



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:33 PM UTC

PDB ID : 1BVP / pdb_00001bvp
Title : THE CRYSTAL STRUCTURE OF BLUETONGUE VIRUS VP7
Authors : Stuart, D.; Grimes, J.
Deposited on : 1995-02-17
Resolution : 2.60 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

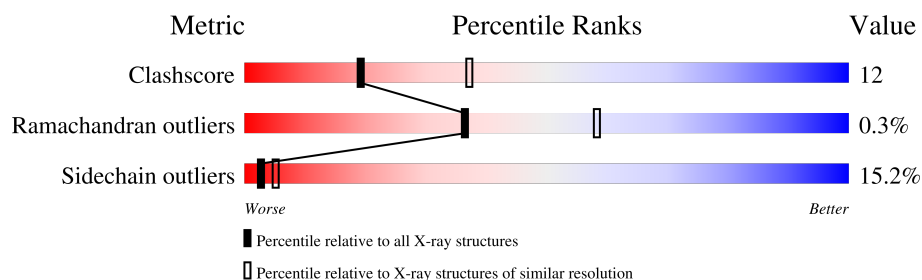
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	1	349	67% 26% 6% •
1	2	349	67% 26% 6% •
1	3	349	69% 25% 5% •
1	4	349	68% 26% 6% •
1	5	349	67% 26% 6% •
1	6	349	69% 24% 6% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16218 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 BLUETONGUE VIRUS COAT PROTEIN VP7.

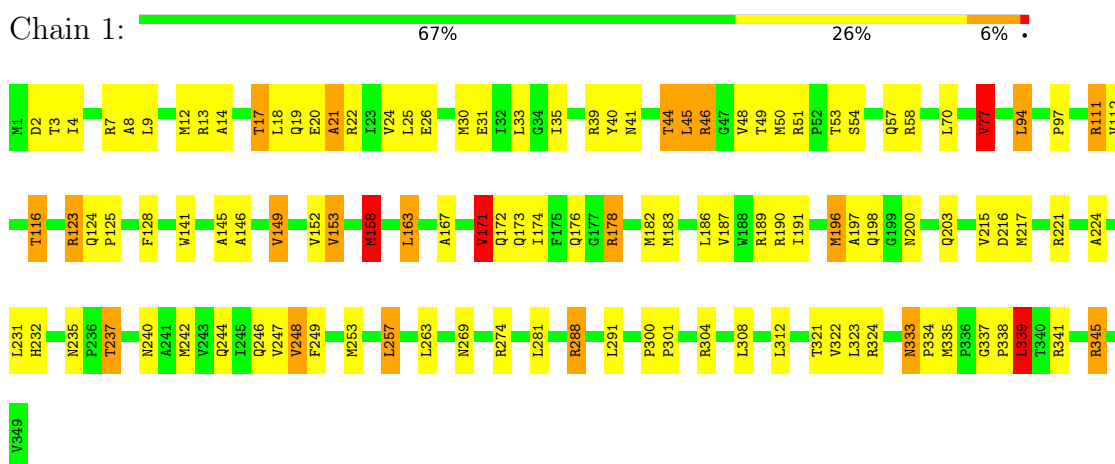
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	349	Total	C	N	O	S	9	0	0
			2703	1712	477	492	22			
1	2	349	Total	C	N	O	S	9	0	0
			2703	1712	477	492	22			
1	3	349	Total	C	N	O	S	9	0	0
			2703	1712	477	492	22			
1	4	349	Total	C	N	O	S	9	0	0
			2703	1712	477	492	22			
1	5	349	Total	C	N	O	S	9	0	0
			2703	1712	477	492	22			
1	6	349	Total	C	N	O	S	9	0	0
			2703	1712	477	492	22			

3 Residue-property plots

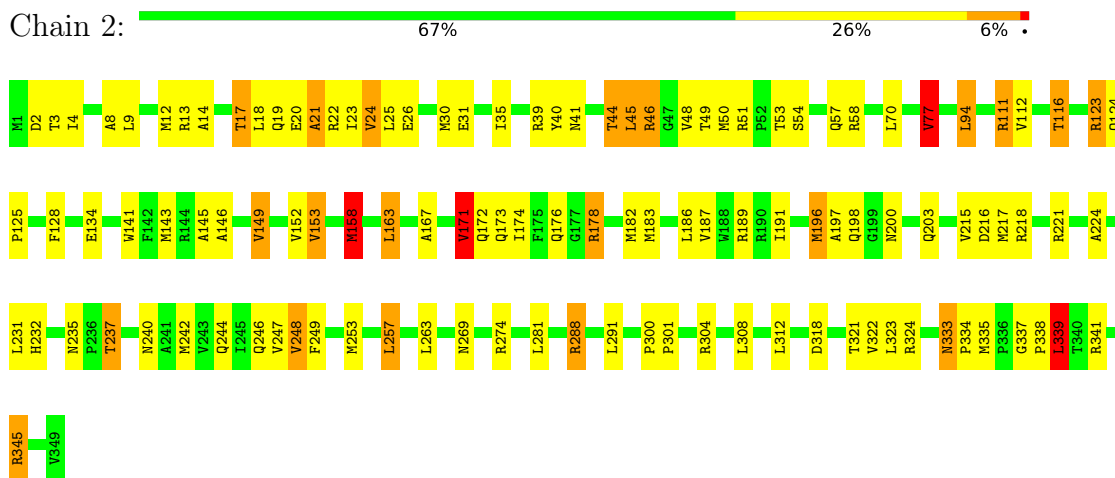
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

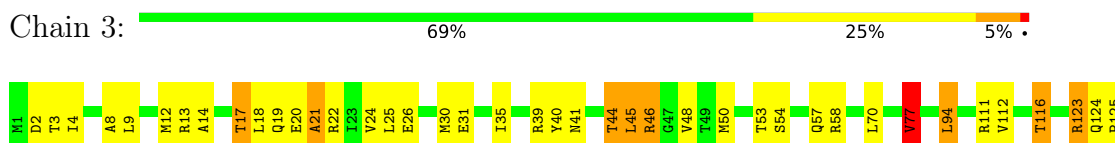
• Molecule 1: BLUETONGUE VIRUS COAT PROTEIN VP7

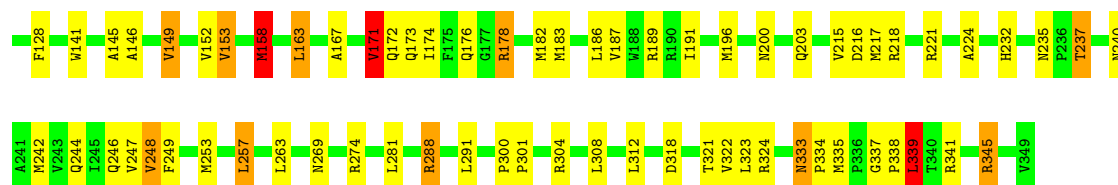


• Molecule 1: BLUETONGUE VIRUS COAT PROTEIN VP7



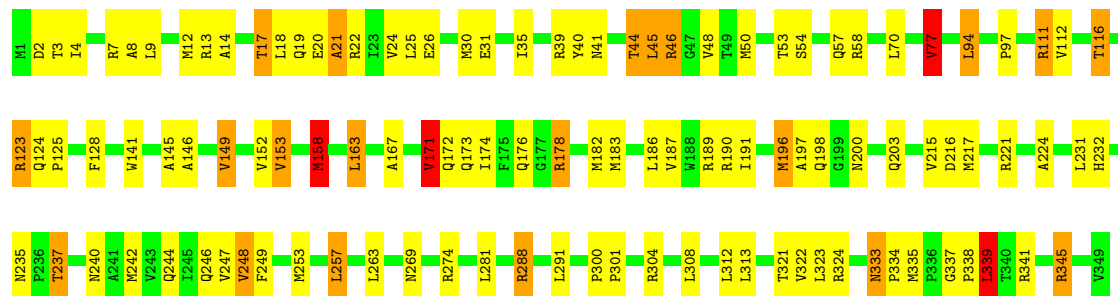
• Molecule 1: BLUETONGUE VIRUS COAT PROTEIN VP7





