



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:45 AM UTC

PDB ID : 1FOD / pdb_00001fod
Title : STRUCTURE OF A MAJOR IMMUNOGENIC SITE ON FOOT-AND-MOUTH DISEASE VIRUS
Authors : Logan, D.T.; Lea, S.; Lewis, R.; Stuart, D.; Fry, E.
Deposited on : 1993-10-27
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

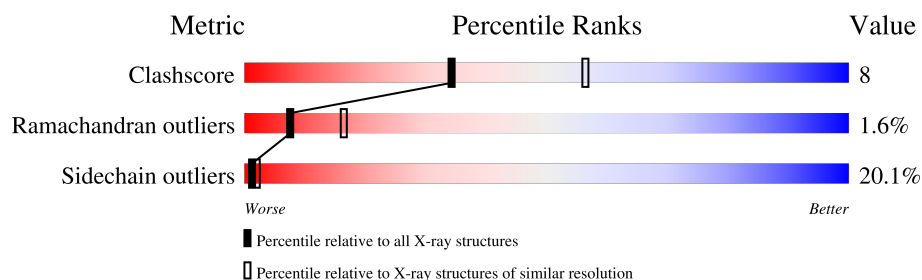
1 Overall quality at a glance

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	213	
2	2	218	
3	3	220	
4	4	85	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5362 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 FOOT AND MOUTH DISEASE VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	210	Total	C	N	O	S	0	0	0
			1651	1041	299	306	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	56	VAL	ILE	conflict	UNP Q84771
1	64	GLY	ALA	conflict	UNP Q84771
1	137	SER	ASN	conflict	UNP Q84771

- Molecule 2 is a protein called FOOT AND MOUTH DISEASE VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	214	Total	C	N	O	S	0	0	0
			1676	1065	286	318	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	130	CYS	TYR	conflict	UNP Q84771

- Molecule 3 is a protein called FOOT AND MOUTH DISEASE VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	220	Total	C	N	O	S	0	0	0
			1681	1075	275	322	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	85	HIS	GLN	conflict	UNP Q84771

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Chain	Residue	Modelled	Actual	Comment	Reference
3	168	THR	ALA	conflict	UNP Q84771
3	173	ASP	GLY	conflict	UNP Q84771

- Molecule 4 is a protein called FOOT AND MOUTH DISEASE VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	47	Total	C	N	O	S	0	0	1
			354	222	58	72	2			

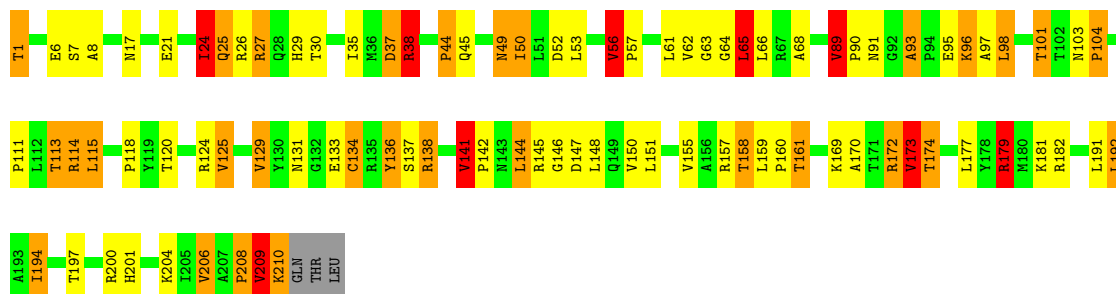
3 Residue-property plots

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.

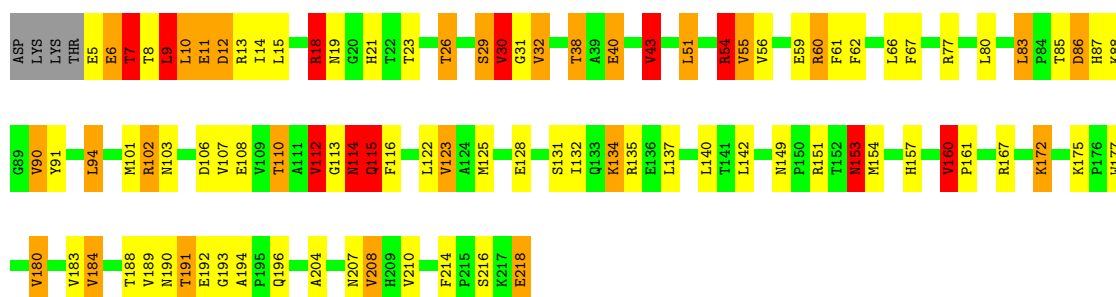
• Molecule 1: FOOT AND MOUTH DISEASE VIRUS

Chain 1: 



