



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:24 AM UTC

PDB ID : 1BBT / pdb_00001bbt
Title : METHODS USED IN THE STRUCTURE DETERMINATION OF FOOT
AND MOUTH DISEASE VIRUS
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Deposited on : 1992-05-18
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

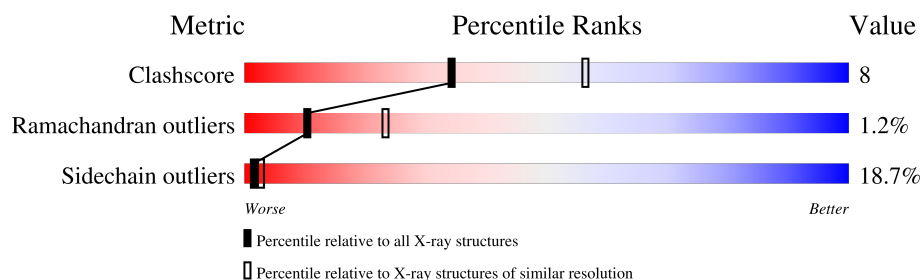
1 Overall quality at a glance

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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5142 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 (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	186	Total	C	N	O	S	0	0	0
			1456	920	257	274	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 (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	210	Total	C	N	O	S	0	0	0
			1652	1052	282	311	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 (SUBUNIT VP3).

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 (SUBUNIT VP4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	46	Total	C	N	O	S	0	0	0
			353	222	57	72	2			

There are 2 discrepancies between the modelled and reference sequences:

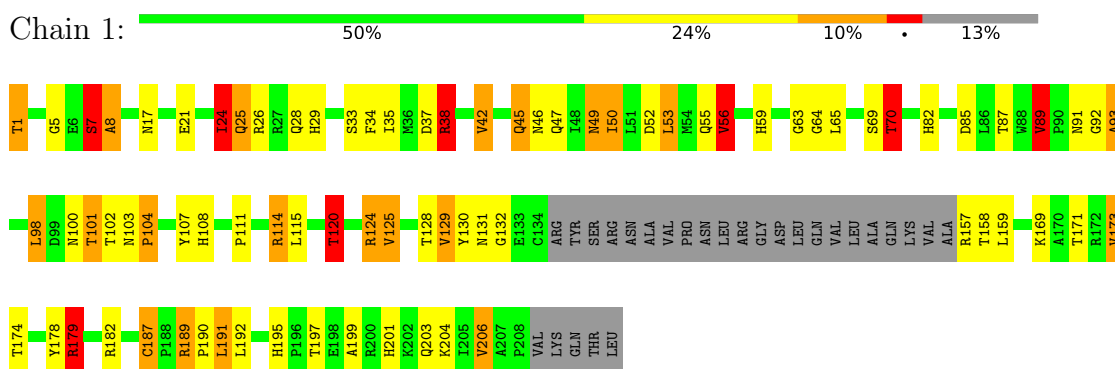
Chain	Residue	Modelled	Actual	Comment	Reference
4	40	ASN	ASP	conflict	UNP O90754
4	41	ASP	ASN	conflict	UNP O90754

3 Residue-property plots

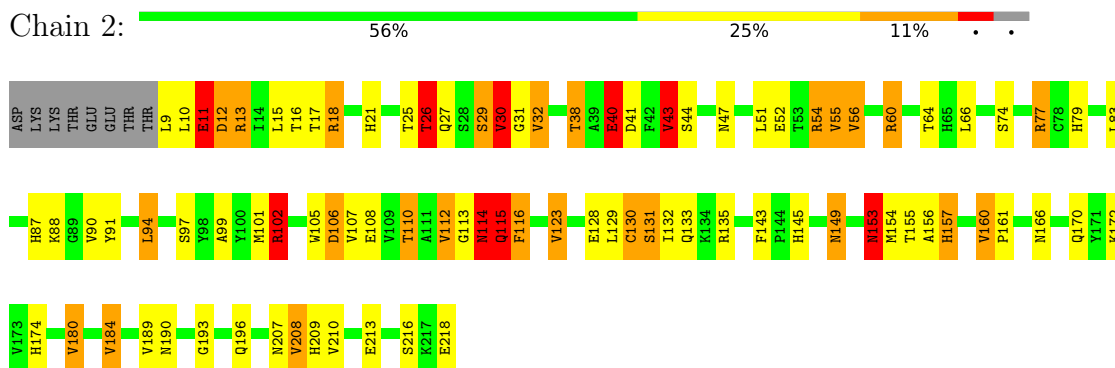
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

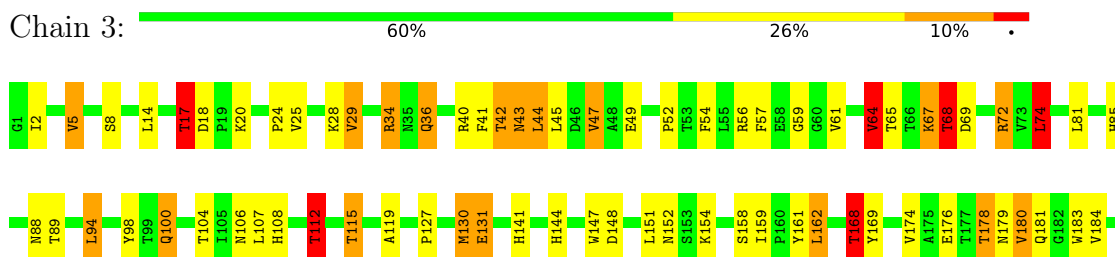
- Molecule 1: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP1)