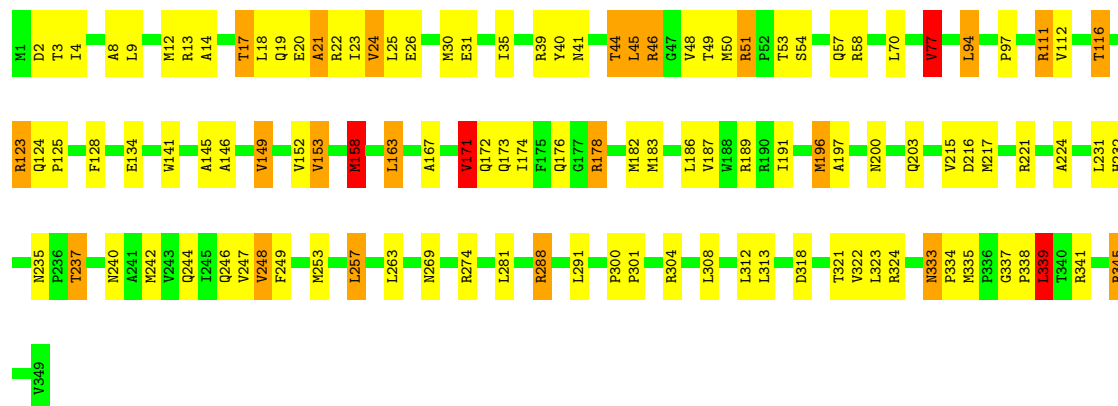
• Molecule 1: BLUETONGUE VIRUS COAT PROTEIN VP7

Chain 4: 68% 26% 6% •



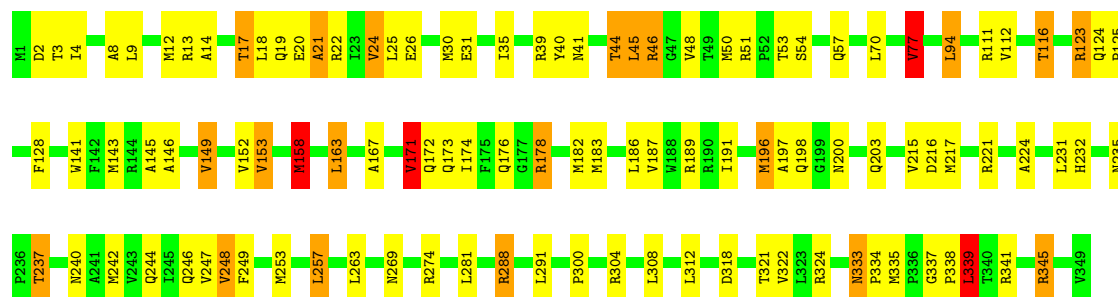
• Molecule 1: BLUETONGUE VIRUS COAT PROTEIN VP7

Chain 5: 67% 26% 6% •



• Molecule 1: BLUETONGUE VIRUS COAT PROTEIN VP7

Chain 6: 69% 24% 6% •



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.60Å 110.20Å 129.80Å 90.00° 103.10° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.60)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16218	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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	1	0.89	5/2762 (0.2%)	1.19	22/3765 (0.6%)
1	2	0.89	5/2762 (0.2%)	1.19	22/3765 (0.6%)
1	3	0.89	5/2762 (0.2%)	1.19	22/3765 (0.6%)
1	4	0.89	5/2762 (0.2%)	1.19	22/3765 (0.6%)
1	5	0.89	5/2762 (0.2%)	1.19	24/3765 (0.6%)
1	6	0.89	5/2762 (0.2%)	1.19	24/3765 (0.6%)
All	All	0.89	30/16572 (0.2%)	1.19	136/22590 (0.6%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	153	VAL	CA-CB	7.33	1.63	1.54
1	6	153	VAL	CA-CB	7.32	1.63	1.54
1	4	153	VAL	CA-CB	7.30	1.63	1.54
1	1	153	VAL	CA-CB	7.30	1.63	1.54
1	3	153	VAL	CA-CB	7.28	1.63	1.54
1	2	153	VAL	CA-CB	7.26	1.63	1.54
1	4	196	MET	SD-CE	6.30	1.95	1.79
1	3	196	MET	SD-CE	6.29	1.95	1.79
1	1	196	MET	SD-CE	6.26	1.95	1.79
1	2	196	MET	SD-CE	6.25	1.95	1.79
1	6	196	MET	SD-CE	6.25	1.95	1.79
1	5	196	MET	SD-CE	6.24	1.95	1.79
1	3	50	MET	SD-CE	5.99	1.94	1.79
1	2	50	MET	SD-CE	5.98	1.94	1.79
1	4	50	MET	SD-CE	5.98	1.94	1.79
1	1	50	MET	SD-CE	5.97	1.94	1.79
1	5	50	MET	SD-CE	5.95	1.94	1.79
1	6	50	MET	SD-CE	5.95	1.94	1.79
1	5	30	MET	SD-CE	5.69	1.93	1.79
1	1	30	MET	SD-CE	5.67	1.93	1.79
1	2	30	MET	SD-CE	5.67	1.93	1.79
1	3	30	MET	SD-CE	5.66	1.93	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	30	MET	SD-CE	5.66	1.93	1.79
1	4	30	MET	SD-CE	5.66	1.93	1.79
1	2	158	MET	SD-CE	-5.41	1.66	1.79
1	4	158	MET	SD-CE	-5.41	1.66	1.79
1	1	158	MET	SD-CE	-5.39	1.66	1.79
1	5	158	MET	SD-CE	-5.39	1.66	1.79
1	3	158	MET	SD-CE	-5.38	1.66	1.79
1	6	158	MET	SD-CE	-5.38	1.66	1.79

