



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:11 AM UTC

PDB ID : 1ABI / pdb_00001abi
Title : STRUCTURE OF THE HIRULOG 3-THROMBIN COMPLEX AND NATURE OF THE S' SUBSITES OF SUBSTRATES AND INHIBITORS
Authors : Qiu, X.; Tulinsky, A.
Deposited on : 1992-08-24
Resolution : 2.30 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

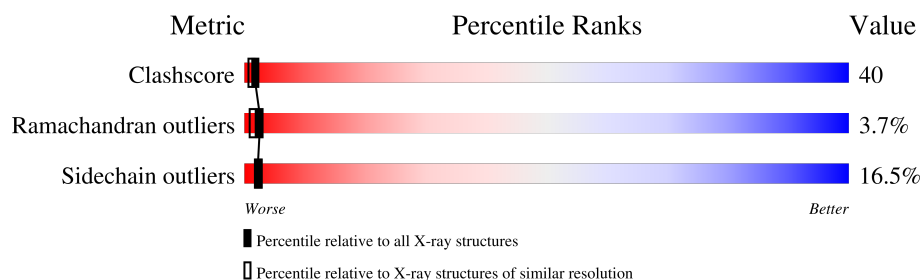
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	
3	I	20	

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	DPN	I	56	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2703 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 ALPHA-THROMBIN (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	33	Total	C	N	O	S	0	0	0
			265	162	45	57	1			

- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	252	Total	C	N	O	S	0	0	0
			2039	1299	360	366	14			

- Molecule 3 is a protein called HIRULOG 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	20	Total	C	N	O	0	0	0
			153	96	24	33			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	29	Total	O	0	0
			29	29		
4	H	199	Total	O	0	0
			199	199		
4	I	18	Total	O	0	0
			18	18		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

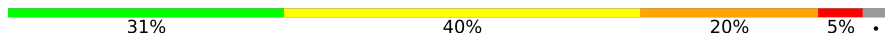
Note EDS was not executed.

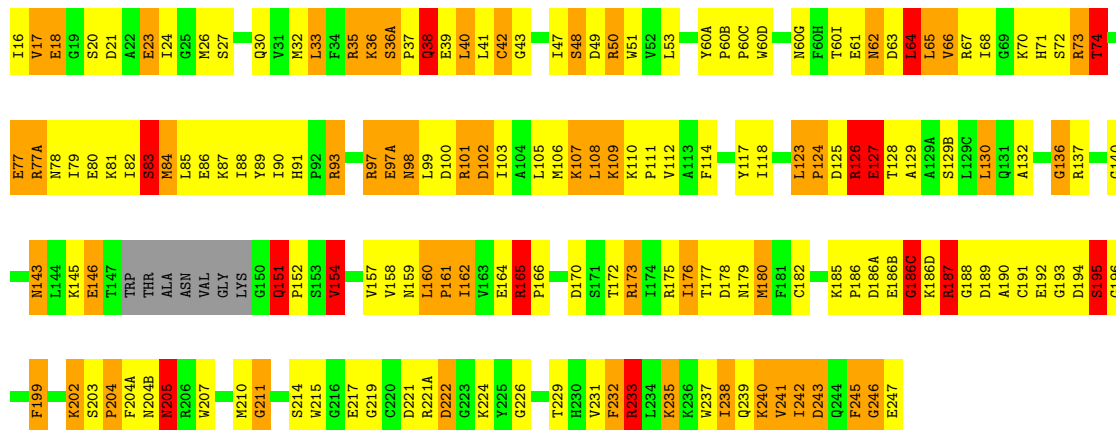
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 



• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 



• Molecule 3: HIRULOG 3

Chain I: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.44Å 72.10Å 73.07Å 90.00° 101.02° 90.00°	Depositor
Resolution (Å)	7.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.132 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2703	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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: HMR, DPN

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	L	1.22	1/267 (0.4%)	2.72	21/353 (5.9%)
2	H	1.42	7/2091 (0.3%)	2.56	155/2823 (5.5%)
3	I	1.19	0/119	2.36	3/154 (1.9%)
All	All	1.39	8/2477 (0.3%)	2.57	179/3330 (5.4%)

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
2	H	0	1
3	I	1	1
All	All	1	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	78	ASN	N-CA	8.41	1.56	1.46
2	H	77(A)	ARG	C-O	8.18	1.34	1.24
2	H	219	GLY	N-CA	5.98	1.55	1.45
2	H	27	SER	N-CA	5.83	1.53	1.46
2	H	238	ILE	CA-CB	5.81	1.61	1.54
1	L	1(A)	ASP	N-CA	5.40	1.52	1.46
2	H	24	ILE	CA-CB	5.40	1.60	1.54
2	H	62	ASN	CA-CB	5.14	1.61	1.53