- Molecule 2: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP2)

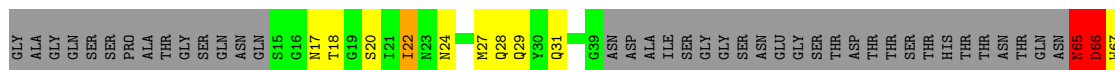
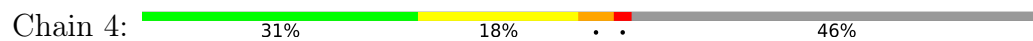


- Molecule 3: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP3)





- Molecule 4: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP4)



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}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5142	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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	1.40	13/1490 (0.9%)	2.29	90/2035 (4.4%)
2	2	1.48	23/1695 (1.4%)	2.24	99/2314 (4.3%)
3	3	1.37	10/1729 (0.6%)	2.17	100/2361 (4.2%)
4	4	1.40	2/359 (0.6%)	2.24	19/481 (4.0%)
All	All	1.42	48/5273 (0.9%)	2.23	308/7191 (4.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	69	SER	CA-CB	-8.65	1.39	1.53
2	2	123	VAL	CA-CB	8.38	1.64	1.54
2	2	55	VAL	CA-CB	8.33	1.62	1.53
3	3	29	VAL	CA-CB	8.26	1.64	1.54
2	2	112	VAL	CA-CB	8.08	1.63	1.54
2	2	87	HIS	CD2-NE2	-7.22	1.29	1.37
1	1	56	VAL	CA-CB	7.11	1.63	1.54
2	2	131	SER	CA-C	6.96	1.62	1.52
1	1	21	GLU	CA-CB	-6.92	1.42	1.53
1	1	173	VAL	CA-CB	6.88	1.62	1.54
3	3	200	VAL	CA-CB	6.80	1.63	1.54
4	4	27	MET	CA-CB	-6.59	1.42	1.53
2	2	32	VAL	CA-CB	6.45	1.63	1.54
2	2	30	VAL	N-CA	6.39	1.54	1.46
2	2	97	SER	CA-CB	-6.35	1.45	1.54
2	2	29	SER	N-CA	-6.28	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	208	VAL	CA-CB	6.28	1.62	1.54
2	2	174	HIS	CD2-NE2	-6.25	1.30	1.37
1	1	201	HIS	CD2-NE2	-6.13	1.31	1.37
2	2	12	ASP	CA-CB	6.09	1.62	1.53
2	2	174	HIS	CG-ND1	-6.07	1.31	1.38
1	1	85	ASP	CA-CB	-6.03	1.44	1.53
3	3	217	ALA	C-N	5.97	1.39	1.33
3	3	108	HIS	CD2-NE2	-5.89	1.31	1.37
1	1	82	HIS	CD2-NE2	-5.88	1.31	1.37
3	3	144	HIS	CD2-NE2	-5.78	1.31	1.37
1	1	47	GLN	CA-CB	-5.72	1.46	1.53
1	1	50	ILE	CB-CG1	-5.63	1.42	1.53
2	2	184	VAL	CA-CB	5.63	1.62	1.54
1	1	29	HIS	CD2-NE2	-5.46	1.31	1.37
3	3	47	VAL	CA-CB	5.38	1.61	1.54
3	3	191	HIS	CD2-NE2	-5.38	1.31	1.37
2	2	79	HIS	CD2-NE2	-5.35	1.31	1.37
2	2	133	GLN	CA-CB	-5.34	1.44	1.53
2	2	157	HIS	CD2-NE2	-5.33	1.31	1.37
2	2	106	ASP	CA-CB	-5.30	1.46	1.53
3	3	188	GLN	CA-CB	-5.30	1.46	1.53
3	3	168	THR	CA-CB	-5.28	1.45	1.53
2	2	13	ARG	CA-CB	-5.25	1.44	1.53
2	2	154	MET	CA-CB	-5.22	1.46	1.54
2	2	21	HIS	CD2-NE2	-5.18	1.32	1.37
1	1	59	HIS	CD2-NE2	-5.12	1.32	1.37
1	1	108	HIS	CD2-NE2	-5.07	1.32	1.37
1	1	34	PHE	CA-CB	-5.05	1.45	1.53
2	2	145	HIS	CG-ND1	-5.05	1.32	1.38
3	3	24	PRO	CA-CB	-5.04	1.47	1.53
1	1	46	ASN	CA-C	-5.01	1.46	1.52
2	2	180	VAL	CA-CB	5.01	1.61	1.54