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	172	GLN	N-CA-C	8.21	121.27	111.33
1	1	172	GLN	N-CA-C	8.21	121.26	111.33
1	6	172	GLN	N-CA-C	8.20	121.25	111.33
1	2	172	GLN	N-CA-C	8.19	121.24	111.33
1	4	172	GLN	N-CA-C	8.18	121.23	111.33
1	5	172	GLN	N-CA-C	8.17	121.22	111.33
1	2	125	PRO	N-CA-C	7.76	123.80	113.40
1	6	125	PRO	N-CA-C	7.76	123.80	113.40
1	5	125	PRO	N-CA-C	7.75	123.78	113.40
1	3	125	PRO	N-CA-C	7.74	123.78	113.40
1	1	125	PRO	N-CA-C	7.74	123.77	113.40
1	4	125	PRO	N-CA-C	7.71	123.73	113.40
1	3	26	GLU	N-CA-C	-7.59	99.04	110.28
1	4	26	GLU	N-CA-C	-7.58	99.06	110.28
1	5	26	GLU	N-CA-C	-7.58	99.07	110.28
1	1	26	GLU	N-CA-C	-7.57	99.07	110.28
1	2	26	GLU	N-CA-C	-7.56	99.09	110.28
1	6	26	GLU	N-CA-C	-7.56	99.09	110.28
1	3	182	MET	N-CA-C	-7.30	104.89	113.88
1	6	182	MET	N-CA-C	-7.30	104.90	113.88
1	5	182	MET	N-CA-C	-7.29	104.91	113.88
1	2	182	MET	N-CA-C	-7.28	104.92	113.88
1	4	182	MET	N-CA-C	-7.28	104.93	113.88
1	1	182	MET	N-CA-C	-7.28	104.93	113.88
1	4	124	GLN	CA-C-N	7.26	126.77	118.85
1	4	124	GLN	C-N-CA	7.26	126.77	118.85
1	3	124	GLN	CA-C-N	7.24	126.74	118.85
1	3	124	GLN	C-N-CA	7.24	126.74	118.85
1	1	124	GLN	CA-C-N	7.24	126.74	118.85
1	1	124	GLN	C-N-CA	7.24	126.74	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	124	GLN	CA-C-N	7.24	126.74	118.85
1	2	124	GLN	C-N-CA	7.24	126.74	118.85
1	5	124	GLN	CA-C-N	7.22	126.72	118.85
1	5	124	GLN	C-N-CA	7.22	126.72	118.85
1	6	124	GLN	CA-C-N	7.21	126.70	118.85
1	6	124	GLN	C-N-CA	7.21	126.70	118.85
1	3	21	ALA	N-CA-C	6.32	117.96	111.14
1	1	21	ALA	N-CA-C	6.30	117.95	111.14
1	5	21	ALA	N-CA-C	6.30	117.94	111.14
1	6	21	ALA	N-CA-C	6.29	117.94	111.14
1	2	21	ALA	N-CA-C	6.28	117.93	111.14
1	4	21	ALA	N-CA-C	6.27	117.91	111.14
1	4	77	VAL	N-CA-C	6.24	118.85	111.05
1	2	334	PRO	N-CA-C	6.24	121.01	111.15
1	2	77	VAL	N-CA-C	6.24	118.84	111.05
1	3	77	VAL	N-CA-C	6.24	118.84	111.05
1	5	334	PRO	N-CA-C	6.23	121.00	111.15
1	1	77	VAL	N-CA-C	6.22	118.82	111.05
1	1	334	PRO	N-CA-C	6.21	120.96	111.15
1	2	22	ARG	N-CA-C	6.21	120.86	113.16
1	6	77	VAL	N-CA-C	6.21	118.81	111.05
1	6	334	PRO	N-CA-C	6.21	120.96	111.15
1	5	77	VAL	N-CA-C	6.20	118.80	111.05
1	2	335	MET	CA-C-N	6.20	127.59	119.84
1	2	335	MET	C-N-CA	6.20	127.59	119.84
1	4	22	ARG	N-CA-C	6.20	120.85	113.16
1	6	158	MET	N-CA-C	6.20	118.73	108.99
1	5	335	MET	CA-C-N	6.20	127.59	119.84
1	5	335	MET	C-N-CA	6.20	127.59	119.84
1	2	158	MET	N-CA-C	6.19	118.71	108.99
1	4	334	PRO	N-CA-C	6.19	120.93	111.15
1	5	158	MET	N-CA-C	6.19	118.71	108.99
1	1	22	ARG	N-CA-C	6.19	120.84	113.16
1	4	158	MET	N-CA-C	6.19	118.71	108.99
1	6	22	ARG	N-CA-C	6.19	120.83	113.16
1	3	158	MET	N-CA-C	6.19	118.70	108.99
1	3	334	PRO	N-CA-C	6.18	120.92	111.15
1	1	158	MET	N-CA-C	6.18	118.69	108.99
1	3	171	VAL	N-CA-CB	-6.18	104.98	112.33
1	5	22	ARG	N-CA-C	6.18	120.82	113.16
1	4	335	MET	CA-C-N	6.17	127.55	119.84
1	4	335	MET	C-N-CA	6.17	127.55	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	171	VAL	N-CA-CB	-6.17	104.99	112.33
1	1	335	MET	CA-C-N	6.16	127.54	119.84
1	1	335	MET	C-N-CA	6.16	127.54	119.84
1	6	333	ASN	CA-C-N	6.16	126.19	119.90
1	6	333	ASN	C-N-CA	6.16	126.19	119.90
1	3	22	ARG	N-CA-C	6.16	120.80	113.16
1	3	335	MET	CA-C-N	6.15	127.53	119.84
1	3	335	MET	C-N-CA	6.15	127.53	119.84
1	2	171	VAL	N-CA-CB	-6.13	105.03	112.33
1	4	171	VAL	N-CA-CB	-6.13	105.03	112.33
1	1	171	VAL	N-CA-CB	-6.13	105.03	112.33
1	4	333	ASN	CA-C-N	6.13	126.15	119.90
1	4	333	ASN	C-N-CA	6.13	126.15	119.90
1	6	335	MET	CA-C-N	6.12	127.50	119.84
1	6	335	MET	C-N-CA	6.12	127.50	119.84
1	2	333	ASN	CA-C-N	6.12	126.14	119.90
1	2	333	ASN	C-N-CA	6.12	126.14	119.90
1	1	333	ASN	CA-C-N	6.12	126.14	119.90
1	1	333	ASN	C-N-CA	6.12	126.14	119.90
1	5	333	ASN	CA-C-N	6.12	126.14	119.90
1	5	333	ASN	C-N-CA	6.12	126.14	119.90
1	3	333	ASN	CA-C-N	6.10	126.13	119.90
1	3	333	ASN	C-N-CA	6.10	126.13	119.90
1	6	77	VAL	CB-CA-C	-6.10	102.70	112.16
1	6	171	VAL	N-CA-CB	-6.10	105.07	112.33
1	2	77	VAL	CB-CA-C	-6.10	102.71	112.16
1	4	77	VAL	CB-CA-C	-6.09	102.71	112.16
1	3	77	VAL	CB-CA-C	-6.09	102.72	112.16
1	1	77	VAL	CB-CA-C	-6.08	102.74	112.16
1	5	77	VAL	CB-CA-C	-6.08	102.74	112.16
1	3	232	HIS	N-CA-C	5.42	117.36	108.52
1	2	232	HIS	N-CA-C	5.41	117.33	108.52
1	4	232	HIS	N-CA-C	5.40	117.33	108.52
1	5	232	HIS	N-CA-C	5.40	117.32	108.52
1	1	232	HIS	N-CA-C	5.40	117.32	108.52
1	6	232	HIS	N-CA-C	5.38	117.28	108.52
1	2	167	ALA	N-CA-C	5.17	117.35	110.53
1	3	167	ALA	N-CA-C	5.17	117.35	110.53
1	6	167	ALA	N-CA-C	5.16	117.34	110.53
1	1	167	ALA	N-CA-C	5.16	117.34	110.53
1	4	167	ALA	N-CA-C	5.16	117.34	110.53
1	5	167	ALA	N-CA-C	5.15	117.33	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	176	GLN	N-CA-C	5.12	117.47	110.55
1	4	176	GLN	N-CA-C	5.12	117.46	110.55
1	1	176	GLN	N-CA-C	5.10	117.44	110.55
1	2	153	VAL	N-CA-CB	5.10	116.28	110.72
1	3	176	GLN	N-CA-C	5.10	117.43	110.55
1	6	176	GLN	N-CA-C	5.10	117.43	110.55
1	1	153	VAL	N-CA-CB	5.08	116.26	110.72
1	2	176	GLN	N-CA-C	5.08	117.41	110.55
1	6	153	VAL	N-CA-CB	5.08	116.25	110.72
1	3	153	VAL	N-CA-CB	5.07	116.25	110.72
1	5	153	VAL	N-CA-CB	5.07	116.25	110.72
1	4	153	VAL	N-CA-CB	5.07	116.24	110.72
1	4	2	ASP	N-CA-C	-5.05	105.86	111.36
1	2	2	ASP	N-CA-C	-5.04	105.86	111.36
1	5	51	ARG	CA-C-N	5.04	124.80	119.76
1	5	51	ARG	C-N-CA	5.04	124.80	119.76
1	1	2	ASP	N-CA-C	-5.04	105.87	111.36
1	6	51	ARG	CA-C-N	5.03	124.79	119.76
1	6	51	ARG	C-N-CA	5.03	124.79	119.76
1	6	2	ASP	N-CA-C	-5.03	105.88	111.36
1	5	2	ASP	N-CA-C	-5.01	105.90	111.36
1	3	2	ASP	N-CA-C	-5.00	105.91	111.36

