



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:52 AM UTC

PDB ID : 4TNC / pdb_00004tnc
Title : REFINED STRUCTURE OF CHICKEN SKELETAL MUSCLE TROPONIN C IN THE TWO-CALCIUM STATE AT 2-ANGSTROMS RESOLUTION
Authors : Sundaralingam, M.
Deposited on : 1987-09-28
Resolution : 2.00 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
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

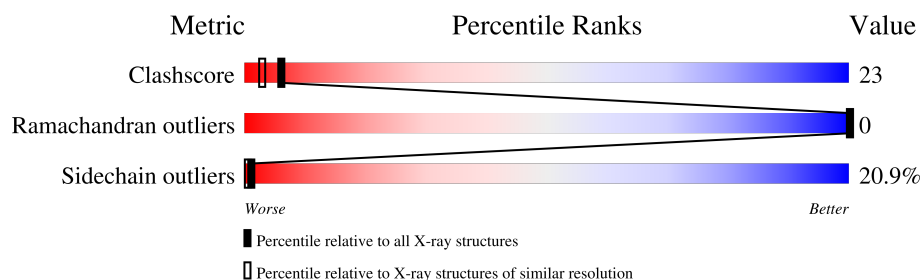
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	A	162	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1327 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 TROPONIN C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1257	774	199	272	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	MET	conflict	UNP P02588
A	4	MET	THR	conflict	UNP P02588
A	100	ASP	ASN	conflict	UNP P02588

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is water.

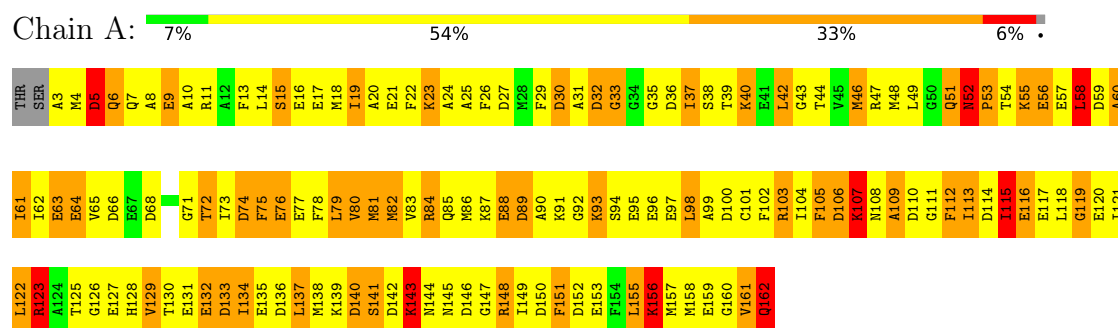
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		

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: TROPONIN C



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	66.70Å 66.70Å 60.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1327	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: CA

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	2.87	106/1269 (8.4%)	4.31	323/1694 (19.1%)

