E:116:GLN:OE1	2.16	0.46
3:G:105:ALA:CA	3:G:108:ARG:HH21	2.28	0.46
4:D:41:GLY:O	4:D:42:GLU:C	2.54	0.46
3:G:128:VAL:CG1	3:G:128:VAL:O	2.64	0.46
1:I:43:ARG:HD3	2:J:60:CYS:O	2.15	0.45
2:F:205:ARG:NH1	4:H:82:ASP:OD1	2.50	0.45
2:B:8:TYR:CG	2:B:93:PRO:HD3	2.52	0.45
2:B:28:ASP:HB3	2:B:31:ARG:HE	1.81	0.45
1:E:542:ARG:HB3	1:E:544:ASP:OD1	2.16	0.45
1:A:52:GLY:HA2	1:A:141:THR:HG21	1.99	0.45
3:K:37:THR:O	3:K:41:VAL:HG23	2.16	0.45
1:E:20:MET:CE	1:E:146:LEU:HD12	2.47	0.45
1:I:266:ASN:HB2	1:I:301:ARG:O	2.16	0.45
3:G:127:LEU:HD11	4:H:37:PHE:HB3	1.99	0.45
2:F:169:PHE:CD1	2:F:205:ARG:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:55:CYS:O	2:J:56:ARG:HD2	2.17	0.45
2:F:119:PRO:HA	2:F:181:PHE:CE2	2.51	0.45
2:B:113:GLN:HA	2:B:113:GLN:OE1	2.16	0.45
1:I:391:CYS:SG	1:I:393:SER:HB2	2.57	0.45
2:B:234:LEU:HD23	4:D:13:VAL:HG13	1.98	0.45
1:A:266:ASN:HB2	1:A:301:ARG:O	2.17	0.44
3:C:128:VAL:CG1	3:C:128:VAL:O	2.66	0.44
2:F:2:ARG:HH11	2:F:24:THR:HG21	1.82	0.44
12:K:1130:CBE:O9	12:K:1130:CBE:C16	2.51	0.44
5:A:601:FAD:N5	6:A:1589:TEO:H2	2.31	0.44
1:A:491:ARG:HD2	13:A:2044:HOH:O	2.16	0.44
2:B:42:LEU:HA	2:B:42:LEU:HD23	1.85	0.44
1:I:54:THR:HG23	1:I:133:ARG:HG3	1.98	0.44
1:I:54:THR:OG1	1:I:402:GLY:HA3	2.17	0.44
1:E:394:VAL:HG23	1:E:395:HIS:CE1	2.51	0.44
1:E:24:LEU:CD1	1:E:156:ASN:OD1	2.66	0.44
2:F:216:CYS:HA	9:F:303:SF4:S3	2.58	0.44
1:I:472:SER:OG	1:I:473:VAL:N	2.47	0.44
4:H:73:TRP:CH2	4:H:94:GLN:HG2	2.53	0.44
1:E:100:GLU:HG3	1:E:114:ILE:HD11	2.00	0.44
1:A:294:MET:O	1:A:298:ARG:HG3	2.18	0.44
3:K:127:LEU:HD23	3:K:127:LEU:O	2.17	0.44
1:E:147:HIS:O	1:E:151:GLN:HG3	2.17	0.44
1:E:43:ARG:HD3	2:F:60:CYS:O	2.17	0.43
4:D:115:VAL:O	4:D:115:VAL:HG12	2.18	0.43
1:E:170:VAL:HG23	1:E:180:CYS:HA	1.99	0.43
2:B:117:ILE:HD12	2:B:117:ILE:C	2.38	0.43
2:F:117:ILE:C	2:F:117:ILE:HD12	2.39	0.43
4:L:69:LEU:HD12	4:L:101:LEU:HB3	1.99	0.43
3:G:128:VAL:HG12	3:G:128:VAL:O	2.16	0.43
1:I:1:MET:CE	1:I:1:MET:HA	2.47	0.43
1:I:286:ARG:HH12	6:I:1589:TEO:C4	2.32	0.43
1:I:350:ILE:HG13	1:I:351:PRO:HD2	2.01	0.43
2:J:8:TYR:CG	2:J:93:PRO:HD3	2.54	0.43
1:I:49:ALA:HB3	1:I:142:GLY:HA3	2.01	0.43
1:E:1:MET:CE	1:E:1:MET:HA	2.48	0.43
1:I:100:GLU:HG3	1:I:114:ILE:HD11	2.00	0.43
4:L:85:LYS:N	4:L:86:PRO:CD	2.81	0.43
2:B:5:PHE:HB2	2:B:23:TYR:HB2	2.01	0.43
5:E:601:FAD:H1'1	5:E:601:FAD:H9	1.69	0.43
1:I:404:SER:HB3	5:I:601:FAD:N1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:CYS:SG	2:B:173:ALA:HB2	2.59	0.43
2:F:1:MET:HG3	2:F:1:MET:O	2.18	0.43
1:E:164:TRP:CH2	1:E:184:CYS:HB2	2.54	0.42
2:J:2:ARG:NH1	2:J:24:THR:HG21	2.31	0.42
1:I:294:MET:O	1:I:298:ARG:HG3	2.19	0.42
