



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:46 PM UTC

PDB ID : 1DU4 / pdb_00001du4
Title : THE STRUCTURAL ORIGINS OF INTERFACIAL ACTIVATION IN THERMOMYCES (HUMICOLA) LANUGINOSA LIPASE OTHER STRUCTURE DETAILS
Authors : Brozozowski, A.M.; Savage, H.
Deposited on : 2000-01-14
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 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

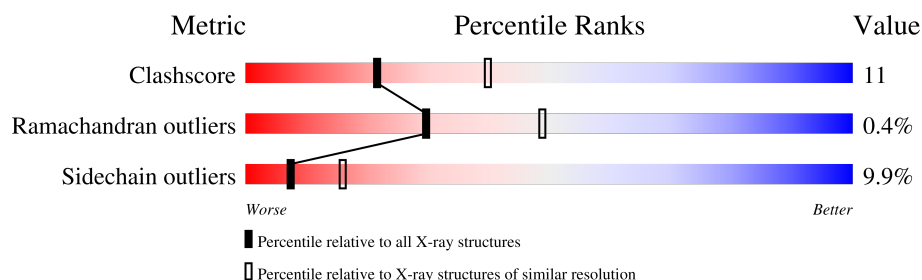
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 ≥ 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	269	 66% 27% 6% .
1	B	269	 62% 29% 6% .
1	C	269	 67% 25% 7% .
1	D	269	 68% 24% 7% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8935 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 LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	B	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	C	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	D	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			

- Molecule 2 is water.

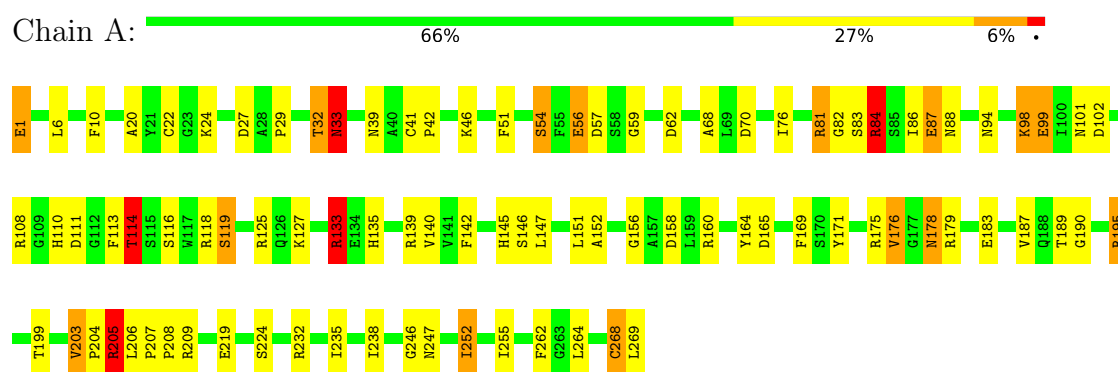
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	179	Total	O	0	0
			179	179		
2	B	162	Total	O	0	0
			162	162		
2	C	173	Total	O	0	0
			173	173		
2	D	137	Total	O	0	0
			137	137		

3 Residue-property plots

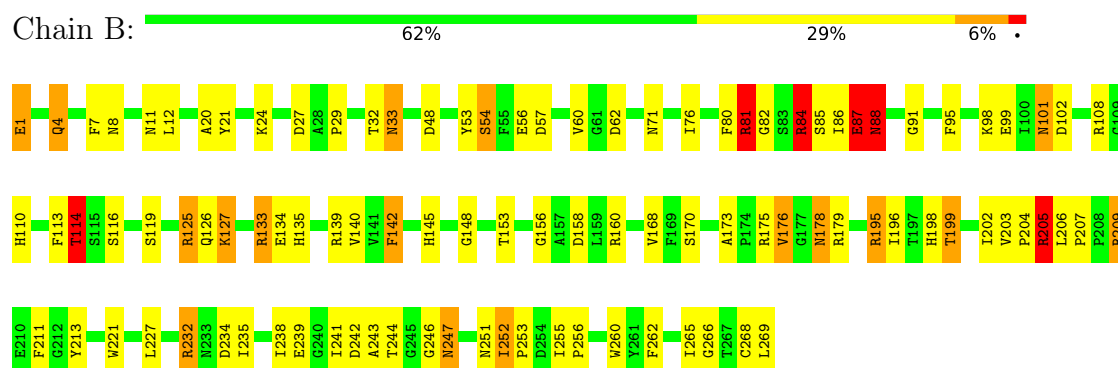
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

