



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:21 AM UTC

PDB ID : 1ALA / pdb_00001ala
Title : STRUCTURE OF CHICKEN ANNEXIN V AT 2.25-ANGSTROMS RESOLUTION
Authors : Waller, D.A.; Bewley, M.C.; Huber, R.
Deposited on : 1993-01-14
Resolution : 2.25 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

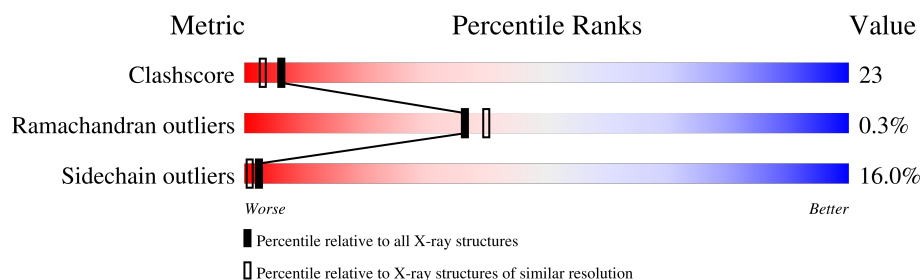
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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	321	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2587 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 ANNEXIN V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2503	1575	436	481	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	GLU	ASP	conflict	UNP P17153

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is water.

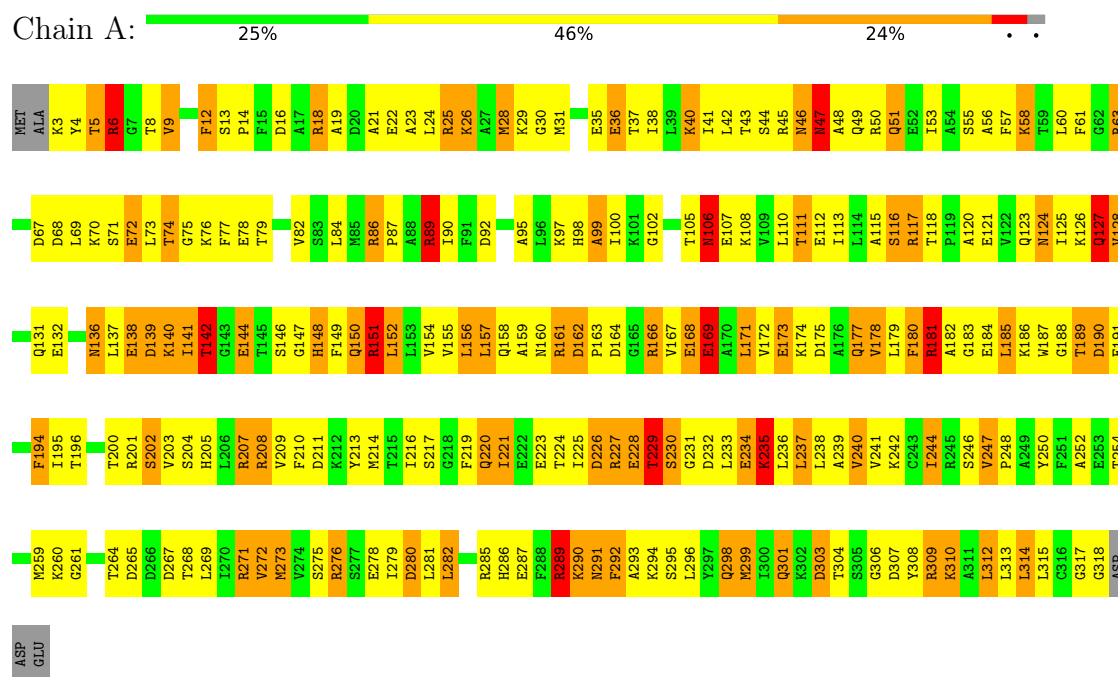
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		

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: ANNEXIN V



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	99.40Å 99.40Å 96.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2587	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.25	2/2537 (0.1%)	3.07	331/3412 (9.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	ILE	CA-CB	5.44	1.60	1.54
1	A	89	ARG	C-N	-5.09	1.27	1.33