1:A:490:ILE:CG2	1:A:520:MET:CE	2.97	0.42
4:H:73:TRP:HH2	4:H:94:GLN:HG2	1.83	0.42
1:I:542:ARG:HB3	1:I:544:ASP:OD1	2.19	0.42
3:C:45:LEU:HA	3:C:45:LEU:HD23	1.82	0.42
3:G:13:LEU:HA	3:G:13:LEU:HD12	1.81	0.42
11:G:1129:HEM:CHA	11:G:1129:HEM:HBA2	2.48	0.42
4:D:32:TYR:HH	4:D:57:THR:HG1	1.66	0.42
3:K:45:LEU:HA	3:K:45:LEU:HD23	1.76	0.42
2:J:28:ASP:HB3	2:J:31:ARG:HE	1.84	0.42
5:I:601:FAD:H9	5:I:601:FAD:H1'1	1.73	0.42
2:J:56:ARG:HG2	2:J:56:ARG:O	2.20	0.42
1:I:173:GLN:CD	1:I:430:ARG:HH11	2.21	0.42
4:H:69:LEU:HD12	4:H:101:LEU:HB3	2.02	0.42
1:E:345:GLU:HA	1:E:346:PRO:HD3	1.91	0.42
3:K:13:LEU:HD12	3:K:13:LEU:HA	1.82	0.42
1:I:20:MET:HE3	1:I:146:LEU:HD12	2.02	0.42
2:J:94:LEU:HA	2:J:95:PRO:HD3	1.89	0.42
2:J:205:ARG:HA	2:J:205:ARG:HD3	1.75	0.42
1:I:20:MET:CE	1:I:146:LEU:CD1	2.98	0.42
1:A:214:ASN:HD22	1:A:214:ASN:N	2.18	0.42
1:A:105:PRO:HD2	1:A:144:ALA:HB1	2.00	0.42
1:A:164:TRP:CH2	1:A:184:CYS:HB2	2.55	0.42
1:E:52:GLY:HA2	1:E:141:THR:HG21	2.01	0.42
2:J:58:GLY:HA2	8:J:302:FES:S1	2.60	0.41
2:J:53:ARG:HD3	2:J:53:ARG:O	2.19	0.41
1:I:20:MET:HE3	1:I:146:LEU:HD11	2.03	0.41
2:F:8:TYR:CG	2:F:93:PRO:HD3	2.54	0.41
1:A:227:ILE:HG23	1:A:561:PRO:HB3	2.01	0.41
1:A:20:MET:HE2	1:A:146:LEU:HD11	2.03	0.41
2:B:169:PHE:CE2	2:B:171:GLY:HA2	2.56	0.41
2:B:146:LEU:CD1	2:B:183:ILE:HD11	2.51	0.41
1:I:171:LYS:HA	1:I:176:ALA:O	2.21	0.41
2:B:1:MET:HG3	2:B:1:MET:O	2.21	0.41
1:I:451:ARG:HD3	1:I:451:ARG:HA	1.93	0.41
3:K:82:ALA:O	3:K:86:VAL:HG23	2.21	0.41
1:E:173:GLN:CD	1:E:430:ARG:HH11	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:LEU:HA	2:B:95:PRO:HD3	1.88	0.41
1:A:100:GLU:HG3	1:A:114:ILE:HD11	2.03	0.41
2:F:5:PHE:HB2	2:F:23:TYR:HB2	2.03	0.41
4:L:66:PHE:O	4:L:69:LEU:HB3	2.21	0.41
1:A:472:SER:OG	1:A:473:VAL:N	2.50	0.41
1:E:554:LEU:HA	1:E:554:LEU:HD12	1.85	0.41
12:G:1130:CBE:O9	12:G:1130:CBE:C16	2.62	0.40
1:E:54:THR:HG1	1:E:402:GLY:HA3	1.86	0.40
1:A:274:GLU:HG2	1:A:281:LYS:CE	2.51	0.40
2:J:17:ALA:HB1	2:J:18:PRO:HD2	2.03	0.40
1:A:404:SER:OG	5:A:601:FAD:H2'	2.21	0.40
3:G:37:THR:O	3:G:41:VAL:HG23	2.21	0.40
1:A:26:ILE:HG12	1:A:419:LEU:HD22	2.02	0.40
3:G:127:LEU:O	3:G:127:LEU:HD23	2.20	0.40
3:C:128:VAL:HG12	3:C:128:VAL:O	2.22	0.40
1:A:383:LEU:C	1:A:384:PHE:CD2	2.95	0.40
4:D:19:VAL:HG23	4:D:74:ILE:HB	2.03	0.40
2:J:42:LEU:HD23	2:J:42:LEU:HA	1.86	0.40
11:K:1129:HEM:CAC	4:L:23:ALA:HB1	2.52	0.40
1:I:14:GLY:HA2	5:I:601:FAD:H1B	2.03	0.40
2:J:150:ILE:HG13	2:J:152:CYS:HB3	2.02	0.40
4:H:19:VAL:HG12	4:H:20:ARG:HG3	2.02	0.40
3:K:128:VAL:O	3:K:128:VAL:CG1	2.69	0.40
1:A:287:ASP:N	1:A:287:ASP:OD1	2.55	0.40
1:A:60:THR:HG22	1:A:60:THR:O	2.22	0.40