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	78	ASN	CA-CB-CG	14.16	126.76	112.60
1	L	15	ARG	CD-NE-CZ	12.57	142.00	124.40
2	H	127	GLU	CB-CG-CD	12.33	133.56	112.60
2	H	175	ARG	CA-C-N	11.36	136.43	120.98
2	H	175	ARG	C-N-CA	11.36	136.43	120.98
2	H	93	ARG	CD-NE-CZ	10.76	139.46	124.40
1	L	14(D)	ARG	CD-NE-CZ	10.69	139.37	124.40
2	H	61	GLU	CA-C-N	10.36	134.16	120.28
2	H	61	GLU	C-N-CA	10.36	134.16	120.28
1	L	1(A)	ASP	CB-CA-C	10.16	127.48	111.02
1	L	14(K)	ILE	CB-CA-C	9.96	127.62	111.29
1	L	14(E)	GLU	CB-CG-CD	9.83	129.31	112.60
2	H	77(A)	ARG	CA-C-N	-9.61	107.13	122.79
2	H	77(A)	ARG	C-N-CA	-9.61	107.13	122.79
2	H	74	THR	N-CA-C	9.49	125.17	113.50
2	H	170	ASP	CA-CB-CG	-9.48	103.12	112.60
2	H	140	GLY	CA-C-O	9.45	131.60	121.96
2	H	232	PHE	CA-CB-CG	-9.33	104.47	113.80
2	H	186(D)	LYS	N-CA-C	-9.23	93.59	108.55
1	L	14(K)	ILE	CA-C-O	9.11	132.16	120.78
2	H	187	ARG	NE-CZ-NH1	9.09	130.59	121.50
1	L	1(A)	ASP	N-CA-C	-9.04	100.66	112.41
2	H	243	ASP	CA-CB-CG	8.98	121.58	112.60
2	H	74	THR	CA-CB-OG1	-8.97	96.14	109.60
2	H	21	ASP	CA-CB-CG	8.95	121.55	112.60
3	I	63	TYR	CA-C-N	8.93	137.78	121.70
3	I	63	TYR	C-N-CA	8.93	137.78	121.70
2	H	187	ARG	NE-CZ-NH2	-8.91	111.18	119.20
2	H	101	ARG	NE-CZ-NH2	-8.79	111.29	119.20
2	H	97	ARG	CD-NE-CZ	-8.58	112.38	124.40
2	H	114	PHE	O-C-N	8.45	132.42	122.79
2	H	77	GLU	CB-CG-CD	8.26	126.64	112.60
2	H	97(A)	GLU	CA-C-O	-8.24	109.83	119.64
2	H	186(A)	ASP	CA-CB-CG	8.20	120.80	112.60
1	L	13	GLU	CA-CB-CG	8.17	130.44	114.10
2	H	154	VAL	N-CA-CB	-8.14	98.80	112.47
2	H	27	SER	N-CA-CB	-8.06	101.60	110.71
2	H	27	SER	CB-CA-C	7.91	120.96	111.15
2	H	101	ARG	NE-CZ-NH1	7.91	129.41	121.50
2	H	83	SER	CA-C-O	7.75	130.15	121.40
1	L	1(B)	ALA	CA-C-O	7.54	131.29	120.51
2	H	132	ALA	CA-C-O	-7.53	112.86	121.15
2	H	233	ARG	NE-CZ-NH2	-7.51	112.44	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	62	ASN	CA-CB-CG	-7.43	105.17	112.60
2	H	38	GLN	N-CA-C	-7.33	98.82	109.59
2	H	80	GLU	CB-CG-CD	7.23	124.89	112.60
2	H	172	THR	CA-C-O	-7.19	113.46	121.51
1	L	14(A)	LYS	CA-C-O	-7.17	112.00	120.10
2	H	205	ASN	CA-CB-CG	7.13	119.73	112.60
2	H	161	PRO	CA-C-O	-7.08	113.27	121.98
2	H	73	ARG	NE-CZ-NH1	7.06	128.56	121.50
2	H	221(A)	ARG	NE-CZ-NH2	7.01	125.51	119.20
2	H	176	ILE	CA-CB-CG2	7.00	122.40	110.50
2	H	165	ARG	CD-NE-CZ	-6.97	114.64	124.40
2	H	231	VAL	CA-C-O	-6.91	113.76	120.95
2	H	62	ASN	CB-CA-C	-6.89	99.35	110.79
2	H	60(B)	PRO	N-CA-C	6.88	119.10	110.70
2	H	102	ASP	CA-CB-CG	-6.84	105.75	112.60
