



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:46 pm GMT

PDB ID : 1BBT
Title : METHODS USED IN THE STRUCTURE DETERMINATION OF FOOT
AND MOUTH DISEASE VIRUS
Authors : Acharya, K.R.; Fry, E.E.; Logan, D.T.; Stuart, D.I.
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

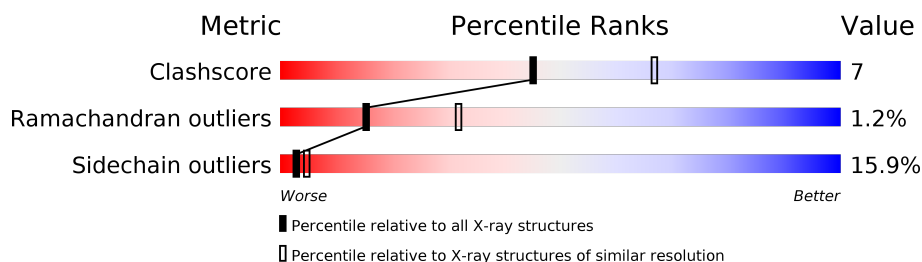
1 Overall quality at a glance

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	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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:

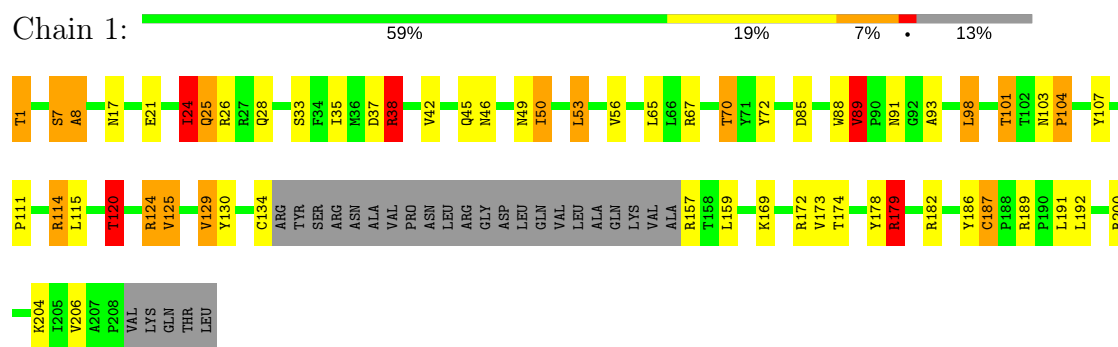
Chain	Residue	Modelled	Actual	Comment	Reference
4	40	ASN	ASP	CONFLICT	UNP O90754
4	41	ASP	ASN	CONFLICT	UNP O90754

3 Residue-property plots [i](#)

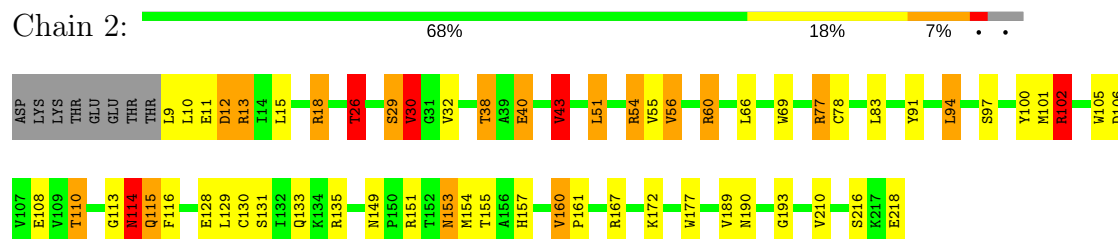
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

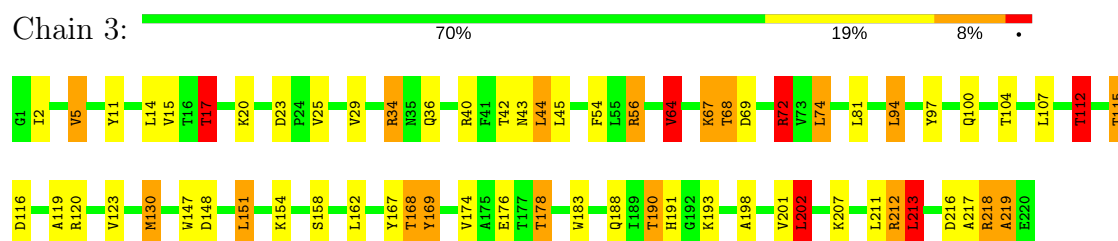
• Molecule 1: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP1)