1:E:171:LYS:HA	1:E:176:ALA:O	2.21	0.40
1:A:437:VAL:O	1:A:440:SER:HB2	2.21	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	586/588 (100%)	569 (97%)	17 (3%)	0	100	100
1	E	586/588 (100%)	569 (97%)	17 (3%)	0	100	100
1	I	586/588 (100%)	571 (97%)	15 (3%)	0	100	100
2	B	236/238 (99%)	227 (96%)	9 (4%)	0	100	100
2	F	236/238 (99%)	223 (94%)	13 (6%)	0	100	100
2	J	236/238 (99%)	225 (95%)	11 (5%)	0	100	100
3	C	120/129 (93%)	116 (97%)	4 (3%)	0	100	100
3	G	120/129 (93%)	117 (98%)	3 (2%)	0	100	100
3	K	120/129 (93%)	119 (99%)	1 (1%)	0	100	100
4	D	103/115 (90%)	97 (94%)	5 (5%)	1 (1%)	19	45
4	H	103/115 (90%)	98 (95%)	4 (4%)	1 (1%)	19	45
4	L	103/115 (90%)	98 (95%)	4 (4%)	1 (1%)	19	45
All	All	3135/3210 (98%)	3029 (97%)	103 (3%)	3 (0%)	56	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	42	GLU
4	L	42	GLU
4	H	42	GLU

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	473/473 (100%)	464 (98%)	9 (2%)	65	88
1	E	473/473 (100%)	463 (98%)	10 (2%)	61	87
1	I	473/473 (100%)	463 (98%)	10 (2%)	61	87
2	B	208/208 (100%)	198 (95%)	10 (5%)	31	62
2	F	208/208 (100%)	199 (96%)	9 (4%)	35	66
2	J	208/208 (100%)	198 (95%)	10 (5%)	31	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	102/109 (94%)	100 (98%)	2 (2%)	63 87
3	G	102/109 (94%)	99 (97%)	3 (3%)	50 80
3	K	102/109 (94%)	99 (97%)	3 (3%)	50 80
4	D	88/96 (92%)	86 (98%)	2 (2%)	58 85
4	H	88/96 (92%)	85 (97%)	3 (3%)	44 75
4	L	88/96 (92%)	85 (97%)	3 (3%)	44 75
All	All	2613/2658 (98%)	2539 (97%)	74 (3%)	51 81

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	119	PHE
1	A	196	ARG
1	A	304	ASP
1	A	451	ARG
1	A	506	PHE
1	A	541	SER
1	A	568	ARG
1	A	578	ARG
2	B	1	MET
2	B	16	ASP
2	B	31	ARG
2	B	45	LYS
2	B	53	ARG
2	B	56	ARG
2	B	87	LYS
2	B	120	TYR
2	B	180	ARG
2	B	212	CYS
3	C	27	SER
3	C	129	TRP
4	D	19	VAL
4	D	60	PHE
1	E	43	ARG
1	E	119	PHE
1	E	196	ARG
1	E	304	ASP
1	E	374	LYS
1	E	451	ARG

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Mol	Chain	Res	Type
1	E	491	ARG
1	E	506	PHE
1	E	541	SER
1	E	568	ARG
2	F	16	ASP
2	F	31	ARG
2	F	45	LYS
2	F	53	ARG
2	F	56	ARG
2	F	87	LYS
2	F	180	ARG
2	F	205	ARG
2	F	212	CYS
3	G	8	GLN
3	G	27	SER
3	G	129	TRP
4	H	19	VAL
4	H	60	PHE
4	H	109	PHE
1	I	43	ARG
1	I	119	PHE
1	I	304	ASP
1	I	325	SER
1	I	373	GLU
1	I	374	LYS
1	I	451	ARG
1	I	491	ARG
1	I	506	PHE
1	I	541	SER
2	J	1	MET
2	J	16	ASP
2	J	31	ARG
2	J	45	LYS
2	J	53	ARG
2	J	56	ARG
2	J	87	LYS
2	J	180	ARG
2	J	205	ARG
2	J	212	CYS
3	K	8	GLN
3	K	27	SER
3	K	129	TRP

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Mol	Chain	Res	Type
4	L	19	VAL
4	L	60	PHE
4	L	109	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	78	GLN