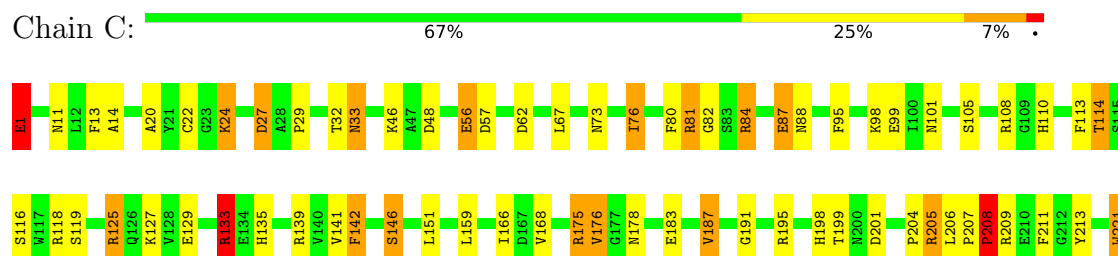
• Molecule 1: LIPASE



• Molecule 1: LIPASE



• Molecule 1: LIPASE



[illegible]

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.56Å 171.16Å 77.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.2 (30.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8935	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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	A	0.76	0/2121	2.00	50/2887 (1.7%)
1	B	0.70	0/2121	1.94	67/2887 (2.3%)
1	C	0.68	0/2121	1.89	48/2887 (1.7%)
1	D	0.67	1/2121 (0.0%)	1.90	41/2887 (1.4%)
All	All	0.70	1/8484 (0.0%)	1.93	206/11548 (1.8%)

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	2
1	B	0	2
1	C	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175	ARG	CD-NE	-5.12	1.39	1.46