All (331) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ARG	CD-NE-CZ	18.82	150.75	124.40
1	A	78	GLU	CB-CG-CD	15.85	139.54	112.60
1	A	208	ARG	CA-C-N	15.04	139.51	120.56
1	A	208	ARG	C-N-CA	15.04	139.51	120.56
1	A	89	ARG	CA-C-N	14.26	138.82	121.85
1	A	89	ARG	C-N-CA	14.26	138.82	121.85
1	A	6	ARG	NH1-CZ-NH2	-12.97	102.44	119.30
1	A	6	ARG	NE-CZ-NH1	12.92	134.42	121.50
1	A	285	ARG	NE-CZ-NH1	12.76	134.26	121.50
1	A	86	ARG	CD-NE-CZ	12.49	141.89	124.40
1	A	211	ASP	CA-CB-CG	12.42	125.02	112.60
1	A	230	SER	N-CA-C	11.49	127.71	109.79
1	A	285	ARG	NE-CZ-NH2	-11.40	108.94	119.20
1	A	195	ILE	CA-C-N	11.25	135.06	120.44
1	A	195	ILE	C-N-CA	11.25	135.06	120.44
1	A	292	PHE	CA-CB-CG	-11.20	102.60	113.80
1	A	301	GLN	OE1-CD-NE2	11.20	133.79	122.60
1	A	207	ARG	NE-CZ-NH2	10.87	128.99	119.20
1	A	172	VAL	CA-C-O	10.87	132.35	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	ASP	CA-CB-CG	-10.61	101.99	112.60
1	A	50	ARG	NE-CZ-NH2	10.57	128.72	119.20
1	A	68	ASP	CA-CB-CG	10.39	122.99	112.60
1	A	24	LEU	CA-C-N	10.29	133.81	120.44
1	A	24	LEU	C-N-CA	10.29	133.81	120.44
1	A	291	ASN	OD1-CG-ND2	-10.25	112.35	122.60
1	A	127	GLN	OE1-CD-NE2	10.23	132.83	122.60
1	A	99	ALA	CA-C-O	10.20	132.17	119.11
1	A	73	LEU	CA-C-O	10.12	133.74	121.89
1	A	3	LYS	CA-CB-CG	9.91	133.92	114.10
1	A	90	ILE	N-CA-CB	-9.88	98.71	112.35
1	A	55	SER	O-C-N	9.75	132.62	122.09
1	A	166	ARG	CD-NE-CZ	9.73	138.02	124.40
1	A	189	THR	O-C-N	9.71	134.26	123.10
1	A	28	MET	CA-C-O	9.67	129.78	119.14
1	A	161	ARG	CD-NE-CZ	9.60	137.84	124.40
1	A	30	GLY	CA-C-N	9.58	135.03	121.24
1	A	30	GLY	C-N-CA	9.58	135.03	121.24
1	A	138	GLU	CA-C-N	9.56	133.09	120.28
1	A	138	GLU	C-N-CA	9.56	133.09	120.28
1	A	21	ALA	CA-C-O	9.39	130.71	120.10
1	A	92	ASP	CA-CB-CG	9.35	121.95	112.60
1	A	25	ARG	NE-CZ-NH1	9.33	130.83	121.50
1	A	42	LEU	CA-C-O	-9.28	109.61	120.10
1	A	6	ARG	CG-CD-NE	9.21	132.25	112.00
1	A	307	ASP	CA-C-O	-9.20	109.71	120.10
1	A	307	ASP	O-C-N	9.11	132.88	122.22
1	A	28	MET	N-CA-CB	-9.02	97.28	110.53
1	A	149	PHE	N-CA-C	-8.89	101.28	110.97
1	A	190	ASP	N-CA-C	-8.89	99.73	111.74
1	A	99	ALA	CA-C-N	8.88	132.04	123.08
1	A	99	ALA	C-N-CA	8.88	132.04	123.08
1	A	70	LYS	CA-CB-CG	-8.84	96.42	114.10
1	A	158	GLN	OE1-CD-NE2	-8.73	113.86	122.60
1	A	209	VAL	N-CA-CB	8.73	120.76	110.55
1	A	280	ASP	CA-C-O	-8.59	110.58	119.51
1	A	207	ARG	CA-C-O	8.59	129.80	120.10
1	A	317	GLY	N-CA-C	8.54	125.24	115.08
1	A	116	SER	N-CA-C	8.51	123.78	113.23
1	A	242	LYS	CA-C-O	-8.51	110.19	119.97
1	A	48	ALA	CA-C-O	8.49	129.55	120.55
1	A	166	ARG	CA-CB-CG	8.47	131.05	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	GLU	CB-CA-C	-8.46	93.89	109.29
1	A	237	LEU	CA-C-N	8.41	131.37	120.44
1	A	237	LEU	C-N-CA	8.41	131.37	120.44
1	A	148	HIS	CA-CB-CG	-8.36	105.44	113.80
1	A	40	LYS	N-CA-CB	8.36	122.19	110.07
1	A	126	LYS	CA-C-O	8.36	129.41	120.55
1	A	175	ASP	CA-CB-CG	8.35	120.95	112.60
1	A	12	PHE	CA-C-O	8.31	131.03	121.47
1	A	18	ARG	CD-NE-CZ	8.18	135.85	124.40
1	A	230	SER	CA-C-N	8.17	137.43	121.41
1	A	230	SER	C-N-CA	8.17	137.43	121.41
1	A	75	GLY	O-C-N	7.98	131.47	122.62
1	A	171	LEU	O-C-N	7.94	131.20	122.15
1	A	280	ASP	O-C-N	7.89	132.88	122.15
1	A	188	GLY	CA-C-O	-7.84	111.70	120.09
1	A	107	GLU	CB-CG-CD	7.83	125.91	112.60
1	A	140	LYS	CB-CA-C	-7.83	98.82	110.95
1	A	106	ASN	CA-C-N	7.79	131.05	120.38
1	A	106	ASN	C-N-CA	7.79	131.05	120.38
1	A	4	TYR	N-CA-C	-7.78	94.40	108.02
1	A	40	LYS	CA-C-O	-7.76	112.71	120.70