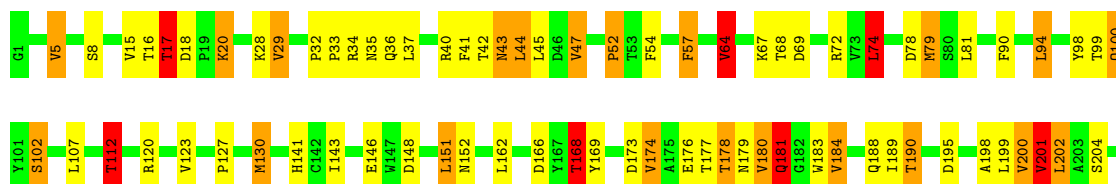
• Molecule 2: FOOT AND MOUTH DISEASE VIRUS

Chain 2: 



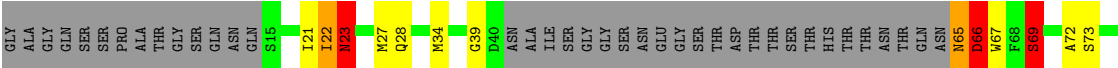
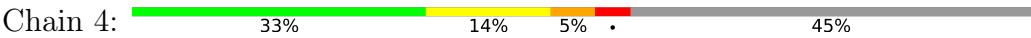
• Molecule 3: FOOT AND MOUTH DISEASE VIRUS

Chain 3: 





● Molecule 4: FOOT AND MOUTH DISEASE VIRUS



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	345.00Å 345.00Å 345.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5362	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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	1.46	11/1688 (0.7%)	2.22	87/2303 (3.8%)
2	2	1.54	16/1719 (0.9%)	2.18	74/2346 (3.2%)
3	3	1.45	8/1729 (0.5%)	2.26	83/2361 (3.5%)
4	4	1.36	3/360 (0.8%)	2.30	17/483 (3.5%)
All	All	1.47	38/5496 (0.7%)	2.22	261/7493 (3.5%)

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
3	3	0	1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	55	VAL	CA-CB	12.10	1.66	1.53
2	2	112	VAL	CA-CB	12.05	1.68	1.54
2	2	14	ILE	CA-CB	11.57	1.68	1.53
1	1	173	VAL	CA-CB	10.42	1.67	1.54
2	2	32	VAL	CA-CB	9.98	1.68	1.54
2	2	184	VAL	CA-CB	9.44	1.65	1.54
3	3	29	VAL	CA-CB	9.38	1.66	1.54
3	3	47	VAL	CA-CB	9.05	1.65	1.54
3	3	184	VAL	CA-CB	7.55	1.63	1.54
2	2	208	VAL	CA-CB	7.45	1.63	1.54
1	1	56	VAL	CA-CB	7.42	1.63	1.54
2	2	6	GLU	CA-C	7.27	1.60	1.52
3	3	200	VAL	CA-CB	7.23	1.63	1.54
1	1	24	ILE	CA-CB	7.17	1.64	1.54
2	2	123	VAL	CA-CB	7.14	1.63	1.54
2	2	132	ILE	CA-CB	7.06	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	201	VAL	CA-CB	7.05	1.64	1.54
3	3	180	VAL	CA-CB	6.92	1.63	1.54
2	2	90	VAL	CA-CB	6.91	1.64	1.54
4	4	69	SER	CA-CB	-6.71	1.42	1.53
2	2	167	ARG	CZ-NH2	6.63	1.42	1.33
2	2	30	VAL	N-CA	6.63	1.54	1.46
4	4	21	ILE	CA-CB	6.40	1.62	1.54
3	3	218	ARG	CA-C	6.38	1.61	1.52
1	1	50	ILE	CB-CG1	-6.06	1.41	1.53
1	1	50	ILE	CA-CB	6.00	1.62	1.54
1	1	161	THR	CA-CB	5.87	1.62	1.53
1	1	21	GLU	CA-CB	-5.78	1.44	1.53
2	2	9	LEU	CA-CB	5.68	1.63	1.53
2	2	180	VAL	CA-CB	5.67	1.61	1.54
1	1	209	VAL	CA-CB	5.50	1.61	1.54
1	1	137	SER	CA-CB	5.49	1.59	1.52
2	2	7	THR	N-CA	5.35	1.53	1.46
2	2	67	PHE	CA-CB	5.26	1.61	1.53
1	1	93	ALA	CA-CB	-5.24	1.45	1.53
3	3	188	GLN	CA-CB	-5.21	1.45	1.53
1	1	134	CYS	CA-C	5.14	1.59	1.52
4	4	39	GLY	C-N	-5.09	1.26	1.33

