



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 10:35 AM EDT

PDB ID : 2HNT  
Title : CRYSTALLOGRAPHIC STRUCTURE OF HUMAN GAMMA-THROMBIN  
Authors : Tulinsky, A.  
Deposited on : 1994-08-23  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

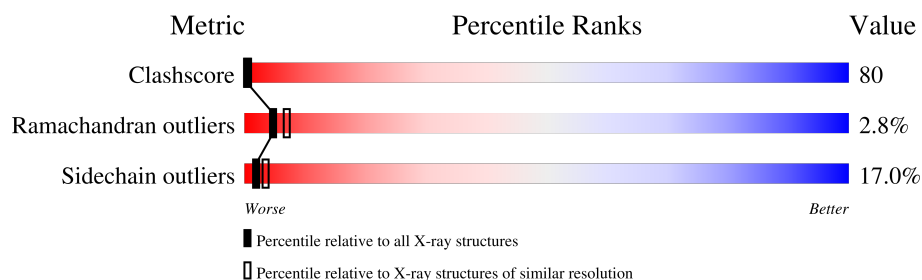
# 1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	C	70	
3	E	81	
4	F	105	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2299 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 GAMMA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	28	Total	C	N	O	S	0	0	0
			230	144	37	48	1			

- Molecule 2 is a protein called GAMMA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	67	Total	C	N	O	S	0	0	0
			532	342	90	96	4			

- Molecule 3 is a protein called GAMMA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	67	Total	C	N	O	S	0	0	0
			549	354	97	95	3			

- Molecule 4 is a protein called GAMMA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	100	Total	C	N	O	S	0	0	0
			802	509	142	144	7			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	12	Total	O	0	0
			12	12		
5	C	47	Total	O	0	0
			47	47		
5	E	54	Total	O	0	0
			54	54		
5	F	73	Total	O	0	0
			73	73		

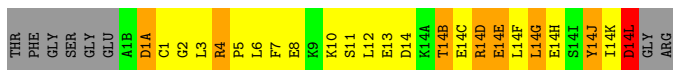
### 3 Residue-property plots

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.

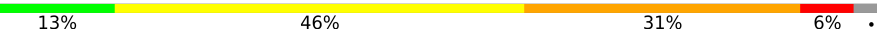
Note EDS was not executed.

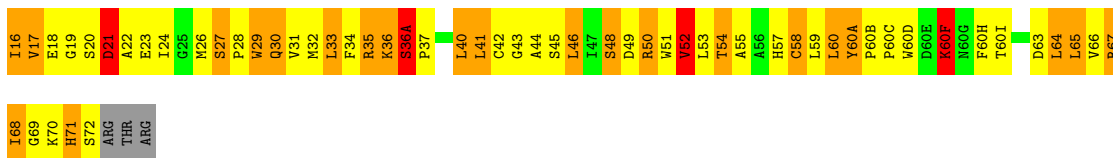
#### • Molecule 1: GAMMA-THROMBIN

Chain L: 




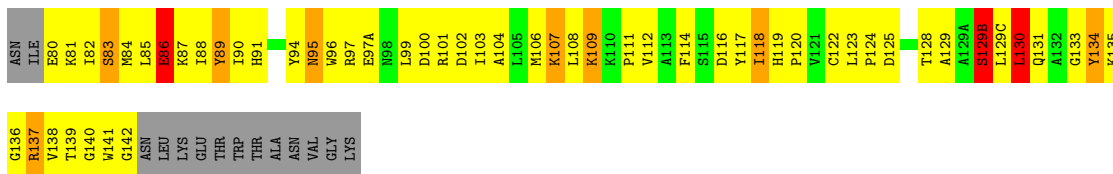
#### • Molecule 2: GAMMA-THROMBIN

Chain C: 



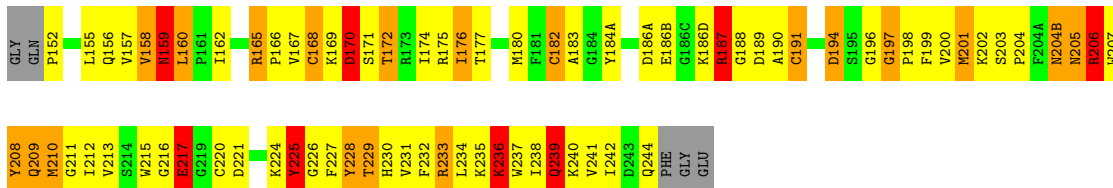
#### • Molecule 3: GAMMA-THROMBIN

Chain E: 



#### • Molecule 4: GAMMA-THROMBIN

Chain F: 



## 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, $\alpha$ , $\beta$ , $\gamma$	126.45Å 48.23Å 52.43Å 90.00° 96.20° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, $R_{free}$	0.156 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2299	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	1.00	0/232	2.22	12/309 (3.9%)
2	C	0.94	0/546	2.00	19/742 (2.6%)
3	E	0.91	0/563	1.97	18/760 (2.4%)
4	F	0.87	1/823 (0.1%)	1.93	22/1108 (2.0%)
All	All	0.92	1/2164 (0.0%)	1.99	71/2919 (2.4%)