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ARG	CD-NE-CZ	28.64	164.49	124.40
1	D	175	ARG	CD-NE-CZ	28.31	164.04	124.40
1	C	175	ARG	CD-NE-CZ	26.59	161.62	124.40
1	C	195	ARG	CD-NE-CZ	24.81	159.14	124.40
1	B	195	ARG	CD-NE-CZ	17.05	148.27	124.40
1	A	205	ARG	CD-NE-CZ	17.05	148.26	124.40
1	D	195	ARG	CD-NE-CZ	16.85	147.99	124.40
1	A	195	ARG	CD-NE-CZ	14.79	145.10	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	205	ARG	CD-NE-CZ	13.84	143.77	124.40
1	B	84	ARG	NE-CZ-NH2	-12.56	107.89	119.20
1	B	175	ARG	NE-CZ-NH1	-11.94	109.56	121.50
1	B	205	ARG	CD-NE-CZ	11.87	141.01	124.40
1	A	195	ARG	NE-CZ-NH2	-11.59	108.77	119.20
1	D	175	ARG	NE-CZ-NH2	-11.31	109.03	119.20
1	B	87	GLU	CB-CG-CD	-10.79	94.25	112.60
1	B	87	GLU	OE1-CD-OE2	10.49	148.09	122.90
1	A	84	ARG	NE-CZ-NH1	10.46	131.96	121.50
1	C	195	ARG	NE-CZ-NH2	-10.40	109.84	119.20
1	B	205	ARG	NE-CZ-NH1	10.07	131.57	121.50
1	A	33	ASN	CA-CB-CG	9.78	122.38	112.60
1	A	84	ARG	NE-CZ-NH2	-9.65	110.51	119.20
1	C	176	VAL	N-CA-CB	-9.31	100.25	112.36
1	D	81	ARG	NE-CZ-NH1	9.13	130.63	121.50
1	C	205	ARG	CD-NE-CZ	9.09	137.12	124.40
1	B	176	VAL	N-CA-CB	-8.95	100.72	112.36
1	D	9	GLN	CA-C-O	-8.78	111.60	120.82
1	C	251	ASN	CA-C-O	-8.55	111.91	121.40
1	A	70	ASP	CA-CB-CG	8.29	120.89	112.60
1	C	205	ARG	NE-CZ-NH1	8.15	129.65	121.50
1	B	205	ARG	NE-CZ-NH2	-8.11	111.90	119.20
1	D	108	ARG	CD-NE-CZ	8.02	135.63	124.40
1	D	176	VAL	N-CA-CB	-7.87	102.11	112.26
1	B	195	ARG	NE-CZ-NH2	-7.81	112.17	119.20
1	B	232	ARG	CD-NE-CZ	7.77	135.28	124.40
1	B	262	PHE	CA-C-N	7.73	133.18	121.04
1	B	262	PHE	C-N-CA	7.73	133.18	121.04
1	B	11	ASN	OD1-CG-ND2	7.71	130.31	122.60
1	B	80	PHE	CA-C-O	7.70	129.35	120.80
1	B	84	ARG	CD-NE-CZ	7.70	135.17	124.40
1	C	262	PHE	CA-C-N	7.69	133.37	121.37
1	C	262	PHE	C-N-CA	7.69	133.37	121.37
1	A	176	VAL	N-CA-CB	-7.45	102.68	112.36
1	B	11	ASN	CA-CB-CG	-7.40	105.20	112.60
1	B	87	GLU	CG-CD-OE2	-7.40	101.38	118.40
1	C	249	GLN	O-C-N	7.40	127.64	121.35
1	A	171	TYR	CA-C-O	-7.38	112.65	120.40
1	C	88	ASN	OD1-CG-ND2	7.34	129.94	122.60
1	A	175	ARG	NE-CZ-NH2	-7.34	112.59	119.20
1	D	7	PHE	CA-CB-CG	-7.32	106.48	113.80
1	B	247	ASN	CA-CB-CG	7.25	119.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ARG	CA-C-N	7.11	130.11	120.38
1	A	118	ARG	C-N-CA	7.11	130.11	120.38
1	A	209	ARG	CD-NE-CZ	7.10	134.34	124.40
1	A	169	PHE	CA-CB-CG	7.01	120.81	113.80
1	B	84	ARG	NE-CZ-NH1	6.93	128.43	121.50
1	C	175	ARG	N-CA-C	-6.93	100.72	110.50
1	A	10	PHE	CA-C-N	6.92	129.88	120.54
1	A	10	PHE	C-N-CA	6.92	129.88	120.54
1	B	175	ARG	CD-NE-CZ	6.92	134.09	124.40
1	C	118	ARG	CA-C-N	6.89	129.82	120.38
1	C	118	ARG	C-N-CA	6.89	129.82	120.38
1	A	113	PHE	CA-C-O	6.89	128.05	120.82
1	B	178	ASN	CA-CB-CG	6.88	119.48	112.60
1	A	142	PHE	CA-CB-CG	6.84	120.64	113.80
1	B	81	ARG	NE-CZ-NH1	6.82	128.32	121.50
1	C	252	ILE	N-CA-CB	6.80	117.50	110.23
1	D	4	GLN	CA-C-O	-6.79	112.42	120.10
1	A	262	PHE	CA-CB-CG	-6.79	107.01	113.80
1	B	4	GLN	CA-C-O	-6.79	113.36	120.55
1	A	203	VAL	O-C-N	-6.75	113.40	121.10
1	D	201	ASP	CA-CB-CG	6.63	119.23	112.60
1	B	179	ARG	NE-CZ-NH2	-6.62	113.25	119.20
1	A	114	THR	N-CA-CB	-6.59	100.45	110.01
1	C	95	PHE	CA-CB-CG	6.56	120.36	113.80
1	A	224	SER	CA-C-N	6.55	127.94	120.53
1	A	224	SER	C-N-CA	6.55	127.94	120.53
1	C	225	GLY	N-CA-C	6.53	119.51	112.33
1	B	158	ASP	N-CA-C	6.47	118.41	111.36
1	B	176	VAL	CB-CA-C	6.40	117.97	110.93
1	B	203	VAL	CA-C-N	6.36	127.17	120.12
1	B	203	VAL	C-N-CA	6.36	127.17	120.12
1	B	175	ARG	NH1-CZ-NH2	6.35	127.56	119.30
1	C	76	ILE	CA-C-O	-6.35	113.79	120.39
1	D	146	SER	CB-CA-C	-6.32	109.30	116.63
1	B	101	ASN	CA-CB-CG	-6.28	106.33	112.60
1	A	187	VAL	N-CA-CB	-6.27	103.79	111.94
1	A	22	CYS	CA-C-N	6.25	127.03	120.03
1	A	22	CYS	C-N-CA	6.25	127.03	120.03
1	C	142	PHE	CA-CB-CG	6.23	120.03	113.80
1	D	84	ARG	NE-CZ-NH1	6.17	127.67	121.50
1	B	142	PHE	CA-CB-CG	6.16	119.96	113.80
1	D	113	PHE	CA-C-O	6.13	127.26	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	ARG	CD-NE-CZ	6.13	132.98	124.40
1	D	90	ILE	N-CA-C	6.12	116.30	110.42
1	B	209	ARG	NE-CZ-NH2	-6.11	113.70	119.20
1	A	133	ARG	CD-NE-CZ	6.11	132.95	124.40
1	D	183	GLU	CA-C-O	6.07	127.19	120.82
1	B	211	PHE	CA-C-O	6.06	126.65	119.56
1	D	110	HIS	CA-CB-CG	6.05	119.85	113.80
1	C	48	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	27	ASP	CA-C-O	6.02	127.27	121.67
1	A	94	ASN	CA-CB-CG	-5.97	106.62	112.60
1	B	7	PHE	CA-CB-CG	-5.96	107.84	113.80