1	A	166	ARG	CA-C-N	-7.70	113.23	122.93
1	A	166	ARG	C-N-CA	-7.70	113.23	122.93
1	A	177	GLN	OE1-CD-NE2	-7.69	114.91	122.60
1	A	211	ASP	CA-C-N	7.67	130.40	120.44
1	A	211	ASP	C-N-CA	7.67	130.40	120.44
1	A	234	GLU	O-C-N	7.62	129.92	122.07
1	A	127	GLN	CB-CG-CD	-7.59	99.70	112.60
1	A	50	ARG	NE-CZ-NH1	-7.57	113.93	121.50
1	A	156	LEU	CA-C-O	-7.45	112.65	120.55
1	A	82	VAL	CB-CA-C	7.40	122.43	112.22
1	A	161	ARG	NE-CZ-NH1	-7.34	114.16	121.50
1	A	67	ASP	CA-CB-CG	-7.33	105.27	112.60
1	A	226	ASP	CA-C-O	7.30	128.96	120.49
1	A	242	LYS	O-C-N	7.27	131.22	122.27
1	A	213	TYR	CA-C-N	7.26	130.01	120.28
1	A	213	TYR	C-N-CA	7.26	130.01	120.28
1	A	155	VAL	CA-C-N	7.25	130.00	120.28
1	A	155	VAL	C-N-CA	7.25	130.00	120.28
1	A	60	LEU	CA-C-O	-7.20	112.85	120.55
1	A	278	GLU	CB-CG-CD	7.16	124.78	112.60
1	A	286	HIS	CA-CB-CG	-7.16	106.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	LYS	O-C-N	7.10	130.25	122.15
1	A	63	ARG	CD-NE-CZ	7.10	134.34	124.40
1	A	202	SER	CA-C-O	-7.05	114.06	122.03
1	A	282	LEU	CA-C-O	7.02	128.07	119.79
1	A	240	VAL	O-C-N	7.00	128.77	121.91
1	A	102	GLY	O-C-N	6.96	129.82	122.86
1	A	229	THR	CA-CB-CG2	6.96	122.33	110.50
1	A	187	TRP	CA-C-N	6.94	129.09	120.34
1	A	187	TRP	C-N-CA	6.94	129.09	120.34
1	A	236	LEU	CB-CA-C	6.94	121.87	110.90
1	A	36	GLU	O-C-N	-6.93	114.25	122.15
1	A	271	ARG	NE-CZ-NH2	-6.93	112.96	119.20
1	A	301	GLN	CA-C-O	6.90	127.86	120.55
1	A	261	GLY	CA-C-O	-6.85	115.50	122.56
1	A	301	GLN	CB-CG-CD	-6.84	100.97	112.60
1	A	183	GLY	CA-C-O	6.81	127.76	120.75
1	A	21	ALA	O-C-N	-6.80	114.26	122.22
1	A	234	GLU	CA-C-O	-6.80	113.68	120.82
1	A	205	HIS	O-C-N	-6.79	114.40	122.15
1	A	118	THR	CA-C-N	6.79	127.35	119.47
1	A	118	THR	C-N-CA	6.79	127.35	119.47
1	A	290	LYS	CA-CB-CG	6.79	127.67	114.10
1	A	269	LEU	CB-CA-C	6.76	121.49	110.88
1	A	63	ARG	CB-CG-CD	6.75	126.82	111.30
1	A	287	GLU	CA-C-O	6.72	127.70	119.97
1	A	9	VAL	CA-CB-CG1	6.71	121.81	110.40
1	A	210	PHE	CA-CB-CG	6.70	120.50	113.80
1	A	307	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	177	GLN	CB-CG-CD	6.68	123.97	112.60
1	A	196	THR	N-CA-CB	6.68	119.70	110.01
1	A	57	PHE	N-CA-C	-6.67	103.94	111.07
1	A	201	ARG	CA-C-O	-6.65	114.31	121.56
1	A	139	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	194	PHE	CB-CA-C	6.63	123.86	109.99
1	A	3	LYS	CA-C-N	6.60	132.71	123.07
1	A	3	LYS	C-N-CA	6.60	132.71	123.07
1	A	25	ARG	CB-CA-C	-6.60	100.52	110.88
1	A	216	ILE	CA-C-N	6.59	131.84	120.58
1	A	216	ILE	C-N-CA	6.59	131.84	120.58
1	A	89	ARG	N-CA-C	6.56	119.42	111.82
1	A	159	ALA	CA-C-N	6.54	133.45	122.79
1	A	159	ALA	C-N-CA	6.54	133.45	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ARG	NE-CZ-NH1	-6.54	114.96	121.50
1	A	112	GLU	CA-C-O	6.53	127.67	120.82
1	A	271	ARG	NH1-CZ-NH2	6.52	127.77	119.30
1	A	239	ALA	CA-C-O	-6.51	113.52	120.42
1	A	247	VAL	CA-C-N	6.50	126.26	119.05
1	A	247	VAL	C-N-CA	6.50	126.26	119.05
1	A	26	LYS	CA-C-O	-6.48	113.55	120.42
1	A	26	LYS	CB-CA-C	-6.46	99.87	110.85
1	A	235	LYS	CB-CA-C	-6.45	100.08	110.79
1	A	89	ARG	CD-NE-CZ	6.45	133.43	124.40
1	A	47	ASN	CB-CA-C	6.44	121.49	110.79
1	A	6	ARG	CA-CB-CG	6.41	126.92	114.10
1	A	180	PHE	CA-C-O	6.40	127.75	120.90
1	A	3	LYS	N-CA-CB	6.38	121.35	110.50
1	A	79	THR	O-C-N	6.38	128.64	122.07
1	A	201	ARG	CD-NE-CZ	6.37	133.32	124.40
1	A	84	LEU	CA-C-O	6.36	127.29	120.55
1	A	296	LEU	N-CA-C	-6.34	104.29	111.07
1	A	229	THR	N-CA-CB	6.32	121.17	110.49
1	A	209	VAL	N-CA-C	-6.31	104.36	110.42