All (308) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	12	ASP	CA-CB-CG	14.54	127.14	112.60
3	3	218	ARG	N-CA-C	-13.22	88.43	108.00
1	1	17	ASN	OD1-CG-ND2	-12.69	109.91	122.60
1	1	50	ILE	CB-CG1-CD1	-11.92	88.78	113.80
2	2	160	VAL	N-CA-CB	-11.33	95.35	111.21
2	2	133	GLN	CA-CB-CG	-11.17	91.77	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	29	SER	CA-C-O	-10.90	108.14	120.24
3	3	36	GLN	CA-CB-CG	-10.76	92.58	114.10
1	1	101	THR	CA-CB-OG1	-10.02	94.57	109.60
2	2	11	GLU	N-CA-C	9.74	123.94	109.24
2	2	38	THR	CA-CB-OG1	-9.61	95.19	109.60
2	2	166	ASN	OD1-CG-ND2	-9.37	113.23	122.60
3	3	74	LEU	N-CA-C	-9.33	101.45	113.12
1	1	24	ILE	CB-CG1-CD1	-9.32	94.22	113.80
2	2	154	MET	N-CA-CB	-9.32	98.68	110.98
3	3	130	MET	CG-SD-CE	-9.24	80.56	100.90
2	2	115	GLN	OE1-CD-NE2	-9.17	113.43	122.60
1	1	174	THR	CA-CB-OG1	-9.11	95.94	109.60
1	1	89	VAL	N-CA-CB	-9.05	98.54	111.21
2	2	114	ASN	OD1-CG-ND2	-8.98	113.62	122.60
2	2	114	ASN	CB-CG-ND2	8.89	129.73	116.40
3	3	217	ALA	N-CA-C	8.81	123.90	111.30
3	3	112	THR	N-CA-CB	-8.71	96.61	110.98
1	1	64	GLY	N-CA-C	-8.55	102.58	112.50
2	2	26	THR	CB-CA-C	-8.42	91.78	109.38
2	2	135	ARG	NE-CZ-NH2	-8.37	111.67	119.20
3	3	193	LYS	CB-CG-CD	-8.37	92.06	111.30
3	3	217	ALA	CA-C-N	8.33	139.61	122.04
3	3	217	ALA	C-N-CA	8.33	139.61	122.04
3	3	17	THR	N-CA-CB	-8.28	95.87	111.43
1	1	101	THR	CA-CB-CG2	8.25	124.53	110.50
1	1	120	THR	N-CA-CB	-8.25	95.92	111.43
3	3	148	ASP	CA-CB-CG	8.25	120.85	112.60
3	3	64	VAL	N-CA-CB	-8.22	96.72	111.93
2	2	157	HIS	CB-CG-CD2	-8.21	120.53	131.20
4	4	31	GLN	OE1-CD-NE2	-8.13	114.47	122.60
3	3	190	THR	OG1-CB-CG2	8.12	125.55	109.30
2	2	29	SER	N-CA-C	8.09	121.64	111.69
3	3	42	THR	CA-CB-OG1	-7.96	97.65	109.60
2	2	27	GLN	OE1-CD-NE2	-7.93	114.67	122.60
2	2	135	ARG	NE-CZ-NH1	7.81	129.31	121.50
2	2	26	THR	N-CA-CB	7.79	125.55	111.37
1	1	179	ARG	NE-CZ-NH1	7.72	129.22	121.50
1	1	8	ALA	CB-CA-C	-7.71	98.95	110.06
1	1	33	SER	CA-CB-OG	-7.69	95.72	111.10
1	1	206	VAL	N-CA-CB	-7.65	98.61	111.23
1	1	55	GLN	OE1-CD-NE2	-7.64	114.95	122.60
4	4	82	ALA	N-CA-C	-7.64	97.22	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	49	ASN	CA-C-N	-7.58	110.38	122.50
1	1	49	ASN	C-N-CA	-7.58	110.38	122.50
2	2	87	HIS	CB-CG-CD2	-7.50	121.45	131.20
3	3	178	THR	CA-CB-OG1	-7.50	98.35	109.60
3	3	100	GLN	OE1-CD-NE2	-7.50	115.11	122.60
3	3	43	ASN	CA-CB-CG	-7.49	105.11	112.60
2	2	21	HIS	N-CA-C	-7.44	105.08	112.97
3	3	190	THR	CB-CA-C	-7.40	97.13	111.78
2	2	196	GLN	CG-CD-NE2	7.37	127.45	116.40
3	3	36	GLN	N-CA-C	7.33	122.18	113.23
3	3	217	ALA	CA-C-O	-7.33	112.70	121.34
2	2	110	THR	CA-CB-OG1	-7.32	98.62	109.60
2	2	56	VAL	N-CA-CB	-7.31	99.07	110.54
1	1	42	VAL	N-CA-CB	-7.30	100.17	112.44
1	1	63	GLY	CA-C-N	7.29	128.04	119.94
1	1	63	GLY	C-N-CA	7.29	128.04	119.94
3	3	85	HIS	CB-CG-CD2	-7.29	121.73	131.20
2	2	196	GLN	OE1-CD-NE2	-7.28	115.32	122.60
2	2	10	LEU	CA-C-O	-7.25	111.82	121.47
1	1	46	ASN	CB-CA-C	-7.25	98.75	110.79
3	3	179	ASN	OD1-CG-ND2	-7.20	115.40	122.60
3	3	183	TRP	CA-C-N	-7.18	113.84	123.10
3	3	183	TRP	C-N-CA	-7.18	113.84	123.10
2	2	207	ASN	CA-CB-CG	-7.16	105.44	112.60
2	2	54	ARG	CA-C-N	-7.15	116.17	122.96
2	2	54	ARG	C-N-CA	-7.15	116.17	122.96
1	1	38	ARG	NE-CZ-NH2	-7.14	112.77	119.20
2	2	157	HIS	CB-CG-ND1	7.14	133.41	122.70