1	B	148	GLY	CA-C-N	5.92	126.51	119.94
1	B	148	GLY	C-N-CA	5.92	126.51	119.94
1	C	11	ASN	CA-CB-CG	-5.91	106.69	112.60
1	C	221	TRP	N-CA-C	5.91	118.36	108.73
1	C	146	SER	CB-CA-C	-5.90	109.79	116.63
1	A	84	ARG	CD-NE-CZ	5.88	132.63	124.40
1	D	211	PHE	CA-C-N	5.86	129.58	121.26
1	D	211	PHE	C-N-CA	5.86	129.58	121.26
1	D	158	ASP	N-CA-C	5.83	117.71	111.36
1	A	114	THR	O-C-N	-5.80	116.09	122.07
1	A	135	HIS	CA-C-N	5.80	125.48	119.56
1	A	135	HIS	C-N-CA	5.80	125.48	119.56
1	A	139	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	D	22	CYS	CA-C-N	5.80	126.53	120.03
1	D	22	CYS	C-N-CA	5.80	126.53	120.03
1	A	232	ARG	CD-NE-CZ	5.80	132.52	124.40
1	A	88	ASN	OD1-CG-ND2	5.75	128.35	122.60
1	C	241	ILE	CB-CG1-CD1	5.71	125.79	113.80
1	D	268	CYS	CA-C-O	-5.70	114.42	120.92
1	B	232	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	C	201	ASP	CA-CB-CG	5.69	118.29	112.60
1	D	151	LEU	CA-C-N	5.65	127.79	120.44
1	D	151	LEU	C-N-CA	5.65	127.79	120.44
1	B	244	THR	CA-C-O	-5.64	112.75	119.35
1	B	211	PHE	CA-CB-CG	-5.63	108.17	113.80
1	B	140	VAL	CA-C-O	5.63	127.27	120.85
1	D	84	ARG	CD-NE-CZ	5.62	132.27	124.40
1	D	10	PHE	CA-CB-CG	5.61	119.41	113.80
1	B	173	ALA	CA-C-O	5.58	124.88	120.19
1	B	54	SER	CA-C-O	-5.56	114.69	120.70
1	C	73	ASN	CA-CB-CG	-5.56	107.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	ASN	OD1-CG-ND2	5.55	128.15	122.60
1	A	255	ILE	O-C-N	-5.53	114.80	121.10
1	B	87	GLU	O-C-N	-5.52	116.27	122.12
1	B	153	THR	CA-C-O	5.52	126.61	120.82
1	D	175	ARG	NH1-CZ-NH2	5.49	126.44	119.30
1	D	178	ASN	CA-CB-CG	5.49	118.08	112.60
1	A	39	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	C	14	ALA	CA-C-O	5.47	126.35	120.55
1	B	81	ARG	CB-CG-CD	-5.46	98.73	111.30
1	B	243	ALA	CA-C-O	-5.46	115.76	121.55
1	A	133	ARG	CB-CG-CD	5.44	123.81	111.30
1	C	244	THR	CA-C-O	-5.44	112.99	119.35
1	C	142	PHE	N-CA-CB	5.43	119.44	110.69
1	C	252	ILE	CA-C-O	5.43	123.92	119.47
1	A	133	ARG	NH1-CZ-NH2	-5.42	112.26	119.30
1	D	262	PHE	CA-C-N	5.41	129.33	120.51
1	D	262	PHE	C-N-CA	5.41	129.33	120.51
1	B	8	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	C	208	PRO	CA-C-O	-5.40	115.20	121.95
1	A	268	CYS	CA-C-O	-5.39	114.77	120.92
1	B	234	ASP	CA-CB-CG	-5.39	107.21	112.60
1	A	152	ALA	CA-C-O	-5.39	114.84	120.55
1	C	22	CYS	CA-C-N	5.38	126.06	120.03
1	C	22	CYS	C-N-CA	5.38	126.06	120.03
1	B	244	THR	N-CA-C	5.38	119.94	113.17
1	B	88	ASN	OD1-CG-ND2	5.37	127.97	122.60
1	C	76	ILE	N-CA-C	-5.36	99.92	107.75
1	D	233	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	A	195	ARG	NH1-CZ-NH2	5.34	126.24	119.30
1	B	81	ARG	CB-CA-C	5.34	118.64	109.51
1	A	158	ASP	N-CA-C	5.33	116.77	111.07
1	C	113	PHE	CA-C-O	5.33	126.41	120.82
1	D	195	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	D	60	VAL	N-CA-C	5.31	115.97	110.82
1	C	135	HIS	CA-C-N	5.30	124.97	119.56
1	C	135	HIS	C-N-CA	5.30	124.97	119.56
1	D	224	SER	CB-CA-C	5.29	119.09	109.62
1	B	196	ILE	N-CA-CB	-5.29	104.96	110.72
1	B	203	VAL	N-CA-C	5.27	118.68	112.35
1	D	211	PHE	CA-C-O	5.27	127.34	119.23
1	C	11	ASN	O-C-N	-5.25	116.55	122.12
1	C	187	VAL	N-CA-C	5.25	117.44	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	THR	O-C-N	-5.24	116.56	122.12
1	B	88	ASN	CA-C-O	5.24	125.97	120.42
1	D	231	THR	N-CA-CB	5.23	118.77	110.87
1	B	71	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	B	91	GLY	CA-C-O	5.21	125.65	119.50
1	B	60	VAL	N-CA-C	5.21	116.67	111.00
1	C	27	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	1	GLU	CA-C-N	-5.20	115.11	122.34
1	C	1	GLU	C-N-CA	-5.20	115.11	122.34
1	C	129	GLU	CB-CG-CD	5.20	121.43	112.60
1	A	6	LEU	CA-C-O	5.19	126.00	120.24
1	B	251	ASN	CA-C-O	-5.19	115.32	121.60
1	D	179	ARG	NE-CZ-NH2	-5.18	114.53	119.20
1	B	86	ILE	O-C-N	-5.18	116.37	121.96
1	A	219	GLU	CA-C-O	-5.16	114.72	120.66
1	C	80	PHE	CA-CB-CG	5.16	118.96	113.80
1	B	135	HIS	CA-C-N	5.15	124.82	119.56
1	B	135	HIS	C-N-CA	5.15	124.82	119.56
1	B	48	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	86	ILE	CB-CG1-CD1	5.15	124.61	113.80
1	A	114	THR	CA-CB-CG2	5.13	119.22	110.50
1	D	4	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	A	178	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	76	ILE	O-C-N	5.10	128.45	122.99
1	A	183	GLU	O-C-N	-5.09	116.01	122.27
1	D	248	ASN	OD1-CG-ND2	5.07	127.67	122.60
1	C	195	ARG	NH1-CZ-NH2	5.05	125.87	119.30
1	C	252	ILE	CB-CA-C	5.01	115.60	110.94
1	B	113	PHE	CA-C-N	5.00	126.98	120.28
1	B	113	PHE	C-N-CA	5.00	126.98	120.28