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	1	2703	0	2703	68	2
1	2	2703	0	2703	75	0
1	3	2703	0	2703	62	2
1	4	2703	0	2703	74	0
1	5	2703	0	2703	65	0
1	6	2703	0	2703	64	0
All	All	16218	0	16218	379	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (379) 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)
1:2:198:GLN:OE1	1:4:198:GLN:O	1.86	0.93
1:2:198:GLN:O	1:4:198:GLN:OE1	1.89	0.90
1:1:112:VAL:O	1:1:116:THR:HB	1.84	0.78
1:3:112:VAL:O	1:3:116:THR:HB	1.84	0.77
1:4:112:VAL:O	1:4:116:THR:HB	1.85	0.77
1:5:112:VAL:O	1:5:116:THR:HB	1.84	0.77
1:6:112:VAL:O	1:6:116:THR:HB	1.84	0.77
1:2:112:VAL:O	1:2:116:THR:HB	1.84	0.77
1:1:269:ASN:HD21	1:1:274:ARG:HH22	1.36	0.73
1:4:269:ASN:HD21	1:4:274:ARG:HH22	1.36	0.73
1:6:257:LEU:HD13	1:6:300:PRO:HB3	1.71	0.72
1:1:189:ARG:HD2	1:1:244:GLN:HE21	1.55	0.72
1:3:257:LEU:HD13	1:3:300:PRO:HB3	1.71	0.72
1:2:189:ARG:HD2	1:2:244:GLN:HE21	1.55	0.72
1:2:269:ASN:HD21	1:2:274:ARG:HH22	1.36	0.72
1:4:257:LEU:HD13	1:4:300:PRO:HB3	1.71	0.72
1:1:257:LEU:HD13	1:1:300:PRO:HB3	1.71	0.72
1:3:189:ARG:HD2	1:3:244:GLN:HE21	1.55	0.72
1:5:257:LEU:HD13	1:5:300:PRO:HB3	1.71	0.71
1:5:269:ASN:HD21	1:5:274:ARG:HH22	1.36	0.71
1:2:257:LEU:HD13	1:2:300:PRO:HB3	1.71	0.71
1:3:116:THR:HG21	1:3:304:ARG:HB2	1.72	0.71
1:5:189:ARG:HD2	1:5:244:GLN:HE21	1.55	0.71
1:6:189:ARG:HD2	1:6:244:GLN:HE21	1.55	0.71
1:6:116:THR:HG21	1:6:304:ARG:HB2	1.72	0.71
1:4:288:ARG:NH1	1:4:288:ARG:HG3	2.05	0.71
1:1:288:ARG:NH1	1:1:288:ARG:HG3	2.05	0.71
1:2:288:ARG:NH1	1:2:288:ARG:HG3	2.05	0.71
1:4:116:THR:HG21	1:4:304:ARG:HB2	1.72	0.71
1:1:116:THR:HG21	1:1:304:ARG:HB2	1.72	0.71
1:4:189:ARG:HD2	1:4:244:GLN:HE21	1.54	0.71
1:2:14:ALA:O	1:2:17:THR:HB	1.91	0.71
1:6:14:ALA:O	1:6:17:THR:HB	1.91	0.70
1:2:288:ARG:HG3	1:2:288:ARG:HH11	1.57	0.70
1:3:14:ALA:O	1:3:17:THR:HB	1.91	0.70
1:5:288:ARG:HG3	1:5:288:ARG:HH11	1.57	0.70
1:5:288:ARG:HG3	1:5:288:ARG:NH1	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:288:ARG:HG3	1:1:288:ARG:HH11	1.57	0.70
1:4:14:ALA:O	1:4:17:THR:HB	1.91	0.70
1:6:288:ARG:HG3	1:6:288:ARG:HH11	1.57	0.70
1:3:269:ASN:HD21	1:3:274:ARG:HH22	1.36	0.70
1:2:116:THR:HG21	1:2:304:ARG:HB2	1.72	0.70
1:5:116:THR:HG21	1:5:304:ARG:HB2	1.72	0.70
1:5:14:ALA:O	1:5:17:THR:HB	1.91	0.69
1:6:269:ASN:HD21	1:6:274:ARG:HH22	1.36	0.69
1:3:288:ARG:HG3	1:3:288:ARG:NH1	2.05	0.69
1:1:123:ARG:HG3	1:1:123:ARG:HH11	1.57	0.69
1:4:123:ARG:HG3	1:4:123:ARG:HH11	1.58	0.69
1:5:44:THR:HG22	1:5:46:ARG:H	1.58	0.69
1:3:288:ARG:HG3	1:3:288:ARG:HH11	1.57	0.69
1:3:20:GLU:HG2	1:3:21:ALA:N	2.08	0.69
1:4:288:ARG:HG3	1:4:288:ARG:HH11	1.57	0.69
1:6:20:GLU:HG2	1:6:21:ALA:N	2.08	0.69
1:1:14:ALA:O	1:1:17:THR:HB	1.91	0.69
1:4:20:GLU:HG2	1:4:21:ALA:N	2.08	0.69
1:5:20:GLU:HG2	1:5:21:ALA:N	2.08	0.69
1:6:44:THR:HG22	1:6:46:ARG:H	1.58	0.69
1:3:123:ARG:HG3	1:3:123:ARG:HH11	1.57	0.69
1:6:123:ARG:HG3	1:6:123:ARG:HH11	1.58	0.69
1:1:20:GLU:HG2	1:1:21:ALA:N	2.08	0.68
1:6:288:ARG:HG3	1:6:288:ARG:NH1	2.05	0.68
1:3:44:THR:HG22	1:3:46:ARG:H	1.58	0.68
1:2:20:GLU:HG2	1:2:21:ALA:N	2.08	0.68
1:2:44:THR:HG22	1:2:46:ARG:H	1.58	0.68
1:1:44:THR:HG22	1:1:46:ARG:H	1.58	0.67
1:5:123:ARG:HG3	1:5:123:ARG:HH11	1.57	0.67
1:4:44:THR:HG22	1:4:46:ARG:H	1.58	0.67
1:2:123:ARG:HG3	1:2:123:ARG:HH11	1.57	0.67
1:4:40:TYR:O	1:4:44:THR:HB	1.97	0.65
1:1:40:TYR:O	1:1:44:THR:HB	1.97	0.65
1:1:235:ASN:OD1	1:1:237:THR:HB	1.97	0.64
1:5:235:ASN:OD1	1:5:237:THR:HB	1.97	0.64
1:3:53:THR:H	1:3:57:GLN:NE2	1.96	0.64
1:6:235:ASN:OD1	1:6:237:THR:HB	1.97	0.64
1:3:235:ASN:OD1	1:3:237:THR:HB	1.98	0.64
1:4:53:THR:H	1:4:57:GLN:NE2	1.96	0.64
1:1:53:THR:H	1:1:57:GLN:NE2	1.96	0.64
1:2:235:ASN:OD1	1:2:237:THR:HB	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:40:TYR:O	1:3:44:THR:HB	1.97	0.64
1:4:235:ASN:OD1	1:4:237:THR:HB	1.97	0.64
1:6:53:THR:H	1:6:57:GLN:NE2	1.96	0.64
1:5:40:TYR:O	1:5:44:THR:HB	1.97	0.64
1:6:20:GLU:HG2	1:6:21:ALA:H	1.63	0.64
1:6:40:TYR:O	1:6:44:THR:HB	1.97	0.64
1:2:40:TYR:O	1:2:44:THR:HB	1.97	0.63
1:5:20:GLU:HG2	1:5:21:ALA:H	1.63	0.63
1:2:53:THR:H	1:2:57:GLN:NE2	1.96	0.63
1:5:53:THR:H	1:5:57:GLN:NE2	1.96	0.63
1:3:20:GLU:HG2	1:3:21:ALA:H	1.63	0.62
1:1:20:GLU:HG2	1:1:21:ALA:H	1.63	0.61
1:4:20:GLU:HG2	1:4:21:ALA:H	1.63	0.61
1:5:338:PRO:O	1:5:339:LEU:HB2	2.01	0.61
1:2:31:GLU:O	1:2:35:ILE:HG13	2.01	0.61
1:1:31:GLU:O	1:1:35:ILE:HG13	2.01	0.61
1:3:31:GLU:O	1:3:35:ILE:HG13	2.01	0.61
1:4:31:GLU:O	1:4:35:ILE:HG13	2.01	0.60
1:6:31:GLU:O	1:6:35:ILE:HG13	2.01	0.60
1:2:20:GLU:HG2	1:2:21:ALA:H	1.63	0.60
1:5:253:MET:HE3	1:6:341:ARG:HG3	1.83	0.60
1:2:338:PRO:O	1:2:339:LEU:HB2	2.01	0.60
1:6:158:MET:CE	1:6:246:GLN:HB2	2.32	0.60
1:5:31:GLU:O	1:5:35:ILE:HG13	2.01	0.59
1:3:338:PRO:O	1:3:339:LEU:HB2	2.01	0.59
1:3:217:MET:HA	1:3:217:MET:HE3	1.85	0.59
1:6:338:PRO:O	1:6:339:LEU:HB2	2.01	0.59
1:1:158:MET:CE	1:1:246:GLN:HB2	2.32	0.59
1:1:338:PRO:O	1:1:339:LEU:HB2	2.01	0.59
1:4:158:MET:CE	1:4:246:GLN:HB2	2.32	0.59
1:6:217:MET:HE3	1:6:217:MET:HA	1.85	0.59
1:3:158:MET:CE	1:3:246:GLN:HB2	2.32	0.58
1:4:253:MET:HE3	1:5:341:ARG:HG3	1.85	0.58
1:5:158:MET:CE	1:5:246:GLN:HB2	2.32	0.58
1:2:158:MET:CE	1:2:246:GLN:HB2	2.32	0.58
1:4:338:PRO:O	1:4:339:LEU:HB2	2.01	0.58
1:4:341:ARG:HG3	1:6:253:MET:HE3	1.84	0.58
1:4:158:MET:HE1	1:4:246:GLN:HB2	1.86	0.58
1:6:158:MET:HE1	1:6:246:GLN:HB2	1.86	0.58
1:1:158:MET:HE1	1:1:246:GLN:HB2	1.86	0.58
1:3:158:MET:HE1	1:3:246:GLN:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:217:MET:HE3	1:1:217:MET:HA	1.85	0.58
1:1:4:ILE:HG23	1:1:94:LEU:HB3	1.86	0.58
1:2:4:ILE:HG23	1:2:94:LEU:HB3	1.86	0.58
1:2:158:MET:HE1	1:2:246:GLN:HB2	1.86	0.58
1:5:4:ILE:HG23	1:5:94:LEU:HB3	1.86	0.58
1:5:158:MET:HE1	1:5:246:GLN:HB2	1.86	0.58
1:4:4:ILE:HG23	1:4:94:LEU:HB3	1.86	0.57
1:4:217:MET:HE3	1:4:217:MET:HA	1.85	0.57