4	H	78	GLN
4	L	78	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
6	TEO	A	1589	-	0,8,8	0.00	-	1,10,10	2.61	1 (100%)
5	FAD	A	601	1	48,58,58	1.28	6 (12%)	54,89,89	2.41	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	FES	B	302	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	B	303	2	0,12,12	0.00	-	0,24,24	0.00	-
10	F3S	B	304	2	0,9,9	0.00	-	0,15,15	0.00	-
11	HEM	C	1129	3,4	30,50,50	2.07	9 (30%)	24,82,82	2.50	14 (58%)
12	CBE	C	1130	-	15,17,17	1.25	1 (6%)	17,22,22	2.09	4 (23%)
6	TEO	E	1589	-	0,8,8	0.00	-	1,10,10	0.11	0
5	FAD	E	601	1	48,58,58	1.34	5 (10%)	54,89,89	2.35	7 (12%)
8	FES	F	302	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	F	303	2	0,12,12	0.00	-	0,24,24	0.00	-
10	F3S	F	304	2	0,9,9	0.00	-	0,15,15	0.00	-
11	HEM	G	1129	3,4	30,50,50	2.11	6 (20%)	24,82,82	2.27	9 (37%)
12	CBE	G	1130	-	15,17,17	1.32	1 (6%)	17,22,22	1.77	3 (17%)
6	TEO	I	1589	-	0,8,8	0.00	-	1,10,10	1.35	0
5	FAD	I	601	1	48,58,58	1.27	4 (8%)	54,89,89	2.25	9 (16%)
8	FES	J	302	2	0,4,4	0.00	-	0,4,4	0.00	-
9	SF4	J	303	2	0,12,12	0.00	-	0,24,24	0.00	-
10	F3S	J	304	2	0,9,9	0.00	-	0,15,15	0.00	-
11	HEM	K	1129	3,4	30,50,50	1.90	6 (20%)	24,82,82	2.76	11 (45%)
12	CBE	K	1130	-	15,17,17	1.25	1 (6%)	17,22,22	2.19	3 (17%)

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
6	TEO	A	1589	-	-	0/1/8/8	0/0/0/0
5	FAD	A	601	1	-	0/30/50/50	0/6/6/6
8	FES	B	302	2	-	0/0/4/4	0/1/1/1
9	SF4	B	303	2	-	0/0/48/48	0/6/5/5
10	F3S	B	304	2	-	0/0/24/24	0/0/3/3
11	HEM	C	1129	3,4	-	0/10/54/54	0/0/8/8
12	CBE	C	1130	-	-	0/6/19/19	0/1/2/2
6	TEO	E	1589	-	-	0/1/8/8	0/0/0/0
5	FAD	E	601	1	-	0/30/50/50	0/6/6/6
8	FES	F	302	2	-	0/0/4/4	0/1/1/1
9	SF4	F	303	2	-	0/0/48/48	0/6/5/5
10	F3S	F	304	2	-	0/0/24/24	0/0/3/3
11	HEM	G	1129	3,4	-	0/10/54/54	0/0/8/8
12	CBE	G	1130	-	-	0/6/19/19	0/1/2/2
6	TEO	I	1589	-	-	0/1/8/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	I	601	1	-	0/30/50/50	0/6/6/6
8	FES	J	302	2	-	0/0/4/4	0/1/1/1
9	SF4	J	303	2	-	0/0/48/48	0/6/5/5
10	F3S	J	304	2	-	0/0/24/24	0/0/3/3
11	HEM	K	1129	3,4	-	0/10/54/54	0/0/8/8
12	CBE	K	1130	-	-	0/6/19/19	0/1/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	1129	HEM	C3B-C4B	-8.27	1.44	1.51
11	K	1129	HEM	C3B-C4B	-6.59	1.46	1.51
11	C	1129	HEM	C3B-C4B	-5.54	1.46	1.51
11	C	1129	HEM	C3D-C4D	-4.89	1.45	1.51
11	G	1129	HEM	C3D-C4D	-4.04	1.46	1.51
12	G	1130	CBE	C11-N10	-3.98	1.34	1.41
11	K	1129	HEM	C3D-C4D	-3.65	1.46	1.51
12	C	1130	CBE	C11-N10	-3.55	1.34	1.41
11	K	1129	HEM	C2C-C1C	-3.42	1.46	1.52
11	G	1129	HEM	C2C-C1C	-3.38	1.46	1.52
12	K	1130	CBE	C11-N10	-3.37	1.35	1.41
11	C	1129	HEM	C2C-C1C	-2.58	1.47	1.52