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	VAL	Mainchain
1	A	68	ALA	Mainchain
1	B	170	SER	Mainchain
1	B	76	ILE	Mainchain
1	C	208	PRO	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	2071	0	1965	44	0
1	B	2071	0	1965	42	0
1	C	2071	0	1965	47	0
1	D	2071	0	1965	42	0
2	A	179	0	0	6	0
2	B	162	0	0	8	0
2	C	173	0	0	5	0
2	D	137	0	0	6	0
All	All	8935	0	7860	175	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 11.

All (175) 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:33:ASN:HD22	1:A:33:ASN:H	1.22	0.86
1:B:20:ALA:HB1	1:B:81:ARG:HB2	1.64	0.80
1:B:87:GLU:HG2	2:B:430:HOH:O	1.83	0.77
1:C:20:ALA:HB1	1:C:81:ARG:HB2	1.69	0.74
1:C:84:ARG:HD3	1:C:84:ARG:O	1.86	0.74
1:B:81:ARG:HD3	1:B:82:GLY:O	1.87	0.73
1:C:209:ARG:HD2	1:C:213:TYR:O	1.90	0.71
1:B:84:ARG:O	1:B:84:ARG:HD3	1.90	0.71
1:A:84:ARG:O	1:A:84:ARG:HD3	1.91	0.70
1:A:110:HIS:O	1:A:114:THR:HB	1.90	0.70
1:C:27:ASP:HB2	2:C:330:HOH:O	1.89	0.70
1:A:81:ARG:HD3	1:A:82:GLY:O	1.92	0.70
1:A:99:GLU:OE1	1:A:101:ASN:ND2	2.24	0.69
1:A:33:ASN:HD22	1:A:33:ASN:N	1.92	0.68
1:C:125:ARG:HD3	1:C:159:LEU:HD22	1.76	0.67
1:D:1:GLU:HB2	1:D:235:ILE:O	1.95	0.66
1:C:110:HIS:O	1:C:114:THR:HB	1.95	0.65
1:D:208:PRO:HD2	1:D:211:PHE:HD1	1.60	0.65
1:A:20:ALA:HB1	1:A:81:ARG:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:HG3	1:A:178:ASN:ND2	2.12	0.65
1:C:33:ASN:HD22	1:C:33:ASN:H	1.45	0.63
1:C:81:ARG:HD3	1:C:82:GLY:O	1.98	0.63
1:A:206:LEU:HA	1:A:207:PRO:C	2.25	0.62
1:B:232:ARG:HD3	2:B:281:HOH:O	1.99	0.61
1:D:125:ARG:HD3	1:D:159:LEU:HD22	1.83	0.60
1:D:84:ARG:NH2	1:D:268:CYS:O	2.34	0.60
1:D:33:ASN:H	1:D:33:ASN:HD22	1.49	0.59
1:C:108:ARG:HG3	1:C:178:ASN:ND2	2.18	0.58
1:C:183:GLU:HG3	1:C:241:ILE:HD12	1.85	0.57
1:C:133:ARG:HG2	1:C:133:ARG:HH11	1.70	0.57
1:B:239:GLU:HG3	2:B:296:HOH:O	2.05	0.57
1:D:110:HIS:O	1:D:114:THR:HB	2.04	0.57
1:C:238:ILE:HD13	1:C:246:GLY:CA	2.35	0.56
1:C:206:LEU:HA	1:C:207:PRO:C	2.31	0.56
1:B:85:SER:OG	1:B:88:ASN:HB2	2.04	0.56
1:D:84:ARG:O	1:D:84:ARG:HD3	2.06	0.56
1:B:110:HIS:O	1:B:114:THR:HB	2.05	0.56
1:A:29:PRO:O	1:A:32:THR:HB	2.06	0.55
1:C:84:ARG:NH2	1:C:268:CYS:O	2.39	0.55
1:A:1:GLU:HB2	1:A:235:ILE:O	2.05	0.55
1:A:81:ARG:NH2	1:A:84:ARG:HG2	2.21	0.55
1:C:1:GLU:HB2	1:C:235:ILE:O	2.07	0.55
1:C:133:ARG:HD3	2:C:376:HOH:O	2.06	0.55
1:B:126:GLN:HB2	2:B:412:HOH:O	2.06	0.55
1:A:165:ASP:OD1	1:A:190:GLY:HA2	2.07	0.55
1:B:133:ARG:HG2	1:B:133:ARG:HH11	1.72	0.55
1:D:108:ARG:HG3	1:D:178:ASN:ND2	2.22	0.54
1:A:133:ARG:HH11	1:A:133:ARG:HG3	1.72	0.54
1:C:116:SER:O	1:C:119:SER:HB2	2.08	0.54
1:A:87:GLU:HB3	2:A:321:HOH:O	2.07	0.54
1:D:85:SER:HB2	2:D:293:HOH:O	2.07	0.54
1:A:57:ASP:OD1	1:A:62:ASP:HB3	2.08	0.54
1:D:73:ASN:O	1:D:74:LYS:HB2	2.09	0.52
1:B:1:GLU:HB2	1:B:235:ILE:O	2.09	0.52
1:A:57:ASP:HA	1:A:62:ASP:HA	1.91	0.52
1:B:206:LEU:HA	1:B:207:PRO:C	2.34	0.52
1:C:13:PHE:CE1	1:C:141:VAL:HG11	2.46	0.51
1:D:20:ALA:HB1	1:D:81:ARG:HB2	1.93	0.51
1:D:53:TYR:CD1	1:D:127:LYS:HE3	2.46	0.51
1:D:189:THR:HA	2:D:351:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ARG:NH2	1:B:268:CYS:O	2.40	0.50
1:D:206:LEU:HA	1:D:207:PRO:C	2.36	0.50
1:C:252:ILE:HD12	1:C:253:PRO:O	2.12	0.50
1:D:5:ASP:O	1:D:9:GLN:HG3	2.11	0.50
1:A:33:ASN:H	1:A:33:ASN:ND2	2.02	0.50
1:D:204:PRO:HB2	1:D:247:ASN:OD1	2.12	0.50
1:A:133:ARG:HH11	1:A:133:ARG:CG	2.25	0.50
1:B:29:PRO:O	1:B:32:THR:HB	2.12	0.50
1:A:87:GLU:H	1:A:87:GLU:CD	2.20	0.49
1:B:252:ILE:HD11	2:B:340:HOH:O	2.11	0.49
1:B:125:ARG:HG2	2:B:371:HOH:O	2.11	0.49
1:D:261:TYR:O	1:D:262:PHE:HB2	2.12	0.49
1:A:156:GLY:O	1:A:160:ARG:HG3	2.12	0.49
1:C:101:ASN:OD1	1:C:105:SER:HA	2.12	0.49
1:D:179:ARG:HD2	1:D:241:ILE:HG21	1.95	0.49
1:A:204:PRO:HB2	1:A:247:ASN:OD1	2.13	0.48
1:D:130:ASP:O	1:D:133:ARG:HG2	2.14	0.48
1:C:238:ILE:HD13	1:C:246:GLY:HA3	1.95	0.48
1:B:12:LEU:HD13	2:B:310:HOH:O	2.14	0.48
1:C:228:VAL:CG1	1:C:229:PRO:HD2	2.43	0.48
1:D:27:ASP:HB2	2:D:288:HOH:O	2.13	0.48
1:B:238:ILE:HD13	1:B:246:GLY:HA3	1.96	0.48
1:D:246:GLY:O	1:D:249:GLN:HG3	2.14	0.48
1:A:84:ARG:NH2	1:A:268:CYS:O	2.42	0.47
1:A:41:CYS:N	1:A:42:PRO:CD	2.78	0.47
1:A:32:THR:HG22	1:A:51:PHE:CD2	2.50	0.47
1:C:204:PRO:HB2	1:C:247:ASN:OD1	2.14	0.47