1	A	161	ARG	CG-CD-NE	6.30	125.87	112.00
1	A	35	GLU	N-CA-CB	6.30	120.09	110.14
1	A	74	THR	N-CA-C	6.28	118.85	108.99
1	A	201	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	A	8	THR	CA-C-O	-6.26	112.01	119.15
1	A	124	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	A	74	THR	N-CA-CB	-6.23	99.93	111.52
1	A	265	ASP	N-CA-C	-6.23	96.27	107.98
1	A	296	LEU	CB-CA-C	6.22	120.65	110.88
1	A	142	THR	CA-C-O	6.21	127.01	119.49
1	A	140	LYS	O-C-N	6.21	128.74	122.03
1	A	317	GLY	CA-C-O	-6.17	112.85	119.27
1	A	67	ASP	CA-C-N	6.16	128.81	120.44
1	A	67	ASP	C-N-CA	6.16	128.81	120.44
1	A	72	GLU	CB-CA-C	-6.16	99.44	110.70
1	A	56	ALA	CA-C-N	6.15	128.44	120.44
1	A	56	ALA	C-N-CA	6.15	128.44	120.44
1	A	173	GLU	CA-CB-CG	-6.15	101.81	114.10
1	A	55	SER	CB-CA-C	-6.13	101.21	110.90
1	A	77	PHE	N-CA-C	-6.11	104.53	111.07
1	A	138	GLU	N-CA-C	6.10	118.71	111.33
1	A	167	VAL	CB-CA-C	6.10	119.13	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ASN	N-CA-C	6.10	120.47	111.87
1	A	161	ARG	N-CA-CB	-6.09	101.55	110.26
1	A	9	VAL	CA-C-O	6.07	126.70	120.39
1	A	238	LEU	CA-C-O	-6.01	114.51	120.82
1	A	254	THR	CA-CB-CG2	6.01	120.72	110.50
1	A	142	THR	O-C-N	-6.01	114.58	122.39
1	A	190	ASP	O-C-N	5.97	130.42	122.41
1	A	308	TYR	N-CA-C	-5.97	104.77	111.28
1	A	55	SER	CA-C-O	-5.94	114.58	120.70
1	A	276	ARG	O-C-N	5.94	129.76	122.34
1	A	201	ARG	NE-CZ-NH1	-5.93	115.57	121.50
1	A	310	LYS	CB-CA-C	-5.93	99.29	110.67
1	A	107	GLU	CG-CD-OE1	5.92	132.03	118.40
1	A	292	PHE	N-CA-C	5.91	120.49	113.28
1	A	299	MET	CA-C-N	5.91	128.81	120.42
1	A	299	MET	C-N-CA	5.91	128.81	120.42
1	A	105	THR	O-C-N	5.91	130.09	123.48
1	A	141	ILE	CA-C-O	5.89	127.39	121.27
1	A	286	HIS	N-CA-CB	5.88	118.87	110.16
1	A	182	ALA	CA-C-N	5.87	126.50	119.98
1	A	182	ALA	C-N-CA	5.87	126.50	119.98
1	A	252	ALA	CA-C-O	5.85	126.96	120.82
1	A	188	GLY	O-C-N	5.84	129.06	122.34
1	A	285	ARG	CA-C-O	5.83	126.72	120.55
1	A	291	ASN	CA-C-O	-5.83	114.70	120.70
1	A	221	ILE	N-CA-C	5.82	117.26	110.62
1	A	230	SER	N-CA-CB	-5.80	102.10	110.45
1	A	95	ALA	CA-C-O	-5.79	114.41	120.55
1	A	151	ARG	CD-NE-CZ	-5.79	116.30	124.40
1	A	37	THR	CA-C-N	5.78	128.34	120.77
1	A	37	THR	C-N-CA	5.78	128.34	120.77
1	A	86	ARG	NE-CZ-NH1	5.77	127.27	121.50
1	A	181	ARG	NE-CZ-NH2	-5.77	114.01	119.20
1	A	125	ILE	CB-CA-C	-5.75	104.61	111.97
1	A	173	GLU	CA-C-O	-5.75	114.33	120.42
1	A	117	ARG	NE-CZ-NH2	-5.74	114.04	119.20
1	A	273	MET	N-CA-CB	5.74	118.49	109.94
1	A	43	THR	CA-CB-OG1	-5.72	101.02	109.60
1	A	45	ARG	N-CA-C	-5.72	100.86	109.95
1	A	227	ARG	CA-C-N	5.71	128.25	120.54
1	A	227	ARG	C-N-CA	5.71	128.25	120.54
1	A	98	HIS	N-CA-C	5.71	120.25	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ARG	NE-CZ-NH1	5.70	127.20	121.50
1	A	105	THR	CA-C-N	-5.70	114.34	122.77
1	A	105	THR	C-N-CA	-5.70	114.34	122.77
1	A	314	LEU	CA-C-O	-5.68	114.40	120.42
1	A	144	GLU	OE1-CD-OE2	5.68	136.52	122.90
1	A	89	ARG	CA-C-O	5.67	126.50	119.97
1	A	106	ASN	O-C-N	-5.67	115.71	122.63
1	A	286	HIS	CA-C-O	-5.65	114.44	120.42
1	A	110	LEU	CA-C-O	5.63	127.26	121.07
1	A	200	THR	N-CA-C	5.62	121.16	113.97
1	A	19	ALA	O-C-N	-5.61	115.38	122.27
1	A	232	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	233	LEU	O-C-N	5.58	128.52	122.15
1	A	124	ASN	CA-C-O	-5.56	114.52	120.42
1	A	25	ARG	CD-NE-CZ	5.55	132.17	124.40
1	A	111	THR	N-CA-C	5.54	117.00	111.07
1	A	148	HIS	O-C-N	5.54	129.08	122.27
1	A	142	THR	N-CA-CB	-5.51	100.95	110.32
1	A	178	VAL	CA-C-O	-5.50	114.31	120.25