11	C	1129	HEM	C2D-C1D	-2.40	1.44	1.51
11	G	1129	HEM	C2B-C1B	-2.27	1.44	1.51
11	K	1129	HEM	C2B-C1B	-2.02	1.45	1.51
11	C	1129	HEM	CAA-C2A	2.04	1.55	1.52
11	G	1129	HEM	FE-NC	2.08	2.04	1.95
11	G	1129	HEM	C3B-CAB	2.09	1.55	1.51
5	A	601	FAD	C10-N1	2.19	1.39	1.35
11	C	1129	HEM	C3B-CAB	2.20	1.55	1.51
5	A	601	FAD	C2A-N1A	2.24	1.38	1.33
5	A	601	FAD	C4-N3	2.27	1.37	1.33
11	K	1129	HEM	FE-NB	2.27	2.09	1.97
5	I	601	FAD	C10-N1	2.50	1.39	1.35
5	A	601	FAD	C5X-N5	2.52	1.39	1.35
5	E	601	FAD	C1'-N10	2.59	1.51	1.48
11	K	1129	HEM	FE-ND	2.65	2.11	1.97
5	E	601	FAD	C10-N1	2.69	1.40	1.35
5	A	601	FAD	C2A-N3A	2.88	1.37	1.32
5	E	601	FAD	C4-N3	3.00	1.38	1.33
5	E	601	FAD	C2A-N3A	3.17	1.37	1.32
11	C	1129	HEM	FE-ND	3.19	2.14	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	601	FAD	C4-N3	3.34	1.39	1.33
11	C	1129	HEM	FE-NB	3.59	2.16	1.97
11	C	1129	HEM	C1C-NC	3.73	1.40	1.36
5	I	601	FAD	C2A-N3A	3.82	1.38	1.32
5	I	601	FAD	C4X-N5	4.15	1.39	1.33
5	E	601	FAD	C4X-N5	4.23	1.40	1.33
5	A	601	FAD	C4X-N5	4.58	1.40	1.33

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	601	FAD	N3A-C2A-N1A	-13.16	118.82	128.89
5	I	601	FAD	N3A-C2A-N1A	-11.02	120.45	128.89
5	A	601	FAD	N3A-C2A-N1A	-10.77	120.65	128.89
11	K	1129	HEM	CBA-CAA-C2A	-5.60	102.48	112.53
11	K	1129	HEM	C3C-CAC-CBC	-4.71	117.23	124.46
11	K	1129	HEM	C3B-CAB-CBB	-4.52	117.52	124.46
11	C	1129	HEM	C3C-CAC-CBC	-4.19	118.02	124.46
12	C	1130	CBE	C11-N10-C8	-4.11	120.38	127.61
11	G	1129	HEM	CBA-CAA-C2A	-3.85	105.62	112.53
5	A	601	FAD	C4X-C4-N3	-3.76	118.45	123.59
11	G	1129	HEM	C3C-CAC-CBC	-3.71	118.77	124.46
12	K	1130	CBE	C11-N10-C8	-3.58	121.32	127.61
5	A	601	FAD	C4A-C5A-N7A	-3.54	106.23	109.48
5	I	601	FAD	C4-C4X-C10	-3.29	117.84	119.94
12	G	1130	CBE	C3-C8-N10	-3.16	109.88	115.61
11	C	1129	HEM	CAA-C2A-C1A	-2.97	123.79	127.01
5	A	601	FAD	O3P-PA-O5B	-2.95	95.11	102.94
11	C	1129	HEM	C3B-C4B-NB	-2.78	106.31	111.63
5	E	601	FAD	O3P-PA-O5B	-2.73	95.70	102.94
12	G	1130	CBE	C11-N10-C8	-2.73	122.82	127.61
5	E	601	FAD	C4X-C4-N3	-2.65	119.96	123.59
5	A	601	FAD	C1B-N9A-C4A	-2.62	122.99	126.94
5	E	601	FAD	C1B-N9A-C4A	-2.52	123.14	126.94
5	I	601	FAD	O3B-C3B-C4B	-2.52	103.51	111.05
12	C	1130	CBE	C3-C8-N10	-2.43	111.19	115.61
5	I	601	FAD	C4X-C4-N3	-2.37	120.34	123.59
11	K	1129	HEM	CMA-C3A-C4A	-2.33	124.51	128.36
12	K	1130	CBE	C1-C2-C3	-2.23	118.87	123.97
5	I	601	FAD	C4A-C5A-N7A	-2.21	107.45	109.48
5	A	601	FAD	O3'-C3'-C4'	-2.16	103.31	108.75
5	A	601	FAD	O5B-PA-O1A	-2.14	101.33	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	1129	HEM	CAD-CBD-CGD	-2.12	104.38	113.02