1:5:141:TRP:CZ3	1:5:240:ASN:HB3	2.39	0.57
1:2:141:TRP:CZ3	1:2:240:ASN:HB3	2.39	0.57
1:2:217:MET:HE3	1:2:217:MET:HA	1.85	0.57
1:5:217:MET:HE3	1:5:217:MET:HA	1.85	0.57
1:6:141:TRP:CZ3	1:6:240:ASN:HB3	2.39	0.57
1:3:141:TRP:CZ3	1:3:240:ASN:HB3	2.39	0.57
1:2:253:MET:HE3	1:3:341:ARG:HG3	1.86	0.56
1:3:4:ILE:HG23	1:3:94:LEU:HB3	1.86	0.56
1:1:141:TRP:CZ3	1:1:240:ASN:HB3	2.39	0.56
1:6:4:ILE:HG23	1:6:94:LEU:HB3	1.86	0.56
1:4:41:ASN:HD21	1:4:48:VAL:H	1.53	0.56
1:5:41:ASN:HD21	1:5:48:VAL:H	1.54	0.56
1:1:41:ASN:HD21	1:1:48:VAL:H	1.54	0.56
1:2:41:ASN:HD21	1:2:48:VAL:H	1.54	0.56
1:4:141:TRP:CZ3	1:4:240:ASN:HB3	2.39	0.55
1:4:97:PRO:O	1:5:24:VAL:HG13	2.05	0.55
1:5:171:VAL:O	1:5:174:ILE:HG22	2.07	0.55
1:1:44:THR:HG22	1:1:46:ARG:N	2.22	0.55
1:3:44:THR:HG22	1:3:46:ARG:N	2.22	0.55
1:1:97:PRO:O	1:2:24:VAL:HG13	2.06	0.55
1:5:253:MET:CE	1:6:341:ARG:HG3	2.37	0.55
1:6:44:THR:HG22	1:6:46:ARG:N	2.22	0.55
1:2:171:VAL:O	1:2:174:ILE:HG22	2.07	0.55
1:2:44:THR:HG22	1:2:46:ARG:N	2.22	0.54
1:6:41:ASN:HD21	1:6:48:VAL:H	1.54	0.54
1:3:41:ASN:HD21	1:3:48:VAL:H	1.54	0.54
1:3:200:ASN:H	1:3:200:ASN:HD22	1.56	0.54
1:4:288:ARG:HH11	1:4:288:ARG:CG	2.21	0.54
1:1:341:ARG:HG3	1:3:253:MET:HE3	1.88	0.54
1:1:345:ARG:HG3	1:1:345:ARG:HH11	1.73	0.54
1:4:171:VAL:O	1:4:174:ILE:HG22	2.07	0.54
1:6:200:ASN:HD22	1:6:200:ASN:H	1.56	0.54
1:2:288:ARG:HH11	1:2:288:ARG:CG	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:345:ARG:HH11	1:3:345:ARG:HG3	1.73	0.54
1:6:171:VAL:O	1:6:174:ILE:HG22	2.07	0.54
1:2:345:ARG:HG3	1:2:345:ARG:HH11	1.73	0.53
1:4:44:THR:HG22	1:4:46:ARG:N	2.22	0.53
1:1:171:VAL:O	1:1:174:ILE:HG22	2.07	0.53
1:2:200:ASN:HD22	1:2:200:ASN:H	1.55	0.53
1:3:171:VAL:O	1:3:174:ILE:HG22	2.07	0.53
1:4:200:ASN:HD22	1:4:200:ASN:H	1.56	0.53
1:5:200:ASN:H	1:5:200:ASN:HD22	1.56	0.53
1:5:288:ARG:HH11	1:5:288:ARG:CG	2.21	0.53
1:6:145:ALA:O	1:6:146:ALA:HB3	2.09	0.53
1:1:200:ASN:HD22	1:1:200:ASN:H	1.56	0.53
1:4:145:ALA:O	1:4:146:ALA:HB3	2.09	0.53
1:2:253:MET:CE	1:3:341:ARG:HG3	2.39	0.53
1:6:345:ARG:HG3	1:6:345:ARG:HH11	1.73	0.53
1:1:145:ALA:O	1:1:146:ALA:HB3	2.09	0.53
1:1:288:ARG:HH11	1:1:288:ARG:CG	2.21	0.52
1:3:145:ALA:O	1:3:146:ALA:HB3	2.09	0.52
1:5:145:ALA:O	1:5:146:ALA:HB3	2.09	0.52
1:2:145:ALA:O	1:2:146:ALA:HB3	2.09	0.52
1:5:345:ARG:HG3	1:5:345:ARG:HH11	1.73	0.52
1:4:345:ARG:HG3	1:4:345:ARG:HH11	1.73	0.52
1:1:183:MET:HE3	1:1:224:ALA:HB1	1.92	0.52
1:2:198:GLN:O	1:4:198:GLN:CD	2.51	0.52
1:4:183:MET:HE3	1:4:224:ALA:HB1	1.92	0.52
1:1:111:ARG:NH1	1:2:318:ASP:OD2	2.42	0.52
1:3:183:MET:HE3	1:3:224:ALA:HB1	1.92	0.52
1:3:288:ARG:HH11	1:3:288:ARG:CG	2.21	0.52
1:2:183:MET:HE3	1:2:224:ALA:HB1	1.92	0.52
1:4:253:MET:CE	1:5:341:ARG:HG3	2.40	0.52
1:6:288:ARG:HH11	1:6:288:ARG:CG	2.21	0.52
1:6:183:MET:HE3	1:6:224:ALA:HB1	1.92	0.52
1:5:44:THR:HG22	1:5:46:ARG:N	2.22	0.51
1:5:183:MET:HE3	1:5:224:ALA:HB1	1.92	0.51
1:1:253:MET:HE3	1:2:341:ARG:HG3	1.93	0.51
1:3:200:ASN:H	1:3:200:ASN:ND2	2.09	0.51
1:6:200:ASN:H	1:6:200:ASN:ND2	2.09	0.51
1:4:111:ARG:NH1	1:5:318:ASP:OD2	2.44	0.51
1:4:341:ARG:HG3	1:6:253:MET:CE	2.41	0.51
1:2:200:ASN:H	1:2:200:ASN:ND2	2.09	0.51
1:1:200:ASN:H	1:1:200:ASN:ND2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:248:VAL:HG22	1:3:249:PHE:HD1	1.77	0.50
1:1:173:GLN:CD	1:1:173:GLN:H	2.20	0.50
1:5:200:ASN:H	1:5:200:ASN:ND2	2.09	0.50
1:2:248:VAL:HG22	1:2:249:PHE:HD1	1.77	0.50
1:5:248:VAL:HG22	1:5:249:PHE:HD1	1.77	0.50
1:4:200:ASN:H	1:4:200:ASN:ND2	2.09	0.50
1:3:173:GLN:CD	1:3:173:GLN:H	2.20	0.50
1:4:173:GLN:H	1:4:173:GLN:CD	2.20	0.50
1:4:248:VAL:HG22	1:4:249:PHE:HD1	1.77	0.50
1:6:173:GLN:CD	1:6:173:GLN:H	2.20	0.50
1:6:248:VAL:HG22	1:6:249:PHE:HD1	1.77	0.49
1:1:248:VAL:HG22	1:1:249:PHE:HD1	1.77	0.49
1:2:173:GLN:CD	1:2:173:GLN:H	2.20	0.49
1:5:173:GLN:CD	1:5:173:GLN:H	2.20	0.49
1:6:191:ILE:HD12	1:6:242:MET:HB3	1.96	0.48
1:1:191:ILE:HD12	1:1:242:MET:HB3	1.96	0.48
1:3:191:ILE:HD12	1:3:242:MET:HB3	1.96	0.48
1:4:190:ARG:NH1	1:5:134:GLU:HG2	2.29	0.48
1:4:191:ILE:HD12	1:4:242:MET:HB3	1.96	0.48
1:2:198:GLN:CD	1:4:198:GLN:O	2.57	0.47
1:4:7:ARG:NH2	1:5:23:ILE:HG22	2.30	0.47
1:5:191:ILE:HD12	1:5:242:MET:HB3	1.96	0.47
1:1:341:ARG:HG3	1:3:253:MET:CE	2.44	0.47
1:2:191:ILE:HD12	1:2:242:MET:HB3	1.96	0.47
1:1:300:PRO:HA	1:1:301:PRO:HD3	1.83	0.47
1:2:9:LEU:O	1:2:13:ARG:HG3	2.15	0.47
1:1:9:LEU:O	1:1:13:ARG:HG3	2.15	0.46
1:4:9:LEU:O	1:4:13:ARG:HG3	2.15	0.46
1:5:9:LEU:O	1:5:13:ARG:HG3	2.15	0.46
1:2:53:THR:H	1:2:57:GLN:HE21	1.62	0.46
1:2:300:PRO:HA	1:2:301:PRO:HD3	1.83	0.46
1:1:53:THR:H	1:1:57:GLN:HE21	1.62	0.46
1:3:9:LEU:O	1:3:13:ARG:HG3	2.15	0.46
1:3:53:THR:H	1:3:57:GLN:HE21	1.61	0.46
1:4:300:PRO:HA	1:4:301:PRO:HD3	1.83	0.46
1:5:231:LEU:HD12	1:5:231:LEU:HA	1.76	0.46
1:2:70:LEU:HD13	1:2:77:VAL:HG22	1.97	0.46
1:5:300:PRO:HA	1:5:301:PRO:HD3	1.83	0.46
1:5:70:LEU:HD13	1:5:77:VAL:HG22	1.98	0.46
1:6:9:LEU:O	1:6:13:ARG:HG3	2.15	0.46
1:6:53:THR:H	1:6:57:GLN:HE21	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:218:ARG:HE	1:3:218:ARG:HB3	1.63	0.46
1:4:70:LEU:HD13	1:4:77:VAL:HG22	1.97	0.46
1:2:345:ARG:HG3	1:2:345:ARG:NH1	2.31	0.45
1:5:53:THR:H	1:5:57:GLN:HE21	1.62	0.45
1:6:70:LEU:HD13	1:6:77:VAL:HG22	1.97	0.45
1:3:70:LEU:HD13	1:3:77:VAL:HG22	1.98	0.45
1:1:190:ARG:NH1	1:2:134:GLU:HG2	2.31	0.45
1:2:111:ARG:NH1	1:3:318:ASP:OD2	2.49	0.45
1:4:345:ARG:HG3	1:4:345:ARG:NH1	2.31	0.45
1:6:345:ARG:HG3	1:6:345:ARG:NH1	2.31	0.45
1:1:70:LEU:HD13	1:1:77:VAL:HG22	1.98	0.45
1:2:178:ARG:CZ	1:2:178:ARG:HB3	2.47	0.45
1:3:345:ARG:HG3	1:3:345:ARG:NH1	2.31	0.45
1:5:178:ARG:CZ	1:5:178:ARG:HB3	2.47	0.45
1:1:178:ARG:HB3	1:1:178:ARG:CZ	2.47	0.45
1:5:345:ARG:HG3	1:5:345:ARG:NH1	2.31	0.45
1:1:345:ARG:HG3	1:1:345:ARG:NH1	2.31	0.45
1:4:53:THR:H	1:4:57:GLN:HE21	1.61	0.45
1:2:198:GLN:NE2	1:6:198:GLN:O	2.50	0.45