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	C	0	2
4	F	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	220	CYS	CA-C	5.10	1.66	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	65	LEU	CA-CB-CG	9.39	136.89	115.30
4	F	194	ASP	CB-CG-OD2	9.21	126.59	118.30
1	L	4	ARG	CB-CA-C	8.88	128.15	110.40
4	F	182	CYS	CA-CB-SG	8.86	129.95	114.00
3	E	134	TYR	CB-CG-CD2	-8.80	115.72	121.00
3	E	125	ASP	CB-CG-OD1	8.33	125.79	118.30
2	C	58	CYS	O-C-N	7.84	135.25	122.70
4	F	183	ALA	N-CA-CB	7.70	120.88	110.10
3	E	137	ARG	NE-CZ-NH1	7.56	124.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	52	VAL	CB-CA-C	7.50	125.65	111.40
2	C	67	ARG	NE-CZ-NH2	-7.45	116.58	120.30
3	E	137	ARG	NE-CZ-NH2	-7.40	116.60	120.30
3	E	134	TYR	CB-CG-CD1	7.40	125.44	121.00
2	C	60(F)	LYS	CA-CB-CG	7.28	129.42	113.40
3	E	125	ASP	CB-CG-OD2	-7.13	111.89	118.30
1	L	14(C)	GLU	CA-CB-CG	7.03	128.86	113.40
4	F	208	TYR	CB-CG-CD2	6.99	125.19	121.00
4	F	233	ARG	CD-NE-CZ	6.81	133.13	123.60
4	F	168	CYS	CA-CB-SG	6.77	126.19	114.00
3	E	97	ARG	NE-CZ-NH2	6.75	123.68	120.30
1	L	14(D)	ARG	N-CA-CB	6.75	122.75	110.60
2	C	21	ASP	CB-CG-OD1	6.65	124.28	118.30
1	L	14(B)	THR	N-CA-CB	6.63	122.90	110.30
4	F	208	TYR	CB-CG-CD1	-6.57	117.06	121.00
4	F	228	TYR	CB-CG-CD2	-6.56	117.06	121.00
2	C	60	LEU	N-CA-CB	-6.50	97.41	110.40
4	F	206	ARG	NE-CZ-NH2	6.43	123.52	120.30
4	F	209	GLN	O-C-N	6.42	132.97	122.70
2	C	44	ALA	O-C-N	6.39	132.92	122.70
4	F	187	ARG	NE-CZ-NH1	-6.28	117.16	120.30
3	E	86	GLU	CG-CD-OE1	-6.16	105.97	118.30
1	L	1(A)	ASP	CB-CG-OD2	6.15	123.83	118.30
2	C	35	ARG	NE-CZ-NH2	6.09	123.35	120.30
1	L	14(L)	ASP	CB-CA-C	6.08	122.55	110.40
3	E	130	LEU	O-C-N	6.07	132.41	122.70
3	E	129(B)	SER	O-C-N	6.00	132.29	122.70
2	C	60(A)	TYR	CB-CG-CD2	-5.98	117.41	121.00
4	F	210	MET	CG-SD-CE	-5.97	90.64	100.20
4	F	187	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	L	14(J)	TYR	O-C-N	5.80	131.99	122.70
1	L	14(E)	GLU	CA-CB-CG	5.78	126.11	113.40
4	F	160	LEU	CA-CB-CG	5.75	128.51	115.30
3	E	80	GLU	CA-CB-CG	5.67	125.87	113.40
3	E	133	GLY	O-C-N	5.65	131.74	122.70
1	L	14(E)	GLU	CG-CD-OE2	5.58	129.47	118.30
2	C	17	VAL	C-N-CA	5.57	135.62	121.70
2	C	41	LEU	CB-CA-C	-5.53	99.69	110.20
3	E	123	LEU	CB-CA-C	5.52	120.69	110.20
3	E	123	LEU	CA-CB-CG	5.52	127.99	115.30
3	E	129(B)	SER	N-CA-CB	5.49	118.73	110.50
2	C	60(A)	TYR	CA-CB-CG	5.48	123.82	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	4	ARG	N-CA-CB	-5.46	100.77	110.60
4	F	225	TYR	CB-CG-CD1	-5.46	117.72	121.00
2	C	67	ARG	N-CA-CB	5.44	120.40	110.60
4	F	170	ASP	N-CA-CB	-5.41	100.86	110.60
3	E	100	ASP	CB-CA-C	5.41	121.21	110.40
1	L	14(G)	LEU	CB-CA-C	5.39	120.44	110.20
4	F	229	THR	N-CA-CB	5.36	120.48	110.30
2	C	21	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	L	14(D)	ARG	CA-CB-CG	5.29	125.05	113.40
4	F	239	GLN	CA-C-N	-5.28	105.58	117.20
2	C	17	VAL	CA-CB-CG2	5.26	118.79	110.90
2	C	30	GLN	CA-C-O	5.24	131.10	120.10
4	F	159	ASN	CB-CG-OD1	-5.23	111.13	121.60
2	C	68	ILE	CB-CA-C	5.23	122.06	111.60
2	C	36(A)	SER	O-C-N	-5.20	111.22	121.10
3	E	140	GLY	CA-C-O	5.16	129.89	120.60
4	F	228	TYR	CB-CG-CD1	5.16	124.10	121.00
3	E	86	GLU	OE1-CD-OE2	5.16	129.49	123.30
4	F	236	LYS	CA-CB-CG	5.07	124.56	113.40
4	F	217	GLU	OE1-CD-OE2	5.05	129.36	123.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	41	LEU	Mainchain
2	C	52	VAL	Mainchain
4	F	225	TYR	Sidechain
4	F	232	PHE	Sidechain