2	H	77(A)	ARG	CA-C-O	-6.78	110.81	120.51
2	H	77	GLU	CA-C-O	6.78	130.61	122.41
2	H	42	CYS	CA-C-O	6.75	128.53	121.31
2	H	165	ARG	NE-CZ-NH2	6.75	125.27	119.20
2	H	246	GLY	O-C-N	6.73	131.19	123.58
2	H	173	ARG	N-CA-C	-6.70	105.14	113.38
2	H	245	PHE	N-CA-C	6.67	121.86	109.24
2	H	63	ASP	CA-C-N	-6.67	111.40	122.21
2	H	63	ASP	C-N-CA	-6.67	111.40	122.21
2	H	83	SER	N-CA-CB	6.67	123.30	111.69
1	L	14(A)	LYS	N-CA-CB	6.64	120.44	110.22
2	H	80	GLU	CA-C-O	6.61	129.07	121.47
2	H	23	GLU	N-CA-C	-6.52	102.12	110.53
2	H	33	LEU	CA-CB-CG	6.51	139.10	116.30
2	H	62	ASN	OD1-CG-ND2	6.51	129.11	122.60
2	H	214	SER	N-CA-C	6.50	120.89	111.02
2	H	74	THR	OG1-CB-CG2	6.47	122.24	109.30
2	H	35	ARG	NE-CZ-NH2	-6.45	113.39	119.20
2	H	74	THR	N-CA-CB	-6.44	101.07	110.53
2	H	97	ARG	CA-C-O	-6.43	113.60	120.42
2	H	196	GLY	N-CA-C	-6.37	106.89	115.36
2	H	38	GLN	CA-C-O	-6.33	113.24	120.58
2	H	62	ASN	N-CA-C	6.31	118.16	111.28
2	H	73	ARG	NE-CZ-NH2	-6.30	113.53	119.20
2	H	231	VAL	O-C-N	6.27	127.95	121.87
2	H	114	PHE	CA-CB-CG	-6.25	107.55	113.80
2	H	233	ARG	CA-C-O	-6.23	113.06	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	64	LEU	N-CA-CB	-6.18	100.00	110.50
1	L	14(C)	GLU	CG-CD-OE1	-6.17	104.21	118.40
2	H	64	LEU	O-C-N	6.13	130.59	123.17
2	H	190	ALA	N-CA-C	-6.11	101.74	110.59
2	H	118	ILE	CA-C-O	6.10	126.29	120.31
2	H	186(D)	LYS	N-CA-CB	6.09	121.77	110.99
2	H	64	LEU	N-CA-C	6.08	118.43	109.24
2	H	154	VAL	CB-CA-C	6.08	119.66	110.90
2	H	186(C)	GLY	C-N-CA	6.07	136.88	121.70
2	H	151	GLN	CB-CA-C	6.05	117.59	109.42
1	L	9	LYS	CA-C-N	6.04	131.85	122.49
1	L	9	LYS	C-N-CA	6.04	131.85	122.49
2	H	137	ARG	CA-C-O	-6.01	113.65	120.32
1	L	14(M)	GLY	N-CA-C	5.99	127.37	113.18
2	H	195	SER	CA-C-O	5.99	127.91	121.44
2	H	129(B)	SER	N-CA-CB	5.97	119.49	110.30
2	H	66	VAL	CB-CA-C	5.97	119.46	110.63
2	H	126	ARG	CA-C-N	5.95	128.74	120.29
2	H	126	ARG	C-N-CA	5.95	128.74	120.29
2	H	193	GLY	CA-C-O	-5.94	113.09	119.27
2	H	193	GLY	N-CA-C	-5.93	108.02	115.08
2	H	112	VAL	CB-CA-C	5.92	119.66	111.49
2	H	186(D)	LYS	CA-C-O	-5.89	113.48	120.43
2	H	128	THR	CB-CA-C	5.87	120.83	110.85
1	L	1(C)	GLU	CA-C-O	-5.87	112.12	120.51
2	H	117	TYR	O-C-N	5.86	129.56	122.35
2	H	157	VAL	O-C-N	5.85	129.44	123.00
2	H	123	LEU	N-CA-C	-5.84	102.25	110.31
2	H	151	GLN	O-C-N	5.84	126.58	121.39
2	H	68	ILE	O-C-N	-5.83	117.19	123.14
1	L	10	LYS	CB-CA-C	-5.82	100.33	110.17
2	H	32	MET	CG-SD-CE	5.80	113.66	100.90
2	H	108	LEU	N-CA-CB	-5.80	101.48	110.29
2	H	160	LEU	N-CA-CB	-5.71	100.91	111.19