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	ILE	CA-CB	13.75	1.70	1.54
1	A	62	ILE	C-N	-10.71	1.19	1.33
1	A	114	ASP	C-O	10.39	1.37	1.23
1	A	130	THR	C-O	10.29	1.37	1.23
1	A	100	ASP	C-N	-10.02	1.20	1.34
1	A	53	PRO	C-O	9.63	1.35	1.23
1	A	52	ASN	CA-CB	9.56	1.64	1.53
1	A	16	GLU	N-CA	-9.07	1.35	1.46
1	A	76	GLU	N-CA	8.89	1.57	1.46
1	A	17	GLU	N-CA	8.52	1.56	1.46
1	A	29	PHE	N-CA	8.24	1.56	1.46
1	A	36	ASP	N-CA	8.21	1.56	1.45
1	A	20	ALA	N-CA	8.13	1.56	1.46
1	A	99	ALA	C-N	7.95	1.44	1.33
1	A	81	MET	C-N	-7.95	1.23	1.33
1	A	20	ALA	C-O	7.92	1.34	1.24
1	A	137	LEU	C-O	7.89	1.33	1.24
1	A	116	GLU	N-CA	7.87	1.55	1.46
1	A	111	GLY	N-CA	7.78	1.56	1.45
1	A	114	ASP	N-CA	7.70	1.55	1.45
1	A	82	MET	SD-CE	7.61	1.98	1.79
1	A	158	MET	N-CA	-7.57	1.37	1.46
1	A	76	GLU	C-O	7.53	1.33	1.24
1	A	47	ARG	NE-CZ	7.40	1.41	1.33
1	A	52	ASN	C-O	7.33	1.32	1.24
1	A	94	SER	CA-CB	7.25	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	LEU	C-N	7.25	1.43	1.33
1	A	130	THR	N-CA	7.24	1.54	1.45
1	A	113	ILE	C-O	7.22	1.31	1.24
1	A	72	THR	C-N	-7.18	1.24	1.33
1	A	86	MET	C-N	-7.14	1.24	1.33
1	A	27	ASP	CA-CB	7.13	1.65	1.53
1	A	118	LEU	N-CA	7.03	1.54	1.46
1	A	53	PRO	N-CA	6.98	1.55	1.47
1	A	130	THR	CB-OG1	6.97	1.54	1.43
1	A	159	GLU	C-O	6.92	1.32	1.24
1	A	61	ILE	C-N	-6.78	1.25	1.33
1	A	157	MET	N-CA	-6.76	1.38	1.46
1	A	73	ILE	C-N	-6.70	1.23	1.33
1	A	13	PHE	CA-CB	6.62	1.64	1.53
1	A	72	THR	N-CA	6.58	1.54	1.45
1	A	37	ILE	CB-CG1	6.53	1.66	1.53
1	A	74	ASP	C-O	-6.49	1.15	1.23
1	A	84	ARG	CD-NE	-6.48	1.37	1.46
1	A	13	PHE	C-O	6.42	1.32	1.24
1	A	139	LYS	CA-C	-6.42	1.44	1.52
1	A	129	VAL	N-CA	-6.38	1.38	1.46
1	A	147	GLY	C-O	6.30	1.33	1.24
1	A	127	GLU	N-CA	-6.30	1.38	1.45
1	A	62	ILE	C-O	6.23	1.31	1.24
1	A	65	VAL	CA-CB	6.23	1.63	1.54
1	A	53	PRO	CA-CB	-6.22	1.45	1.53
1	A	161	VAL	N-CA	-6.21	1.37	1.46
1	A	133	ASP	CA-C	6.20	1.60	1.52
1	A	157	MET	CG-SD	6.19	1.96	1.80
1	A	21	GLU	C-O	6.16	1.31	1.24
1	A	51	GLN	N-CA	6.15	1.52	1.45
1	A	136	ASP	C-N	6.07	1.41	1.33
1	A	147	GLY	N-CA	6.03	1.54	1.45
1	A	19	ILE	C-O	-6.02	1.17	1.24
1	A	142	ASP	C-N	-6.02	1.24	1.33
1	A	94	SER	C-N	-6.01	1.25	1.33
1	A	153	GLU	CA-C	6.00	1.60	1.52
1	A	79	LEU	CB-CG	-5.98	1.41	1.53
1	A	18	MET	C-N	-5.97	1.26	1.33
1	A	61	ILE	N-CA	-5.97	1.39	1.46
1	A	11	ARG	C-N	-5.96	1.25	1.34
1	A	48	MET	N-CA	-5.94	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	ALA	C-O	5.92	1.31	1.24
1	A	142	ASP	C-O	5.89	1.31	1.23
1	A	56	GLU	C-O	5.89	1.30	1.24
1	A	118	LEU	C-N	5.84	1.41	1.33
1	A	143	LYS	C-O	5.82	1.31	1.24
1	A	4	MET	C-O	5.81	1.31	1.24
1	A	142	ASP	CG-OD2	5.78	1.36	1.25
1	A	83	VAL	C-N	5.74	1.41	1.33
1	A	132	GLU	C-O	-5.73	1.16	1.24
1	A	102	PHE	CA-C	5.73	1.59	1.52
1	A	159	GLU	C-N	-5.66	1.25	1.33
1	A	71	GLY	C-N	-5.49	1.26	1.33
1	A	84	ARG	CA-C	5.49	1.59	1.52
1	A	151	PHE	C-O	5.48	1.30	1.24
1	A	17	GLU	C-N	5.45	1.41	1.34
1	A	9	GLU	CA-CB	5.44	1.62	1.53
1	A	106	ASP	CA-C	5.42	1.59	1.53
1	A	14	LEU	C-N	5.41	1.40	1.33
1	A	57	GLU	N-CA	5.38	1.52	1.46
1	A	151	PHE	N-CA	5.34	1.52	1.46
1	A	160	GLY	CA-C	-5.31	1.44	1.51
1	A	35	GLY	C-O	5.29	1.31	1.24
1	A	141	SER	C-N	-5.28	1.26	1.33
1	A	145	ASN	N-CA	-5.27	1.38	1.46
1	A	30	ASP	N-CA	5.26	1.53	1.46
1	A	101	CYS	C-O	5.24	1.30	1.24
1	A	135	GLU	N-CA	-5.24	1.40	1.46
1	A	54	THR	CA-CB	5.22	1.61	1.53
1	A	134	ILE	CA-C	-5.22	1.46	1.52
1	A	134	ILE	CA-CB	5.21	1.61	1.54
1	A	38	SER	C-N	-5.20	1.26	1.33
1	A	14	LEU	CA-CB	5.19	1.61	1.53
1	A	37	ILE	CA-CB	5.18	1.63	1.54
1	A	115	ILE	CA-CB	5.17	1.62	1.54
1	A	42	LEU	N-CA	5.11	1.52	1.46
1	A	8	ALA	CA-CB	5.11	1.61	1.53
1	A	93	LYS	C-O	5.03	1.30	1.24
1	A	53	PRO	N-CD	-5.01	1.40	1.47