12	C	1130	CBE	C1-C2-C3	-2.09	119.19	123.97
11	C	1129	HEM	CMA-C3A-C4A	-2.03	125.01	128.36
5	A	601	FAD	C6-C5X-N5	2.06	121.61	118.96
11	C	1129	HEM	CBD-CAD-C3D	2.18	119.89	113.55
11	C	1129	HEM	C2D-C3D-C4D	2.19	105.22	101.50
11	K	1129	HEM	C2D-C3D-C4D	2.21	105.24	101.50
11	C	1129	HEM	CMD-C2D-C3D	2.23	124.19	114.35
5	A	601	FAD	C4-C4X-N5	2.35	121.57	118.72
11	C	1129	HEM	CMC-C2C-C3C	2.38	122.48	116.53
11	G	1129	HEM	C2D-C3D-C4D	2.51	105.76	101.50
11	G	1129	HEM	C2C-C1C-CHC	2.57	127.60	123.68
11	C	1129	HEM	C2C-C1C-CHC	2.59	127.62	123.68
6	A	1589	TEO	O2-C2-C3	2.61	114.95	109.53
5	I	601	FAD	C5X-C9A-N10	2.65	119.63	117.62
11	C	1129	HEM	CAD-C3D-C2D	2.71	121.00	113.22
11	K	1129	HEM	CMD-C2D-C3D	2.79	126.70	114.35
11	C	1129	HEM	CMB-C2B-C3B	2.89	123.75	116.53
11	G	1129	HEM	CMD-C2D-C3D	3.04	127.78	114.35
11	G	1129	HEM	CMC-C2C-C3C	3.10	124.28	116.53
11	G	1129	HEM	CMB-C2B-C3B	3.14	124.36	116.53
5	A	601	FAD	C5X-C9A-N10	3.21	120.06	117.62
5	A	601	FAD	C4X-N5-C5X	3.30	120.56	116.76
11	K	1129	HEM	CMC-C2C-C3C	3.31	124.80	116.53
11	K	1129	HEM	CMB-C2B-C3B	3.54	125.37	116.53
5	E	601	FAD	C4X-N5-C5X	3.59	120.89	116.76
11	K	1129	HEM	CAD-C3D-C2D	3.65	123.70	113.22
5	I	601	FAD	C4-C4X-N5	3.77	123.29	118.72
5	E	601	FAD	C5X-C9A-N10	3.86	120.56	117.62
5	I	601	FAD	C4X-N5-C5X	3.90	121.25	116.76
11	K	1129	HEM	C3B-C4B-CHC	3.94	128.71	123.16
11	C	1129	HEM	C3B-C4B-CHC	4.38	129.33	123.16
11	G	1129	HEM	CAD-C3D-C2D	4.38	125.81	113.22
11	G	1129	HEM	CAD-C3D-C4D	4.53	128.43	112.47
11	K	1129	HEM	CAD-C3D-C4D	5.26	131.04	112.47
12	G	1130	CBE	O7-C2-C1	5.45	115.74	109.44
5	E	601	FAD	C4-N3-C2	5.93	120.37	115.25
11	C	1129	HEM	CAD-C3D-C4D	5.99	133.59	112.47
12	C	1130	CBE	O7-C2-C1	6.40	116.84	109.44
5	I	601	FAD	C4-N3-C2	6.94	121.25	115.25
12	K	1130	CBE	O7-C2-C1	7.40	118.00	109.44
5	A	601	FAD	C4-N3-C2	8.98	123.01	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1589	TEO	2	0
5	A	601	FAD	7	0
11	C	1129	HEM	2	0
12	C	1130	CBE	2	0
6	E	1589	TEO	2	0
5	E	601	FAD	5	0
9	F	303	SF4	1	0
11	G	1129	HEM	7	0
12	G	1130	CBE	2	0
6	I	1589	TEO	2	0
5	I	601	FAD	7	0
8	J	302	FES	1	0
11	K	1129	HEM	7	0
12	K	1130	CBE	2	0

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

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	588/588 (100%)	-0.09	7 (1%) 81 81	35, 50, 67, 78	0
1	E	588/588 (100%)	0.14	25 (4%) 39 38	42, 60, 85, 94	0
1	I	588/588 (100%)	0.43	63 (10%) 8 6	47, 72, 101, 120	0
2	B	238/238 (100%)	-0.07	9 (3%) 44 44	36, 47, 67, 82	0
2	F	238/238 (100%)	-0.01	11 (4%) 36 35	45, 56, 88, 104	0
2	J	238/238 (100%)	0.09	16 (6%) 21 19	48, 61, 101, 120	0
3	C	122/129 (94%)	0.15	9 (7%) 17 15	51, 68, 106, 119	0