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	180	VAL	CA-C-O	14.09	134.50	120.27
1	1	147	ASP	CA-CB-CG	13.95	126.55	112.60
2	2	7	THR	N-CA-C	12.84	138.16	110.80
2	2	6	GLU	N-CA-C	12.83	129.82	107.49
2	2	12	ASP	CA-CB-CG	12.64	125.24	112.60
3	3	219	ALA	N-CA-C	12.14	136.67	110.80
3	3	102	SER	CA-CB-OG	-11.67	87.76	111.10
1	1	208	PRO	O-C-N	11.46	138.12	122.64
3	3	42	THR	CA-CB-OG1	-11.25	92.73	109.60
3	3	218	ARG	N-CA-C	-11.03	87.32	110.80
4	4	65	ASN	CA-CB-CG	10.76	123.36	112.60
1	1	89	VAL	N-CA-CB	-10.14	97.02	111.21
2	2	11	GLU	N-CA-C	10.00	124.09	108.79
3	3	218	ARG	CA-CB-CG	9.77	133.64	114.10
2	2	29	SER	CA-C-O	-9.77	110.10	120.55
2	2	29	SER	N-CA-C	9.73	123.27	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	69	ASP	CA-CB-CG	9.69	122.29	112.60
2	2	135	ARG	NE-CZ-NH1	9.46	130.96	121.50
3	3	43	ASN	CA-CB-CG	-9.37	103.23	112.60
4	4	65	ASN	CA-C-O	-9.12	105.29	120.80
1	1	50	ILE	CB-CG1-CD1	-9.09	94.71	113.80
3	3	42	THR	CA-CB-CG2	9.06	125.91	110.50
3	3	217	ALA	CA-C-N	8.89	138.52	121.54
3	3	217	ALA	C-N-CA	8.89	138.52	121.54
3	3	64	VAL	N-CA-CB	-8.88	95.94	111.39
3	3	173	ASP	CA-CB-CG	8.80	121.40	112.60
2	2	160	VAL	N-CA-CB	-8.63	99.12	111.21
4	4	80	PHE	CA-CB-CG	8.55	122.35	113.80
3	3	28	LYS	CA-C-O	-8.41	111.82	121.65
3	3	17	THR	N-CA-CB	-8.35	94.98	111.60
2	2	184	VAL	N-CA-C	-8.32	104.65	111.81
3	3	176	GLU	CA-C-N	8.30	131.75	120.54
3	3	176	GLU	C-N-CA	8.30	131.75	120.54
1	1	209	VAL	CA-C-O	-8.30	110.41	120.78
3	3	173	ASP	O-C-N	8.24	131.98	122.25
3	3	28	LYS	CA-C-N	-8.23	112.48	123.10
3	3	28	LYS	C-N-CA	-8.23	112.48	123.10
3	3	68	THR	OG1-CB-CG2	8.19	125.69	109.30
3	3	148	ASP	CA-CB-CG	8.17	120.77	112.60
2	2	6	GLU	CA-C-N	8.07	136.94	121.54
2	2	6	GLU	C-N-CA	8.07	136.94	121.54
1	1	101	THR	N-CA-CB	-8.01	96.70	110.32
1	1	141	VAL	CB-CA-C	8.01	118.73	110.88
3	3	36	GLN	N-CA-C	8.00	122.34	112.58
2	2	172	LYS	CB-CG-CD	8.00	129.69	111.30
1	1	101	THR	CA-CB-OG1	-8.00	97.60	109.60
1	1	96	LYS	CA-CB-CG	8.00	130.09	114.10
2	2	61	PHE	CA-CB-CG	7.91	121.71	113.80
3	3	64	VAL	CB-CA-C	7.88	122.36	110.62
3	3	36	GLN	CA-CB-CG	-7.87	98.37	114.10
2	2	218	GLU	CA-CB-CG	7.79	129.69	114.10
3	3	179	ASN	CA-CB-CG	7.77	120.37	112.60
1	1	182	ARG	CA-CB-CG	7.74	129.57	114.10
2	2	114	ASN	CB-CG-ND2	7.67	127.90	116.40
2	2	115	GLN	OE1-CD-NE2	-7.65	114.95	122.60
1	1	141	VAL	N-CA-CB	-7.60	100.98	110.33
3	3	112	THR	N-CA-CB	-7.55	98.73	111.27
2	2	14	ILE	CB-CA-C	-7.53	101.20	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	220	GLU	CA-CB-CG	7.52	129.14	114.10
1	1	206	VAL	N-CA-CB	-7.52	98.83	111.23
3	3	98	TYR	CA-C-O	-7.49	112.37	121.06
4	4	82	ALA	N-CA-C	-7.49	97.20	109.40
2	2	135	ARG	NE-CZ-NH2	-7.43	112.51	119.20
3	3	57	PHE	CA-CB-CG	-7.42	106.38	113.80
1	1	101	THR	CA-CB-CG2	7.38	123.05	110.50
1	1	200	ARG	CD-NE-CZ	7.38	134.73	124.40