All (323) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ARG	CD-NE-CZ	30.59	167.22	124.40
1	A	5	ASP	CA-C-O	24.15	145.57	120.70
1	A	103	ARG	NE-CZ-NH1	22.20	143.70	121.50
1	A	161	VAL	N-CA-C	-21.55	91.41	111.45
1	A	115	ILE	O-C-N	17.15	139.19	121.87
1	A	143	LYS	CB-CG-CD	16.39	149.00	111.30
1	A	112	PHE	CA-CB-CG	16.12	129.92	113.80
1	A	123	ARG	NE-CZ-NH1	-15.81	105.69	121.50
1	A	139	LYS	CA-C-O	15.73	137.73	120.90
1	A	75	PHE	O-C-N	15.67	138.73	122.12
1	A	63	GLU	CB-CG-CD	15.41	138.79	112.60
1	A	93	LYS	O-C-N	15.34	139.63	122.15
1	A	160	GLY	CA-C-N	14.87	143.66	121.65
1	A	160	GLY	C-N-CA	14.87	143.66	121.65
1	A	104	ILE	CA-C-N	14.52	139.32	120.44
1	A	104	ILE	C-N-CA	14.52	139.32	120.44
1	A	152	ASP	CA-CB-CG	-13.72	98.88	112.60
1	A	129	VAL	O-C-N	13.72	137.47	122.93
1	A	159	GLU	CA-C-O	-13.15	106.61	120.55
1	A	115	ILE	CA-C-O	-12.87	106.80	120.57
1	A	11	ARG	CD-NE-CZ	12.70	142.19	124.40
1	A	158	MET	CA-C-O	12.42	133.70	120.90
1	A	76	GLU	CB-CG-CD	12.42	133.71	112.60
1	A	31	ALA	CA-C-N	12.36	138.07	120.28
1	A	31	ALA	C-N-CA	12.36	138.07	120.28
1	A	116	GLU	O-C-N	-12.27	109.11	122.12
1	A	113	ILE	CA-C-O	-12.23	106.33	120.65
1	A	75	PHE	CA-C-O	-11.91	107.93	120.55
1	A	151	PHE	CA-CB-CG	-11.69	102.11	113.80
1	A	122	LEU	CA-C-O	11.66	133.19	120.24
1	A	129	VAL	CA-C-O	-11.55	107.44	120.84
1	A	101	CYS	CA-C-O	-11.52	107.08	120.10
1	A	99	ALA	CA-C-O	11.52	132.76	120.55
1	A	27	ASP	CA-CB-CG	-11.46	101.14	112.60
1	A	100	ASP	CA-C-O	-11.29	108.45	120.42
1	A	111	GLY	O-C-N	-11.26	108.13	122.43
1	A	76	GLU	CG-CD-OE1	11.22	144.20	118.40
1	A	160	GLY	N-CA-C	10.96	139.17	113.18
1	A	19	ILE	O-C-N	10.96	133.12	121.83
1	A	64	GLU	O-C-N	-10.94	109.68	122.15
1	A	68	ASP	CA-CB-CG	10.90	123.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ASP	OD1-CG-OD2	10.85	148.93	122.90
1	A	111	GLY	CA-C-O	10.76	131.11	119.06
1	A	103	ARG	NE-CZ-NH2	-10.69	109.58	119.20
1	A	116	GLU	CA-C-N	10.68	135.45	120.29
1	A	116	GLU	C-N-CA	10.68	135.45	120.29
1	A	107	LYS	CB-CA-C	-10.67	93.08	110.79
1	A	139	LYS	O-C-N	-10.65	111.01	122.09
1	A	108	ASN	O-C-N	10.64	135.64	122.34
1	A	33	GLY	O-C-N	10.46	132.09	122.57
1	A	85	GLN	O-C-N	-10.43	111.07	122.12
1	A	84	ARG	CD-NE-CZ	10.38	138.92	124.40
1	A	94	SER	CA-C-O	-10.30	109.64	120.55
1	A	159	GLU	CB-CA-C	10.29	127.88	110.79
1	A	162	GLN	CA-C-O	-10.23	103.41	120.80
1	A	120	GLU	O-C-N	-10.12	111.64	122.07
1	A	157	MET	O-C-N	-10.01	110.73	122.15
1	A	144	ASN	CA-C-N	9.99	136.35	122.07
1	A	144	ASN	C-N-CA	9.99	136.35	122.07
1	A	24	ALA	O-C-N	-9.85	111.85	122.09
1	A	103	ARG	NH1-CZ-NH2	-9.69	106.70	119.30
1	A	101	CYS	O-C-N	9.58	133.43	122.22
1	A	37	ILE	CA-C-O	9.54	131.69	121.67
1	A	159	GLU	N-CA-C	-9.53	100.89	111.28