3	3	64	VAL	CB-CA-C	7.11	122.06	110.69
1	1	101	THR	N-CA-CB	-7.09	97.41	110.32
3	3	42	THR	OG1-CB-CG2	7.07	123.45	109.30
1	1	174	THR	CA-CB-CG2	7.01	122.41	110.50
2	2	143	PHE	CA-CB-CG	-7.00	106.80	113.80
2	2	132	ILE	O-C-N	-6.91	115.72	123.18
3	3	127	PRO	CB-CA-C	6.89	119.32	110.92
4	4	27	MET	CG-SD-CE	-6.88	85.75	100.90
3	3	176	GLU	N-CA-CB	-6.85	100.74	110.46
3	3	218	ARG	CD-NE-CZ	6.84	133.98	124.40
4	4	68	PHE	CA-CB-CG	-6.82	106.98	113.80
1	1	5	GLY	O-C-N	-6.80	114.95	122.84
4	4	72	ALA	O-C-N	-6.76	115.11	122.07
2	2	38	THR	N-CA-CB	-6.71	100.47	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	5	VAL	N-CA-CB	-6.69	98.92	111.62
2	2	54	ARG	NE-CZ-NH2	6.66	125.19	119.20
3	3	25	VAL	O-C-N	-6.65	114.25	122.57
1	1	49	ASN	OD1-CG-ND2	-6.64	115.96	122.60
2	2	79	HIS	CA-CB-CG	-6.64	107.16	113.80
1	1	197	THR	CA-CB-OG1	-6.62	99.67	109.60
3	3	152	ASN	OD1-CG-ND2	-6.61	115.99	122.60
1	1	182	ARG	NE-CZ-NH1	6.56	128.06	121.50
4	4	29	GLN	N-CA-CB	-6.54	99.53	110.39
2	2	38	THR	CA-CB-CG2	6.54	121.62	110.50
3	3	180	VAL	N-CA-CB	-6.54	101.64	110.54
1	1	55	GLN	CG-CD-NE2	6.54	126.21	116.40
1	1	101	THR	N-CA-C	6.53	120.71	112.87
1	1	158	THR	CB-CA-C	6.51	121.44	109.46
3	3	218	ARG	CA-CB-CG	6.51	127.11	114.10
3	3	106	ASN	OD1-CG-ND2	-6.50	116.10	122.60
3	3	147	TRP	CG-CD2-CE3	6.47	140.38	133.90
3	3	40	ARG	NE-CZ-NH2	6.41	124.97	119.20
3	3	64	VAL	N-CA-C	-6.41	98.42	108.86
2	2	130	CYS	CA-C-O	-6.39	114.65	122.64
1	1	125	VAL	N-CA-CB	-6.39	98.90	112.00
3	3	181	GLN	CG-CD-NE2	6.37	125.96	116.40
3	3	18	ASP	CA-CB-CG	6.35	118.95	112.60
3	3	69	ASP	CA-CB-CG	6.33	118.93	112.60
4	4	67	TRP	CG-CD2-CE3	6.33	140.23	133.90
1	1	63	GLY	CA-C-O	-6.32	114.24	120.75
2	2	190	ASN	CB-CG-ND2	6.28	125.83	116.40
1	1	131	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	1	131	ASN	N-CA-CB	-6.27	102.89	110.53
1	1	182	ARG	NE-CZ-NH2	-6.24	113.58	119.20
3	3	34	ARG	CG-CD-NE	-6.21	98.34	112.00
1	1	70	THR	CB-CA-C	6.18	120.05	109.24
1	1	64	GLY	O-C-N	-6.16	116.27	122.18
3	3	28	LYS	CA-C-N	-6.14	115.58	123.19
3	3	28	LYS	C-N-CA	-6.14	115.58	123.19
2	2	21	HIS	CE1-NE2-CD2	6.14	115.14	109.00
1	1	7	SER	CA-C-O	-6.13	112.55	119.79
1	1	45	GLN	O-C-N	-6.13	115.86	122.85
3	3	218	ARG	CB-CG-CD	6.13	125.40	111.30
1	1	132	GLY	O-C-N	-6.12	114.74	122.70
3	3	141	HIS	CA-CB-CG	-6.12	107.68	113.80
2	2	40	GLU	CA-CB-CG	-6.10	101.90	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	149	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	1	17	ASN	CB-CG-ND2	6.02	125.43	116.40
3	3	65	THR	CA-CB-OG1	-6.00	100.59	109.60
1	1	52	ASP	CA-CB-CG	6.00	118.59	112.60
3	3	34	ARG	CA-C-O	5.98	125.73	119.51
4	4	24	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	1	59	HIS	CB-CG-CD2	-5.98	123.42	131.20
1	1	129	VAL	N-CA-CB	-5.98	101.55	111.36
3	3	147	TRP	CB-CG-CD1	-5.98	117.93	126.90
3	3	20	LYS	CB-CG-CD	-5.96	97.59	111.30
3	3	115	THR	CA-CB-OG1	-5.95	100.68	109.60
3	3	217	ALA	N-CA-CB	-5.95	102.63	111.43
3	3	144	HIS	CB-CG-CD2	-5.93	123.50	131.20
1	1	100	ASN	OD1-CG-ND2	-5.92	116.67	122.60
1	1	93	ALA	CA-C-N	5.92	125.94	119.90
1	1	93	ALA	C-N-CA	5.92	125.94	119.90
1	1	124	ARG	NE-CZ-NH1	5.92	127.42	121.50
3	3	108	HIS	CB-CG-CD2	-5.92	123.51	131.20
3	3	154	LYS	CB-CG-CD	-5.89	97.76	111.30
3	3	131	GLU	CA-C-N	5.88	123.95	119.66