1:3:178:ARG:CZ	1:3:178:ARG:HB3	2.47	0.45
1:3:123:ARG:HG3	1:3:123:ARG:NH1	2.30	0.45
1:3:300:PRO:HA	1:3:301:PRO:HD3	1.83	0.45
1:6:149:VAL:HB	1:6:163:LEU:HD13	1.99	0.44
1:6:178:ARG:HB3	1:6:178:ARG:CZ	2.47	0.44
1:1:149:VAL:HB	1:1:163:LEU:HD13	1.99	0.44
1:5:149:VAL:HB	1:5:163:LEU:HD13	1.99	0.44
1:5:337:GLY:CA	1:5:339:LEU:H	2.31	0.44
1:6:337:GLY:CA	1:6:339:LEU:H	2.31	0.44
1:1:123:ARG:HG3	1:1:123:ARG:NH1	2.30	0.44
1:3:149:VAL:HB	1:3:163:LEU:HD13	1.99	0.44
1:3:337:GLY:CA	1:3:339:LEU:H	2.31	0.44
1:4:337:GLY:CA	1:4:339:LEU:H	2.31	0.44
1:4:44:THR:O	1:4:45:LEU:HB2	2.18	0.44
1:4:149:VAL:HB	1:4:163:LEU:HD13	1.99	0.44
1:4:178:ARG:CZ	1:4:178:ARG:HB3	2.47	0.44
1:1:231:LEU:HD12	1:1:231:LEU:HA	1.76	0.44
1:2:149:VAL:HB	1:2:163:LEU:HD13	1.99	0.44
1:4:123:ARG:HG3	1:4:123:ARG:NH1	2.30	0.44
1:1:7:ARG:NH2	1:2:23:ILE:HG22	2.33	0.44
1:1:54:SER:H	1:1:57:GLN:HE21	1.66	0.44
1:4:54:SER:H	1:4:57:GLN:HE21	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:44:THR:O	1:3:45:LEU:HB2	2.18	0.43
1:6:231:LEU:HD12	1:6:231:LEU:HA	1.76	0.43
1:1:337:GLY:CA	1:1:339:LEU:H	2.31	0.43
1:2:44:THR:O	1:2:45:LEU:HB2	2.18	0.43
1:5:44:THR:O	1:5:45:LEU:HB2	2.18	0.43
1:6:8:ALA:O	1:6:12:MET:HG3	2.19	0.43
1:6:41:ASN:ND2	1:6:48:VAL:H	2.16	0.43
1:4:8:ALA:O	1:4:12:MET:HG3	2.18	0.43
1:1:44:THR:O	1:1:45:LEU:HB2	2.18	0.43
1:2:8:ALA:O	1:2:12:MET:HG3	2.19	0.43
1:2:41:ASN:ND2	1:2:48:VAL:H	2.16	0.43
1:5:111:ARG:NH1	1:6:318:ASP:OD2	2.51	0.43
1:1:8:ALA:O	1:1:12:MET:HG3	2.19	0.43
1:5:41:ASN:ND2	1:5:48:VAL:H	2.16	0.43
1:5:54:SER:H	1:5:57:GLN:HE21	1.66	0.43
1:6:44:THR:O	1:6:45:LEU:HB2	2.18	0.43
1:2:54:SER:H	1:2:57:GLN:HE21	1.66	0.43
1:2:337:GLY:CA	1:2:339:LEU:H	2.31	0.43
1:2:218:ARG:HE	1:2:218:ARG:HB3	1.63	0.43
1:4:231:LEU:HA	1:4:231:LEU:HD12	1.76	0.43
1:5:158:MET:HE3	1:5:246:GLN:HB2	2.01	0.43
1:3:41:ASN:ND2	1:3:48:VAL:H	2.16	0.42
1:3:158:MET:HE3	1:3:246:GLN:HB2	2.01	0.42
1:5:8:ALA:O	1:5:12:MET:HG3	2.19	0.42
1:5:158:MET:HE2	1:5:244:GLN:CD	2.44	0.42
1:6:54:SER:H	1:6:57:GLN:HE21	1.66	0.42
1:6:123:ARG:HG3	1:6:123:ARG:NH1	2.30	0.42
1:6:158:MET:HE3	1:6:246:GLN:HB2	2.01	0.42
1:2:116:THR:HG21	1:2:304:ARG:CB	2.47	0.42
1:2:158:MET:HE2	1:2:244:GLN:CD	2.44	0.42
1:3:158:MET:HE2	1:3:244:GLN:CD	2.44	0.42
1:1:33:LEU:HD23	1:1:33:LEU:HA	1.84	0.42
1:2:231:LEU:HA	1:2:231:LEU:HD12	1.76	0.42
1:3:41:ASN:HD21	1:3:48:VAL:HG23	1.85	0.42
1:6:41:ASN:HD21	1:6:48:VAL:HG23	1.85	0.42
1:6:116:THR:CG2	1:6:304:ARG:HB2	2.46	0.42
1:1:253:MET:CE	1:2:341:ARG:HG3	2.48	0.42
1:1:41:ASN:HD21	1:1:48:VAL:HG23	1.85	0.42
1:3:8:ALA:O	1:3:12:MET:HG3	2.19	0.42
1:4:41:ASN:ND2	1:4:48:VAL:H	2.16	0.42
1:4:116:THR:HG21	1:4:304:ARG:CB	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:158:MET:HE3	1:4:246:GLN:HB2	2.01	0.42
1:3:54:SER:H	1:3:57:GLN:HE21	1.66	0.42
1:5:41:ASN:HD21	1:5:48:VAL:HG23	1.85	0.42
1:6:128:PHE:HB2	1:6:247:VAL:HG11	2.02	0.42
1:1:41:ASN:ND2	1:1:48:VAL:H	2.16	0.42
1:2:116:THR:CG2	1:2:304:ARG:HB2	2.46	0.42
1:3:128:PHE:HB2	1:3:247:VAL:HG11	2.02	0.42
1:4:158:MET:HE2	1:4:244:GLN:CD	2.44	0.42
1:5:97:PRO:O	1:6:24:VAL:HG13	2.19	0.42
1:1:158:MET:HE2	1:1:244:GLN:CD	2.44	0.42
1:4:41:ASN:HD21	1:4:48:VAL:HG23	1.85	0.42
1:4:116:THR:CG2	1:4:304:ARG:HB2	2.46	0.42
1:2:41:ASN:HD21	1:2:48:VAL:HG23	1.85	0.41
1:1:158:MET:HE3	1:1:246:GLN:HB2	2.01	0.41
1:2:128:PHE:HB2	1:2:247:VAL:HG11	2.02	0.41
1:4:58:ARG:HD2	1:4:323:LEU:O	2.20	0.41
1:5:58:ARG:HD2	1:5:323:LEU:O	2.21	0.41
1:5:128:PHE:HB2	1:5:247:VAL:HG11	2.02	0.41
1:3:116:THR:CG2	1:3:304:ARG:HB2	2.46	0.41
1:6:158:MET:HE2	1:6:244:GLN:CD	2.44	0.41
1:1:128:PHE:HB2	1:1:247:VAL:HG11	2.02	0.41
1:1:198:GLN:O	1:4:198:GLN:NE2	2.53	0.41
1:2:158:MET:HE3	1:2:246:GLN:HB2	2.01	0.41
1:4:54:SER:H	1:4:57:GLN:NE2	2.19	0.41
1:1:49:THR:HG22	1:1:51:ARG:H	1.86	0.41
1:2:58:ARG:HD2	1:2:323:LEU:O	2.21	0.41
1:4:196:MET:HE3	1:4:197:ALA:H	1.86	0.41
1:1:58:ARG:HD2	1:1:323:LEU:O	2.20	0.41
1:2:54:SER:H	1:2:57:GLN:NE2	2.19	0.41
1:2:196:MET:HE3	1:2:197:ALA:H	1.86	0.41
1:4:128:PHE:HB2	1:4:247:VAL:HG11	2.02	0.41
1:6:54:SER:H	1:6:57:GLN:NE2	2.19	0.41
1:6:143:MET:HE2	1:6:143:MET:HB2	1.93	0.41
1:6:196:MET:HE3	1:6:197:ALA:H	1.86	0.41
1:1:116:THR:CG2	1:1:304:ARG:HB2	2.46	0.41
1:2:337:GLY:HA3	1:2:339:LEU:N	2.36	0.41
1:5:196:MET:HE3	1:5:197:ALA:H	1.86	0.41
1:2:49:THR:HG22	1:2:51:ARG:H	1.86	0.40
1:2:143:MET:HE2	1:2:143:MET:HB2	1.93	0.40
1:3:337:GLY:HA3	1:3:339:LEU:N	2.36	0.40
1:4:337:GLY:HA3	1:4:339:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:248:VAL:HG22	1:3:249:PHE:CD1	2.55	0.40
1:2:158:MET:HE3	1:2:246:GLN:CA	2.52	0.40
1:3:54:SER:H	1:3:57:GLN:NE2	2.19	0.40
1:5:49:THR:HG22	1:5:51:ARG:H	1.86	0.40
1:1:158:MET:HE3	1:1:246:GLN:CA	2.52	0.40
1:3:58:ARG:HD2	1:3:323:LEU:O	2.20	0.40
1:5:158:MET:HE3	1:5:246:GLN:CA	2.52	0.40
1:6:248:VAL:HG22	1:6:249:PHE:CD1	2.55	0.40
1:1:196:MET:HE3	1:1:197:ALA:H	1.86	0.40
1:1:248:VAL:HG22	1:1:249:PHE:CD1	2.55	0.40
1:4:35:ILE:HG13	1:4:35:ILE:H	1.72	0.40
1:4:158:MET:HE3	1:4:246:GLN:CA	2.52	0.40
1:4:248:VAL:HG22	1:4:249:PHE:CD1	2.55	0.40
1:6:158:MET:HE3	1:6:246:GLN:CA	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:288:ARG:NH1	1:3:288:ARG:NH1[2_457]	1.94	0.26
1:1:288:ARG:CZ	1:3:288:ARG:NH1[2_457]	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	1	347/349 (99%)	330 (95%)	16 (5%)	1 (0%)	36 58
1	2	347/349 (99%)	330 (95%)	16 (5%)	1 (0%)	36 58
1	3	347/349 (99%)	330 (95%)	16 (5%)	1 (0%)	36 58
1	4	347/349 (99%)	330 (95%)	16 (5%)	1 (0%)	36 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	347/349 (99%)	330 (95%)	16 (5%)	1 (0%)	36	58
1	6	347/349 (99%)	330 (95%)	16 (5%)	1 (0%)	36	58
All	All	2082/2094 (99%)	1980 (95%)	96 (5%)	6 (0%)	36	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	339	LEU
1	2	339	LEU
1	3	339	LEU
1	4	339	LEU
1	5	339	LEU
1	6	339	LEU

