



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2018 – 09:44 pm GMT

PDB ID : 1D4D
Title : CRYSTAL STRUCTURE OF THE SUCCINATE COMPLEXED FORM OF THE FLAVOCYTOCHROME C FUMARATE REDUCTASE OF SHEWANELLA PUTREFACIENS STRAIN MR-1
Authors : Leys, D.; Tsapin, A.S.; Meyer, T.E.; Cusanovich, M.A.; Van Beeumen, J.J.
Deposited on : 1999-10-03
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

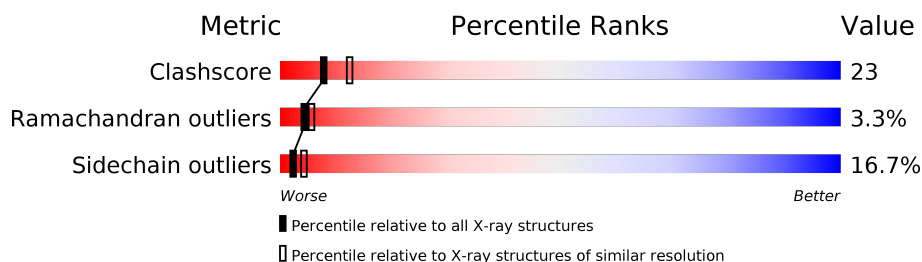
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	122078	4826 (2.50-2.50)
Ramachandran outliers	120005	4734 (2.50-2.50)
Sidechain outliers	119972	4736 (2.50-2.50)

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.

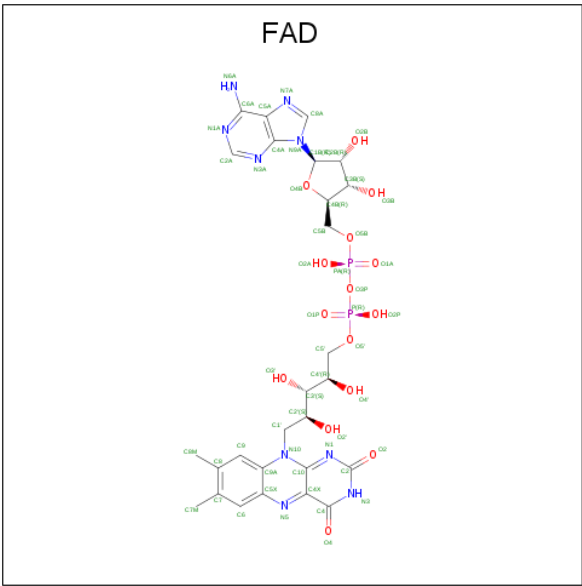
Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	572	

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

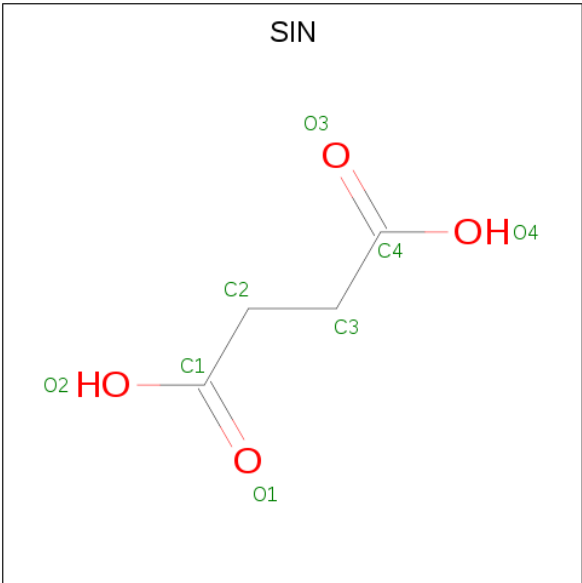
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FAD	A	600	X	-	-	-
4	SIN	A	700	-	-	X	-

C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is SUCCINIC ACID (three-letter code: SIN) (formula: C₄H₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is water.