3	3	131	GLU	C-N-CA	5.88	123.95	119.66
2	2	110	THR	N-CA-CB	-5.88	100.61	110.83
2	2	166	ASN	CB-CG-ND2	5.86	125.19	116.40
2	2	115	GLN	CG-CD-NE2	5.86	125.19	116.40
3	3	188	GLN	CB-CG-CD	-5.86	102.65	112.60
3	3	152	ASN	CB-CG-ND2	5.85	125.18	116.40
4	4	79	LEU	O-C-N	-5.85	114.81	122.59
2	2	30	VAL	CA-CB-CG2	-5.85	100.46	110.40
2	2	55	VAL	CA-C-O	5.84	127.28	121.09
2	2	149	ASN	CB-CG-ND2	5.83	125.15	116.40
2	2	29	SER	O-C-N	-5.83	114.65	122.23
2	2	131	SER	N-CA-C	5.81	123.17	110.80
3	3	43	ASN	OD1-CG-ND2	-5.80	116.80	122.60
3	3	61	VAL	N-CA-C	-5.80	104.44	109.19
3	3	8	SER	N-CA-C	5.79	119.07	109.46
2	2	113	GLY	N-CA-C	-5.78	99.48	113.18
2	2	108	GLU	N-CA-CB	-5.78	101.64	110.65
1	1	190	PRO	CA-C-O	-5.77	114.84	121.36
2	2	11	GLU	CA-C-N	5.77	130.08	122.06
2	2	11	GLU	C-N-CA	5.77	130.08	122.06
1	1	64	GLY	CA-C-O	5.75	127.21	121.00
1	1	195	HIS	CB-CG-CD2	-5.75	123.72	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	73	SER	CA-CB-OG	-5.75	99.60	111.10
1	1	46	ASN	N-CA-C	5.75	117.54	111.28
2	2	102	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	1	201	HIS	CB-CG-CD2	-5.73	123.75	131.20
4	4	65	ASN	CA-CB-CG	5.71	118.31	112.60
2	2	30	VAL	CA-CB-CG1	5.70	120.10	110.40
1	1	120	THR	CB-CA-C	5.70	120.49	110.35
3	3	42	THR	CA-CB-CG2	5.69	120.17	110.50
2	2	170	GLN	OE1-CD-NE2	-5.68	116.92	122.60
2	2	110	THR	CA-CB-CG2	5.67	120.15	110.50
2	2	77	ARG	NE-CZ-NH2	-5.67	114.10	119.20
3	3	162	LEU	O-C-N	-5.66	116.65	123.27
1	1	82	HIS	CB-CG-CD2	-5.64	123.86	131.20
1	1	120	THR	CA-CB-CG2	5.64	120.09	110.50
2	2	47	ASN	OD1-CG-ND2	-5.64	116.96	122.60
2	2	207	ASN	CA-C-N	-5.63	113.89	121.66
2	2	207	ASN	C-N-CA	-5.63	113.89	121.66
3	3	141	HIS	CB-CG-CD2	-5.63	123.88	131.20
2	2	116	PHE	CA-CB-CG	-5.62	108.17	113.80
2	2	13	ARG	N-CA-C	-5.61	95.83	107.67
3	3	98	TYR	CA-C-O	-5.61	115.06	121.40
1	1	129	VAL	O-C-N	-5.61	116.59	123.09
2	2	114	ASN	CA-CB-CG	5.60	118.20	112.60
3	3	115	THR	CA-CB-CG2	5.59	120.01	110.50
4	4	17	ASN	N-CA-CB	-5.59	102.27	110.49
3	3	131	GLU	CA-CB-CG	-5.59	102.92	114.10
2	2	21	HIS	CB-CG-CD2	-5.58	123.94	131.20
3	3	57	PHE	CA-CB-CG	-5.57	108.23	113.80
1	1	120	THR	CA-CB-OG1	-5.57	101.25	109.60
2	2	41	ASP	O-C-N	-5.57	115.19	122.59
3	3	190	THR	N-CA-CB	5.56	121.27	111.49
1	1	25	GLN	CA-CB-CG	5.54	125.19	114.10
2	2	25	THR	CA-C-O	-5.54	114.29	120.66
3	3	131	GLU	CB-CG-CD	-5.49	103.26	112.60
3	3	42	THR	N-CA-CB	-5.49	103.29	110.59
1	1	69	SER	CA-C-N	-5.48	112.28	122.09
1	1	69	SER	C-N-CA	-5.48	112.28	122.09
2	2	132	ILE	N-CA-C	5.48	116.37	108.48
4	4	31	GLN	CG-CD-NE2	5.47	124.60	116.40
3	3	183	TRP	CG-CD2-CE3	5.46	139.36	133.90
3	3	68	THR	OG1-CB-CG2	5.45	120.20	109.30
1	1	203	GLN	CB-CG-CD	-5.45	103.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	69	ASP	N-CA-C	-5.45	99.41	108.07
2	2	131	SER	O-C-N	-5.42	115.38	122.59
3	3	89	THR	CA-CB-OG1	-5.42	101.47	109.60
3	3	202	LEU	CA-CB-CG	5.41	135.22	116.30
1	1	114	ARG	N-CA-C	-5.40	100.38	109.07
2	2	64	THR	CA-CB-OG1	-5.39	101.51	109.60
1	1	102	THR	CA-CB-OG1	-5.39	101.52	109.60
1	1	108	HIS	CB-CG-CD2	-5.39	124.19	131.20
2	2	156	ALA	N-CA-C	-5.38	100.64	109.40
1	1	195	HIS	CG-CD2-NE2	-5.37	101.83	107.20
2	2	30	VAL	O-C-N	-5.37	115.86	122.57
2	2	107	VAL	N-CA-C	5.36	115.61	108.11
2	2	129	LEU	CA-C-O	5.35	127.39	121.39
2	2	160	VAL	CB-CA-C	5.34	121.08	111.36