1	A	72	THR	CA-CB-OG1	-9.51	95.33	109.60
1	A	5	ASP	O-C-N	-9.47	111.86	122.09
1	A	120	GLU	CA-C-O	9.44	130.73	120.82
1	A	32	ASP	CA-CB-CG	9.43	122.03	112.60
1	A	135	GLU	N-CA-CB	9.35	124.00	110.16
1	A	140	ASP	CB-CG-OD2	-9.34	96.91	118.40
1	A	94	SER	CA-CB-OG	-9.34	92.42	111.10
1	A	11	ARG	CA-C-N	9.25	133.61	120.28
1	A	11	ARG	C-N-CA	9.25	133.61	120.28
1	A	130	THR	CA-CB-OG1	-9.22	95.77	109.60
1	A	144	ASN	O-C-N	-9.21	111.29	122.34
1	A	87	LYS	O-C-N	9.08	131.42	122.07
1	A	148	ARG	NE-CZ-NH1	-9.06	112.44	121.50
1	A	88	GLU	CA-C-N	9.01	132.69	120.44
1	A	88	GLU	C-N-CA	9.01	132.69	120.44
1	A	82	MET	CA-C-O	9.00	130.27	120.82
1	A	103	ARG	CA-C-O	8.98	130.33	120.63
1	A	59	ASP	CA-C-N	8.86	131.96	120.44
1	A	59	ASP	C-N-CA	8.86	131.96	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	MET	CA-C-O	8.85	130.37	120.90
1	A	81	MET	CA-C-N	8.81	131.90	120.44
1	A	81	MET	C-N-CA	8.81	131.90	120.44
1	A	80	VAL	O-C-N	-8.80	113.33	121.87
1	A	117	GLU	CG-CD-OE1	8.76	138.55	118.40
1	A	54	THR	O-C-N	-8.74	111.89	122.65
1	A	57	GLU	N-CA-CB	8.72	122.66	110.01
1	A	72	THR	CA-CB-CG2	8.70	125.29	110.50
1	A	58	LEU	CA-C-O	8.63	129.70	120.55
1	A	55	LYS	CG-CD-CE	8.62	131.13	111.30
1	A	155	LEU	CA-C-O	-8.57	111.47	120.55
1	A	107	LYS	N-CA-C	8.51	120.56	111.28
1	A	98	LEU	O-C-N	8.45	131.08	122.12
1	A	92	GLY	CA-C-N	8.43	132.27	120.29
1	A	92	GLY	C-N-CA	8.43	132.27	120.29
1	A	26	PHE	O-C-N	-8.42	113.07	122.08
1	A	143	LYS	CG-CD-CE	8.40	130.61	111.30
1	A	151	PHE	N-CA-CB	-8.35	97.84	110.12
1	A	48	MET	CA-C-N	8.35	136.92	122.56
1	A	48	MET	C-N-CA	8.35	136.92	122.56
1	A	66	ASP	CA-CB-CG	-8.31	104.29	112.60
1	A	76	GLU	OE1-CD-OE2	-8.22	103.17	122.90
1	A	162	GLN	OE1-CD-NE2	-8.19	114.41	122.60
1	A	115	ILE	CB-CA-C	-8.15	99.53	112.16
1	A	63	GLU	CA-C-O	8.13	129.04	120.42
1	A	59	ASP	CB-CG-OD1	8.12	137.07	118.40
1	A	106	ASP	CA-C-O	8.07	131.65	122.37
1	A	157	MET	CA-C-O	8.06	128.96	120.42
1	A	118	LEU	O-C-N	-8.05	113.77	122.07
1	A	108	ASN	CA-C-O	-8.02	109.97	119.35
1	A	44	THR	O-C-N	-8.02	113.81	122.07
1	A	148	ARG	NE-CZ-NH2	8.00	126.40	119.20
1	A	113	ILE	CB-CG1-CD1	-7.98	97.04	113.80
1	A	52	ASN	CA-CB-CG	-7.89	104.71	112.60
1	A	149	ILE	O-C-N	7.87	133.19	122.88
1	A	23	LYS	CA-C-N	7.85	131.14	120.54
1	A	23	LYS	C-N-CA	7.85	131.14	120.54
1	A	57	GLU	CB-CA-C	-7.84	98.58	110.88
1	A	80	VAL	CA-C-N	7.76	130.99	120.44
1	A	80	VAL	C-N-CA	7.76	130.99	120.44
1	A	148	ARG	CA-C-O	7.71	130.53	121.58
1	A	151	PHE	CB-CA-C	7.69	123.56	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	THR	CA-C-O	7.69	128.89	120.82
1	A	114	ASP	CA-C-O	-7.66	111.92	121.88
1	A	123	ARG	NH1-CZ-NH2	7.64	129.24	119.30
1	A	155	LEU	O-C-N	7.62	130.20	122.12