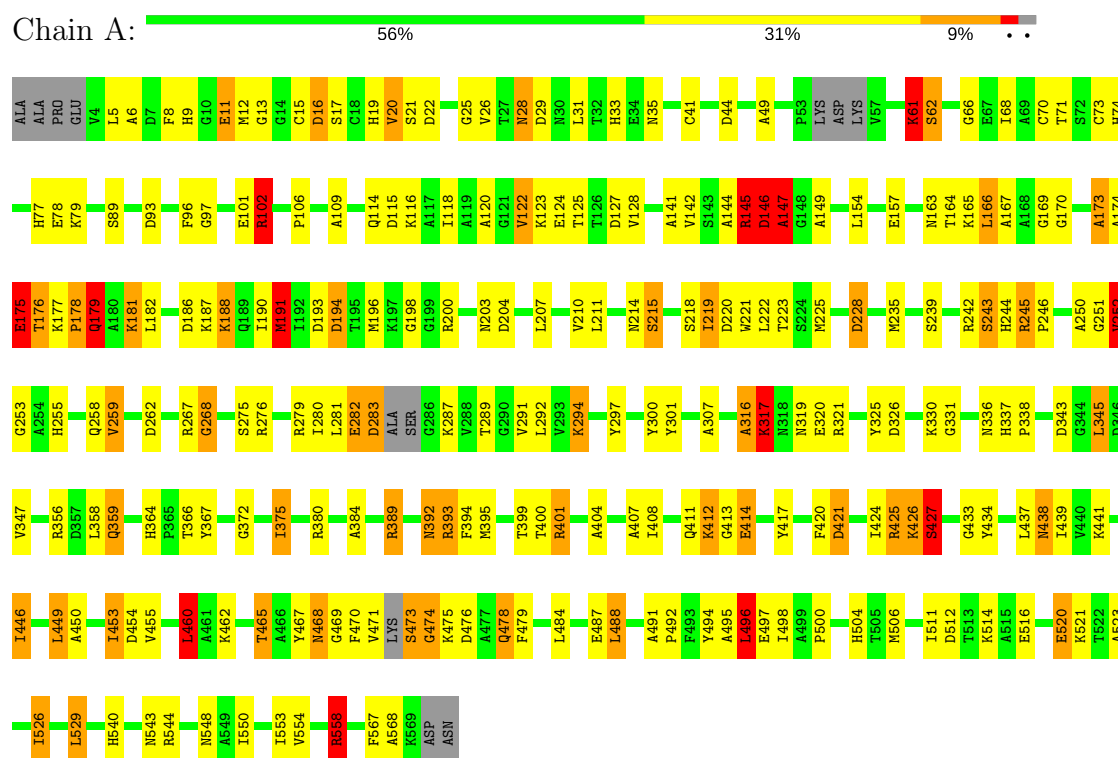
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	72.86 Å 72.86 Å 216.47 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.50 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.50-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.239 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4254	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SIN, 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	0.57	0/4029	1.69	70/5478 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	ARG	NE-CZ-NH1	14.64	127.62	120.30
1	A	356	ARG	NE-CZ-NH1	-13.00	113.80	120.30
1	A	200	ARG	NE-CZ-NH2	10.10	125.35	120.30
1	A	393	ARG	NE-CZ-NH2	10.06	125.33	120.30
1	A	558	ARG	CD-NE-CZ	8.93	136.09	123.60
1	A	175	GLU	C-N-CA	8.40	142.70	121.70
1	A	174	ALA	CA-C-N	-8.27	99.02	117.20
1	A	267	ARG	CA-C-N	7.96	132.12	116.20
1	A	145	ARG	NE-CZ-NH1	-7.94	116.33	120.30
1	A	122	VAL	N-CA-CB	7.78	128.61	111.50
1	A	438	ASN	CA-CB-CG	7.77	130.49	113.40
1	A	262	ASP	CB-CG-OD1	7.76	125.28	118.30
1	A	178	PRO	C-N-CA	7.62	140.75	121.70
1	A	491	ALA	CA-C-O	-7.62	104.11	120.10
1	A	102	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	A	146	ASP	CB-CG-OD2	-7.19	111.83	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	A	242	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	A	326	ASP	CB-CG-OD2	6.95	124.56	118.30
1	A	421	ASP	N-CA-CB	-6.92	98.15	110.60
1	A	425	ARG	CD-NE-CZ	6.89	133.25	123.60
1	A	147	ALA	CB-CA-C	6.83	120.34	110.10
1	A	317	LYS	N-CA-CB	6.65	122.57	110.60
1	A	11	GLU	CA-CB-CG	6.59	127.89	113.40
1	A	19	HIS	CA-CB-CG	-6.41	102.71	113.60
1	A	147	ALA	CA-C-N	-6.34	103.51	116.20
1	A	426	LYS	CA-C-N	6.18	130.81	117.20
1	A	169	GLY	N-CA-C	6.15	128.47	113.10
1	A	242	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	A	494	TYR	CB-CG-CD2	-6.11	117.33	121.00