3	G	122/129 (94%)	0.45	15 (12%) 5 4	59, 81, 118, 129	0
3	K	122/129 (94%)	0.65	18 (14%) 3 2	70, 86, 125, 134	0
4	D	105/115 (91%)	0.11	7 (6%) 21 19	47, 66, 106, 125	0
4	H	105/115 (91%)	0.31	9 (8%) 13 10	53, 71, 138, 161	0
4	L	105/115 (91%)	0.26	6 (5%) 27 26	60, 77, 137, 159	0
All	All	3159/3210 (98%)	0.16	195 (6%) 24 23	35, 61, 104, 161	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	129	TRP	7.4
1	I	1	MET	7.2
4	D	41	GLY	6.9
1	E	1	MET	6.4
3	K	129	TRP	6.3
3	G	68	PHE	6.3
3	C	129	TRP	6.0
3	K	69	PHE	6.0
3	K	68	PHE	5.3
4	L	37	PHE	5.1
1	I	266	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
1	I	301	ARG	4.7
2	J	85	PRO	4.7
2	J	31	ARG	4.7
2	B	86	GLY	4.5
3	K	126	VAL	4.5
1	I	306	PRO	4.4
2	J	30	GLY	4.3
4	D	42	GLU	4.3
4	H	51	PHE	4.3
2	F	29	GLU	4.2
1	I	204	GLY	4.2
2	J	29	GLU	4.2
1	A	268	HIS	4.0
3	C	68	PHE	4.0
4	H	42	GLU	3.9
1	I	268	HIS	3.9
1	I	276	TYR	3.9
2	J	14	VAL	3.9
4	L	42	GLU	3.8
4	H	40	SER	3.8
3	G	69	PHE	3.8
4	L	38	ALA	3.6
2	F	31	ARG	3.6
3	G	64	ILE	3.6
1	I	496	ASN	3.6
1	I	295	ILE	3.6
4	D	49	ILE	3.6
1	I	452	ASN	3.5
1	E	449	ASN	3.5
3	K	98	TYR	3.5
1	E	451	ARG	3.5
1	A	300	GLY	3.5
1	I	265	LEU	3.5
4	H	52	PHE	3.4
4	L	115	VAL	3.4
3	K	108	ARG	3.4
4	H	49	ILE	3.4
4	H	41	GLY	3.4
1	I	307	TRP	3.3
1	I	340	VAL	3.3
3	K	72	PHE	3.3
3	G	126	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
4	D	43	LEU	3.3
2	B	30	GLY	3.3
4	H	47	VAL	3.3
3	C	69	PHE	3.3
1	A	1	MET	3.2
1	I	524	TYR	3.2
2	B	85	PRO	3.2
2	F	30	GLY	3.2
4	D	40	SER	3.2
1	I	213	THR	3.2
3	K	56	GLU	3.2
1	I	267	LYS	3.2
1	I	451	ARG	3.1
2	B	2	ARG	3.1
1	I	303	CYS	3.1
1	I	270	GLU	3.1
2	J	2	ARG	3.1
1	A	373	GLU	3.1
2	B	1	MET	3.1
1	I	299	GLU	3.0
1	E	46	THR	3.0
3	K	107	LYS	3.0
1	I	345	GLU	2.9
2	F	28	ASP	2.9
2	J	28	ASP	2.9
3	G	72	PHE	2.9
1	E	528	VAL	2.9
2	B	14	VAL	2.9
3	K	64	ILE	2.9
1	I	302	GLY	2.9
1	E	496	ASN	2.9
1	I	203	GLY	2.9
3	K	128	VAL	2.9
2	F	12	PRO	2.9
1	I	205	ALA	2.8
1	I	45	HIS	2.8
2	F	18	PRO	2.8
1	I	381	PRO	2.8
2	F	27	ALA	2.8
1	I	300	GLY	2.8
4	L	43	LEU	2.8
1	I	489	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	55	CYS	2.8
2	J	86	GLY	2.8
1	I	562	GLU	2.7
3	G	98	TYR	2.7
1	E	531	ASN	2.7
1	I	373	GLU	2.7
3	K	99	LEU	2.7
3	K	100	GLU	2.7
1	I	297	ILE	2.7
2	F	10	TYR	2.7
3	C	127	LEU	2.6
2	J	18	PRO	2.6
1	I	214	ASN	2.6
1	I	588	TYR	2.6
1	E	345	GLU	2.6
1	I	421	GLU	2.6
3	G	127	LEU	2.6
1	I	344	LYS	2.6
3	C	59	GLU	2.6
1	E	373	GLU	2.6
1	I	143	HIS	2.5
3	C	67	SER	2.5
4	H	43	LEU	2.5
1	I	419	LEU	2.5
1	I	275	ARG	2.5
1	E	499	LEU	2.4
1	I	281	LYS	2.4
3	K	125	GLY	2.4
1	I	218	ASN	2.4
4	D	48	TRP	2.4
1	E	2	LYS	2.4
4	L	41	GLY	2.4
3	G	65	MET	2.4