## 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	230	0	229	35	0
2	C	532	0	525	109	0
3	E	549	0	556	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	802	0	779	139	0
5	C	47	0	0	7	0
5	E	54	0	0	12	0
5	F	73	0	0	5	0
5	L	12	0	0	5	0
All	All	2299	0	2089	314	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 80.

All (314) 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)
4:F:201:MET:HG3	4:F:210:MET:CE	1.63	1.28
4:F:201:MET:CG	4:F:210:MET:HE3	1.62	1.27
2:C:60(A):TYR:CE1	2:C:60(C):PRO:HG2	1.77	1.19
3:E:137:ARG:HD3	4:F:159:ASN:HD21	1.12	1.13
3:E:137:ARG:HD3	4:F:159:ASN:ND2	1.65	1.12
2:C:60(A):TYR:CD1	2:C:60(C):PRO:HG2	1.85	1.10
2:C:36:LYS:HG2	2:C:36:LYS:O	1.35	1.10
2:C:23:GLU:H	2:C:26:MET:HE3	1.15	1.07
1:L:6:LEU:CD1	3:E:116:ASP:HB3	1.83	1.07
3:E:137:ARG:HD2	4:F:157:VAL:CG1	1.86	1.04
3:E:139:THR:CG2	4:F:157:VAL:HG22	1.87	1.04
3:E:139:THR:HG22	4:F:157:VAL:HG22	0.99	0.97
2:C:36:LYS:O	2:C:36:LYS:CG	2.11	0.97
3:E:139:THR:HG22	4:F:157:VAL:CG2	1.95	0.95
4:F:176:ILE:HG13	4:F:227:PHE:CE2	2.01	0.95
4:F:176:ILE:HG13	4:F:227:PHE:HE2	1.29	0.95
2:C:32:MET:SD	2:C:70:LYS:HD3	2.07	0.93
2:C:23:GLU:H	2:C:26:MET:CE	1.83	0.92
3:E:129(B):SER:HA	5:E:320:HOH:O	1.67	0.92
2:C:50:ARG:NH1	3:E:109:LYS:O	2.05	0.88
2:C:23:GLU:N	2:C:26:MET:HE3	1.89	0.88
4:F:211:GLY:HA2	4:F:231:VAL:HG23	1.56	0.88
3:E:138:VAL:N	4:F:158:VAL:O	2.06	0.87
2:C:67:ARG:HG2	3:E:82:ILE:HG13	1.57	0.87
1:L:8:GLU:OE2	4:F:202:LYS:NZ	2.08	0.86
3:E:114:PHE:HA	3:E:118:ILE:HG22	1.57	0.86
1:L:14(L):ASP:OD1	1:L:14(L):ASP:N	2.08	0.85
3:E:119:HIS:ND1	5:E:396:HOH:O	2.08	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:4:ARG:HH11	2:C:26:MET:HA	1.41	0.85
2:C:60(B):PRO:N	2:C:60(C):PRO:HD2	1.91	0.84
4:F:177:THR:HB	4:F:180:MET:CE	2.09	0.83
1:L:6:LEU:HD11	3:E:116:ASP:HB3	1.61	0.83
3:E:136:GLY:HA3	4:F:199:PHE:CZ	2.14	0.82
2:C:46:LEU:HD13	2:C:48:SER:O	1.79	0.82
3:E:129:ALA:O	3:E:130:LEU:HB2	1.80	0.81
3:E:86:GLU:HG3	3:E:109:LYS:HE3	1.63	0.80
2:C:17:VAL:HG11	4:F:221:ASP:HB2	1.61	0.80
4:F:177:THR:HB	4:F:180:MET:HE2	1.65	0.79
1:L:6:LEU:HD13	3:E:116:ASP:HB3	1.65	0.79
3:E:86:GLU:HG3	3:E:109:LYS:HD2	1.65	0.79
4:F:198:PRO:HB3	4:F:209:GLN:NE2	1.97	0.79
3:E:94:TYR:CE2	3:E:96:TRP:HB3	2.18	0.78
3:E:128:THR:O	3:E:129(C):LEU:HB2	1.83	0.78
2:C:64:LEU:O	5:C:324:HOH:O	2.00	0.78
4:F:200:VAL:HG12	4:F:209:GLN:HA	1.64	0.77
3:E:128:THR:HG22	3:E:129(C):LEU:HD12	1.67	0.76
4:F:198:PRO:HA	4:F:209:GLN:NE2	2.00	0.76
3:E:86:GLU:HG3	3:E:109:LYS:CD	2.16	0.76
1:L:12:LEU:HD23	1:L:13:GLU:H	1.52	0.75
3:E:86:GLU:CG	3:E:109:LYS:HE3	2.16	0.75
2:C:46:LEU:CD1	2:C:48:SER:O	2.34	0.75
3:E:124:PRO:O	4:F:235:LYS:HE3	1.87	0.75
3:E:128:THR:CG2	3:E:129(C):LEU:HD12	2.17	0.74
2:C:60(B):PRO:N	2:C:60(C):PRO:CD	2.50	0.74
3:E:141:TRP:O	4:F:152:PRO:HD3	1.89	0.73