2	H	30	GLN	CB-CA-C	5.69	119.00	109.89
2	H	151	GLN	N-CA-C	-5.69	100.29	109.40
2	H	97(A)	GLU	CA-CB-CG	5.66	125.42	114.10
1	L	14(K)	ILE	N-CA-CB	-5.66	101.90	111.23
2	H	129(B)	SER	CA-C-O	-5.65	113.12	119.79
2	H	146	GLU	O-C-N	5.65	128.11	122.12
2	H	189	ASP	O-C-N	5.63	130.07	122.59
2	H	124	PRO	CB-CA-C	-5.63	103.58	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	114	PHE	CA-C-O	-5.62	115.35	121.87
2	H	217	GLU	CB-CG-CD	5.62	122.15	112.60
2	H	242	ILE	CB-CA-C	5.61	119.96	112.22
2	H	136	GLY	N-CA-C	-5.58	102.99	111.14
2	H	173	ARG	CG-CD-NE	5.55	124.21	112.00
2	H	170	ASP	N-CA-C	5.53	119.64	113.01
1	L	14(B)	THR	CA-C-O	-5.52	112.66	119.18
2	H	80	GLU	O-C-N	-5.50	116.75	122.96
2	H	125	ASP	N-CA-C	-5.47	101.67	110.14
2	H	127	GLU	CA-CB-CG	5.46	125.03	114.10
1	L	14(G)	LEU	CB-CA-C	5.46	119.86	110.79
2	H	211	GLY	O-C-N	5.46	128.35	123.60
2	H	179	ASN	CA-CB-CG	-5.43	107.17	112.60
1	L	14(E)	GLU	CA-C-O	5.41	126.29	120.55
2	H	18	GLU	CA-C-N	5.41	128.33	122.16
2	H	18	GLU	C-N-CA	5.41	128.33	122.16
2	H	67	ARG	NH1-CZ-NH2	-5.39	112.29	119.30
2	H	132	ALA	O-C-N	5.39	129.55	122.97
2	H	90	ILE	O-C-N	-5.39	117.22	122.93
2	H	33	LEU	N-CA-C	-5.38	99.74	108.41
2	H	164	GLU	CB-CG-CD	5.37	121.73	112.60
2	H	199	PHE	N-CA-C	-5.37	98.49	107.99
2	H	143	ASN	OD1-CG-ND2	5.36	127.96	122.60
2	H	73	ARG	CA-C-O	5.36	126.22	120.70
2	H	158	VAL	CA-C-N	5.36	130.54	122.99
2	H	158	VAL	C-N-CA	5.36	130.54	122.99
2	H	173	ARG	O-C-N	5.33	129.41	122.42
2	H	77	GLU	CB-CA-C	5.32	120.34	111.83
2	H	118	ILE	N-CA-CB	-5.28	105.35	112.10
2	H	146	GLU	N-CA-CB	5.28	117.87	110.12
2	H	219	GLY	O-C-N	-5.27	117.90	122.91
2	H	123	LEU	CB-CA-C	5.27	116.00	108.68
2	H	38	GLN	CB-CG-CD	5.25	121.52	112.60
2	H	43	GLY	N-CA-C	-5.25	103.54	112.51
2	H	93	ARG	N-CA-C	5.24	118.98	112.59
2	H	40	LEU	N-CA-CB	5.22	117.68	109.69
2	H	60(D)	TRP	N-CA-CB	5.18	119.53	110.98
2	H	151	GLN	OE1-CD-NE2	5.18	127.78	122.60
2	H	114	PHE	N-CA-CB	5.16	117.74	110.36
2	H	162	ILE	N-CA-C	-5.14	102.97	109.80
2	H	20	SER	CA-CB-OG	-5.13	100.85	111.10
2	H	204	PRO	N-CA-C	-5.11	107.07	114.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	98	ASN	N-CA-CB	-5.08	101.48	111.60
2	H	222	ASP	CA-CB-CG	-5.08	107.52	112.60
2	H	17	VAL	N-CA-C	5.08	114.88	107.37
2	H	93	ARG	NE-CZ-NH1	5.07	126.57	121.50
2	H	189	ASP	CA-CB-CG	5.07	117.67	112.60
2	H	130	LEU	N-CA-CB	-5.06	101.94	110.49
2	H	67	ARG	NE-CZ-NH1	5.05	126.55	121.50
2	H	73	ARG	O-C-N	-5.03	116.65	122.09
2	H	110	LYS	O-C-N	5.03	127.22	121.94
2	H	33	LEU	N-CA-CB	5.02	118.19	110.21