2	2	18	ARG	CA-CB-CG	-7.36	99.38	114.10
2	2	114	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	1	114	ARG	CA-CB-CG	7.25	128.59	114.10
3	3	20	LYS	N-CA-CB	-7.25	98.94	111.55
1	1	113	THR	CA-C-O	-7.24	112.54	120.36
1	1	37	ASP	CA-CB-CG	7.24	119.84	112.60
2	2	13	ARG	N-CA-C	-7.23	90.92	107.48
3	3	35	ASN	CA-CB-CG	7.15	119.75	112.60
4	4	65	ASN	N-CA-CB	7.14	122.64	110.50
2	2	153	ASN	CA-CB-CG	7.13	119.73	112.60
2	2	26	THR	CB-CA-C	-7.12	95.31	109.33
2	2	194	ALA	N-CA-C	-7.11	100.80	109.83
3	3	143	ILE	N-CA-C	-7.06	99.40	108.93
3	3	100	GLN	OE1-CD-NE2	-7.05	115.55	122.60
2	2	103	ASN	OD1-CG-ND2	-7.00	115.60	122.60
3	3	123	VAL	CG1-CB-CG2	6.92	126.02	110.80
1	1	63	GLY	CA-C-O	-6.89	113.56	121.00
2	2	55	VAL	CA-C-O	6.83	128.34	121.09
1	1	62	VAL	CA-C-O	-6.77	113.67	120.85
3	3	72	ARG	NE-CZ-NH2	-6.77	113.11	119.20
3	3	127	PRO	CB-CA-C	6.75	119.16	110.92
2	2	26	THR	N-CA-CB	6.74	122.60	111.08
3	3	218	ARG	NE-CZ-NH1	-6.71	114.79	121.50
2	2	30	VAL	CA-CB-CG1	6.70	121.78	110.40
1	1	172	ARG	CA-CB-CG	6.68	127.45	114.10
1	1	138	ARG	N-CA-C	-6.65	99.46	108.24
3	3	54	PHE	CA-CB-CG	6.64	120.44	113.80
2	2	7	THR	CA-CB-OG1	6.62	119.52	109.60
3	3	190	THR	CB-CA-C	-6.61	98.70	111.78
1	1	27	ARG	N-CA-C	6.56	119.98	112.57
3	3	130	MET	CA-CB-CG	6.55	127.21	114.10
1	1	29	HIS	CA-C-O	-6.53	110.76	119.11
1	1	50	ILE	CB-CA-C	6.52	120.14	111.21
1	1	95	GLU	CA-C-O	-6.50	112.75	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	54	ARG	NE-CZ-NH2	6.47	125.03	119.20
3	3	189	ILE	N-CA-C	-6.46	104.55	110.82
2	2	43	VAL	N-CA-CB	-6.41	97.01	111.87
3	3	32	PRO	O-C-N	-6.39	118.37	121.31
2	2	218	GLU	CB-CG-CD	6.37	123.44	112.60
2	2	62	PHE	CA-CB-CG	6.34	120.14	113.80
2	2	5	GLU	CA-C-O	-6.32	110.06	120.80
4	4	73	SER	CA-CB-OG	-6.31	98.47	111.10
3	3	181	GLN	CG-CD-NE2	6.28	125.82	116.40
1	1	17	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	1	125	VAL	N-CA-CB	-6.25	99.18	112.00
1	1	182	ARG	CD-NE-CZ	6.24	133.13	124.40
3	3	183	TRP	CA-C-N	-6.20	115.51	123.19
3	3	183	TRP	C-N-CA	-6.20	115.51	123.19
2	2	18	ARG	NE-CZ-NH2	-6.19	113.63	119.20
2	2	30	VAL	CA-CB-CG2	-6.17	99.91	110.40
1	1	49	ASN	CA-C-N	-6.16	112.64	122.50
1	1	49	ASN	C-N-CA	-6.16	112.64	122.50
1	1	52	ASP	CA-CB-CG	6.16	118.76	112.60
3	3	68	THR	N-CA-CB	-6.16	101.61	111.58
1	1	64	GLY	O-C-N	-6.14	114.72	122.70
2	2	110	THR	CA-CB-OG1	-6.14	100.39	109.60
4	4	72	ALA	O-C-N	-6.13	115.16	122.15
3	3	151	LEU	CA-C-N	6.12	130.56	122.30
3	3	151	LEU	C-N-CA	6.12	130.56	122.30
1	1	170	ALA	N-CA-C	-6.09	99.88	108.96
2	2	10	LEU	CA-C-O	-6.09	111.80	120.51
2	2	38	THR	CA-CB-OG1	-6.08	100.48	109.60
3	3	216	ASP	O-C-N	-6.06	116.12	123.27
3	3	74	LEU	N-CA-CB	-6.05	101.24	110.26
2	2	18	ARG	CA-C-O	-6.03	113.85	120.36
2	2	191	THR	OG1-CB-CG2	-5.99	97.32	109.30
1	1	131	ASN	CA-CB-CG	5.97	118.57	112.60