1	1	92	GLY	O-C-N	-5.33	116.25	122.60
1	1	199	ALA	N-CA-C	5.33	118.88	112.38
3	3	178	THR	CA-CB-CG2	5.32	119.55	110.50
4	4	22	ILE	CB-CG1-CD1	-5.32	102.64	113.80
2	2	52	GLU	O-C-N	-5.31	116.80	122.85
2	2	153	ASN	OD1-CG-ND2	-5.30	117.30	122.60
2	2	87	HIS	CB-CG-ND1	5.30	130.65	122.70
3	3	49	GLU	CB-CA-C	-5.30	101.00	110.70
3	3	64	VAL	O-C-N	-5.30	117.33	123.00
3	3	41	PHE	CA-CB-CG	5.28	119.08	113.80
1	1	189	ARG	CA-C-N	5.28	125.28	119.90
1	1	189	ARG	C-N-CA	5.28	125.28	119.90
2	2	16	THR	CA-CB-OG1	-5.27	101.69	109.60
2	2	129	LEU	O-C-N	5.27	129.06	122.63
1	1	21	GLU	N-CA-CB	-5.27	102.50	110.77
3	3	191	HIS	CA-C-O	-5.26	115.65	121.33
4	4	67	TRP	CB-CG-CD1	-5.25	119.02	126.90
3	3	141	HIS	CB-CG-ND1	5.25	130.58	122.70
3	3	141	HIS	CE1-NE2-CD2	5.25	114.25	109.00
2	2	88	LYS	CA-CB-CG	-5.25	103.60	114.10
2	2	99	ALA	O-C-N	-5.24	115.31	122.33
3	3	159	ILE	CB-CA-C	-5.24	106.07	110.94
2	2	105	TRP	CG-CD1-NE1	-5.24	103.39	110.20
2	2	132	ILE	N-CA-CB	-5.22	102.30	111.39
1	1	206	VAL	CB-CA-C	5.22	119.85	111.29
2	2	64	THR	CA-CB-CG2	5.21	119.35	110.50
1	1	47	GLN	CB-CA-C	-5.20	104.35	112.31
3	3	88	ASN	OD1-CG-ND2	-5.20	117.40	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	209	HIS	CB-CG-CD2	-5.20	124.45	131.20
1	1	191	LEU	N-CA-C	-5.19	98.93	108.02
1	1	195	HIS	O-C-N	-5.19	117.03	121.23
3	3	161	TYR	O-C-N	-5.19	116.64	123.02
1	1	7	SER	CA-C-N	-5.18	117.28	126.45
1	1	7	SER	C-N-CA	-5.18	117.28	126.45
1	1	179	ARG	CB-CG-CD	5.18	123.22	111.30
3	3	65	THR	CA-CB-CG2	5.18	119.31	110.50
4	4	65	ASN	CB-CA-C	5.18	119.95	110.10
1	1	46	ASN	O-C-N	5.17	127.60	122.12
1	1	182	ARG	CA-CB-CG	5.16	124.41	114.10
2	2	43	VAL	N-CA-CB	-5.15	97.69	111.75
2	2	17	THR	N-CA-C	-5.14	101.31	109.59
1	1	197	THR	N-CA-CB	-5.14	102.61	110.26
1	1	50	ILE	CB-CA-C	5.13	118.24	111.21
3	3	181	GLN	OE1-CD-NE2	-5.13	117.47	122.60
4	4	80	PHE	N-CA-C	-5.13	99.88	110.80
1	1	87	THR	CA-CB-OG1	-5.13	101.91	109.60
1	1	128	THR	N-CA-C	-5.10	107.06	113.28
1	1	124	ARG	CB-CG-CD	5.10	123.02	111.30
3	3	183	TRP	CB-CG-CD1	-5.09	119.26	126.90
1	1	157	ARG	CA-C-O	-5.09	112.15	120.80
1	1	171	THR	CA-C-O	-5.09	115.48	120.82
1	1	46	ASN	CA-CB-CG	-5.08	107.52	112.60
2	2	170	GLN	CA-CB-CG	-5.08	103.94	114.10
3	3	28	LYS	CA-C-O	-5.08	115.23	121.28
3	3	5	VAL	CA-CB-CG2	-5.08	101.77	110.40
4	4	82	ALA	O-C-N	-5.08	117.25	123.19
2	2	31	GLY	CA-C-O	-5.08	117.33	122.56
2	2	44	SER	CB-CA-C	-5.07	102.71	111.23
2	2	160	VAL	CG1-CB-CG2	5.07	121.96	110.80
2	2	26	THR	OG1-CB-CG2	5.07	119.43	109.30
2	2	74	SER	N-CA-CB	-5.07	103.22	110.87
3	3	72	ARG	NE-CZ-NH1	5.06	126.56	121.50
2	2	18	ARG	N-CA-CB	-5.06	102.05	110.80
1	1	178	TYR	CA-C-O	-5.06	115.45	121.16
1	1	130	TYR	O-C-N	-5.05	116.81	123.28
2	2	54	ARG	CA-C-O	-5.05	115.11	120.92
3	3	59	GLY	N-CA-C	-5.05	108.00	114.37
3	3	191	HIS	CB-CG-CD2	-5.05	124.64	131.20
3	3	52	PRO	O-C-N	-5.05	116.75	123.01
2	2	18	ARG	CG-CD-NE	-5.04	100.91	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	27	GLN	O-C-N	-5.04	116.04	122.34
2	2	213	GLU	CA-C-N	5.03	129.08	121.03
2	2	213	GLU	C-N-CA	5.03	129.08	121.03
3	3	152	ASN	CA-C-O	-5.02	114.80	120.43
3	3	127	PRO	N-CA-CB	-5.02	98.21	103.08
3	3	179	ASN	CA-CB-CG	-5.01	107.59	112.60
4	4	22	ILE	O-C-N	5.01	128.87	122.61
3	3	195	ASP	CB-CA-C	-5.00	103.10	110.06