1	A	150	ASP	N-CA-CB	7.59	121.96	110.42
1	A	14	LEU	N-CA-C	7.57	122.36	110.17
1	A	27	ASP	CA-C-O	7.56	128.67	120.20
1	A	84	ARG	N-CA-CB	7.56	120.97	110.01
1	A	131	GLU	N-CA-CB	7.53	121.31	110.16
1	A	101	CYS	CA-CB-SG	7.51	131.68	114.40
1	A	87	LYS	CA-C-O	-7.44	113.00	120.82
1	A	140	ASP	CA-C-O	7.44	128.53	119.97
1	A	79	LEU	O-C-N	-7.41	113.71	122.15
1	A	86	MET	O-C-N	-7.40	114.28	122.12
1	A	13	PHE	O-C-N	7.38	131.35	122.27
1	A	95	GLU	N-CA-CB	7.35	121.04	110.16
1	A	94	SER	N-CA-CB	7.34	120.91	110.12
1	A	9	GLU	N-CA-CB	7.32	121.57	110.30
1	A	117	GLU	OE1-CD-OE2	-7.24	105.53	122.90
1	A	9	GLU	CA-CB-CG	-7.21	99.69	114.10
1	A	61	ILE	N-CA-CB	7.20	118.97	110.55
1	A	40	LYS	O-C-N	-7.17	113.44	122.27
1	A	93	LYS	CA-C-O	-7.15	112.84	120.42
1	A	115	ILE	N-CA-CB	7.13	122.84	110.65
1	A	97	GLU	CA-CB-CG	-7.12	99.87	114.10
1	A	107	LYS	CA-C-N	-7.07	110.88	122.54
1	A	107	LYS	C-N-CA	-7.07	110.88	122.54
1	A	47	ARG	NE-CZ-NH1	7.01	128.51	121.50
1	A	16	GLU	CG-CD-OE1	6.98	134.46	118.40
1	A	60	ALA	CA-C-N	6.98	129.36	120.56
1	A	60	ALA	C-N-CA	6.98	129.36	120.56
1	A	117	GLU	N-CA-CB	6.97	120.48	110.16
1	A	26	PHE	CA-CB-CG	6.96	120.76	113.80
1	A	125	THR	OG1-CB-CG2	6.84	122.98	109.30
1	A	83	VAL	O-C-N	-6.82	114.81	121.83
1	A	47	ARG	NE-CZ-NH2	-6.80	113.08	119.20
1	A	25	ALA	CA-C-N	6.77	130.20	120.79
1	A	25	ALA	C-N-CA	6.77	130.20	120.79
1	A	97	GLU	CA-C-O	6.77	127.75	119.97
1	A	122	LEU	O-C-N	-6.73	113.48	122.23
1	A	65	VAL	CA-C-O	6.72	126.98	119.92
1	A	116	GLU	CA-C-O	6.72	127.67	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	VAL	CA-CB-CG1	6.71	121.81	110.40
1	A	31	ALA	CA-C-O	-6.62	113.41	120.42
1	A	132	GLU	N-CA-CB	-6.59	100.06	110.28
1	A	85	GLN	CA-C-O	6.59	127.54	120.55
1	A	25	ALA	O-C-N	-6.59	114.91	122.03
1	A	62	ILE	CA-C-N	6.57	129.62	120.29
1	A	62	ILE	C-N-CA	6.57	129.62	120.29
1	A	144	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	A	51	GLN	CA-C-O	6.52	129.62	121.66
1	A	119	GLY	CA-C-O	6.52	127.46	120.75
1	A	4	MET	N-CA-CB	-6.51	99.85	110.14
1	A	123	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	A	127	GLU	CA-C-N	-6.50	113.15	122.77
1	A	127	GLU	C-N-CA	-6.50	113.15	122.77
1	A	130	THR	CA-C-O	-6.50	113.64	121.89
1	A	36	ASP	CA-C-O	6.45	128.30	121.33
1	A	148	ARG	CG-CD-NE	-6.45	97.81	112.00
1	A	18	MET	CA-CB-CG	-6.40	101.30	114.10
1	A	125	THR	N-CA-C	6.39	119.06	111.71
1	A	22	PHE	CE1-CZ-CE2	6.37	131.47	120.00
1	A	90	ALA	CA-C-O	-6.37	113.80	120.55
1	A	135	GLU	CB-CA-C	-6.37	100.02	110.85
1	A	93	LYS	N-CA-CB	6.37	119.58	110.16
1	A	140	ASP	N-CA-C	6.37	119.20	111.82
1	A	51	GLN	O-C-N	-6.32	115.89	123.03
1	A	14	LEU	N-CA-CB	-6.31	100.34	110.63
1	A	9	GLU	CG-CD-OE2	-6.30	103.91	118.40
1	A	92	GLY	CA-C-O	-6.30	114.26	120.75