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	56	DPN	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	187	ARG	Sidechain
3	I	2	PRO	Peptide

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	L	265	0	259	43	2
2	H	2039	0	2010	149	1
3	I	153	0	124	33	0
4	H	199	0	0	18	0
4	I	18	0	0	4	0
4	L	29	0	0	13	0
All	All	2703	0	2393	195	2

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 40.

All (195) 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)
2:H:205:ASN:HB3	4:H:593:HOH:O	1.36	1.22
3:I:61:GLU:CD	4:I:572:HOH:O	1.83	1.19
2:H:224:LYS:HE2	4:H:585:HOH:O	1.48	1.12
1:L:1(E):SER:HB2	2:H:123:LEU:O	1.49	1.12
2:H:240:LYS:HZ2	2:H:240:LYS:HB3	0.97	1.11
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.33	1.09
2:H:82:ILE:HD12	3:I:63:TYR:CD2	1.87	1.09
2:H:240:LYS:HB3	2:H:240:LYS:NZ	1.65	1.06
1:L:9:LYS:CD	4:L:526:HOH:O	2.04	1.05
1:L:10:LYS:HE3	4:L:501:HOH:O	1.53	1.04
1:L:15:ARG:HB2	2:H:204:PRO:O	1.57	1.03
1:L:9:LYS:HD2	4:L:526:HOH:O	1.56	1.02
2:H:36:LYS:HG3	2:H:65:LEU:HD22	1.41	1.01
2:H:50:ARG:HH11	2:H:107:LYS:HE2	1.26	0.99
2:H:73:ARG:HD3	2:H:152:PRO:O	1.61	0.97
2:H:65:LEU:HD11	2:H:84:MET:HE2	1.41	0.97
2:H:50:ARG:NH1	2:H:107:LYS:HE2	1.80	0.97
1:L:14(A):LYS:HG2	2:H:23:GLU:OE2	1.67	0.93
1:L:15:ARG:NH1	2:H:204(A):PHE:O	2.00	0.93
2:H:240:LYS:HZ2	2:H:240:LYS:CB	1.81	0.89
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.55	0.88
1:L:10:LYS:CE	4:L:501:HOH:O	2.15	0.86
3:I:53:ASN:O	3:I:55:ASP:N	2.08	0.86
2:H:85:LEU:HD13	2:H:106:MET:CE	2.07	0.83
2:H:17:VAL:O	2:H:188:GLY:HA2	1.78	0.83
2:H:82:ILE:HD12	3:I:63:TYR:HD2	1.38	0.82
2:H:240:LYS:NZ	2:H:240:LYS:CB	2.29	0.80
2:H:187:ARG:NH1	2:H:221:ASP:O	2.16	0.79
2:H:146:GLU:HB2	4:H:624:HOH:O	1.81	0.79
1:L:1(E):SER:CB	2:H:123:LEU:O	2.30	0.78
1:L:14(J):TYR:C	1:L:14(K):ILE:HG13	2.06	0.78
2:H:50:ARG:NH1	2:H:86:GLU:OE1	2.17	0.78
2:H:40:LEU:O	3:I:6:GLY:O	2.04	0.76
2:H:84:MET:HE3	3:I:63:TYR:O	1.86	0.76
1:L:14(J):TYR:O	1:L:14(K):ILE:HG13	1.86	0.75
2:H:65:LEU:HD11	2:H:84:MET:CE	2.16	0.75
1:L:14(D):ARG:O	1:L:14(H):GLU:HG3	1.87	0.74
3:I:53:ASN:C	3:I:55:ASP:H	1.96	0.74
2:H:187:ARG:HD3	2:H:221:ASP:OD2	1.87	0.74
4:L:549:HOH:O	2:H:26:MET:HE1	1.88	0.73
2:H:50:ARG:NH1	2:H:107:LYS:CE	2.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:10:LYS:NZ	4:L:560:HOH:O	2.22	0.72
2:H:129:ALA:O	2:H:130:LEU:HB2	1.89	0.71
2:H:178:ASP:O	2:H:233:ARG:HD2	1.91	0.70
2:H:65:LEU:CD1	2:H:84:MET:HE2	2.18	0.70
2:H:146:GLU:N	4:H:624:HOH:O	2.00	0.70
3:I:54:GLY:O	3:I:56:DPN:N	2.25	0.70
2:H:187:ARG:HH22	2:H:222:ASP:CG	1.99	0.69
2:H:224:LYS:CE	4:H:585:HOH:O	2.19	0.69
1:L:14(A):LYS:HD3	2:H:23:GLU:CD	2.18	0.69
3:I:64:LEU:HD13	3:I:64:LEU:OXT	1.93	0.69
1:L:1(D):GLY:H	2:H:123:LEU:H	1.42	0.68
2:H:143:ASN:ND2	2:H:192:GLU:HG2	2.07	0.68
2:H:109:LYS:HE3	4:H:623:HOH:O	1.92	0.68
1:L:14(J):TYR:C	1:L:14(K):ILE:CG1	2.67	0.67
2:H:35:ARG:O	2:H:38:GLN:HA	1.96	0.66
1:L:15:ARG:NH1	4:L:469:HOH:O	2.28	0.65
2:H:99:LEU:HD21	3:I:2:PRO:HB3	1.77	0.65
2:H:105:LEU:HD12	2:H:241:VAL:CG2	2.27	0.65
1:L:1(C):GLU:OE2	4:L:618:HOH:O	2.15	0.64
3:I:64:LEU:OXT	3:I:64:LEU:CD1	2.47	0.63
1:L:15:ARG:HD2	2:H:204:PRO:O	1.99	0.63