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	107	TYR	Sidechain

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	1456	0	1453	27	0
2	2	1652	0	1610	22	0
3	3	1681	0	1616	24	0
4	4	353	0	324	9	0
All	All	5142	0	5003	77	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 (77) 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)
2:2:11:GLU:HG2	2:2:13:ARG:HD3	1.39	1.04
1:1:70:THR:HG23	1:1:187:CYS:HB2	1.47	0.95
3:3:100:GLN:HE22	3:3:212:ARG:HH21	1.15	0.92
1:1:103:ASN:HD21	3:3:216:ASP:H	1.25	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:115:GLN:NE2	2:2:115:GLN:H	1.82	0.77
2:2:114:ASN:HD21	2:2:193:GLY:HA2	1.51	0.75
2:2:115:GLN:H	2:2:115:GLN:HE21	1.34	0.75
1:1:45:GLN:H	1:1:49:ASN:HD21	1.33	0.75
3:3:100:GLN:NE2	3:3:212:ARG:HH21	1.83	0.75
3:3:43:ASN:HD22	3:3:45:LEU:H	1.36	0.72
2:2:216:SER:OG	2:2:218:GLU:HG2	1.91	0.71
1:1:89:VAL:HG13	1:1:93:ALA:HB3	1.77	0.66
2:2:101:MET:HG2	2:2:210:VAL:HG12	1.79	0.65
4:4:65:ASN:CB	4:4:69:SER:HB2	2.29	0.62
2:2:149:ASN:H	2:2:153:ASN:ND2	1.98	0.61
1:1:70:THR:HB	1:1:189:ARG:HD2	1.82	0.61
1:1:35:ILE:O	1:1:38:ARG:HD2	2.02	0.60
3:3:168:THR:HG22	3:3:169:TYR:H	1.65	0.60
2:2:115:GLN:HE21	2:2:115:GLN:N	2.00	0.59
1:1:91:ASN:H	1:1:120:THR:HG23	1.66	0.59
1:1:91:ASN:H	1:1:120:THR:CG2	2.16	0.59
1:1:91:ASN:HB3	1:1:120:THR:HG23	1.84	0.58
1:1:89:VAL:HB	1:1:98:LEU:HD13	1.86	0.58
3:3:43:ASN:ND2	3:3:45:LEU:H	2.01	0.57
1:1:45:GLN:H	1:1:49:ASN:ND2	2.02	0.57
1:1:89:VAL:HG13	1:1:93:ALA:CB	2.33	0.57
2:2:106:ASP:OD1	2:2:157:HIS:HE1	1.88	0.57
3:3:100:GLN:HE22	3:3:212:ARG:NH2	1.95	0.56
3:3:112:THR:HB	3:3:198:ALA:O	2.07	0.55
1:1:98:LEU:HG	1:1:169:LYS:HB2	1.88	0.55
1:1:45:GLN:N	1:1:49:ASN:HD21	2.05	0.54
1:1:53:LEU:O	1:1:56:VAL:HG13	2.08	0.54
4:4:65:ASN:O	4:4:65:ASN:OD1	2.26	0.53
3:3:68:THR:HG23	3:3:191:HIS:HE2	1.72	0.53
1:1:91:ASN:CB	1:1:120:THR:HG23	2.38	0.53
2:2:149:ASN:H	2:2:153:ASN:HD21	1.56	0.52
1:1:37:ASP:OD1	1:1:179:ARG:HD2	2.08	0.52
4:4:65:ASN:N	4:4:69:SER:HB2	2.26	0.51
1:1:70:THR:CG2	1:1:189:ARG:HH11	2.25	0.49
3:3:43:ASN:HD22	3:3:45:LEU:N	2.07	0.49
3:3:168:THR:HG22	3:3:169:TYR:N	2.27	0.49
2:2:114:ASN:ND2	2:2:116:PHE:H	2.11	0.49
1:1:103:ASN:ND2	3:3:216:ASP:H	2.04	0.49
1:1:129:VAL:HG13	2:2:128:GLU:HB2	1.95	0.48
3:3:64:VAL:HG13	3:3:74:LEU:HG	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:43:VAL:HG22	2:2:102:ARG:HD2	1.94	0.48
1:1:70:THR:HB	1:1:189:ARG:HH11	1.78	0.48
4:4:65:ASN:HB3	4:4:69:SER:HB2	1.94	0.48
2:2:114:ASN:HB2	2:2:115:GLN:NE2	2.28	0.48
3:3:67:LYS:HE2	3:3:67:LYS:HB3	1.66	0.48
2:2:29:SER:O	2:2:30:VAL:HB	2.14	0.47
3:3:44:LEU:HG	3:3:94:LEU:HD21	1.96	0.47
1:1:70:THR:HG22	1:1:187:CYS:O	2.15	0.47
3:3:119:ALA:HA	3:3:191:HIS:HA	1.95	0.47
3:3:104:THR:CG2	3:3:158:SER:HB3	2.46	0.46
2:2:114:ASN:ND2	2:2:193:GLY:HA2	2.24	0.46
1:1:7:SER:O	1:1:8:ALA:HB3	2.15	0.45
2:2:40:GLU:HG2	2:2:102:ARG:NH1	2.31	0.45
4:4:65:ASN:CA	4:4:69:SER:HB2	2.47	0.45
1:1:1:THR:HG21	4:4:76:PHE:HE2	1.82	0.45
2:2:91:TYR:O	2:2:94:LEU:HB2	2.17	0.44
4:4:65:ASN:N	4:4:69:SER:CB	2.80	0.44
3:3:212:ARG:O	3:3:213:LEU:HB2	2.16	0.44
3:3:72:ARG:HG2	3:3:188:GLN:O	2.18	0.43
4:4:65:ASN:O	4:4:65:ASN:CG	2.61	0.43
2:2:60:ARG:HH11	2:2:60:ARG:HD3	1.62	0.43
2:2:94:LEU:HD12	2:2:94:LEU:HA	1.82	0.43
3:3:2:ILE:HD13	3:3:2:ILE:HG21	1.76	0.42
1:1:159:LEU:HD12	1:1:159:LEU:HA	1.87	0.42
2:2:26:THR:HG21	2:2:155:THR:OG1	2.20	0.42
3:3:54:PHE:CD1	3:3:202:LEU:HD13	2.54	0.42
3:3:67:LYS:HD2	3:3:74:LEU:CD1	2.51	0.41
1:1:24:ILE:HD11	1:1:26:ARG:CZ	2.50	0.41
2:2:114:ASN:HB2	2:2:115:GLN:HE21	1.85	0.41
1:1:104:PRO:HG3	3:3:17:THR:HG21	2.03	0.41
3:3:64:VAL:CG1	3:3:74:LEU:HG	2.51	0.41
4:4:65:ASN:O	4:4:66:ASP:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	182/213 (85%)	176 (97%)	4 (2%)	2 (1%)	11	25
2	2	208/218 (95%)	195 (94%)	11 (5%)	2 (1%)	12	28
3	3	218/220 (99%)	211 (97%)	5 (2%)	2 (1%)	14	30
4	4	42/85 (49%)	35 (83%)	5 (12%)	2 (5%)	2	2
All	All	650/736 (88%)	617 (95%)	25 (4%)	8 (1%)	10	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	30	VAL
2	2	131	SER
4	4	80	PHE
1	1	104	PRO
3	3	219	ALA
4	4	66	ASP
1	1	187	CYS
3	3	213	LEU