1	A	140	LYS	CA-CB-CG	-5.50	103.11	114.10
1	A	234	GLU	CA-C-N	5.49	127.64	120.28
1	A	234	GLU	C-N-CA	5.49	127.64	120.28
1	A	219	PHE	N-CA-CB	5.48	121.34	111.37
1	A	4	TYR	CA-C-N	5.47	130.19	122.09
1	A	4	TYR	C-N-CA	5.47	130.19	122.09
1	A	82	VAL	CA-C-O	-5.47	115.05	120.85
1	A	298	GLN	CA-C-O	-5.47	114.62	120.42
1	A	272	VAL	CA-C-O	5.47	127.52	121.18
1	A	289	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	A	309	ARG	CD-NE-CZ	5.46	132.04	124.40
1	A	41	ILE	CA-CB-CG2	5.45	119.77	110.50
1	A	28	MET	CA-CB-CG	5.45	125.00	114.10
1	A	128	VAL	N-CA-C	-5.44	105.22	110.72
1	A	53	ILE	N-CA-C	-5.42	105.25	110.72
1	A	246	SER	CA-C-N	-5.42	116.00	120.33
1	A	246	SER	C-N-CA	-5.42	116.00	120.33
1	A	301	GLN	CG-CD-NE2	-5.42	108.28	116.40
1	A	318	GLY	CA-C-O	-5.42	109.42	120.80
1	A	295	SER	CB-CA-C	5.40	118.72	109.80
1	A	187	TRP	CA-C-O	5.40	127.83	121.08
1	A	289	ARG	NH1-CZ-NH2	5.40	126.32	119.30
1	A	75	GLY	CA-C-O	-5.38	115.00	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ASP	CA-C-N	5.37	127.74	120.38
1	A	16	ASP	C-N-CA	5.37	127.74	120.38
1	A	185	LEU	CB-CA-C	5.37	119.92	110.37
1	A	58	LYS	CA-C-N	5.36	127.90	120.29
1	A	58	LYS	C-N-CA	5.36	127.90	120.29
1	A	149	PHE	CB-CA-C	5.35	119.19	110.96
1	A	157	LEU	CA-C-O	-5.35	112.80	119.38
1	A	6	ARG	O-C-N	-5.33	116.26	123.19
1	A	140	LYS	CA-C-O	-5.33	115.41	120.90
1	A	267	ASP	O-C-N	5.33	127.77	122.12
1	A	179	LEU	CA-C-N	5.32	127.72	120.54
1	A	179	LEU	C-N-CA	5.32	127.72	120.54
1	A	37	THR	CA-CB-OG1	-5.30	101.66	109.60
1	A	3	LYS	CB-CG-CD	5.29	123.47	111.30
1	A	166	ARG	CG-CD-NE	5.29	123.63	112.00
1	A	123	GLN	CB-CA-C	-5.28	102.03	110.79
1	A	61	PHE	N-CA-CB	-5.28	103.34	110.67
1	A	159	ALA	CA-C-O	5.27	127.95	121.84
1	A	181	ARG	NE-CZ-NH1	5.27	126.77	121.50
1	A	276	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	A	69	LEU	O-C-N	5.25	127.48	122.07
1	A	162	ASP	O-C-N	5.25	127.17	121.60
1	A	246	SER	N-CA-C	5.25	116.59	107.93
1	A	242	LYS	CB-CG-CD	-5.25	99.23	111.30
1	A	144	GLU	CG-CD-OE2	-5.24	106.35	118.40
1	A	313	LEU	CA-C-O	-5.23	114.88	120.42
1	A	23	ALA	CA-C-N	5.22	129.50	120.58
1	A	23	ALA	C-N-CA	5.22	129.50	120.58
1	A	76	LYS	CB-CG-CD	-5.22	99.29	111.30
1	A	121	GLU	CA-C-O	-5.20	114.90	120.42
1	A	55	SER	N-CA-CB	5.20	117.61	110.07
1	A	281	LEU	CA-C-O	-5.20	114.23	120.10
1	A	169	GLU	O-C-N	5.18	129.12	122.39
1	A	196	THR	CA-C-N	5.17	127.18	120.56
1	A	196	THR	C-N-CA	5.17	127.18	120.56
1	A	40	LYS	O-C-N	5.17	127.67	122.09
1	A	105	THR	CA-CB-OG1	-5.15	101.88	109.60
1	A	204	SER	CB-CA-C	5.14	119.58	110.85
1	A	47	ASN	N-CA-CB	-5.13	102.58	110.12
1	A	51	GLN	CA-C-O	5.12	125.88	120.10
1	A	150	GLN	CG-CD-NE2	-5.12	108.72	116.40
1	A	190	ASP	CA-C-O	-5.10	115.21	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ALA	N-CA-C	-5.10	105.80	111.36
1	A	42	LEU	CA-C-N	-5.08	113.18	122.38
1	A	42	LEU	C-N-CA	-5.08	113.18	122.38
1	A	177	GLN	N-CA-CB	5.08	118.15	110.28
1	A	152	LEU	CB-CA-C	5.07	119.46	110.85
1	A	45	ARG	CA-C-O	-5.06	115.44	121.16
1	A	14	PRO	CA-C-N	5.06	128.74	121.50
1	A	14	PRO	C-N-CA	5.06	128.74	121.50
1	A	156	LEU	O-C-N	5.06	127.48	122.12
1	A	220	GLN	CA-C-O	-5.05	115.30	121.05
1	A	53	ILE	CA-C-N	5.03	127.01	120.28
1	A	53	ILE	C-N-CA	5.03	127.01	120.28
1	A	132	GLU	CA-C-O	-5.02	115.18	120.55
1	A	107	GLU	CA-C-N	5.01	131.12	121.54
1	A	107	GLU	C-N-CA	5.01	131.12	121.54
1	A	84	LEU	CA-C-N	5.00	129.07	120.72
1	A	84	LEU	C-N-CA	5.00	129.07	120.72
1	A	113	ILE	O-C-N	-5.00	117.01	121.91