1	A	133	ASP	N-CA-CB	6.30	119.48	110.16
1	A	46	MET	O-C-N	6.29	128.79	122.12
1	A	118	LEU	CA-C-N	6.24	126.90	119.98
1	A	118	LEU	C-N-CA	6.24	126.90	119.98
1	A	66	ASP	CA-C-N	-6.20	109.49	121.58
1	A	66	ASP	C-N-CA	-6.20	109.49	121.58
1	A	107	LYS	O-C-N	6.15	128.64	122.12
1	A	103	ARG	O-C-N	-6.14	115.61	122.12
1	A	79	LEU	CA-CB-CG	6.12	137.74	116.30
1	A	94	SER	O-C-N	6.11	128.59	122.12
1	A	130	THR	CA-CB-CG2	6.08	120.84	110.50
1	A	125	THR	CA-C-O	6.08	126.97	120.10
1	A	156	LYS	O-C-N	-6.04	115.27	122.15
1	A	25	ALA	CA-C-O	6.02	127.10	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ARG	CA-CB-CG	-6.01	102.07	114.10
1	A	48	MET	O-C-N	-5.96	115.80	122.12
1	A	125	THR	CA-CB-OG1	-5.94	100.69	109.60
1	A	114	ASP	CA-CB-CG	-5.90	106.70	112.60
1	A	68	ASP	CB-CA-C	5.89	119.90	109.65
1	A	113	ILE	CA-CB-CG2	5.89	120.51	110.50
1	A	64	GLU	CA-C-N	5.88	129.93	120.82
1	A	64	GLU	C-N-CA	5.88	129.93	120.82
1	A	47	ARG	CD-NE-CZ	-5.85	116.21	124.40
1	A	161	VAL	CA-C-O	5.84	127.96	120.83
1	A	11	ARG	CG-CD-NE	-5.84	99.16	112.00
1	A	133	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	94	SER	CB-CA-C	-5.81	101.14	110.79
1	A	136	ASP	CA-CB-CG	-5.80	106.80	112.60
1	A	116	GLU	CB-CG-CD	5.79	122.44	112.60
1	A	78	PHE	CA-C-N	5.76	128.47	120.29
1	A	78	PHE	C-N-CA	5.76	128.47	120.29
1	A	15	SER	CA-CB-OG	-5.73	99.64	111.10
1	A	135	GLU	CA-C-O	-5.73	114.35	120.42
1	A	82	MET	O-C-N	-5.72	116.17	122.07
1	A	108	ASN	OD1-CG-ND2	5.72	128.32	122.60
1	A	79	LEU	N-CA-C	-5.71	105.13	111.36
1	A	126	GLY	N-CA-C	-5.71	107.22	115.27
1	A	8	ALA	N-CA-CB	5.70	119.11	110.28
1	A	162	GLN	CG-CD-NE2	5.68	124.93	116.40
1	A	99	ALA	CA-C-N	-5.68	112.22	120.29
1	A	99	ALA	C-N-CA	-5.68	112.22	120.29
1	A	128	HIS	CA-CB-CG	-5.67	108.13	113.80
1	A	35	GLY	N-CA-C	-5.67	107.36	115.64
1	A	6	GLN	CA-C-N	5.65	127.85	120.28
1	A	6	GLN	C-N-CA	5.65	127.85	120.28
1	A	5	ASP	N-CA-C	5.64	117.24	111.14
1	A	145	ASN	CB-CA-C	-5.64	103.57	111.80
1	A	73	ILE	CA-C-O	-5.63	114.39	120.36
1	A	131	GLU	CG-CD-OE1	5.60	131.28	118.40
1	A	140	ASP	CA-CB-CG	-5.58	107.02	112.60
1	A	35	GLY	O-C-N	5.58	128.69	122.50
1	A	160	GLY	CA-C-O	5.57	130.27	120.57
1	A	142	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	15	SER	CA-C-N	5.56	127.73	120.28
1	A	15	SER	C-N-CA	5.56	127.73	120.28
1	A	109	ALA	N-CA-C	5.54	118.83	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	19	ILE	CA-C-N	-5.52	111.92	120.31
1	A	19	ILE	C-N-CA	-5.52	111.92	120.31
1	A	159	GLU	O-C-N	-5.50	116.29	122.12
1	A	140	ASP	CB-CA-C	-5.49	100.12	110.67
1	A	96	GLU	CG-CD-OE2	-5.49	105.78	118.40
1	A	114	ASP	N-CA-CB	-5.49	101.68	110.51
1	A	55	LYS	CA-C-O	5.48	126.36	120.55
1	A	110	ASP	N-CA-C	-5.48	106.37	113.16