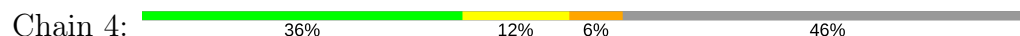
• Molecule 2: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP2)

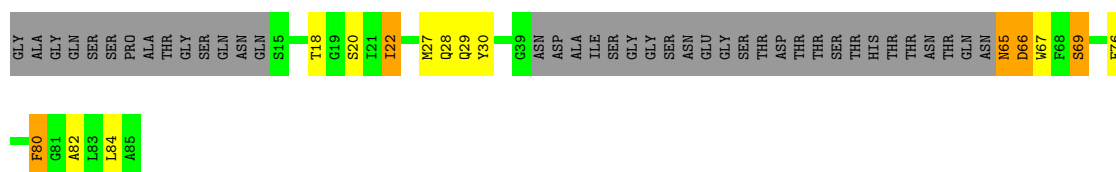


• Molecule 3: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP3)



• 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 [i](#)

5.1 Standard geometry [i](#)

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	1.08	1/1490 (0.1%)	2.04	44/2035 (2.2%)
2	2	1.15	3/1695 (0.2%)	1.98	55/2314 (2.4%)
3	3	1.08	0/1729	1.93	63/2361 (2.7%)
4	4	1.17	2/359 (0.6%)	2.04	10/481 (2.1%)
All	All	1.11	6/5273 (0.1%)	1.99	172/7191 (2.4%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	69	SER	CA-CB	-8.85	1.39	1.52
2	2	167	ARG	CZ-NH2	5.29	1.40	1.33
2	2	97	SER	CA-CB	-5.29	1.45	1.52
2	2	108	GLU	CD-OE2	-5.18	1.20	1.25
1	1	21	GLU	CA-CB	-5.11	1.42	1.53
4	4	27	MET	CA-CB	-5.10	1.42	1.53