3	3	152	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	1	120	THR	CA-C-O	-5.95	112.75	119.95
1	1	208	PRO	CA-C-N	5.94	132.67	121.97
1	1	208	PRO	C-N-CA	5.94	132.67	121.97
1	1	138	ARG	O-C-N	5.93	129.54	122.72
2	2	188	THR	CA-C-O	-5.93	114.42	120.71
4	4	34	MET	O-C-N	-5.92	116.29	123.16
1	1	192	LEU	O-C-N	-5.91	116.48	123.22
1	1	182	ARG	NE-CZ-NH2	-5.88	113.91	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	78	ASP	CA-CB-CG	5.88	118.48	112.60
4	4	80	PHE	N-CA-C	-5.87	106.09	113.72
3	3	181	GLN	CA-CB-CG	5.84	125.78	114.10
1	1	129	VAL	CA-CB-CG2	-5.84	100.48	110.40
2	2	31	GLY	CA-C-N	-5.84	115.01	123.06
2	2	31	GLY	C-N-CA	-5.84	115.01	123.06
2	2	135	ARG	CD-NE-CZ	5.83	132.57	124.40
3	3	52	PRO	CB-CA-C	5.83	118.97	111.21
2	2	190	ASN	CB-CG-ND2	5.82	125.12	116.40
4	4	23	ASN	CB-CG-ND2	5.80	125.09	116.40
2	2	19	ASN	CB-CG-ND2	5.77	125.05	116.40
1	1	133	GLU	CA-C-O	-5.74	114.62	121.11
1	1	155	VAL	N-CA-C	5.73	118.21	111.05
2	2	108	GLU	CA-CB-CG	-5.72	102.65	114.10
1	1	97	ALA	N-CA-C	-5.71	105.58	112.54
1	1	66	LEU	O-C-N	-5.69	116.17	122.09
2	2	51	LEU	N-CA-C	5.68	120.21	113.16
1	1	137	SER	O-C-N	5.68	130.20	122.48
4	4	76	PHE	CA-CB-CG	5.68	119.48	113.80
3	3	217	ALA	N-CA-CB	-5.67	102.55	111.39
4	4	84	LEU	N-CA-C	-5.67	99.95	109.07
1	1	208	PRO	CA-N-CD	-5.66	104.08	112.00
2	2	38	THR	CA-CB-CG2	5.66	120.12	110.50
2	2	38	THR	N-CA-CB	-5.65	102.22	110.53
3	3	5	VAL	N-CA-CB	-5.64	102.11	111.36
3	3	169	TYR	N-CA-C	5.64	118.62	110.28
2	2	54	ARG	CA-C-N	-5.61	117.63	122.96
2	2	54	ARG	C-N-CA	-5.61	117.63	122.96
3	3	8	SER	N-CA-C	5.61	118.77	109.46
1	1	129	VAL	N-CA-CB	-5.60	102.26	111.45
1	1	50	ILE	N-CA-C	-5.59	100.37	108.87
1	1	201	HIS	CA-CB-CG	-5.58	108.22	113.80
1	1	93	ALA	CA-C-N	5.56	125.57	119.90
1	1	93	ALA	C-N-CA	5.56	125.57	119.90
1	1	181	LYS	CB-CG-CD	5.56	124.08	111.30
3	3	74	LEU	N-CA-C	-5.55	104.74	112.45
4	4	22	ILE	O-C-N	5.55	128.75	122.98
3	3	20	LYS	CB-CA-C	5.54	121.14	109.79
2	2	183	VAL	O-C-N	-5.54	116.63	122.83
2	2	14	ILE	CA-C-O	-5.53	114.40	120.48
1	1	182	ARG	CB-CA-C	-5.53	103.88	111.73
3	3	90	PHE	CA-CB-CG	-5.52	108.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	41	PHE	CA-CB-CG	5.51	119.31	113.80
1	1	89	VAL	CB-CA-C	5.50	121.38	111.36
1	1	30	THR	CA-C-O	5.49	126.43	119.95
2	2	88	LYS	CA-CB-CG	5.48	125.06	114.10
1	1	146	GLY	CA-C-N	-5.48	112.22	122.73
1	1	146	GLY	C-N-CA	-5.48	112.22	122.73
3	3	217	ALA	N-CA-C	5.47	119.59	111.87
1	1	182	ARG	NE-CZ-NH1	5.47	126.97	121.50
1	1	157	ARG	CA-C-O	5.47	127.21	120.92
3	3	166	ASP	O-C-N	5.46	129.95	122.46
3	3	33	PRO	N-CD-CG	-5.45	95.02	103.20
1	1	125	VAL	CB-CA-C	5.43	120.25	110.48
3	3	199	LEU	N-CA-C	-5.43	99.67	108.52
1	1	174	THR	CA-CB-OG1	-5.41	101.49	109.60
3	3	202	LEU	CA-CB-CG	5.40	135.20	116.30
3	3	34	ARG	NE-CZ-NH1	5.40	126.90	121.50
1	1	192	LEU	N-CA-CB	-5.39	101.63	110.42
3	3	34	ARG	CG-CD-NE	-5.38	100.16	112.00