2	J	10	TYR	2.4
1	I	312	LYS	2.4
1	I	310	HIS	2.4
2	B	60	CYS	2.4
4	H	37	PHE	2.4
1	I	144	ALA	2.4
3	G	63	ALA	2.4
2	J	12	PRO	2.3
1	I	49	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	304	ASP	2.3
1	I	215	ALA	2.3
1	I	220	GLY	2.3
1	E	44	SER	2.3
1	I	420	GLN	2.3
3	G	67	SER	2.3
3	C	46	TRP	2.3
2	J	16	ASP	2.3
1	A	274	GLU	2.3
2	B	29	GLU	2.3
1	I	48	SER	2.3
3	K	111	LYS	2.3
1	A	543	PHE	2.3
1	I	51	GLY	2.3
3	K	65	MET	2.2
1	I	305	GLY	2.2
1	I	217	ILE	2.2
1	E	450	ASN	2.2
1	E	482	LYS	2.2
2	J	58	GLY	2.2
1	I	430	ARG	2.2
4	D	39	THR	2.2
3	K	58	PHE	2.2
3	G	71	LYS	2.2
1	I	534	THR	2.2
1	E	48	SER	2.2
2	J	55	CYS	2.2
3	C	63	ALA	2.2
1	E	15	ALA	2.1
1	I	46	THR	2.1
1	I	424	ALA	2.1
1	I	52	GLY	2.1
2	J	54	SER	2.1
1	E	218	ASN	2.1
1	I	426	GLN	2.1
2	J	13	ASP	2.1
1	I	405	LEU	2.1
3	C	128	VAL	2.1
3	G	108	ARG	2.1
3	K	97	GLY	2.1
1	E	489	VAL	2.1
1	I	495	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	54	SER	2.1
2	F	14	VAL	2.1
1	E	20	MET	2.1
1	E	532	PHE	2.1
2	F	16	ASP	2.1
1	E	465	GLU	2.1
3	G	97	GLY	2.1
1	I	499	LEU	2.1
1	I	47	VAL	2.1
1	E	217	ILE	2.1
3	G	103	PHE	2.0
1	E	47	VAL	2.0
1	E	520	MET	2.0
1	E	17	GLY	2.0
1	I	313	LEU	2.0
1	A	301	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 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, 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	LLDF	B-factors(Å^2)	Q<0.9
7	NA	I	1590	1/1	0.89	0.52	6.23	49,49,49,49	0
7	NA	E	1590	1/1	0.96	0.33	4.83	37,37,37,37	0
7	NA	A	1590	1/1	0.89	0.30	3.32	31,31,31,31	0
6	TEO	A	1589	9/9	0.98	0.25	2.11	46,48,52,55	0
12	CBE	K	1130	16/16	0.96	0.22	1.67	72,73,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	HEM	G	1129	43/43	0.98	0.19	1.39	62,65,67,72	0
11	HEM	C	1129	43/43	0.97	0.17	1.36	52,55,59,63	0
12	CBE	G	1130	16/16	0.99	0.18	1.18	53,55,58,58	0
9	SF4	F	303	8/8	0.99	0.18	1.05	45,46,49,50	0
6	TEO	I	1589	9/9	0.92	0.27	0.92	68,70,72,74	0
9	SF4	B	303	8/8	0.99	0.19	0.86	38,39,41,41	0
8	FES	F	302	4/4	0.99	0.24	0.61	49,50,51,54	0
9	SF4	J	303	8/8	0.98	0.18	0.39	47,51,52,52	0
6	TEO	E	1589	9/9	0.96	0.18	0.24	45,47,49,53	0
5	FAD	A	601	53/53	0.98	0.21	0.18	30,39,50,55	0
11	HEM	K	1129	43/43	0.98	0.15	-0.06	51,57,63,65	0
10	F3S	B	304	7/7	0.99	0.14	-0.10	41,43,47,49	0
5	FAD	E	601	53/53	0.97	0.24	-0.13	40,52,60,62	0
5	FAD	I	601	53/53	0.97	0.23	-0.35	47,55,62,63	0
8	FES	B	302	4/4	0.99	0.24	-0.37	37,43,45,47	0
8	FES	J	302	4/4	0.98	0.21	-0.60	56,58,59,60	0
12	CBE	C	1130	16/16	0.97	0.13	-0.68	46,49,53,53	0
10	F3S	J	304	7/7	0.99	0.12	-1.03	53,55,59,61	0
10	F3S	F	304	7/7	0.99	0.11	-1.51	50,51,53,54	0

6.5 Other polymers (i)

There are no such residues in this entry.