1	A	252	VAL	CB-CA-C	-6.09	99.82	111.40
1	A	491	ALA	O-C-N	6.09	132.68	121.10
1	A	179	GLN	CB-CG-CD	6.08	127.40	111.60
1	A	427	SER	N-CA-CB	6.06	119.59	110.50
1	A	474	GLY	N-CA-C	6.06	128.25	113.10
1	A	147	ALA	CA-C-O	6.01	132.73	120.10
1	A	492	PRO	N-CA-CB	5.98	110.47	103.30
1	A	268	GLY	CA-C-O	-5.96	109.87	120.60
1	A	193	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	468	ASN	CA-CB-CG	-5.95	100.31	113.40
1	A	145	ARG	NH1-CZ-NH2	5.89	125.88	119.40
1	A	44	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	181	LYS	CA-C-N	5.85	130.07	117.20
1	A	173	ALA	CA-C-N	-5.83	104.37	117.20
1	A	29	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	462	LYS	CA-CB-CG	5.74	126.03	113.40
1	A	316	ALA	CA-C-N	5.73	129.81	117.20
1	A	174	ALA	CA-C-O	5.67	132.00	120.10
1	A	520	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	A	281	LEU	CA-C-O	5.64	131.94	120.10
1	A	16	ASP	N-CA-CB	-5.63	100.46	110.60
1	A	144	ALA	CA-C-O	5.63	131.92	120.10
1	A	13	GLY	N-CA-C	5.62	127.14	113.10
1	A	496	LEU	CA-CB-CG	5.58	128.15	115.30
1	A	222	LEU	CB-CA-C	5.57	120.77	110.20
1	A	191	MET	CA-CB-CG	5.47	122.60	113.30
1	A	182	LEU	CA-CB-CG	5.43	127.80	115.30
1	A	211	LEU	CA-CB-CG	5.40	127.73	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	LYS	CA-CB-CG	5.39	125.25	113.40
1	A	460	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	228	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	492	PRO	CA-N-CD	-5.23	104.18	111.50
1	A	345	LEU	CA-CB-CG	5.20	127.27	115.30
1	A	245	ARG	CA-CB-CG	5.14	124.70	113.40
1	A	251	GLY	C-N-CA	5.12	134.50	121.70
1	A	77	HIS	CA-CB-CG	-5.09	104.94	113.60
1	A	93	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	62	SER	CB-CA-C	-5.04	100.53	110.10
1	A	325	TYR	CB-CA-C	-5.03	100.34	110.40
1	A	145	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	VAL	Mainchain