1:L:14(A):LYS:HD3	2:H:23:GLU:OE1	1.98	0.63
2:H:237:TRP:O	2:H:241:VAL:HG13	1.99	0.63
2:H:60(I):THR:CB	2:H:62:ASN:HD22	2.13	0.62
2:H:85:LEU:CD1	2:H:106:MET:CE	2.78	0.62
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.21	0.62
1:L:5:PRO:HA	1:L:9:LYS:HG3	1.81	0.61
2:H:182:CYS:HA	2:H:226:GLY:O	2.00	0.61
2:H:36:LYS:CG	2:H:65:LEU:HD22	2.26	0.60
2:H:105:LEU:HD12	2:H:241:VAL:HG22	1.82	0.60
2:H:124:PRO:O	2:H:235:LYS:NZ	2.35	0.60
3:I:53:ASN:C	3:I:55:ASP:N	2.57	0.60
3:I:59:ILE:HD11	3:I:64:LEU:CD2	2.32	0.60
1:L:1(D):GLY:HA3	2:H:123:LEU:H	1.67	0.60
2:H:82:ILE:CD1	3:I:63:TYR:CD2	2.76	0.59
3:I:61:GLU:CG	4:I:572:HOH:O	2.31	0.59
2:H:36(A):SER:HA	2:H:37:PRO:C	2.28	0.58
2:H:129:ALA:HA	2:H:210:MET:HE1	1.85	0.58
2:H:35:ARG:NH1	4:H:482:HOH:O	2.36	0.58
1:L:1(E):SER:O	1:L:1(C):GLU:N	2.28	0.58
2:H:36:LYS:HE3	4:H:534:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:91:HIS:CE1	2:H:93:ARG:HB2	2.38	0.57
3:I:59:ILE:HB	3:I:60:PRO:HD2	1.86	0.57
3:I:62:GLU:CD	4:I:568:HOH:O	2.47	0.57
2:H:50:ARG:NH1	2:H:108:LEU:O	2.38	0.57
3:I:61:GLU:HG2	4:I:572:HOH:O	2.00	0.57
2:H:39:GLU:HB2	3:I:8:GLY:HA2	1.86	0.56
2:H:126:ARG:CB	2:H:126:ARG:HH11	2.18	0.56
1:L:1(D):GLY:N	2:H:123:LEU:H	2.02	0.56
1:L:15:ARG:HD3	4:L:591:HOH:O	2.05	0.56
2:H:185:LYS:HB2	2:H:186(B):GLU:CG	2.31	0.56
2:H:51:TRP:HZ2	2:H:246:GLY:HA3	1.70	0.56
2:H:162:ILE:HD11	2:H:199:PHE:CZ	2.41	0.56
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.41	0.55
1:L:1(D):GLY:O	1:L:1(C):GLU:HB2	2.07	0.55
1:L:1(D):GLY:CA	2:H:123:LEU:H	2.21	0.54
1:L:5:PRO:HA	1:L:9:LYS:CG	2.38	0.53
2:H:87:LYS:HD2	2:H:88:ILE:H	1.72	0.53
1:L:1(C):GLU:CB	1:L:1:CYS:HB3	2.39	0.53
2:H:35:ARG:HB3	2:H:37:PRO:O	2.09	0.52
1:L:15:ARG:CZ	4:L:469:HOH:O	2.58	0.52
3:I:59:ILE:HD11	3:I:64:LEU:HD23	1.92	0.52
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.25	0.51
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.45	0.51
2:H:165:ARG:NH1	4:H:613:HOH:O	2.25	0.51
2:H:202:LYS:HG3	2:H:207:TRP:CE2	2.45	0.51
2:H:50:ARG:CD	2:H:108:LEU:O	2.59	0.51
2:H:53:LEU:HD11	2:H:103:ILE:HD11	1.92	0.51
2:H:73:ARG:NE	2:H:151:GLN:HB2	2.26	0.51
2:H:165:ARG:N	2:H:166:PRO:HD2	2.26	0.51
2:H:60(I):THR:HB	2:H:62:ASN:ND2	2.25	0.51
2:H:82:ILE:HD12	3:I:63:TYR:CE2	2.42	0.50
2:H:87:LYS:HG3	2:H:89:TYR:CE1	2.47	0.50
2:H:60(C):PRO:HB2	4:H:464:HOH:O	2.11	0.50
2:H:83:SER:HB3	4:H:445:HOH:O	2.12	0.50
1:L:1(C):GLU:HB3	1:L:1:CYS:HB3	1.95	0.49
2:H:211:GLY:HA2	2:H:229:THR:O	2.11	0.49
2:H:205:ASN:CB	4:H:593:HOH:O	2.18	0.49
1:L:14(D):ARG:HE	1:L:14(H):GLU:CD	2.21	0.49
1:L:14(I):SER:C	1:L:14(K):ILE:H	2.20	0.49
2:H:126:ARG:HH11	2:H:126:ARG:HB3	1.77	0.49
2:H:51:TRP:CZ3	2:H:107:LYS:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.19	0.48
2:H:235:LYS:O	2:H:238:ILE:HB	2.14	0.48
2:H:70:LYS:HE3	2:H:72:SER:O	2.14	0.48
2:H:60(I):THR:HB	2:H:62:ASN:HD22	1.79	0.48
2:H:105:LEU:HD12	2:H:241:VAL:HG21	1.96	0.47
2:H:99:LEU:O	2:H:102:ASP:HB2	2.14	0.47
2:H:16:ILE:N	2:H:194:ASP:OD2	2.47	0.47
2:H:42:CYS:HB3	2:H:195:SER:O	2.14	0.47
2:H:97(A):GLU:HB2	4:H:599:HOH:O	2.15	0.47
1:L:14(E):GLU:HB2	4:L:434:HOH:O	2.14	0.47
2:H:48:SER:OG	2:H:49:ASP:N	2.47	0.47
2:H:39:GLU:HB2	3:I:7:GLY:O	2.14	0.47