2	2	19	ASN	OD1-CG-ND2	-5.37	117.23	122.60
4	4	27	MET	CA-CB-CG	-5.37	103.36	114.10
2	2	108	GLU	N-CA-CB	-5.35	102.36	110.77
1	1	179	ARG	NE-CZ-NH2	-5.35	114.39	119.20
2	2	87	HIS	N-CA-C	-5.35	99.22	108.69
1	1	68	ALA	N-CA-CB	-5.34	103.20	110.56
2	2	30	VAL	N-CA-C	5.33	120.42	109.34
1	1	179	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	1	91	ASN	CB-CG-ND2	-5.32	108.42	116.40
2	2	30	VAL	O-C-N	-5.32	115.93	122.57
3	3	177	THR	N-CA-C	5.32	117.49	111.11
3	3	181	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	1	65	LEU	N-CA-CB	-5.29	102.32	110.20
1	1	114	ARG	CD-NE-CZ	5.29	131.80	124.40
1	1	158	THR	CB-CA-C	5.28	119.03	109.37
3	3	190	THR	N-CA-CB	5.28	120.78	111.49
2	2	21	HIS	CE1-NE2-CD2	5.27	114.27	109.00
1	1	158	THR	N-CA-C	-5.26	101.59	109.95
2	2	86	ASP	CA-CB-CG	5.26	117.86	112.60
3	3	201	VAL	N-CA-C	5.25	116.29	108.46
3	3	168	THR	CA-CB-CG2	-5.25	101.57	110.50
2	2	207	ASN	OD1-CG-ND2	5.23	127.83	122.60
3	3	174	VAL	CB-CA-C	-5.23	102.71	111.29
1	1	114	ARG	CA-C-N	5.23	130.78	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	114	ARG	C-N-CA	5.23	130.78	122.94
2	2	113	GLY	N-CA-C	-5.22	100.80	113.18
1	1	177	LEU	CD1-CG-CD2	-5.22	99.32	110.80
1	1	38	ARG	CA-CB-CG	5.21	124.52	114.10
1	1	96	LYS	CG-CD-CE	5.20	123.27	111.30
1	1	173	VAL	CA-C-N	5.20	131.10	121.52
1	1	173	VAL	C-N-CA	5.20	131.10	121.52
2	2	151	ARG	N-CA-C	-5.20	106.20	112.54
2	2	160	VAL	CB-CA-C	5.20	120.82	111.36
1	1	194	ILE	CA-CB-CG1	-5.18	101.59	110.40
3	3	141	HIS	ND1-CE1-NE2	-5.17	103.23	108.40
3	3	178	THR	N-CA-CB	-5.15	101.84	110.39
2	2	204	ALA	O-C-N	-5.12	116.84	121.39
3	3	40	ARG	CA-CB-CG	5.11	124.33	114.10
2	2	26	THR	OG1-CB-CG2	5.11	119.51	109.30
4	4	65	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	1	136	TYR	O-C-N	5.09	128.01	122.11
3	3	34	ARG	NH1-CZ-NH2	-5.08	112.69	119.30
2	2	21	HIS	ND1-CE1-NE2	-5.08	103.32	108.40
1	1	172	ARG	N-CA-C	-5.08	99.34	108.48
3	3	173	ASP	N-CA-C	5.08	119.93	113.18
1	1	179	ARG	CB-CG-CD	5.08	122.97	111.30
2	2	40	GLU	CA-CB-CG	5.07	124.25	114.10
2	2	196	GLN	CG-CD-NE2	5.07	124.01	116.40
1	1	145	ARG	NE-CZ-NH2	-5.06	114.65	119.20
4	4	69	SER	CB-CA-C	-5.06	102.91	110.90
3	3	190	THR	OG1-CB-CG2	5.05	119.41	109.30
2	2	192	GLU	N-CA-C	5.04	120.05	113.30
1	1	206	VAL	CB-CA-C	5.04	119.55	111.29
4	4	67	TRP	CA-C-O	-5.04	115.71	120.90
1	1	209	VAL	N-CA-C	5.03	119.80	109.34
1	1	62	VAL	CA-C-N	5.03	125.52	119.94
1	1	62	VAL	C-N-CA	5.03	125.52	119.94
3	3	42	THR	OG1-CB-CG2	5.02	119.35	109.30
2	2	60	ARG	NE-CZ-NH1	-5.02	116.48	121.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	16	THR	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	1	1651	0	1670	30	0
2	2	1676	0	1625	32	0
3	3	1681	0	1616	23	0
4	4	354	0	324	7	0
All	All	5362	0	5235	80	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 8.