1:D:87:GLU:H	1:D:87:GLU:CD	2.22	0.47
1:A:98:LYS:HG2	1:A:111:ASP:HA	1.97	0.47
1:A:238:ILE:HD13	1:A:246:GLY:CA	2.45	0.47
1:D:4:GLN:OE1	1:D:232:ARG:HD2	2.15	0.46
1:B:57:ASP:HA	1:B:62:ASP:HA	1.98	0.46
1:B:145:HIS:HB2	1:B:265:ILE:HD11	1.97	0.46
1:D:33:ASN:ND2	1:D:33:ASN:N	2.63	0.46
1:A:116:SER:O	1:A:119:SER:HB2	2.15	0.46
1:A:145:HIS:CE1	1:A:146:SER:HB2	2.50	0.46
1:B:252:ILE:HD12	1:B:253:PRO:O	2.15	0.46
1:D:20:ALA:O	1:D:81:ARG:HG3	2.16	0.46
1:D:81:ARG:HD2	1:D:82:GLY:O	2.16	0.46
1:A:252:ILE:HD11	2:A:317:HOH:O	2.16	0.46
1:C:57:ASP:HA	1:C:62:ASP:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:PRO:O	1:C:32:THR:HB	2.15	0.46
1:A:54:SER:HB2	2:A:396:HOH:O	2.15	0.45
1:D:21:TYR:CD2	1:D:266:GLY:HA2	2.52	0.45
1:B:207:PRO:HG2	1:B:213:TYR:CZ	2.52	0.45
1:B:116:SER:O	1:B:119:SER:HB2	2.16	0.45
1:B:255:ILE:N	1:B:256:PRO:CD	2.79	0.45
1:D:207:PRO:HG2	1:D:213:TYR:CZ	2.51	0.45
1:A:205:ARG:HG3	2:A:295:HOH:O	2.17	0.45
1:B:84:ARG:HD3	1:B:84:ARG:C	2.39	0.45
1:C:226:THR:HG22	1:C:227:LEU:HG	1.99	0.45
1:B:57:ASP:OD1	1:B:62:ASP:HB3	2.17	0.45
1:B:108:ARG:HG3	1:B:178:ASN:ND2	2.31	0.45
1:D:179:ARG:HB3	2:D:337:HOH:O	2.15	0.45
1:B:33:ASN:HD22	1:B:33:ASN:H	1.65	0.45
1:D:160:ARG:NH1	1:D:188:GLN:OE1	2.50	0.45
1:A:206:LEU:HD23	1:A:208:PRO:HD3	1.98	0.44
1:B:21:TYR:CE2	1:B:266:GLY:HA2	2.53	0.44
1:D:126:GLN:HG2	2:D:381:HOH:O	2.17	0.44
1:C:175:ARG:HD2	1:C:213:TYR:HB3	2.00	0.44
1:A:32:THR:HG22	1:A:51:PHE:HD2	1.81	0.44
1:B:53:TYR:CD2	1:B:127:LYS:HD3	2.52	0.44
1:B:142:PHE:O	1:B:168:VAL:HA	2.17	0.44
1:A:27:ASP:OD1	1:A:56:GLU:OE1	2.35	0.44
1:C:46:LYS:HE2	2:C:379:HOH:O	2.18	0.44
1:C:33:ASN:H	1:C:33:ASN:ND2	2.13	0.44
1:B:4:GLN:OE1	1:B:232:ARG:HD2	2.18	0.44
1:D:99:GLU:HB2	2:D:353:HOH:O	2.17	0.43
1:D:99:GLU:OE1	1:D:101:ASN:ND2	2.50	0.43
1:D:57:ASP:HA	1:D:62:ASP:HA	2.01	0.43
1:D:175:ARG:HG2	1:D:215:HIS:CE1	2.52	0.43
1:C:67:LEU:HD11	1:C:76:ILE:HG22	2.01	0.43
1:D:133:ARG:HG2	1:D:133:ARG:HH11	1.83	0.43
1:A:147:LEU:HD12	1:A:147:LEU:O	2.18	0.43
1:B:156:GLY:O	1:B:160:ARG:HG3	2.18	0.43
1:D:166:ILE:O	1:D:191:GLY:HA3	2.19	0.43
1:C:33:ASN:ND2	1:C:33:ASN:N	2.66	0.43
1:C:87:GLU:H	1:C:87:GLU:CD	2.26	0.43
1:D:81:ARG:CD	1:D:82:GLY:O	2.66	0.43
1:A:1:GLU:HG3	1:A:235:ILE:O	2.19	0.42
1:B:241:ILE:O	1:B:242:ASP:HB2	2.18	0.42
1:B:202:ILE:HB	1:B:253:PRO:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:LYS:HG2	2:C:419:HOH:O	2.18	0.42
1:D:33:ASN:H	1:D:33:ASN:ND2	2.15	0.42
1:D:221:TRP:CE3	1:D:246:GLY:HA2	2.54	0.42
1:B:198:HIS:O	1:B:199:THR:C	2.63	0.42
1:C:198:HIS:O	1:C:199:THR:C	2.62	0.42
1:A:81:ARG:CD	1:A:82:GLY:O	2.63	0.42
1:D:255:ILE:N	1:D:256:PRO:CD	2.83	0.42
1:C:166:ILE:O	1:C:191:GLY:HA3	2.20	0.42
1:B:221:TRP:CE3	1:B:246:GLY:HA2	2.55	0.41
1:C:227:LEU:HD23	1:C:260:TRP:CE3	2.55	0.41
1:C:187:VAL:HG22	1:C:187:VAL:O	2.20	0.41
1:A:238:ILE:HD13	1:A:246:GLY:HA3	2.02	0.41
1:A:140:VAL:HG21	1:A:164:TYR:CD2	2.54	0.41
1:C:207:PRO:HB2	1:C:213:TYR:CD1	2.55	0.41
1:A:179:ARG:NH1	2:A:325:HOH:O	2.54	0.41
1:B:195:ARG:HG3	2:B:379:HOH:O	2.21	0.41
1:D:142:PHE:O	1:D:168:VAL:HA	2.21	0.41
1:A:59:GLY:HA3	1:A:119:SER:HB3	2.03	0.41
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.90	0.41
1:A:195:ARG:HG3	2:A:366:HOH:O	2.19	0.41
1:C:27:ASP:OD2	1:C:56:GLU:OE1	2.38	0.41
1:C:253:PRO:HD2	2:C:420:HOH:O	2.20	0.41
1:C:142:PHE:O	1:C:168:VAL:HA	2.21	0.41
1:C:221:TRP:CE3	1:C:246:GLY:HA2	2.56	0.41
1:C:227:LEU:HA	1:C:260:TRP:CE2	2.56	0.41
1:B:202:ILE:O	1:B:205:ARG:HB2	2.20	0.40
1:B:227:LEU:H	1:B:260:TRP:CG	2.39	0.40
1:B:204:PRO:HB2	1:B:247:ASN:OD1	2.20	0.40
1:C:227:LEU:H	1:C:260:TRP:CG	2.39	0.40
1:C:255:ILE:N	1:C:256:PRO:CD	2.85	0.40
1:B:95:PHE:CD1	1:B:207:PRO:HB3	2.57	0.40
1:C:151:LEU:HD23	1:C:151:LEU:HA	1.92	0.40
1:C:208:PRO:HG2	1:C:211:PHE:CE1	2.57	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	A	267/269 (99%)	258 (97%)	8 (3%)	1 (0%)	30	49
1	B	267/269 (99%)	260 (97%)	6 (2%)	1 (0%)	30	49
1	C	267/269 (99%)	257 (96%)	9 (3%)	1 (0%)	30	49
1	D	267/269 (99%)	260 (97%)	6 (2%)	1 (0%)	30	49
All	All	1068/1076 (99%)	1035 (97%)	29 (3%)	4 (0%)	30	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	199	THR
1	A	199	THR
1	D	262	PHE
1	C	262	PHE