2:H:74:THR:OG1	3:I:56:DPN:HA	2.15	0.47
2:H:88:ILE:HD13	2:H:88:ILE:HG21	1.73	0.47
2:H:186(B):GLU:O	2:H:186(C):GLY:C	2.57	0.47
3:I:54:GLY:C	3:I:56:DPN:N	2.73	0.46
2:H:39:GLU:OE1	3:I:8:GLY:HA2	2.14	0.46
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.51	0.46
2:H:203:SER:O	2:H:205:ASN:HA	2.16	0.46
1:L:1(D):GLY:HA3	2:H:123:LEU:N	2.30	0.46
2:H:146:GLU:CB	4:H:624:HOH:O	2.47	0.46
3:I:61:GLU:O	3:I:62:GLU:O	2.33	0.46
2:H:165:ARG:NH2	2:H:180:MET:O	2.49	0.46
2:H:60(G):ASN:ND2	4:H:436:HOH:O	2.27	0.46
2:H:126:ARG:HA	2:H:232:PHE:CZ	2.52	0.45
2:H:73:ARG:CZ	2:H:151:GLN:HB2	2.46	0.45
2:H:107:LYS:HB2	2:H:107:LYS:HE3	1.48	0.45
3:I:61:GLU:O	3:I:62:GLU:C	2.59	0.45
3:I:59:ILE:CG1	3:I:64:LEU:HD23	2.47	0.45
2:H:215:TRP:HB2	3:I:1:DPN:O	2.17	0.45
2:H:176:ILE:N	2:H:176:ILE:HD13	2.31	0.45
2:H:17:VAL:O	2:H:18:GLU:HB2	2.18	0.44
2:H:51:TRP:CZ2	2:H:246:GLY:HA3	2.50	0.44
2:H:126:ARG:NH1	2:H:126:ARG:CG	2.78	0.44
2:H:127:GLU:H	2:H:127:GLU:CD	2.25	0.44
2:H:224:LYS:O	4:H:421:HOH:O	2.21	0.44
2:H:70:LYS:HB2	4:H:592:HOH:O	2.17	0.44
2:H:152:PRO:HB2	2:H:154:VAL:O	2.18	0.44
2:H:97:ARG:HH11	2:H:97:ARG:HD2	1.40	0.43
2:H:136:GLY:O	2:H:159:ASN:HA	2.18	0.43
2:H:50:ARG:HD3	2:H:108:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:15:ARG:HG2	4:L:591:HOH:O	2.18	0.43
3:I:62:GLU:O	3:I:64:LEU:N	2.52	0.43
1:L:9:LYS:CE	4:L:526:HOH:O	2.58	0.43
2:H:100:ASP:CG	2:H:177:THR:HG21	2.44	0.43
2:H:107:LYS:NZ	2:H:246:GLY:HA2	2.34	0.43
2:H:191:CYS:O	2:H:194:ASP:HB2	2.18	0.43
2:H:151:GLN:H	2:H:151:GLN:HG2	1.49	0.43
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.54	0.43
2:H:143:ASN:ND2	2:H:192:GLU:CG	2.79	0.43
2:H:186:PRO:HD3	4:H:449:HOH:O	2.18	0.42
2:H:64:LEU:HD12	2:H:85:LEU:HD12	2.00	0.42
1:L:14(G):LEU:HD22	1:L:14(G):LEU:N	2.34	0.42
2:H:82:ILE:HG13	3:I:63:TYR:CE2	2.53	0.42
2:H:232:PHE:O	2:H:235:LYS:HB2	2.19	0.42
2:H:177:THR:HG23	2:H:180:MET:HE3	2.02	0.42
2:H:98:ASN:HD21	2:H:177:THR:CG2	2.33	0.41
1:L:14(A):LYS:CG	2:H:23:GLU:OE2	2.54	0.41
1:L:3:LEU:O	1:L:9:LYS:HE3	2.21	0.41
2:H:126:ARG:HB3	2:H:127:GLU:OE1	2.21	0.41
1:L:1(E):SER:C	1:L:1(C):GLU:H	2.25	0.41
2:H:87:LYS:HE3	2:H:88:ILE:O	2.21	0.41
1:L:3:LEU:HD23	1:L:3:LEU:HA	1.72	0.41
1:L:14(A):LYS:CD	2:H:23:GLU:CD	2.92	0.41
2:H:160:LEU:HA	2:H:161:PRO:HD3	1.90	0.41
2:H:36(A):SER:CA	2:H:37:PRO:C	2.92	0.40
2:H:38:GLN:HE22	3:I:64:LEU:HD21	1.86	0.40
2:H:204(B):ASN:ND2	2:H:204(B):ASN:C	2.76	0.40
2:H:49:ASP:OD2	2:H:111:PRO:HB3	2.21	0.40
2:H:77:GLU:O	2:H:77(A):ARG:C	2.64	0.40
2:H:98:ASN:HA	3:I:1:DPN:HZ	2.02	0.40
2:H:187:ARG:NH2	2:H:222:ASP:OD1	2.50	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14(M):GLY:O	2:H:173:ARG:NE[4_556]	2.09	0.11
1:L:14(H):GLU:OE2	1:L:14(L):ASP:OD2[2_556]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	L	31/36 (86%)	22 (71%)	4 (13%)	5 (16%)	0	0
2	H	248/259 (96%)	227 (92%)	20 (8%)	1 (0%)	30	38
3	I	16/20 (80%)	10 (62%)	1 (6%)	5 (31%)	0	0
All	All	295/315 (94%)	259 (88%)	25 (8%)	11 (4%)	2	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(D)	GLY
1	L	1(C)	GLU
1	L	14(M)	GLY
3	I	54	GLY
3	I	55	ASP
3	I	63	TYR
1	L	14(L)	ASP
3	I	62	GLU
3	I	7	GLY
1	L	1(B)	ALA
2	H	186(C)	GLY