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	1	286/286 (100%)	243 (85%)	43 (15%)	3	5
1	2	286/286 (100%)	243 (85%)	43 (15%)	3	5
1	3	286/286 (100%)	243 (85%)	43 (15%)	3	5
1	4	286/286 (100%)	242 (85%)	44 (15%)	2	5
1	5	286/286 (100%)	242 (85%)	44 (15%)	2	5
1	6	286/286 (100%)	243 (85%)	43 (15%)	3	5
All	All	1716/1716 (100%)	1456 (85%)	260 (15%)	3	5

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	3	THR
1	1	17	THR
1	1	18	LEU
1	1	19	GLN

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Mol	Chain	Res	Type
1	1	24	VAL
1	1	25	LEU
1	1	39	ARG
1	1	44	THR
1	1	45	LEU
1	1	46	ARG
1	1	77	VAL
1	1	94	LEU
1	1	111	ARG
1	1	116	THR
1	1	123	ARG
1	1	149	VAL
1	1	152	VAL
1	1	153	VAL
1	1	158	MET
1	1	163	LEU
1	1	171	VAL
1	1	178	ARG
1	1	186	LEU
1	1	187	VAL
1	1	203	GLN
1	1	215	VAL
1	1	216	ASP
1	1	221	ARG
1	1	237	THR
1	1	248	VAL
1	1	257	LEU
1	1	263	LEU
1	1	281	LEU
1	1	288	ARG
1	1	291	LEU
1	1	308	LEU
1	1	312	LEU
1	1	321	THR
1	1	322	VAL
1	1	324	ARG
1	1	333	ASN
1	1	339	LEU
1	1	345	ARG
1	2	3	THR
1	2	17	THR
1	2	18	LEU