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	220/220 (100%)	194 (88%)	26 (12%)	5	11
1	B	220/220 (100%)	196 (89%)	24 (11%)	6	13
1	C	220/220 (100%)	201 (91%)	19 (9%)	10	21
1	D	220/220 (100%)	202 (92%)	18 (8%)	10	23
All	All	880/880 (100%)	793 (90%)	87 (10%)	7	16

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	24	LYS
1	A	32	THR
1	A	33	ASN
1	A	46	LYS
1	A	54	SER
1	A	56	GLU
1	A	81	ARG
1	A	83	SER
1	A	84	ARG
1	A	86	ILE
1	A	87	GLU
1	A	98	LYS
1	A	99	GLU
1	A	102	ASP
1	A	114	THR
1	A	119	SER
1	A	125	ARG
1	A	127	LYS
1	A	133	ARG
1	A	176	VAL
1	A	189	THR
1	A	205	ARG
1	A	252	ILE
1	A	264	LEU
1	A	269	LEU
1	B	1	GLU
1	B	24	LYS
1	B	33	ASN
1	B	54	SER
1	B	56	GLU
1	B	81	ARG
1	B	84	ARG
1	B	87	GLU
1	B	88	ASN
1	B	98	LYS
1	B	99	GLU
1	B	101	ASN
1	B	102	ASP
1	B	114	THR
1	B	125	ARG
1	B	127	LYS