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	2503	0	2536	114	0
2	A	3	0	0	0	0
3	A	81	0	0	5	3
All	All	2587	0	2536	114	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 (114) 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:106:ASN:HD21	1:A:108:LYS:HB3	1.08	1.17
1:A:5:THR:HG23	1:A:279:ILE:O	1.45	1.16
1:A:28:MET:HG3	1:A:72:GLU:HG3	1.28	1.10
1:A:106:ASN:ND2	1:A:108:LYS:HB3	1.65	1.10
1:A:226:ASP:OD2	1:A:229:THR:CG2	2.05	1.05
1:A:89:ARG:NH1	3:A:448:HOH:O	1.89	1.03
1:A:136:ASN:HD21	1:A:138:GLU:HB3	1.28	0.97
1:A:226:ASP:OD2	1:A:229:THR:HG22	1.64	0.96
1:A:36:GLU:HG2	1:A:40:LYS:HE2	1.49	0.95
1:A:227:ARG:HG3	1:A:228:GLU:H	1.35	0.91
1:A:139:ASP:O	1:A:142:THR:HG22	1.70	0.90
1:A:5:THR:CG2	1:A:279:ILE:O	2.21	0.89
1:A:28:MET:CG	1:A:72:GLU:HG3	2.03	0.88
1:A:139:ASP:C	1:A:142:THR:HG22	2.01	0.86
1:A:226:ASP:OD2	1:A:229:THR:HG23	1.73	0.86
1:A:25:ARG:O	1:A:29:LYS:HB2	1.76	0.84
1:A:36:GLU:CG	1:A:40:LYS:HE2	2.07	0.84
1:A:28:MET:HG3	1:A:72:GLU:CG	2.08	0.81
1:A:18:ARG:O	1:A:22:GLU:HG3	1.79	0.81
1:A:127:GLN:O	1:A:131:GLN:HG3	1.81	0.81
1:A:181:ARG:HH11	1:A:181:ARG:HG2	1.49	0.78
1:A:89:ARG:NH2	1:A:128:VAL:HG22	1.99	0.78
1:A:229:THR:OG1	1:A:230:SER:N	2.16	0.78
1:A:100:ILE:HG12	1:A:144:GLU:HG3	1.66	0.77
1:A:148:HIS:CD2	3:A:482:HOH:O	2.38	0.77
1:A:148:HIS:HD2	3:A:482:HOH:O	1.69	0.75
1:A:177:GLN:OE1	1:A:181:ARG:NE	2.21	0.73
1:A:268:THR:O	1:A:272:VAL:HG23	1.90	0.72
1:A:180:PHE:CD2	1:A:181:ARG:HD2	2.27	0.70
1:A:164:ASP:OD1	1:A:202:SER:HB2	1.90	0.70
1:A:191:GLU:HA	1:A:194:PHE:CE2	2.26	0.70
1:A:162:ASP:HB3	1:A:163:PRO:HD2	1.73	0.69
1:A:240:VAL:O	1:A:244:ILE:HD12	1.93	0.69
1:A:136:ASN:ND2	1:A:138:GLU:HB3	2.05	0.69
1:A:177:GLN:O	1:A:181:ARG:HD3	1.94	0.68
1:A:47:ASN:O	1:A:51:GLN:HG2	1.92	0.68
1:A:181:ARG:HG2	1:A:181:ARG:NH1	2.07	0.68
1:A:137:LEU:O	1:A:140:LYS:HB2	1.95	0.67
1:A:229:THR:HG1	1:A:230:SER:H	1.45	0.65
1:A:147:GLY:O	1:A:151:ARG:HD2	1.97	0.64
1:A:231:GLY:HA3	1:A:234:GLU:OE1	1.99	0.63
1:A:276:ARG:HB3	1:A:280:ASP:OD1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLN:O	1:A:154:VAL:HG23	2.00	0.62
1:A:151:ARG:HD3	3:A:482:HOH:O	2.02	0.60
1:A:180:PHE:HD2	1:A:181:ARG:HD2	1.67	0.59
1:A:6:ARG:HD3	1:A:282:LEU:HD23	1.85	0.58
1:A:106:ASN:HD22	1:A:106:ASN:C	2.12	0.57
1:A:227:ARG:HG3	1:A:228:GLU:N	2.15	0.56
1:A:228:GLU:HG3	1:A:229:THR:N	2.21	0.56
1:A:220:GLN:HB2	1:A:223:GLU:HG3	1.88	0.55
1:A:304:THR:O	1:A:309:ARG:HD3	2.07	0.55
1:A:247:VAL:O	1:A:250:TYR:HB3	2.07	0.54
1:A:292:PHE:O	1:A:293:ALA:HB3	2.06	0.54
1:A:46:ASN:HD21	1:A:49:GLN:HG3	1.73	0.54
1:A:89:ARG:NH2	1:A:128:VAL:CG2	2.70	0.53
1:A:138:GLU:O	1:A:142:THR:HB	2.08	0.53
1:A:148:HIS:HA	1:A:151:ARG:HD2	1.91	0.53