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	3965	0	3739	179	0
2	A	172	0	120	21	0
3	A	53	0	31	8	0
4	A	8	0	4	6	0
5	A	56	0	0	1	0
All	All	4254	0	3894	186	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 23.

All (186) 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:15:CYS:SG	2:A:603:HEM:HAB	1.29	1.71
3:A:600:FAD:C1'	3:A:600:FAD:C2'	1.79	1.53
1:A:73:CYS:SG	2:A:602:HEM:HAC	1.50	1.51
1:A:41:CYS:SG	2:A:604:HEM:HAC	1.51	1.50
1:A:15:CYS:SG	2:A:603:HEM:CAB	2.10	1.40
1:A:73:CYS:HG	2:A:602:HEM:CAC	1.52	1.17
1:A:15:CYS:HG	2:A:603:HEM:CAB	1.53	1.09
1:A:359:GLN:H	1:A:359:GLN:HE21	1.11	0.99
1:A:395:MET:HE3	1:A:408:ILE:HG13	1.64	0.80
1:A:154:LEU:HD23	1:A:275:SER:HB3	1.63	0.80
1:A:426:LYS:O	1:A:427:SER:HB3	1.81	0.79
1:A:558:ARG:HG2	1:A:558:ARG:HH11	1.47	0.79
1:A:446:ILE:HG23	1:A:460:LEU:HD13	1.65	0.77
1:A:453:ILE:HG23	1:A:455:VAL:HG13	1.68	0.76
1:A:412:LYS:HD2	1:A:412:LYS:H	1.53	0.73
1:A:401:ARG:HH12	4:A:700:SIN:H22	1.52	0.72
1:A:567:PHE:O	1:A:568:ALA:HB3	1.89	0.72
1:A:449:LEU:HD11	1:A:495:ALA:HB2	1.71	0.72
1:A:41:CYS:SG	2:A:604:HEM:C3C	2.84	0.71
1:A:393:ARG:HD3	1:A:478:GLN:HE22	1.57	0.69
1:A:165:LYS:HG3	1:A:166:LEU:HD23	1.76	0.67
1:A:359:GLN:HE21	1:A:359:GLN:N	1.87	0.67
3:A:600:FAD:C3'	3:A:600:FAD:C1'	2.72	0.67
1:A:145:ARG:HD2	1:A:268:GLY:H	1.59	0.66
1:A:141:ALA:O	1:A:145:ARG:HB2	1.95	0.66
1:A:228:ASP:N	1:A:255:HIS:NE2	2.43	0.66
1:A:245:ARG:HB2	1:A:246:PRO:HD2	1.78	0.65
1:A:392:ASN:HD22	1:A:393:ARG:H	1.44	0.65
1:A:190:ILE:O	1:A:194:ASP:OD1	2.15	0.65
1:A:395:MET:CE	1:A:407:ALA:HB3	2.28	0.64
1:A:73:CYS:SG	2:A:602:HEM:C3C	2.91	0.64
1:A:114:GLN:O	1:A:118:ILE:HG13	1.97	0.64
1:A:467:TYR:O	1:A:471:VAL:HG23	1.99	0.63
1:A:142:VAL:HG11	1:A:225:MET:CE	2.29	0.63
1:A:359:GLN:NE2	1:A:359:GLN:H	1.90	0.63
1:A:316:ALA:O	1:A:317:LYS:CB	2.47	0.62
1:A:170:GLY:HA2	1:A:252:VAL:HG21	1.80	0.62
1:A:245:ARG:HB2	1:A:246:PRO:CD	2.29	0.62
1:A:345:LEU:HD11	1:A:358:LEU:HD21	1.82	0.62
1:A:41:CYS:HG	2:A:604:HEM:HAC	1.54	0.61
1:A:49:ALA:HB1	1:A:61:LYS:HD3	1.81	0.61
3:A:600:FAD:O2'	3:A:600:FAD:C1'	2.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ASN:ND2	1:A:331:GLY:H	1.97	0.61
1:A:343:ASP:HB2	5:A:704:HOH:O	2.00	0.61
1:A:426:LYS:O	1:A:427:SER:CB	2.46	0.60
1:A:319:ASN:HD21	1:A:330:LYS:HA	1.65	0.60
3:A:600:FAD:N10	3:A:600:FAD:C2'	2.60	0.60
1:A:102:ARG:NH2	1:A:157:GLU:OE1	2.35	0.60
1:A:146:ASP:O	1:A:147:ALA:HB3	2.02	0.60
1:A:142:VAL:HG11	1:A:225:MET:HE1	1.85	0.58
1:A:506:MET:HG3	1:A:540:HIS:HB2	1.86	0.58
1:A:142:VAL:O	1:A:146:ASP:HB2	2.04	0.58
1:A:395:MET:HE2	1:A:407:ALA:HB3	1.86	0.58
1:A:433:GLY:CA	2:A:601:HEM:HBA2	2.33	0.58
1:A:35:ASN:HD21	1:A:71:THR:H	1.49	0.58
1:A:300:TYR:O	1:A:301:TYR:HB3	2.03	0.57
1:A:62:SER:CB	2:A:601:HEM:HBB2	2.35	0.57
1:A:8:PHE:O	1:A:11:GLU:HG2	2.05	0.57