3:E:131:GLN:O	3:E:134:TYR:HB2	1.88	0.72
1:L:12:LEU:CD2	1:L:13:GLU:H	2.02	0.72
2:C:36:LYS:O	2:C:36(A):SER:HB2	1.88	0.72
3:E:130:LEU:O	3:E:131:GLN:HG3	1.90	0.72
4:F:199:PHE:O	4:F:210:MET:N	2.23	0.72
3:E:141:TRP:CZ3	4:F:155:LEU:HD13	2.24	0.71
4:F:182:CYS:HB2	4:F:225:TYR:HB2	1.72	0.71
4:F:224:LYS:O	5:F:357:HOH:O	2.09	0.70
3:E:101:ARG:HG3	3:E:101:ARG:HH11	1.56	0.70
4:F:182:CYS:HB2	4:F:225:TYR:CB	2.22	0.70
4:F:203:SER:O	4:F:204(B):ASN:O	2.09	0.69
3:E:128:THR:HG22	3:E:129(C):LEU:CD1	2.21	0.69
2:C:17:VAL:N	4:F:189:ASP:O	2.24	0.69
4:F:221:ASP:HB3	5:F:329:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:136:GLY:O	4:F:159:ASN:HA	1.94	0.67
3:E:137:ARG:HD2	4:F:157:VAL:HG11	1.74	0.67
4:F:174:ILE:HG22	4:F:175:ARG:N	2.08	0.67
4:F:199:PHE:HB3	4:F:211:GLY:H	1.59	0.67
3:E:86:GLU:HG3	3:E:109:LYS:CE	2.23	0.67
2:C:60(A):TYR:C	2:C:60(C):PRO:HD2	2.15	0.67
4:F:198:PRO:CA	4:F:209:GLN:NE2	2.58	0.66
3:E:85:LEU:HD22	3:E:106:MET:HB3	1.78	0.66
4:F:198:PRO:CB	4:F:209:GLN:NE2	2.58	0.66
3:E:128:THR:CG2	3:E:129(C):LEU:CD1	2.74	0.66
4:F:240:LYS:O	4:F:244:GLN:CG	2.44	0.65
3:E:94:TYR:CZ	3:E:96:TRP:HB3	2.31	0.65
4:F:199:PHE:HD2	4:F:210:MET:HB3	1.63	0.64
2:C:57:HIS:ND1	3:E:102:ASP:OD2	2.24	0.64
2:C:43:GLY:HA2	5:C:312:HOH:O	1.97	0.64
2:C:31:VAL:HG11	2:C:52:VAL:HG11	1.78	0.64
2:C:23:GLU:N	2:C:26:MET:CE	2.54	0.63
2:C:60(A):TYR:CE1	2:C:60(C):PRO:CG	2.69	0.63
3:E:85:LEU:CD1	3:E:106:MET:HE2	2.27	0.63
2:C:60(B):PRO:CD	2:C:60(C):PRO:HD2	2.29	0.63
4:F:169:LYS:HE2	5:F:429:HOH:O	1.97	0.63
4:F:201:MET:SD	4:F:210:MET:HG2	2.39	0.63
3:E:85:LEU:CD2	3:E:106:MET:HB3	2.28	0.62
4:F:172:THR:HG23	4:F:174:ILE:N	2.15	0.62
4:F:174:ILE:CG2	4:F:175:ARG:N	2.62	0.62
2:C:68:ILE:HG22	3:E:118:ILE:HG13	1.80	0.61
4:F:171:SER:O	4:F:224:LYS:NZ	2.33	0.61
4:F:236:LYS:O	4:F:239:GLN:HB2	2.01	0.61
4:F:211:GLY:HA2	4:F:231:VAL:CG2	2.30	0.61
4:F:230:HIS:ND1	4:F:233:ARG:HD2	2.15	0.61
2:C:50:ARG:NH1	3:E:109:LYS:C	2.54	0.61
4:F:165:ARG:HD3	5:F:429:HOH:O	2.01	0.60
4:F:198:PRO:CA	4:F:209:GLN:HE21	2.14	0.60
1:L:14(K):ILE:C	1:L:14(L):ASP:OD1	2.40	0.60
2:C:31:VAL:HG13	2:C:66:VAL:CG1	2.32	0.59
4:F:165:ARG:CB	4:F:166:PRO:CD	2.79	0.59
3:E:86:GLU:CG	3:E:109:LYS:CD	2.79	0.59
1:L:4:ARG:H	1:L:8:GLU:HB2	1.67	0.59
2:C:31:VAL:HG11	2:C:52:VAL:CG1	2.32	0.59
4:F:216:GLY:O	4:F:217:GLU:HG3	2.03	0.59
1:L:1:CYS:C	3:E:122:CYS:SG	2.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:29:TRP:O	2:C:31:VAL:HG23	2.03	0.59
3:E:84:MET:O	3:E:109:LYS:HB2	2.03	0.59
2:C:65:LEU:CB	5:C:364:HOH:O	2.51	0.58
3:E:136:GLY:O	4:F:160:LEU:N	2.32	0.58
3:E:124:PRO:O	4:F:235:LYS:CE	2.50	0.58
4:F:198:PRO:HA	4:F:209:GLN:HE21	1.67	0.58
1:L:5:PRO:HG3	5:E:396:HOH:O	2.03	0.58
2:C:60:LEU:HA	2:C:60(F):LYS:O	2.03	0.58
4:F:199:PHE:HB3	4:F:211:GLY:N	2.17	0.58