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	L	29/31 (94%)	28 (97%)	1 (3%)	32	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	220/225 (98%)	183 (83%)	37 (17%)	2	2
3	I	11/11 (100%)	6 (54%)	5 (46%)	0	0
All	All	260/267 (97%)	217 (84%)	43 (16%)	2	2

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	15	ARG
2	H	33	LEU
2	H	36	LYS
2	H	36(A)	SER
2	H	38	GLN
2	H	41	LEU
2	H	47	ILE
2	H	48	SER
2	H	50	ARG
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	74	THR
2	H	79	ILE
2	H	81	LYS
2	H	83	SER
2	H	84	MET
2	H	107	LYS
2	H	109	LYS
2	H	126	ARG
2	H	127	GLU
2	H	145	LYS
2	H	151	GLN
2	H	154	VAL
2	H	165	ARG
2	H	180	MET
2	H	195	SER
2	H	202	LYS
2	H	205	ASN
2	H	233	ARG
2	H	235	LYS
2	H	239	GLN
2	H	240	LYS
2	H	241	VAL

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Mol	Chain	Res	Type
2	H	242	ILE
2	H	243	ASP
2	H	245	PHE
2	H	247	GLU
3	I	53	ASN
3	I	55	ASP
3	I	59	ILE
3	I	63	TYR
3	I	64	LEU

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

Mol	Chain	Res	Type
2	H	62	ASN
2	H	204(B)	ASN
2	H	244	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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	HMR	I	3	3	11,11,12	0.81	0	9,12,14	2.65	2 (22%)

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	DPN	I	56	3	1/1/1/2	-	-
3	HMR	I	3	3	-	3/10/10/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	3	HMR	CB-CA-C	-6.84	101.13	112.17
3	I	3	HMR	O-C-CA	-2.85	117.09	125.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	56	DPN	CA

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	3	HMR	CA-CB-CC-CG
3	I	3	HMR	N-CB-CC-CG
3	I	3	HMR	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	56	DPN	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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

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.