1:A:128:VAL:HG22	1:A:307:ALA:HB3	1.86	0.57
1:A:433:GLY:HA3	2:A:601:HEM:HBA2	1.85	0.57
1:A:175:GLU:OE2	1:A:187:LYS:HA	2.05	0.57
1:A:170:GLY:HA3	1:A:243:SER:OG	2.05	0.57
1:A:170:GLY:HA2	1:A:244:HIS:O	2.05	0.57
1:A:364:HIS:O	1:A:500:PRO:HA	2.05	0.56
1:A:319:ASN:HD21	1:A:331:GLY:H	1.52	0.56
1:A:28:ASN:HD22	1:A:28:ASN:H	1.53	0.55
1:A:401:ARG:HH22	4:A:700:SIN:C1	2.19	0.55
1:A:468:ASN:ND2	1:A:487:GLU:HG2	2.22	0.55
1:A:343:ASP:HB3	3:A:600:FAD:H61A	1.71	0.55
1:A:294:LYS:HG2	1:A:300:TYR:CE2	2.41	0.55
1:A:6:ALA:HA	2:A:603:HEM:HBC2	1.89	0.54
1:A:218:SER:HB2	1:A:554:VAL:HG12	1.90	0.54
1:A:246:PRO:HG2	1:A:250:ALA:HB3	1.90	0.54
1:A:550:ILE:HA	1:A:553:ILE:HG12	1.90	0.54
1:A:62:SER:HB3	2:A:601:HEM:HBB2	1.90	0.54
1:A:393:ARG:HH11	1:A:478:GLN:NE2	2.06	0.54
1:A:467:TYR:CZ	1:A:484:LEU:HD23	2.43	0.54
1:A:487:GLU:O	1:A:488:LEU:HB2	2.07	0.54
1:A:389:ARG:HD2	1:A:412:LYS:O	2.09	0.53
1:A:337:HIS:HB2	1:A:338:PRO:HD2	1.89	0.53
1:A:66:GLY:H	1:A:258:GLN:HE22	1.56	0.52
1:A:417:TYR:CE2	1:A:497:GLU:HB2	2.44	0.52
1:A:399:THR:OG1	1:A:400:THR:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ASP:HB2	1:A:424:ILE:HG12	1.92	0.52
1:A:173:ALA:HB3	1:A:244:HIS:CE1	2.44	0.52
1:A:221:TRP:CH2	1:A:558:ARG:HG3	2.45	0.51
1:A:380:ARG:HA	1:A:384:ALA:HB3	1.93	0.51
1:A:395:MET:HE1	1:A:407:ALA:HB3	1.92	0.51
1:A:177:LYS:O	1:A:179:GLN:N	2.44	0.51
1:A:550:ILE:HG12	3:A:600:FAD:C2	2.40	0.51
1:A:35:ASN:ND2	1:A:70:CYS:H	2.09	0.51
1:A:421:ASP:CB	1:A:424:ILE:HG12	2.41	0.50
1:A:20:VAL:HG23	1:A:33:HIS:CD2	2.47	0.50
1:A:127:ASP:CB	1:A:149:ALA:HB1	2.42	0.50
1:A:280:ILE:HD12	1:A:347:VAL:HG12	1.93	0.49
1:A:163:ASN:HD21	1:A:336:ASN:ND2	2.10	0.49
1:A:512:ASP:OD1	1:A:514:LYS:HB2	2.13	0.49
1:A:392:ASN:ND2	1:A:393:ARG:H	2.10	0.48
1:A:167:ALA:HB3	1:A:253:GLY:CA	2.44	0.48
1:A:25:GLY:H	2:A:603:HEM:CHB	2.26	0.48
1:A:471:VAL:HG11	1:A:487:GLU:HG3	1.94	0.48
1:A:469:GLY:O	1:A:473:SER:HB2	2.13	0.48
1:A:245:ARG:CB	1:A:246:PRO:CD	2.91	0.47
1:A:453:ILE:HG22	1:A:455:VAL:H	1.79	0.47
1:A:173:ALA:HB2	1:A:219:ILE:HD12	1.96	0.47
1:A:283:ASP:HB3	1:A:287:LYS:O	2.13	0.47
1:A:170:GLY:CA	1:A:252:VAL:HG21	2.44	0.47
1:A:26:VAL:HG21	1:A:297:TYR:HB2	1.96	0.47
1:A:219:ILE:HD13	1:A:244:HIS:CD2	2.50	0.47
1:A:395:MET:HE1	1:A:404:ALA:O	2.14	0.47
1:A:407:ALA:O	1:A:411:GLN:HG2	2.15	0.47
1:A:434:TYR:HB3	1:A:439:ILE:HD11	1.97	0.47
1:A:420:PHE:HE1	1:A:496:LEU:HD11	1.79	0.46
1:A:567:PHE:O	1:A:568:ALA:CB	2.53	0.46
1:A:5:LEU:HG	1:A:96:PHE:CD1	2.50	0.46
1:A:196:MET:HE3	1:A:196:MET:HA	1.96	0.46
1:A:413:GLY:O	1:A:414:GLU:HB2	2.16	0.46
1:A:470:PHE:HB3	1:A:476:ASP:HA	1.97	0.46
1:A:450:ALA:HB1	1:A:455:VAL:O	2.15	0.46
1:A:375:ILE:HD12	1:A:434:TYR:CE2	2.51	0.46
1:A:235:MET:CE	4:A:700:SIN:H21	2.46	0.46
1:A:526:ILE:HG13	1:A:529:LEU:HB2	1.97	0.46
1:A:514:LYS:HD3	1:A:516:GLU:OE2	2.17	0.45