3:E:85:LEU:CD1	3:E:106:MET:CE	2.82	0.58
3:E:118:ILE:HD13	5:E:526:HOH:O	2.02	0.58
3:E:137:ARG:HA	4:F:159:ASN:HA	1.85	0.58
3:E:85:LEU:HD13	3:E:106:MET:HE2	1.85	0.57
2:C:36(A):SER:H	2:C:37:PRO:C	2.07	0.57
2:C:18:GLU:HB2	4:F:188:GLY:HA2	1.87	0.57
4:F:172:THR:HG23	4:F:174:ILE:H	1.70	0.57
4:F:165:ARG:HB2	4:F:166:PRO:CD	2.33	0.57
2:C:23:GLU:HG3	2:C:26:MET:HE1	1.84	0.57
2:C:32:MET:SD	2:C:70:LYS:CD	2.88	0.57
1:L:10:LYS:O	1:L:11:SER:C	2.42	0.57
4:F:176:ILE:CG1	4:F:227:PHE:CE2	2.84	0.57
3:E:137:ARG:HD2	4:F:157:VAL:HG12	1.80	0.57
1:L:12:LEU:HD23	1:L:13:GLU:N	2.18	0.56
1:L:14(F):LEU:O	1:L:14(J):TYR:CE1	2.59	0.56
1:L:14(G):LEU:HG	5:L:477:HOH:O	2.04	0.56
2:C:55:ALA:HB3	2:C:58:CYS:SG	2.45	0.56
3:E:129(C):LEU:O	3:E:134:TYR:HD2	1.89	0.56
2:C:60(H):PHE:HD2	2:C:63:ASP:HB3	1.70	0.56
1:L:14(B):THR:CG2	5:L:425:HOH:O	2.53	0.56
4:F:182:CYS:HA	4:F:226:GLY:O	2.07	0.55
2:C:54:THR:HG22	3:E:104:ALA:HB3	1.88	0.55
2:C:60(A):TYR:H	2:C:60(F):LYS:HB3	1.70	0.55
3:E:85:LEU:HD11	3:E:106:MET:CE	2.36	0.55
4:F:182:CYS:CB	4:F:225:TYR:HB2	2.37	0.54
3:E:131:GLN:HB2	3:E:134:TYR:CD2	2.43	0.54
2:C:66:VAL:O	3:E:82:ILE:HA	2.07	0.54
3:E:135:LYS:HG3	5:E:350:HOH:O	2.07	0.54
4:F:166:PRO:O	4:F:170:ASP:HB2	2.07	0.54
2:C:60(B):PRO:CD	2:C:60(C):PRO:CD	2.86	0.54
4:F:184(A):TYR:CE2	4:F:186(D):LYS:HB3	2.42	0.54
4:F:165:ARG:HB2	4:F:166:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:ASP:HA	4:F:156:GLN:NE2	2.22	0.54
2:C:33:LEU:HD11	2:C:59:LEU:HD21	1.89	0.54
2:C:35:ARG:O	2:C:36:LYS:HB3	2.08	0.54
3:E:86:GLU:CG	3:E:109:LYS:CE	2.83	0.53
1:L:7:PHE:HE2	2:C:26:MET:N	2.07	0.53
4:F:229:THR:HG22	4:F:234:LEU:CD1	2.37	0.53
2:C:35:ARG:O	2:C:63:ASP:O	2.26	0.53
1:L:2:GLY:O	4:F:207:TRP:HD1	1.92	0.53
2:C:60(A):TYR:CD1	2:C:60(C):PRO:CG	2.77	0.53
3:E:137:ARG:CD	4:F:159:ASN:HD21	2.03	0.53
3:E:135:LYS:CG	5:E:350:HOH:O	2.56	0.52
2:C:60(C):PRO:HD3	3:E:96:TRP:CE3	2.45	0.52
2:C:60(C):PRO:HD3	3:E:96:TRP:CZ3	2.45	0.52
3:E:137:ARG:HD2	4:F:157:VAL:HG13	1.83	0.52
4:F:199:PHE:CD2	4:F:210:MET:HB3	2.42	0.52
4:F:204(B):ASN:CG	4:F:206:ARG:HG3	2.30	0.52
2:C:23:GLU:O	2:C:26:MET:HB2	2.10	0.52
1:L:14(B):THR:HG21	5:L:425:HOH:O	2.09	0.52
4:F:226:GLY:O	4:F:228:TYR:CE1	2.63	0.52
4:F:240:LYS:O	4:F:244:GLN:HB2	2.09	0.52
3:E:141:TRP:C	3:E:142:GLY:O	2.48	0.52
2:C:68:ILE:N	3:E:81:LYS:O	2.44	0.51
1:L:1:CYS:O	3:E:122:CYS:SG	2.68	0.51
4:F:180:MET:HG3	4:F:227:PHE:HD2	1.74	0.51
4:F:182:CYS:HB2	4:F:225:TYR:HB3	1.92	0.51
2:C:19:GLY:HA2	4:F:158:VAL:HG23	1.91	0.51
2:C:17:VAL:O	4:F:189:ASP:N	2.37	0.51
2:C:23:GLU:CA	2:C:26:MET:HE3	2.41	0.51
1:L:1(A):ASP:HA	4:F:206:ARG:NH2	2.26	0.51
3:E:137:ARG:CD	4:F:159:ASN:ND2	2.56	0.51
1:L:6:LEU:HB2	5:L:301:HOH:O	2.10	0.51
2:C:40:LEU:HD21	2:C:42:CYS:O	2.11	0.51
3:E:130:LEU:HD23	4:F:162:ILE:HD13	1.93	0.51