1	A	4	MET	CA-C-N	5.47	127.88	120.44
1	A	4	MET	C-N-CA	5.47	127.88	120.44
1	A	116	GLU	CG-CD-OE1	5.46	130.97	118.40
1	A	20	ALA	CA-C-O	-5.45	113.71	119.97
1	A	43	GLY	O-C-N	5.43	127.40	122.19
1	A	29	PHE	CA-C-O	5.42	125.90	119.56
1	A	84	ARG	NH1-CZ-NH2	5.42	126.34	119.30
1	A	51	GLN	N-CA-CB	5.41	118.99	110.56
1	A	90	ALA	O-C-N	5.39	127.83	122.12
1	A	5	ASP	CA-C-N	5.37	127.43	120.44
1	A	5	ASP	C-N-CA	5.37	127.43	120.44
1	A	89	ASP	CA-C-O	5.37	126.23	120.70
1	A	104	ILE	CA-C-O	-5.37	115.16	120.85
1	A	97	GLU	N-CA-C	5.37	118.05	111.82
1	A	38	SER	CA-CB-OG	-5.34	100.41	111.10
1	A	9	GLU	CG-CD-OE1	5.34	130.69	118.40
1	A	133	ASP	N-CA-C	-5.34	105.54	111.36
1	A	127	GLU	O-C-N	-5.34	116.56	122.86
1	A	128	HIS	O-C-N	5.33	129.13	122.63
1	A	118	LEU	CA-C-O	5.32	126.41	120.82
1	A	6	GLN	CB-CG-CD	5.31	121.63	112.60
1	A	131	GLU	CA-CB-CG	5.31	124.72	114.10
1	A	102	PHE	N-CA-CB	5.31	117.66	109.91
1	A	52	ASN	N-CA-C	5.30	118.27	108.94
1	A	56	GLU	CG-CD-OE2	-5.30	106.21	118.40
1	A	10	ALA	O-C-N	5.30	128.19	122.15
1	A	81	MET	CG-SD-CE	5.30	112.55	100.90
1	A	157	MET	CA-C-N	5.29	127.83	120.63
1	A	157	MET	C-N-CA	5.29	127.83	120.63
1	A	90	ALA	CA-C-N	-5.27	112.69	120.28
1	A	90	ALA	C-N-CA	-5.27	112.69	120.28
1	A	39	THR	N-CA-CB	5.26	119.27	110.32
1	A	115	ILE	CG1-CB-CG2	5.26	126.48	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ASN	CA-C-N	-5.26	114.83	120.03
1	A	52	ASN	C-N-CA	-5.26	114.83	120.03
1	A	74	ASP	CB-CG-OD2	5.24	130.46	118.40
1	A	26	PHE	CA-C-N	5.24	128.03	120.38
1	A	26	PHE	C-N-CA	5.24	128.03	120.38
1	A	104	ILE	CB-CG1-CD1	-5.22	102.83	113.80
1	A	48	MET	CB-CG-SD	-5.22	97.04	112.70
1	A	47	ARG	CA-CB-CG	-5.21	103.67	114.10
1	A	16	GLU	CA-CB-CG	-5.20	103.70	114.10
1	A	56	GLU	CA-C-O	5.20	126.28	120.82
1	A	23	LYS	CB-CG-CD	5.18	123.22	111.30
1	A	146	ASP	N-CA-C	-5.18	106.81	113.02
1	A	115	ILE	CA-CB-CG2	-5.17	101.72	110.50
1	A	135	GLU	CB-CG-CD	-5.16	103.84	112.60
1	A	42	LEU	N-CA-C	5.15	117.29	111.11
1	A	158	MET	O-C-N	-5.15	116.47	122.03
1	A	55	LYS	CD-CE-NZ	5.14	128.36	111.90
1	A	31	ALA	O-C-N	5.13	128.00	122.15
1	A	14	LEU	CA-C-N	-5.09	110.63	121.32
1	A	14	LEU	C-N-CA	-5.09	110.63	121.32
1	A	33	GLY	N-CA-C	-5.09	104.60	113.76
1	A	95	GLU	CB-CA-C	-5.07	102.23	110.85
1	A	139	LYS	CB-CG-CD	5.07	122.96	111.30
1	A	161	VAL	CA-CB-CG1	5.07	119.01	110.40
1	A	56	GLU	N-CA-C	-5.06	105.66	111.07
1	A	80	VAL	CB-CA-C	-5.06	105.31	112.14
1	A	63	GLU	O-C-N	-5.04	116.40	122.15
1	A	114	ASP	CB-CA-C	5.04	121.69	111.60
1	A	16	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	116	GLU	CG-CD-OE2	-5.03	106.84	118.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1257	0	1178	55	1
2	A	2	0	0	0	0
3	A	68	0	0	5	3
All	All	1327	0	1178	55	3