1:A:167:ALA:HB3	1:A:253:GLY:HA3	1.96	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:600:FAD:O3'	3:A:600:FAD:C1'	2.64	0.45
1:A:316:ALA:O	1:A:317:LYS:HB3	2.17	0.45
1:A:367:TYR:OH	1:A:372:GLY:HA2	2.17	0.45
1:A:453:ILE:CG2	1:A:455:VAL:HG13	2.41	0.45
1:A:142:VAL:HG11	1:A:225:MET:HE2	1.99	0.45
1:A:465:THR:O	1:A:468:ASN:HB2	2.17	0.45
1:A:394:PHE:HA	1:A:479:PHE:CZ	2.52	0.45
1:A:8:PHE:HE2	2:A:604:HEM:HHA	1.81	0.45
1:A:469:GLY:O	1:A:470:PHE:C	2.55	0.44
1:A:453:ILE:HD11	1:A:495:ALA:HB1	1.99	0.44
1:A:511:ILE:HA	1:A:516:GLU:O	2.16	0.44
1:A:66:GLY:H	1:A:258:GLN:NE2	2.16	0.44
1:A:319:ASN:HD21	1:A:331:GLY:N	2.15	0.44
1:A:219:ILE:HD13	1:A:244:HIS:CG	2.53	0.44
1:A:221:TRP:CZ2	1:A:558:ARG:HG3	2.53	0.44
1:A:127:ASP:HB2	1:A:149:ALA:HB1	1.99	0.44
1:A:255:HIS:O	1:A:259:VAL:HG13	2.17	0.44
1:A:420:PHE:HE1	1:A:496:LEU:CD1	2.30	0.44
1:A:145:ARG:HH11	1:A:268:GLY:H	1.65	0.44
1:A:437:LEU:O	1:A:438:ASN:HB2	2.16	0.44
1:A:20:VAL:HG23	1:A:33:HIS:CG	2.53	0.44
1:A:504:HIS:CD2	1:A:544:ARG:HE	2.36	0.44
1:A:188:LYS:O	1:A:191:MET:HB3	2.18	0.43
1:A:5:LEU:HD22	1:A:9:HIS:CE1	2.52	0.43
1:A:20:VAL:HG23	1:A:33:HIS:CE1	2.52	0.43
1:A:163:ASN:O	1:A:164:THR:C	2.56	0.43
1:A:437:LEU:HD21	2:A:601:HEM:C2A	2.53	0.43
1:A:214:ASN:O	1:A:215:SER:C	2.56	0.43
1:A:283:ASP:CB	1:A:289:THR:HG23	2.48	0.43
1:A:146:ASP:O	1:A:147:ALA:CB	2.63	0.43
1:A:115:ASP:O	1:A:116:LYS:C	2.57	0.43
1:A:433:GLY:HA2	2:A:601:HEM:HBA2	1.99	0.43
1:A:204:ASP:HB3	1:A:207:LEU:HD12	2.01	0.42
1:A:401:ARG:HH22	4:A:700:SIN:H22	1.83	0.42
1:A:437:LEU:O	1:A:438:ASN:CB	2.66	0.42
1:A:106:PRO:HG2	1:A:109:ALA:HB2	2.01	0.42
1:A:453:ILE:HG21	1:A:455:VAL:HG22	1.99	0.42
1:A:401:ARG:NH1	4:A:700:SIN:H22	2.26	0.42
1:A:220:ASP:O	1:A:223:THR:HB	2.19	0.42
2:A:604:HEM:HHA	2:A:604:HEM:HAA1	1.97	0.42
1:A:245:ARG:CB	1:A:246:PRO:HD2	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:HD21	2:A:601:HEM:C3A	2.55	0.42
1:A:74:HIS:HB3	2:A:604:HEM:HMB3	2.01	0.42
1:A:198:GLY:O	1:A:543:ASN:HB3	2.19	0.42
1:A:487:GLU:O	1:A:488:LEU:CB	2.68	0.42
1:A:412:LYS:CD	1:A:412:LYS:H	2.27	0.42
1:A:421:ASP:HB3	1:A:424:ILE:H	1.83	0.42
1:A:276:ARG:NH2	1:A:343:ASP:OD1	2.52	0.42
1:A:393:ARG:HD3	1:A:478:GLN:NE2	2.30	0.42
1:A:366:THR:HA	1:A:498:ILE:HB	2.00	0.42
1:A:558:ARG:HG2	1:A:558:ARG:NH1	2.22	0.41
1:A:282:GLU:H	1:A:282:GLU:HG3	1.35	0.41
1:A:145:ARG:HD2	1:A:268:GLY:N	2.30	0.41
1:A:283:ASP:N	1:A:287:LYS:O	2.45	0.41
1:A:394:PHE:CE1	1:A:395:MET:HE2	2.56	0.41
1:A:35:ASN:ND2	1:A:70:CYS:N	2.68	0.41
1:A:498:ILE:HD12	1:A:498:ILE:O	2.21	0.41
1:A:401:ARG:HH22	4:A:700:SIN:C2	2.34	0.41
3:A:600:FAD:H2B	3:A:600:FAD:H8A	1.95	0.40
1:A:283:ASP:HB2	1:A:289:THR:HG23	2.03	0.40
1:A:186:ASP:OD1	1:A:187:LYS:N	2.55	0.40
1:A:392:ASN:HD22	1:A:393:ARG:N	2.17	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	552/572 (96%)	492 (89%)	42 (8%)	18 (3%)	4 5