2:C:24:ILE:CG2	3:E:117:TYR:HE2	2.23	0.51
3:E:89:TYR:N	3:E:89:TYR:CD1	2.79	0.51
2:C:65:LEU:HB3	5:C:364:HOH:O	2.09	0.50
2:C:65:LEU:HD23	3:E:84:MET:HG2	1.94	0.50
3:E:103:ILE:HG13	4:F:212:ILE:CD1	2.41	0.50
4:F:182:CYS:SG	4:F:225:TYR:HB2	2.51	0.50
4:F:169:LYS:HD3	4:F:176:ILE:HB	1.94	0.50
2:C:60(D):TRP:O	2:C:60(D):TRP:CD1	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:50:ARG:NH1	3:E:111:PRO:HD3	2.26	0.50
3:E:86:GLU:HG2	3:E:109:LYS:HE3	1.91	0.50
2:C:19:GLY:CA	4:F:158:VAL:HG23	2.41	0.50
3:E:135:LYS:HE3	5:E:350:HOH:O	2.12	0.49
2:C:68:ILE:HG22	2:C:69:GLY:H	1.77	0.49
5:E:317:HOH:O	4:F:197:GLY:HA3	2.10	0.49
2:C:34:PHE:CE2	2:C:67:ARG:HD2	2.47	0.49
4:F:196:GLY:O	4:F:212:ILE:HG23	2.12	0.49
2:C:29:TRP:O	2:C:45:SER:HA	2.13	0.49
2:C:22:ALA:HB2	4:F:157:VAL:HG23	1.95	0.49
2:C:48:SER:HB3	2:C:51:TRP:HB2	1.95	0.49
2:C:50:ARG:HH11	3:E:109:LYS:C	2.16	0.49
1:L:7:PHE:O	1:L:12:LEU:N	2.46	0.48
4:F:238:ILE:O	4:F:238:ILE:HG22	2.12	0.48
2:C:20:SER:O	4:F:157:VAL:N	2.33	0.48
3:E:141:TRP:CE3	4:F:155:LEU:HD13	2.49	0.48
4:F:229:THR:CG2	4:F:234:LEU:CD1	2.90	0.48
2:C:33:LEU:HD11	2:C:59:LEU:CD2	2.43	0.48
4:F:226:GLY:O	4:F:228:TYR:CD1	2.66	0.48
4:F:165:ARG:CB	4:F:166:PRO:HD3	2.44	0.48
2:C:51:TRP:CH2	3:E:107:LYS:HB2	2.49	0.48
4:F:184(A):TYR:CZ	4:F:186(D):LYS:HB3	2.48	0.48
2:C:31:VAL:HG13	2:C:66:VAL:HG11	1.96	0.48
3:E:86:GLU:CG	3:E:109:LYS:HD2	2.40	0.48
4:F:204(B):ASN:ND2	4:F:206:ARG:HG3	2.29	0.48
4:F:234:LEU:O	4:F:238:ILE:HG13	2.14	0.48
2:C:60(I):THR:HG22	5:C:394:HOH:O	2.12	0.47
3:E:128:THR:O	3:E:129(C):LEU:HD12	2.14	0.47
3:E:128:THR:HG23	3:E:129(C):LEU:CD1	2.44	0.47
3:E:130:LEU:HD13	4:F:230:HIS:HE2	1.79	0.47
4:F:198:PRO:HB3	4:F:209:GLN:HE22	1.78	0.47
2:C:60(B):PRO:HD2	2:C:60(C):PRO:HD2	1.96	0.47
2:C:27:SER:N	2:C:28:PRO:HD3	2.29	0.47
2:C:43:GLY:CA	5:C:312:HOH:O	2.57	0.47
3:E:130:LEU:C	3:E:131:GLN:HG3	2.34	0.47
3:E:122:CYS:HB2	4:F:207:TRP:O	2.15	0.47
3:E:139:THR:HA	4:F:156:GLN:O	2.15	0.47
2:C:65:LEU:HB2	5:C:364:HOH:O	2.12	0.47
3:E:114:PHE:CE1	3:E:120:PRO:HD3	2.50	0.47
2:C:17:VAL:CG1	4:F:221:ASP:HB2	2.37	0.47
4:F:167:VAL:HG12	4:F:167:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:198:PRO:CB	4:F:209:GLN:HE21	2.27	0.47
4:F:241:VAL:HA	4:F:244:GLN:HB2	1.96	0.47
2:C:68:ILE:HG22	2:C:69:GLY:N	2.30	0.46
3:E:130:LEU:HD23	3:E:130:LEU:HA	1.62	0.46
3:E:89:TYR:O	3:E:104:ALA:HA	2.15	0.46
2:C:22:ALA:HB2	4:F:157:VAL:CG2	2.46	0.46
1:L:4:ARG:NH1	2:C:26:MET:HA	2.21	0.46
2:C:36:LYS:HB2	2:C:65:LEU:HD12	1.97	0.46
4:F:200:VAL:HA	4:F:208:TYR:O	2.15	0.46
4:F:234:LEU:O	4:F:237:TRP:HB3	2.16	0.46
2:C:23:GLU:CG	2:C:26:MET:HE1	2.45	0.45
2:C:33:LEU:HD22	2:C:64:LEU:HD22	1.99	0.45
3:E:85:LEU:HD13	3:E:106:MET:CE	2.46	0.45
4:F:165:ARG:O	4:F:168:CYS:HB2	2.17	0.45
2:C:21:ASP:HA	4:F:155:LEU:O	2.16	0.45