1:A:221:ILE:HG23	1:A:241:VAL:HG11	1.91	0.52
1:A:106:ASN:HD21	1:A:108:LYS:CB	2.00	0.52
1:A:259:MET:HG2	1:A:264:THR:HG23	1.91	0.52
1:A:180:PHE:O	1:A:184:GLU:HG2	2.10	0.52
1:A:136:ASN:HD22	1:A:139:ASP:H	1.58	0.51
1:A:89:ARG:CZ	1:A:128:VAL:HG22	2.40	0.51
1:A:231:GLY:O	1:A:235:LYS:HD3	2.11	0.51
1:A:310:LYS:O	1:A:314:LEU:HG	2.10	0.51
1:A:108:LYS:NZ	3:A:439:HOH:O	2.34	0.50
1:A:99:ALA:O	1:A:106:ASN:N	2.30	0.50
1:A:168:GLU:HG2	1:A:171:LEU:H	1.76	0.50
1:A:185:LEU:O	1:A:186:LYS:HB2	2.11	0.49
1:A:36:GLU:OE2	1:A:40:LYS:CE	2.61	0.49
1:A:58:LYS:HE3	1:A:58:LYS:HB2	1.64	0.49
1:A:169:GLU:O	1:A:173:GLU:HB2	2.13	0.49
1:A:240:VAL:HG13	1:A:244:ILE:CD1	2.43	0.48
1:A:5:THR:HG23	1:A:279:ILE:C	2.32	0.48
1:A:152:LEU:O	1:A:156:LEU:HG	2.13	0.48
1:A:247:VAL:N	1:A:248:PRO:CD	2.75	0.48
1:A:191:GLU:HA	1:A:194:PHE:CZ	2.48	0.47
1:A:139:ASP:CA	1:A:142:THR:HG22	2.44	0.47
1:A:306:GLY:O	1:A:309:ARG:HB3	2.15	0.47
1:A:139:ASP:HA	1:A:142:THR:CG2	2.45	0.47
1:A:273:MET:HG3	1:A:312:LEU:HD12	1.97	0.47
1:A:247:VAL:HB	1:A:248:PRO:HD3	1.96	0.47
1:A:227:ARG:NH1	1:A:228:GLU:HB3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASN:ND2	1:A:128:VAL:HG23	2.29	0.46
1:A:124:ASN:HD21	1:A:128:VAL:HG23	1.81	0.46
1:A:203:VAL:O	1:A:207:ARG:HG3	2.16	0.46
1:A:294:LYS:HE2	1:A:294:LYS:HB3	1.79	0.46
1:A:22:GLU:O	1:A:26:LYS:HG3	2.16	0.46
1:A:289:ARG:HA	1:A:294:LYS:O	2.15	0.46
1:A:28:MET:HG3	1:A:72:GLU:CD	2.41	0.45
1:A:224:THR:C	1:A:225:ILE:HG13	2.41	0.45
1:A:6:ARG:O	1:A:280:ASP:HA	2.18	0.44
1:A:46:ASN:ND2	1:A:49:GLN:HG3	2.32	0.44
1:A:290:LYS:HG3	1:A:291:ASN:ND2	2.33	0.44
1:A:6:ARG:HH11	1:A:282:LEU:HD21	1.84	0.43
1:A:86:ARG:HA	1:A:87:PRO:HD3	1.88	0.43
1:A:106:ASN:ND2	1:A:108:LYS:CB	2.58	0.43
1:A:189:THR:HA	1:A:191:GLU:OE1	2.17	0.43
1:A:124:ASN:HD21	1:A:128:VAL:CG2	2.32	0.43
1:A:271:ARG:O	1:A:275:SER:OG	2.29	0.42
1:A:298:GLN:HE21	1:A:298:GLN:HB3	1.49	0.42
1:A:139:ASP:O	1:A:142:THR:CG2	2.55	0.42
1:A:168:GLU:CD	1:A:171:LEU:HB2	2.44	0.42
1:A:240:VAL:CG1	1:A:244:ILE:CD1	2.98	0.42
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.87	0.42
1:A:89:ARG:HE	1:A:89:ARG:HB2	1.49	0.42
1:A:162:ASP:HB3	1:A:163:PRO:CD	2.46	0.42
1:A:289:ARG:HA	1:A:289:ARG:HD2	1.78	0.42
1:A:12:PHE:HB2	1:A:44:SER:O	2.20	0.41
1:A:116:SER:OG	1:A:117:ARG:NH1	2.48	0.41
1:A:139:ASP:HA	1:A:142:THR:HG21	2.03	0.41
1:A:168:GLU:OE2	1:A:171:LEU:HB2	2.21	0.41
1:A:111:THR:O	1:A:115:ALA:HB3	2.20	0.40
1:A:28:MET:SD	1:A:72:GLU:HG3	2.62	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:484:HOH:O	3:A:484:HOH:O[3_555]	1.96	0.24
3:A:432:HOH:O	3:A:483:HOH:O[2_555]	2.05	0.15
3:A:464:HOH:O	3:A:471:HOH:O[6_455]	2.17	0.03