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Mol	Chain	Res	Type
1	2	19	GLN
1	2	24	VAL
1	2	25	LEU
1	2	39	ARG
1	2	44	THR
1	2	45	LEU
1	2	46	ARG
1	2	77	VAL
1	2	94	LEU
1	2	111	ARG
1	2	116	THR
1	2	123	ARG
1	2	149	VAL
1	2	152	VAL
1	2	153	VAL
1	2	158	MET
1	2	163	LEU
1	2	171	VAL
1	2	178	ARG
1	2	186	LEU
1	2	187	VAL
1	2	203	GLN
1	2	215	VAL
1	2	216	ASP
1	2	221	ARG
1	2	237	THR
1	2	248	VAL
1	2	257	LEU
1	2	263	LEU
1	2	281	LEU
1	2	288	ARG
1	2	291	LEU
1	2	308	LEU
1	2	312	LEU
1	2	321	THR
1	2	322	VAL
1	2	324	ARG
1	2	333	ASN
1	2	339	LEU
1	2	345	ARG
1	3	3	THR
1	3	17	THR

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Mol	Chain	Res	Type
1	3	18	LEU
1	3	19	GLN
1	3	24	VAL
1	3	25	LEU
1	3	39	ARG
1	3	44	THR
1	3	45	LEU
1	3	46	ARG
1	3	77	VAL
1	3	94	LEU
1	3	111	ARG
1	3	116	THR
1	3	123	ARG
1	3	149	VAL
1	3	152	VAL
1	3	153	VAL
1	3	158	MET
1	3	163	LEU
1	3	171	VAL
1	3	178	ARG
1	3	186	LEU
1	3	187	VAL
1	3	203	GLN
1	3	215	VAL
1	3	216	ASP
1	3	221	ARG
1	3	237	THR
1	3	248	VAL
1	3	257	LEU
1	3	263	LEU
1	3	281	LEU
1	3	288	ARG
1	3	291	LEU
1	3	308	LEU
1	3	312	LEU
1	3	321	THR
1	3	322	VAL
1	3	324	ARG
1	3	333	ASN
1	3	339	LEU
1	3	345	ARG
1	4	3	THR

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Mol	Chain	Res	Type
1	4	17	THR
1	4	18	LEU
1	4	19	GLN
1	4	24	VAL
1	4	25	LEU
1	4	39	ARG
1	4	44	THR
1	4	45	LEU
1	4	46	ARG
1	4	77	VAL
1	4	94	LEU
1	4	111	ARG
1	4	116	THR
1	4	123	ARG
1	4	149	VAL
1	4	152	VAL
1	4	153	VAL
1	4	158	MET
1	4	163	LEU
1	4	171	VAL
1	4	178	ARG
1	4	186	LEU
1	4	187	VAL
1	4	203	GLN
1	4	215	VAL
1	4	216	ASP
1	4	221	ARG
1	4	237	THR
1	4	248	VAL
1	4	257	LEU
1	4	263	LEU
1	4	281	LEU
1	4	288	ARG
1	4	291	LEU
1	4	308	LEU
1	4	312	LEU
1	4	313	LEU
1	4	321	THR
1	4	322	VAL
1	4	324	ARG
1	4	333	ASN
1	4	339	LEU

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Mol	Chain	Res	Type
1	4	345	ARG
1	5	3	THR
1	5	17	THR
1	5	18	LEU
1	5	19	GLN
1	5	24	VAL
1	5	25	LEU
1	5	39	ARG
1	5	44	THR
1	5	45	LEU
1	5	46	ARG
1	5	77	VAL
1	5	94	LEU
1	5	111	ARG
1	5	116	THR
1	5	123	ARG
1	5	149	VAL
1	5	152	VAL
1	5	153	VAL
1	5	158	MET
1	5	163	LEU
1	5	171	VAL
1	5	178	ARG
1	5	186	LEU
1	5	187	VAL
1	5	203	GLN
1	5	215	VAL
1	5	216	ASP
1	5	221	ARG
1	5	237	THR
1	5	248	VAL
1	5	257	LEU
1	5	263	LEU
1	5	281	LEU
1	5	288	ARG
1	5	291	LEU
1	5	308	LEU
1	5	312	LEU
1	5	313	LEU
1	5	321	THR
1	5	322	VAL
1	5	324	ARG

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Mol	Chain	Res	Type
1	5	333	ASN
1	5	339	LEU
1	5	345	ARG
1	6	3	THR
1	6	17	THR
1	6	18	LEU
1	6	19	GLN
1	6	24	VAL
1	6	25	LEU
1	6	39	ARG
1	6	44	THR
1	6	45	LEU
1	6	46	ARG
1	6	77	VAL
1	6	94	LEU
1	6	111	ARG
1	6	116	THR
1	6	123	ARG
1	6	149	VAL
1	6	152	VAL
1	6	153	VAL
1	6	158	MET
1	6	163	LEU
1	6	171	VAL
1	6	178	ARG
1	6	186	LEU
1	6	187	VAL
1	6	203	GLN
1	6	215	VAL
1	6	216	ASP
1	6	221	ARG
1	6	237	THR
1	6	248	VAL
1	6	257	LEU
1	6	263	LEU
1	6	281	LEU
1	6	288	ARG
1	6	291	LEU
1	6	308	LEU
1	6	312	LEU
1	6	321	THR
1	6	322	VAL

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Mol	Chain	Res	Type
1	6	324	ARG
1	6	333	ASN
1	6	339	LEU
1	6	345	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	41	ASN
1	1	57	GLN
1	1	179	ASN
1	1	200	ASN
1	1	244	GLN
1	1	269	ASN
1	1	276	HIS
1	1	302	ASN
1	2	41	ASN
1	2	57	GLN
1	2	179	ASN
1	2	198	GLN
1	2	200	ASN
1	2	244	GLN
1	2	269	ASN
1	2	276	HIS
1	2	302	ASN
1	3	41	ASN
1	3	57	GLN
1	3	179	ASN
1	3	198	GLN
1	3	200	ASN
1	3	244	GLN
1	3	269	ASN
1	3	276	HIS
1	3	302	ASN
1	4	41	ASN
1	4	57	GLN
1	4	179	ASN
1	4	193	ASN
1	4	200	ASN
1	4	203	GLN
1	4	205	GLN
1	4	244	GLN

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Mol	Chain	Res	Type
1	4	269	ASN
1	4	276	HIS
1	4	302	ASN
1	5	41	ASN
1	5	57	GLN
1	5	179	ASN
1	5	200	ASN
1	5	244	GLN
1	5	269	ASN
1	5	276	HIS
1	5	302	ASN
1	6	41	ASN
1	6	57	GLN
1	6	179	ASN
1	6	200	ASN
1	6	244	GLN
1	6	269	ASN
1	6	276	HIS
1	6	302	ASN

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.