2:C:71:HIS:O	2:C:72:SER:C	2.54	0.45
4:F:187:ARG:HE	4:F:221:ASP:CG	2.20	0.45
4:F:215:TRP:HE3	4:F:216:GLY:N	2.15	0.45
3:E:141:TRP:O	4:F:152:PRO:CD	2.63	0.45
2:C:30:GLN:HG2	4:F:155:LEU:HD22	1.97	0.45
2:C:67:ARG:HA	3:E:81:LYS:O	2.16	0.45
1:L:14(D):ARG:CZ	1:L:14(H):GLU:OE2	2.65	0.44
2:C:48:SER:OG	2:C:49:ASP:N	2.49	0.44
4:F:240:LYS:O	4:F:244:GLN:CB	2.64	0.44
1:L:14(F):LEU:HB3	1:L:14(J):TYR:OH	2.17	0.44
4:F:215:TRP:CE3	4:F:216:GLY:O	2.71	0.44
2:C:60:LEU:HG	2:C:60:LEU:O	2.16	0.44
4:F:208:TYR:HB2	4:F:210:MET:HE1	2.00	0.44
4:F:189:ASP:CG	4:F:190:ALA:H	2.21	0.44
1:L:12:LEU:HD22	1:L:13:GLU:H	1.80	0.44
2:C:23:GLU:O	2:C:26:MET:CB	2.66	0.44
4:F:174:ILE:HG22	4:F:175:ARG:O	2.17	0.44
2:C:55:ALA:HB2	4:F:196:GLY:HA2	2.00	0.43
3:E:95:ASN:O	3:E:99:LEU:N	2.51	0.43
2:C:16:ILE:HG21	4:F:158:VAL:HB	2.00	0.43
1:L:14:ASP:HB2	2:C:23:GLU:OE2	2.18	0.43
1:L:14(G):LEU:CG	5:L:477:HOH:O	2.63	0.43
3:E:109:LYS:HD2	3:E:109:LYS:HA	1.26	0.43
4:F:236:LYS:O	4:F:239:GLN:CB	2.67	0.43
4:F:200:VAL:CG1	4:F:209:GLN:HA	2.42	0.43
2:C:68:ILE:CG2	2:C:69:GLY:H	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:205:ASN:HD22	4:F:205:ASN:HA	1.54	0.43
4:F:240:LYS:O	4:F:244:GLN:HG2	2.18	0.43
2:C:57:HIS:HD1	3:E:102:ASP:CG	2.16	0.43
2:C:70:LYS:O	3:E:141:TRP:HH2	2.02	0.43
2:C:72:SER:H	3:E:141:TRP:HZ2	1.67	0.43
3:E:87:LYS:HB3	3:E:89:TYR:CE1	2.53	0.43
2:C:53:LEU:HD23	4:F:209:GLN:OE1	2.18	0.43
1:L:14(B):THR:O	1:L:14(E):GLU:HB3	2.19	0.42
4:F:177:THR:H	4:F:180:MET:CE	2.32	0.42
2:C:26:MET:C	2:C:28:PRO:HD3	2.40	0.42
3:E:103:ILE:HG13	4:F:212:ILE:HD13	1.99	0.42
1:L:4:ARG:HH11	1:L:4:ARG:HD2	1.64	0.42
3:E:129(B):SER:HB3	5:E:320:HOH:O	2.19	0.42
3:E:135:LYS:CE	5:E:350:HOH:O	2.66	0.42
4:F:200:VAL:HG12	4:F:208:TYR:O	2.20	0.42
2:C:50:ARG:HD2	3:E:108:LEU:O	2.20	0.42
2:C:65:LEU:CD2	3:E:84:MET:HG2	2.50	0.42
4:F:177:THR:CB	4:F:180:MET:CE	2.90	0.42
1:L:3:LEU:HD12	4:F:206:ARG:HH21	1.85	0.42
2:C:66:VAL:O	3:E:83:SER:N	2.48	0.42
4:F:221:ASP:CB	5:F:329:HOH:O	2.58	0.42
3:E:90:ILE:HD13	3:E:104:ALA:HB2	2.01	0.41
1:L:1(A):ASP:HA	4:F:206:ARG:HH22	1.85	0.41
2:C:23:GLU:CB	2:C:26:MET:CE	2.98	0.41
4:F:172:THR:HG22	4:F:174:ILE:O	2.21	0.41
2:C:59:LEU:HD12	3:E:104:ALA:HB1	2.03	0.41
3:E:107:LYS:O	3:E:107:LYS:CG	2.67	0.41
3:E:90:ILE:O	3:E:91:HIS:C	2.59	0.41
1:L:14(J):TYR:HA	3:E:134:TYR:CE1	2.55	0.41
3:E:130:LEU:O	3:E:131:GLN:CG	2.64	0.41
4:F:203:SER:HA	4:F:204:PRO:HD3	1.70	0.41
2:C:49:ASP:O	3:E:112:VAL:HG12	2.20	0.41
3:E:101:ARG:N	5:E:340:HOH:O	2.41	0.41
3:E:130:LEU:HB3	5:E:308:HOH:O	2.21	0.41
4:F:229:THR:HG22	4:F:234:LEU:HD12	2.03	0.41
2:C:51:TRP:CE2	4:F:242:ILE:HG12	2.56	0.41
4:F:191:CYS:O	4:F:194:ASP:HB2	2.21	0.40
3:E:124:PRO:O	4:F:235:LYS:NZ	2.53	0.40
3:E:96:TRP:CE3	3:E:96:TRP:C	2.95	0.40
2:C:50:ARG:HH11	2:C:50:ARG:HD3	1.60	0.40