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	314/321 (98%)	305 (97%)	8 (2%)	1 (0%)	36	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	THR

5.3.2 Protein sidechains [i](#)

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	269/273 (98%)	226 (84%)	43 (16%)	2	1

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

Mol	Chain	Res	Type
1	A	5	THR
1	A	6	ARG
1	A	9	VAL
1	A	13	SER
1	A	31	MET
1	A	46	ASN
1	A	47	ASN
1	A	63	ARG
1	A	71	SER
1	A	74	THR

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Mol	Chain	Res	Type
1	A	89	ARG
1	A	97	LYS
1	A	106	ASN
1	A	127	GLN
1	A	136	ASN
1	A	141	ILE
1	A	142	THR
1	A	146	SER
1	A	151	ARG
1	A	157	LEU
1	A	161	ARG
1	A	166	ARG
1	A	168	GLU
1	A	169	GLU
1	A	174	LYS
1	A	178	VAL
1	A	181	ARG
1	A	190	ASP
1	A	208	ARG
1	A	214	MET
1	A	217	SER
1	A	228	GLU
1	A	229	THR
1	A	235	LYS
1	A	237	LEU
1	A	244	ILE
1	A	260	LYS
1	A	289	ARG
1	A	299	MET
1	A	301	GLN
1	A	303	ASP
1	A	312	LEU
1	A	315	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	47	ASN
1	A	106	ASN
1	A	124	ASN
1	A	136	ASN

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Mol	Chain	Res	Type
1	A	148	HIS
1	A	158	GLN
1	A	291	ASN
1	A	298	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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](#)

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.