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Mol	Chain	Res	Type
1	B	133	ARG
1	B	134	GLU
1	B	139	ARG
1	B	176	VAL
1	B	205	ARG
1	B	209	ARG
1	B	252	ILE
1	B	269	LEU
1	C	1	GLU
1	C	24	LYS
1	C	33	ASN
1	C	56	GLU
1	C	81	ARG
1	C	84	ARG
1	C	87	GLU
1	C	98	LYS
1	C	99	GLU
1	C	114	THR
1	C	125	ARG
1	C	127	LYS
1	C	133	ARG
1	C	139	ARG
1	C	146	SER
1	C	176	VAL
1	C	205	ARG
1	C	241	ILE
1	C	252	ILE
1	D	1	GLU
1	D	24	LYS
1	D	33	ASN
1	D	46	LYS
1	D	56	GLU
1	D	83	SER
1	D	84	ARG
1	D	87	GLU
1	D	98	LYS
1	D	99	GLU
1	D	102	ASP
1	D	114	THR
1	D	125	ARG
1	D	127	LYS
1	D	139	ARG

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Mol	Chain	Res	Type
1	D	176	VAL
1	D	205	ARG
1	D	252	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	39	ASN
1	A	162	ASN
1	B	33	ASN
1	B	92	ASN
1	B	135	HIS
1	B	162	ASN
1	C	26	ASN
1	C	33	ASN
1	C	135	HIS
1	D	26	ASN
1	D	33	ASN
1	D	88	ASN
1	D	162	ASN
1	D	215	HIS

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 ⓘ

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.