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	159/183 (87%)	132 (83%)	27 (17%)	2	4
2	2	183/191 (96%)	148 (81%)	35 (19%)	1	2
3	3	176/176 (100%)	140 (80%)	36 (20%)	1	2
4	4	37/67 (55%)	31 (84%)	6 (16%)	2	4
All	All	555/617 (90%)	451 (81%)	104 (19%)	1	3

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	1	THR
1	1	7	SER
1	1	24	ILE
1	1	25	GLN
1	1	28	GLN
1	1	38	ARG
1	1	42	VAL
1	1	50	ILE
1	1	53	LEU
1	1	56	VAL
1	1	65	LEU
1	1	70	THR
1	1	89	VAL
1	1	98	LEU
1	1	101	THR
1	1	111	PRO
1	1	114	ARG
1	1	115	LEU
1	1	120	THR
1	1	124	ARG
1	1	125	VAL
1	1	173	VAL
1	1	179	ARG
1	1	191	LEU
1	1	192	LEU
1	1	204	LYS
1	1	206	VAL
2	2	9	LEU
2	2	11	GLU
2	2	12	ASP
2	2	15	LEU
2	2	18	ARG
2	2	26	THR
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
2	2	56	VAL
2	2	60	ARG
2	2	66	LEU

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Mol	Chain	Res	Type
2	2	77	ARG
2	2	83	LEU
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	130	CYS
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	208	VAL
3	3	5	VAL
3	3	14	LEU
3	3	17	THR
3	3	29	VAL
3	3	34	ARG
3	3	36	GLN
3	3	42	THR
3	3	44	LEU
3	3	47	VAL
3	3	56	ARG
3	3	64	VAL
3	3	67	LYS
3	3	68	THR
3	3	74	LEU
3	3	81	LEU
3	3	94	LEU
3	3	107	LEU
3	3	112	THR
3	3	115	THR
3	3	130	MET
3	3	131	GLU
3	3	151	LEU
3	3	162	LEU

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Mol	Chain	Res	Type
3	3	168	THR
3	3	174	VAL
3	3	178	THR
3	3	180	VAL
3	3	184	VAL
3	3	190	THR
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	18	THR
4	4	20	SER
4	4	22	ILE
4	4	28	GLN
4	4	65	ASN
4	4	66	ASP

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	29	HIS
1	1	49	ASN
1	1	55	GLN
1	1	103	ASN
1	1	108	HIS
2	2	19	ASN
2	2	65	HIS
2	2	114	ASN
2	2	115	GLN
2	2	133	GLN
2	2	153	ASN
2	2	157	HIS
3	3	43	ASN
3	3	100	GLN
3	3	181	GLN
4	4	17	ASN
4	4	32	ASN

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.