All (80) 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)
1:1:1:THR:HG23	4:4:79:LEU:HA	1.46	0.94
3:3:100:GLN:HE22	3:3:212:ARG:HH21	1.15	0.94
4:4:65:ASN:HA	4:4:69:SER:HB2	1.51	0.93
2:2:114:ASN:HD21	2:2:193:GLY:HA2	1.42	0.82
2:2:115:GLN:HE21	2:2:115:GLN:H	1.28	0.82
3:3:79:MET:HE2	3:3:79:MET:HA	1.64	0.79
3:3:100:GLN:NE2	3:3:212:ARG:HH21	1.85	0.74
3:3:43:ASN:HD22	3:3:45:LEU:H	1.34	0.74
1:1:7:SER:O	1:1:8:ALA:HB3	1.87	0.73
1:1:1:THR:HG23	4:4:79:LEU:CA	2.19	0.73
2:2:18:ARG:HG3	2:2:23:THR:HG22	1.70	0.73
1:1:103:ASN:HD21	3:3:216:ASP:H	1.35	0.72
2:2:6:GLU:HB3	2:2:12:ASP:HB3	1.71	0.72
4:4:65:ASN:CA	4:4:69:SER:HB2	2.20	0.72
1:1:35:ILE:O	1:1:38:ARG:HD2	1.90	0.71
1:1:144:LEU:HG	1:1:150:VAL:HG13	1.76	0.68
3:3:100:GLN:HE22	3:3:212:ARG:NH2	1.91	0.67
2:2:115:GLN:H	2:2:115:GLN:NE2	1.93	0.65
3:3:64:VAL:HG13	3:3:74:LEU:HG	1.80	0.63
3:3:168:THR:HG21	3:3:181:GLN:NE2	2.14	0.62
1:1:98:LEU:HG	1:1:169:LYS:HB2	1.83	0.61
1:1:134:CYS:SG	1:1:161:THR:HG23	2.42	0.59
3:3:52:PRO:HB3	3:3:204:SER:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:7:SER:O	1:1:8:ALA:CB	2.48	0.59
2:2:106:ASP:OD1	2:2:157:HIS:HE1	1.85	0.59
1:1:25:GLN:HG2	1:1:27:ARG:HG3	1.86	0.58
1:1:151:LEU:HD13	2:2:131:SER:HA	1.87	0.57
2:2:114:ASN:ND2	2:2:193:GLY:HA2	2.19	0.55
3:3:64:VAL:CG1	3:3:74:LEU:HG	2.36	0.55
1:1:89:VAL:HB	1:1:98:LEU:HD13	1.88	0.55
1:1:45:GLN:H	1:1:49:ASN:HD21	1.53	0.55
1:1:141:VAL:HG12	2:2:175:LYS:NZ	2.22	0.55
1:1:104:PRO:HG3	3:3:17:THR:HG21	1.89	0.55
1:1:113:THR:HG22	1:1:115:LEU:HD13	1.88	0.54
2:2:114:ASN:ND2	2:2:116:PHE:H	2.06	0.53
2:2:101:MET:HG2	2:2:210:VAL:HG12	1.92	0.52
3:3:44:LEU:HG	3:3:94:LEU:HD21	1.91	0.52
1:1:89:VAL:HG13	1:1:93:ALA:CB	2.40	0.52
2:2:216:SER:OG	2:2:218:GLU:HG2	2.11	0.52
4:4:65:ASN:HA	4:4:69:SER:CB	2.32	0.51
1:1:103:ASN:ND2	3:3:216:ASP:H	2.07	0.51
2:2:107:VAL:O	2:2:157:HIS:HA	2.12	0.48
1:1:61:LEU:O	1:1:65:LEU:HB2	2.14	0.48
1:1:209:VAL:HG12	1:1:210:LYS:HG3	1.95	0.48
1:1:89:VAL:HG13	1:1:93:ALA:HB3	1.95	0.47
3:3:79:MET:HA	3:3:79:MET:CE	2.41	0.47
1:1:6:GLU:HG2	2:2:153:ASN:ND2	2.29	0.47
3:3:15:VAL:HB	3:3:18:ASP:HB3	1.96	0.47
2:2:149:ASN:H	2:2:153:ASN:ND2	2.14	0.46
2:2:43:VAL:HG22	2:2:102:ARG:HD2	1.97	0.46
2:2:114:ASN:HB2	2:2:115:GLN:HE21	1.81	0.45
1:1:44:PRO:HB2	1:1:173:VAL:HG22	1.97	0.45
2:2:101:MET:HE2	2:2:101:MET:HB3	1.80	0.45
3:3:57:PHE:CE2	3:3:201:VAL:HG13	2.52	0.45
1:1:129:VAL:HG13	2:2:128:GLU:HB2	1.99	0.45
1:1:141:VAL:HG12	2:2:175:LYS:HZ3	1.80	0.45
2:2:54:ARG:NH1	2:2:59:GLU:OE1	2.50	0.45
2:2:9:LEU:HD12	2:2:10:LEU:HG	1.99	0.44
2:2:115:GLN:HE21	2:2:115:GLN:N	2.04	0.44
1:1:56:VAL:HA	1:1:57:PRO:HD3	1.84	0.44
2:2:214:PHE:CD1	3:3:130:MET:HG2	2.53	0.44
2:2:122:LEU:HD23	2:2:140:LEU:HD23	1.99	0.43
3:3:18:ASP:OD2	3:3:20:LYS:HE2	2.18	0.43
1:1:90:PRO:HG2	3:3:99:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:120:ARG:HH11	3:3:146:GLU:HG2	1.83	0.43
2:2:112:VAL:HB	2:2:154:MET:SD	2.58	0.43
1:1:24:ILE:HD11	1:1:26:ARG:HG3	2.01	0.43
2:2:83:LEU:HD23	2:2:125:MET:HE1	2.01	0.43
3:3:112:THR:HB	3:3:198:ALA:O	2.18	0.43
2:2:91:TYR:O	2:2:94:LEU:HB2	2.19	0.42
2:2:29:SER:O	2:2:30:VAL:HB	2.20	0.42
1:1:37:ASP:OD1	1:1:179:ARG:HD2	2.21	0.41
2:2:134:LYS:O	2:2:137:LEU:HB2	2.21	0.41
4:4:65:ASN:O	4:4:66:ASP:C	2.64	0.41
3:3:218:ARG:HE	3:3:219:ALA:H	1.68	0.41
4:4:22:ILE:HD12	4:4:23:ASN:O	2.19	0.41
3:3:43:ASN:ND2	3:3:45:LEU:H	2.09	0.41
2:2:142:LEU:HD23	2:2:142:LEU:HA	1.83	0.41
2:2:160:VAL:HG13	2:2:177:TRP:CZ2	2.56	0.40
1:1:142:PRO:HG2	1:1:144:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