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	474	GLY
1	A	120	ALA
1	A	175	GLU
1	A	176	THR
1	A	178	PRO
1	A	317	LYS
1	A	427	SER
1	A	521	LYS
1	A	147	ALA
1	A	181	LYS
1	A	215	SER
1	A	523	ALA
1	A	412	LYS
1	A	488	LEU
1	A	97	GLY
1	A	179	GLN
1	A	122	VAL

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	377/429 (88%)	314 (83%)	63 (17%)	2 4

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	17	SER
1	A	20	VAL
1	A	21	SER
1	A	22	ASP
1	A	28	ASN
1	A	31	LEU
1	A	61	LYS
1	A	68	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	78	GLU
1	A	79	LYS
1	A	89	SER
1	A	101	GLU
1	A	102	ARG
1	A	123	LYS
1	A	124	GLU
1	A	125	THR
1	A	145	ARG
1	A	146	ASP
1	A	166	LEU
1	A	175	GLU
1	A	176	THR
1	A	188	LYS
1	A	191	MET
1	A	194	ASP
1	A	203	ASN
1	A	219	ILE
1	A	239	SER
1	A	243	SER
1	A	252	VAL
1	A	259	VAL
1	A	279	ARG
1	A	282	GLU
1	A	283	ASP
1	A	291	VAL
1	A	292	LEU
1	A	294	LYS
1	A	320	GLU
1	A	321	ARG
1	A	359	GLN
1	A	375	ILE
1	A	389	ARG
1	A	392	ASN
1	A	401	ARG
1	A	414	GLU
1	A	425	ARG
1	A	427	SER
1	A	441	LYS
1	A	446	ILE
1	A	449	LEU
1	A	453	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	454	ASP
1	A	460	LEU
1	A	465	THR
1	A	473	SER
1	A	475	LYS
1	A	478	GLN
1	A	496	LEU
1	A	520	GLU
1	A	526	ILE
1	A	529	LEU
1	A	548	ASN
1	A	558	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	35	ASN
1	A	114	GLN
1	A	172	ASN
1	A	258	GLN
1	A	319	ASN
1	A	336	ASN
1	A	359	GLN
1	A	392	ASN
1	A	411	GLN
1	A	468	ASN
1	A	478	GLN
1	A	543	ASN
1	A	548	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](#)

6 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
3	FAD	A	600	-	51,58,58	1.75	8 (15%)	57,89,89	3.36	26 (45%)
2	HEM	A	601	1	27,50,50	2.25	5 (18%)	17,82,82	2.43	9 (52%)
2	HEM	A	602	1	27,50,50	2.17	5 (18%)	17,82,82	2.34	8 (47%)
2	HEM	A	603	1	27,50,50	2.09	5 (18%)	17,82,82	2.33	9 (52%)
2	HEM	A	604	1	27,50,50	2.02	5 (18%)	17,82,82	4.56	9 (52%)
4	SIN	A	700	-	1,7,7	0.22	0	2,8,8	6.58	2 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	600	-	2/2/9/9	0/28/50/50	0/6/6/6
2	HEM	A	601	1	-	0/6/54/54	0/0/8/8
2	HEM	A	602	1	-	0/6/54/54	0/0/8/8
2	HEM	A	603	1	-	0/6/54/54	0/0/8/8
2	HEM	A	604	1	-	0/6/54/54	0/0/8/8
4	SIN	A	700	-	-	0/1/5/5	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3C-C2C	-5.38	1.32	1.40
2	A	603	HEM	C3C-C2C	-4.92	1.33	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	HEM	C3B-C2B	-4.81	1.33	1.40
2	A	604	HEM	C3C-C2C	-4.76	1.33	1.40
2	A	604	HEM	C3B-C2B	-4.67	1.33	1.40
2	A	601	HEM	C3B-C2B	-4.43	1.34	1.40
2	A	603	HEM	C3B-C2B	-4.21	1.34	1.40
2	A	602	HEM	C3C-C2C	-3.98	1.34	1.40
3	A	600	FAD	C5'-C4'	-2.32	1.48	1.51
3	A	600	FAD	P-O1P	-2.04	1.43	1.50
3	A	600	FAD	C8-C7	2.01	1.46	1.40
2	A	604	HEM	CMD-C2D	2.03	1.55	1.51
3	A	600	FAD	O4B-C1B	2.06	1.44	1.41
2	A	601	HEM	CAA-C2A	2.06	1.55	1.52
2	A	603	HEM	CAA-C2A	2.23	1.55	1.52
2	A	602	HEM	CAA-C2A	2.97	1.57	1.52
3	A	600	FAD	C4-N3	3.34	1.39	1.33
2	A	604	HEM	C3C-CAC	4.12	1.55	1.47
3	A	600	FAD	C4-C4X	4.26	1.48	1.41
2	A	603	HEM	C3C-CAC	4.34	1.56	1.47
2	A	604	HEM	C3B-CAB	4.37	1.56	1.47
3	A	600	FAD	C1'-C2'	4.45	1.79	1.51
2	A	603	HEM	C3B-CAB	4.63	1.57	1.47
2	A	601	HEM	C3B-CAB	4.74	1.57	1.47
2	A	602	HEM	C3C-CAC	4.76	1.57	1.47
2	A	602	HEM	C3B-CAB	5.00	1.57	1.47
2	A	601	HEM	C3C-CAC	5.22	1.58	1.47
3	A	600	FAD	C5B-C4B	6.60	1.72	1.51