There are no symmetry-related clashes.



## 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	26/36 (72%)	19 (73%)	7 (27%)	0	100	100
2	C	65/70 (93%)	50 (77%)	14 (22%)	1 (2%)	10	18
3	E	65/81 (80%)	55 (85%)	9 (14%)	1 (2%)	10	18
4	F	98/105 (93%)	82 (84%)	11 (11%)	5 (5%)	2	2
All	All	254/292 (87%)	206 (81%)	41 (16%)	7 (3%)	5	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	186(B)	GLU
2	C	36(A)	SER
3	E	130	LEU
4	F	197	GLY
4	F	217	GLU
4	F	165	ARG
4	F	213	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	L	26/31 (84%)	25 (96%)	1 (4%)	33	58
2	C	59/62 (95%)	45 (76%)	14 (24%)	1	1
3	E	58/70 (83%)	48 (83%)	10 (17%)	2	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	87/90 (97%)	73 (84%)	14 (16%)	2	4
All	All	230/253 (91%)	191 (83%)	39 (17%)	2	3

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	14(L)	ASP
2	C	16	ILE
2	C	21	ASP
2	C	27	SER
2	C	29	TRP
2	C	33	LEU
2	C	36	LYS
2	C	40	LEU
2	C	46	LEU
2	C	48	SER
2	C	50	ARG
2	C	54	THR
2	C	60(F)	LYS
2	C	64	LEU
2	C	71	HIS
3	E	83	SER
3	E	86	GLU
3	E	88	ILE
3	E	89	TYR
3	E	95	ASN
3	E	97(A)	GLU
3	E	107	LYS
3	E	109	LYS
3	E	118	ILE
3	E	129(B)	SER
4	F	158	VAL
4	F	159	ASN
4	F	170	ASP
4	F	172	THR
4	F	176	ILE
4	F	186(A)	ASP
4	F	187	ARG
4	F	191	CYS
4	F	201	MET
4	F	204(B)	ASN
4	F	205	ASN

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Mol	Chain	Res	Type
4	F	206	ARG
4	F	236	LYS
4	F	239	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	131	GLN
4	F	156	GLN
4	F	159	ASN
4	F	204(B)	ASN
4	F	209	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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 [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.