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	208/213 (98%)	197 (95%)	9 (4%)	2 (1%)	12	28
2	2	212/218 (97%)	195 (92%)	13 (6%)	4 (2%)	6	13
3	3	218/220 (99%)	206 (94%)	9 (4%)	3 (1%)	9	19
4	4	43/85 (51%)	37 (86%)	4 (9%)	2 (5%)	2	2
All	All	681/736 (92%)	635 (93%)	35 (5%)	11 (2%)	7	16

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	209	VAL
2	2	8	THR
2	2	9	LEU
2	2	30	VAL
3	3	174	VAL
4	4	66	ASP
2	2	7	THR
3	3	219	ALA
1	1	104	PRO
3	3	218	ARG
4	4	81	GLY

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	1	180/183 (98%)	141 (78%)	39 (22%)	1	2
2	2	185/191 (97%)	145 (78%)	40 (22%)	1	2
3	3	176/176 (100%)	145 (82%)	31 (18%)	2	3
4	4	37/67 (55%)	31 (84%)	6 (16%)	2	4
All	All	578/617 (94%)	462 (80%)	116 (20%)	1	2

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	1	THR
1	1	24	ILE
1	1	25	GLN
1	1	38	ARG
1	1	44	PRO
1	1	50	ILE
1	1	53	LEU
1	1	56	VAL
1	1	65	LEU
1	1	89	VAL
1	1	96	LYS

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Mol	Chain	Res	Type
1	1	98	LEU
1	1	101	THR
1	1	111	PRO
1	1	114	ARG
1	1	115	LEU
1	1	118	PRO
1	1	124	ARG
1	1	125	VAL
1	1	136	TYR
1	1	138	ARG
1	1	141	VAL
1	1	144	LEU
1	1	148	LEU
1	1	158	THR
1	1	159	LEU
1	1	160	PRO
1	1	172	ARG
1	1	173	VAL
1	1	174	THR
1	1	179	ARG
1	1	191	LEU
1	1	192	LEU
1	1	194	ILE
1	1	197	THR
1	1	204	LYS
1	1	206	VAL
1	1	208	PRO
1	1	210	LYS
2	2	7	THR
2	2	9	LEU
2	2	11	GLU
2	2	15	LEU
2	2	18	ARG
2	2	26	THR
2	2	30	VAL
2	2	32	VAL
2	2	38	THR
2	2	40	GLU
2	2	43	VAL
2	2	51	LEU
2	2	54	ARG
2	2	55	VAL

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Mol	Chain	Res	Type
2	2	56	VAL
2	2	60	ARG
2	2	66	LEU
2	2	77	ARG
2	2	80	LEU
2	2	83	LEU
2	2	85	THR
2	2	86	ASP
2	2	90	VAL
2	2	94	LEU
2	2	102	ARG
2	2	110	THR
2	2	112	VAL
2	2	114	ASN
2	2	115	GLN
2	2	123	VAL
2	2	134	LYS
2	2	153	ASN
2	2	160	VAL
2	2	161	PRO
2	2	172	LYS
2	2	180	VAL
2	2	184	VAL
2	2	189	VAL
2	2	191	THR
2	2	208	VAL
3	3	5	VAL
3	3	17	THR
3	3	29	VAL
3	3	37	LEU
3	3	44	LEU
3	3	47	VAL
3	3	64	VAL
3	3	67	LYS
3	3	74	LEU
3	3	79	MET
3	3	81	LEU
3	3	94	LEU
3	3	102	SER
3	3	107	LEU
3	3	112	THR
3	3	151	LEU

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Mol	Chain	Res	Type
3	3	162	LEU
3	3	168	THR
3	3	178	THR
3	3	180	VAL
3	3	181	GLN
3	3	184	VAL
3	3	190	THR
3	3	195	ASP
3	3	200	VAL
3	3	201	VAL
3	3	202	LEU
3	3	207	LYS
3	3	211	LEU
3	3	213	LEU
3	3	218	ARG
4	4	23	ASN
4	4	28	GLN
4	4	66	ASP
4	4	69	SER
4	4	79	LEU
4	4	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	25	GLN
1	1	49	ASN
1	1	55	GLN
1	1	103	ASN
2	2	19	ASN
2	2	65	HIS
2	2	114	ASN
2	2	115	GLN
2	2	153	ASN
2	2	157	HIS
2	2	166	ASN
2	2	196	GLN
3	3	43	ASN
3	3	76	GLN
3	3	100	GLN
3	3	179	ASN
3	3	181	GLN

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Mol	Chain	Res	Type
4	4	31	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](#)

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.