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	FAD	C5B-C4B-C3B	-10.84	74.49	115.29
3	A	600	FAD	C4B-O4B-C1B	-8.11	101.38	109.83
3	A	600	FAD	C1'-N10-C10	-6.11	112.35	118.46
2	A	603	HEM	CMA-C3A-C4A	-5.49	120.02	128.46
3	A	600	FAD	C4X-C4-N3	-4.93	116.46	123.47
2	A	601	HEM	CMA-C3A-C4A	-4.39	121.72	128.46
2	A	604	HEM	CMD-C2D-C1D	-3.89	122.48	128.46
2	A	602	HEM	CMD-C2D-C1D	-3.86	122.54	128.46
3	A	600	FAD	O4'-C4'-C3'	-3.80	99.71	109.10
2	A	604	HEM	CAA-CBA-CGA	-3.80	106.17	112.66
3	A	600	FAD	O2'-C2'-C1'	-3.66	100.56	109.61
2	A	601	HEM	CMD-C2D-C1D	-3.42	123.22	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	604	HEM	CMA-C3A-C4A	-3.37	123.28	128.46
3	A	600	FAD	C1B-N9A-C4A	-3.35	120.85	126.64
3	A	600	FAD	C4X-C10-N10	-2.93	117.67	120.40
3	A	600	FAD	C6-C5X-N5	-2.92	115.60	118.95
2	A	603	HEM	CMD-C2D-C1D	-2.84	124.11	128.46
3	A	600	FAD	C6-C7-C8	-2.60	115.38	119.94
2	A	602	HEM	CMA-C3A-C4A	-2.56	124.53	128.46
3	A	600	FAD	C9A-C5X-N5	-2.53	118.73	122.32
3	A	600	FAD	C4'-C3'-C2'	-2.46	108.22	113.40
3	A	600	FAD	C9-C9A-C5X	-2.18	116.30	119.89
3	A	600	FAD	O2'-C2'-C3'	-2.11	103.88	109.10
3	A	600	FAD	C9A-N10-C10	-2.05	119.04	121.77
2	A	601	HEM	C3C-C4C-NC	-2.01	107.15	110.94
2	A	603	HEM	C4C-C3C-C2C	2.01	108.30	106.90
2	A	603	HEM	CMC-C2C-C3C	2.01	128.54	124.88
3	A	600	FAD	C9-C8-C7	2.02	123.48	119.94
3	A	600	FAD	C7M-C7-C6	2.02	125.34	120.36
2	A	603	HEM	CAD-CBD-CGD	2.14	116.31	112.66
2	A	604	HEM	CMA-C3A-C2A	2.15	128.99	124.94
2	A	604	HEM	CMB-C2B-C3B	2.15	128.80	124.88
2	A	602	HEM	C4C-C3C-C2C	2.20	108.44	106.90
2	A	604	HEM	CMD-C2D-C3D	2.23	129.14	124.94
2	A	602	HEM	CMD-C2D-C3D	2.33	129.33	124.94
2	A	603	HEM	CMB-C2B-C3B	2.35	129.17	124.88
2	A	601	HEM	CMC-C2C-C3C	2.38	129.22	124.88
2	A	601	HEM	CBA-CAA-C2A	2.39	117.06	112.48
3	A	600	FAD	O5'-C5'-C4'	2.40	115.77	109.36
2	A	603	HEM	CBA-CAA-C2A	2.42	117.11	112.48
2	A	602	HEM	CAD-CBD-CGD	2.49	116.92	112.66
2	A	602	HEM	CMB-C2B-C3B	2.51	129.45	124.88
2	A	604	HEM	CMC-C2C-C3C	2.53	129.49	124.88
3	A	600	FAD	P-O3P-PA	2.62	141.44	132.63
2	A	602	HEM	CMC-C2C-C3C	2.65	129.71	124.88
2	A	603	HEM	CBD-CAD-C3D	2.72	117.65	112.47
3	A	600	FAD	N6A-C6A-N1A	2.75	124.28	118.57
2	A	601	HEM	CMB-C2B-C3B	2.85	130.06	124.88
2	A	601	HEM	CBD-CAD-C3D	2.91	118.02	112.47
2	A	601	HEM	CMA-C3A-C2A	2.94	130.49	124.94
2	A	603	HEM	CMA-C3A-C2A	3.85	132.20	124.94
3	A	600	FAD	C6-C5X-C9A	4.22	124.67	119.01
2	A	601	HEM	C4C-C3C-C2C	4.35	109.93	106.90
3	A	600	FAD	C4X-N5-C5X	4.86	121.85	116.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	SIN	C3-C2-C1	4.96	121.14	112.66
2	A	602	HEM	CBD-CAD-C3D	5.19	122.36	112.47
3	A	600	FAD	C4-N3-C2	5.73	120.02	115.14
3	A	600	FAD	O4B-C4B-C5B	7.08	132.96	109.39
3	A	600	FAD	C1'-N10-C9A	7.21	124.72	118.31
4	A	700	SIN	C2-C3-C4	7.88	126.12	112.66
3	A	600	FAD	O5B-C5B-C4B	8.55	138.74	109.00
2	A	604	HEM	CBA-CAA-C2A	11.34	134.16	112.48
2	A	604	HEM	CBD-CAD-C3D	12.27	135.88	112.47

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	600	FAD	C4'
3	A	600	FAD	C3'

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	FAD	8	0
2	A	601	HEM	7	0
2	A	602	HEM	3	0
2	A	603	HEM	5	0
2	A	604	HEM	6	0
4	A	700	SIN	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.