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 (55) 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:119:GLY:HA2	1:A:134:ILE:HD13	1.24	1.13
1:A:141:SER:O	1:A:143:LYS:HD3	1.61	0.98
1:A:6:GLN:NE2	3:A:199:HOH:O	1.94	0.94
1:A:105:PHE:CE2	1:A:121:ILE:HG21	2.05	0.92
1:A:60:ALA:O	1:A:63:GLU:HG2	1.73	0.88
1:A:151:PHE:O	1:A:155:LEU:HD13	1.74	0.87
1:A:119:GLY:HA2	1:A:134:ILE:CD1	2.05	0.84
1:A:107:LYS:HZ1	1:A:121:ILE:HG12	1.49	0.77
1:A:143:LYS:HE2	1:A:156:LYS:CE	2.16	0.76
1:A:77:GLU:HG2	3:A:188:HOH:O	1.87	0.75
1:A:156:LYS:HG2	1:A:162:GLN:O	1.87	0.75
1:A:143:LYS:HE2	1:A:156:LYS:HE2	1.73	0.70
1:A:60:ALA:O	1:A:63:GLU:CG	2.39	0.70
1:A:105:PHE:CE2	1:A:121:ILE:CG2	2.75	0.69
1:A:51:GLN:NE2	1:A:89:ASP:OD2	2.28	0.67
1:A:107:LYS:NZ	1:A:121:ILE:HG12	2.10	0.65
1:A:5:ASP:O	1:A:9:GLU:HG3	1.97	0.65
1:A:105:PHE:CZ	1:A:121:ILE:HG21	2.34	0.62
1:A:119:GLY:CA	1:A:134:ILE:HD13	2.16	0.61
1:A:77:GLU:CG	3:A:188:HOH:O	2.46	0.60
1:A:151:PHE:CZ	1:A:155:LEU:HD11	2.36	0.60
1:A:63:GLU:HG3	1:A:64:GLU:N	2.16	0.60
1:A:155:LEU:HD12	1:A:155:LEU:N	2.17	0.59
1:A:156:LYS:HA	1:A:162:GLN:HB3	1.83	0.59
1:A:156:LYS:HG2	1:A:162:GLN:C	2.27	0.58
1:A:23:LYS:HD3	1:A:75:PHE:CD2	2.39	0.58
1:A:119:GLY:O	1:A:123:ARG:HD2	2.04	0.57
1:A:143:LYS:HE2	1:A:156:LYS:HE3	1.87	0.56
1:A:56:GLU:CD	1:A:56:GLU:C	2.74	0.56
1:A:63:GLU:HB3	3:A:215:HOH:O	2.05	0.55
1:A:53:PRO:HG2	1:A:58:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:O	1:A:72:THR:HA	2.08	0.53
1:A:60:ALA:C	1:A:63:GLU:HG2	2.33	0.52
1:A:23:LYS:HD3	1:A:75:PHE:CE2	2.45	0.51
1:A:122:LEU:HD11	1:A:137:LEU:HD23	1.92	0.51
1:A:106:ASP:OD1	1:A:109:ALA:HA	2.11	0.50
1:A:30:ASP:OD1	1:A:33:GLY:N	2.46	0.49
1:A:3:ALA:O	1:A:7:GLN:HG3	2.13	0.49
1:A:112:PHE:CD2	1:A:148:ARG:HG3	2.48	0.48
1:A:115:ILE:H	1:A:115:ILE:HG13	1.46	0.47
1:A:80:VAL:O	1:A:84:ARG:HG3	2.15	0.46
1:A:155:LEU:N	1:A:155:LEU:CD1	2.79	0.46
1:A:141:SER:C	1:A:143:LYS:HD3	2.37	0.46
1:A:53:PRO:HG2	1:A:58:LEU:CD2	2.47	0.44
1:A:123:ARG:HH11	1:A:123:ARG:HD3	1.33	0.44
1:A:56:GLU:C	1:A:56:GLU:OE1	2.61	0.43
1:A:42:LEU:HD11	1:A:46:MET:HE3	2.00	0.43
1:A:151:PHE:O	1:A:155:LEU:CD1	2.57	0.43
1:A:121:ILE:HD13	1:A:121:ILE:HA	1.84	0.43
1:A:61:ILE:CG2	1:A:81:MET:HG3	2.50	0.42
1:A:156:LYS:HE2	1:A:156:LYS:HB2	1.67	0.42
1:A:15:SER:O	1:A:19:ILE:HG13	2.20	0.41
1:A:115:ILE:HG13	3:A:170:HOH:O	2.22	0.40
1:A:52:ASN:HD22	1:A:52:ASN:HA	1.43	0.40
1:A:113:ILE:HD13	1:A:113:ILE:HG21	1.65	0.40

All (3) 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)
3:A:236:HOH:O	3:A:239:HOH:O[3_564]	1.54	0.66
3:A:233:HOH:O	3:A:234:HOH:O[6_554]	2.00	0.20
1:A:133:ASP:OD1	3:A:218:HOH:O[2_664]	2.06	0.14

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	158/162 (98%)	156 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/136 (98%)	106 (79%)	28 (21%)	1	0

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	32	ASP
1	A	40	LYS
1	A	49	LEU
1	A	52	ASN
1	A	55	LYS
1	A	58	LEU
1	A	74	ASP
1	A	76	GLU
1	A	79	LEU
1	A	82	MET
1	A	88	GLU
1	A	91	LYS
1	A	93	LYS
1	A	98	LEU
1	A	103	ARG
1	A	105	PHE
1	A	107	LYS
1	A	115	ILE
1	A	116	GLU
1	A	123	ARG

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Mol	Chain	Res	Type
1	A	129	VAL
1	A	132	GLU
1	A	140	ASP
1	A	143	LYS
1	A	156	LYS
1	A	161	VAL
1	A	162	GLN

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

Mol	Chain	Res	Type
1	A	7	GLN
1	A	52	ASN
1	A	162	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	62:ILE	C	63:GLU	N	1.19

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.