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	135	ARG	NE-CZ-NH1	18.03	129.31	120.30
1	1	179	ARG	NE-CZ-NH1	17.84	129.22	120.30
2	2	135	ARG	NE-CZ-NH2	-17.26	111.67	120.30
1	1	182	ARG	NE-CZ-NH1	15.53	128.06	120.30
1	1	38	ARG	NE-CZ-NH2	-15.06	112.77	120.30
1	1	124	ARG	NE-CZ-NH1	14.24	127.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	102	ARG	NE-CZ-NH1	13.89	127.25	120.30
1	1	182	ARG	NE-CZ-NH2	-13.44	113.58	120.30
3	3	72	ARG	NE-CZ-NH1	12.52	126.56	120.30
2	2	77	ARG	NE-CZ-NH2	-12.40	114.10	120.30
3	3	130	MET	CG-SD-CE	-12.27	80.56	100.20
1	1	38	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	1	114	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	1	179	ARG	NE-CZ-NH2	-11.09	114.75	120.30
2	2	77	ARG	NE-CZ-NH1	10.70	125.65	120.30
2	2	133	GLN	CA-CB-CG	-9.83	91.77	113.40
2	2	54	ARG	NE-CZ-NH2	9.79	125.19	120.30
2	2	18	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	1	67	ARG	NE-CZ-NH1	9.60	125.10	120.30
3	3	36	GLN	CA-CB-CG	-9.46	92.58	113.40
3	3	40	ARG	NE-CZ-NH2	9.34	124.97	120.30
2	2	29	SER	CA-C-N	9.08	137.17	117.20
4	4	27	MET	CG-SD-CE	-9.03	85.75	100.20
2	2	105	TRP	CD1-CG-CD2	9.00	113.50	106.30
1	1	50	ILE	CB-CG1-CD1	-8.97	88.78	113.90
3	3	11	TYR	CB-CG-CD2	-8.70	115.78	121.00
3	3	34	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	1	101	THR	CA-CB-CG2	8.66	124.53	112.40
3	3	202	LEU	CA-CB-CG	8.66	135.22	115.30
3	3	72	ARG	NE-CZ-NH2	-8.48	116.06	120.30
4	4	67	TRP	CD1-CG-CD2	8.38	113.00	106.30
3	3	218	ARG	N-CA-C	-8.36	88.43	111.00
3	3	169	TYR	CB-CG-CD2	-8.30	116.02	121.00
4	4	30	TYR	CB-CG-CD2	-8.24	116.06	121.00
2	2	102	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	1	172	ARG	NE-CZ-NH1	8.10	124.35	120.30
2	2	13	ARG	NE-CZ-NH2	-8.06	116.27	120.30
2	2	26	THR	N-CA-CB	8.03	125.55	110.30
2	2	177	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	1	88	TRP	CD1-CG-CD2	7.61	112.39	106.30
3	3	212	ARG	NE-CZ-NH1	7.60	124.10	120.30
3	3	17	THR	N-CA-CB	-7.59	95.87	110.30
1	1	120	THR	N-CA-CB	-7.57	95.92	110.30
3	3	193	LYS	CB-CG-CD	-7.52	92.06	111.60
1	1	8	ALA	CB-CA-C	-7.43	98.95	110.10
3	3	218	ARG	CD-NE-CZ	7.41	133.98	123.60
3	3	183	TRP	CD1-CG-CD2	7.39	112.21	106.30
2	2	26	THR	CB-CA-C	-7.34	91.78	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	160	VAL	N-CA-CB	-7.34	95.35	111.50
1	1	72	TYR	CB-CG-CD1	-7.29	116.62	121.00
4	4	67	TRP	CE2-CD2-CG	-7.25	101.50	107.30
3	3	147	TRP	CE2-CD2-CG	-7.23	101.52	107.30
3	3	112	THR	N-CA-CB	-7.21	96.61	110.30
3	3	147	TRP	CG-CD2-CE3	7.19	140.38	133.90
3	3	217	ALA	C-N-CA	7.17	139.61	121.70
1	1	174	THR	CA-CB-CG2	7.15	122.41	112.40
3	3	147	TRP	CD1-CG-CD2	7.09	111.97	106.30
4	4	67	TRP	CG-CD2-CE3	7.03	140.23	133.90
1	1	24	ILE	CB-CG1-CD1	-7.03	94.22	113.90
2	2	10	LEU	CA-C-N	7.02	132.65	117.20
1	1	88	TRP	CE2-CD2-CG	-7.02	101.69	107.30
1	1	124	ARG	NE-CZ-NH2	-6.99	116.81	120.30
3	3	147	TRP	CB-CG-CD1	-6.97	117.93	127.00
2	2	30	VAL	CA-CB-CG2	-6.96	100.46	110.90
2	2	160	VAL	CG1-CB-CG2	6.91	121.96	110.90
1	1	8	ALA	N-CA-CB	6.91	119.77	110.10
1	1	200	ARG	NE-CZ-NH1	6.90	123.75	120.30
2	2	105	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	1	101	THR	CA-CB-OG1	-6.87	94.57	109.00
1	1	101	THR	N-CA-CB	-6.78	97.41	110.30
3	3	190	THR	OG1-CB-CG2	6.76	125.55	110.00
3	3	64	VAL	N-CA-CB	-6.72	96.72	111.50
2	2	105	TRP	CG-CD1-NE1	-6.71	103.39	110.10
3	3	183	TRP	CE2-CD2-CG	-6.64	101.99	107.30
2	2	154	MET	N-CA-CB	-6.62	98.68	110.60
3	3	97	TYR	CB-CG-CD1	-6.61	117.03	121.00
2	2	38	THR	CA-CB-CG2	6.59	121.62	112.40
2	2	38	THR	CA-CB-OG1	-6.58	95.19	109.00
2	2	151	ARG	NE-CZ-NH1	6.52	123.56	120.30
3	3	34	ARG	CG-CD-NE	-6.41	98.34	111.80
2	2	154	MET	CG-SD-CE	6.38	110.42	100.20
3	3	120	ARG	NE-CZ-NH1	6.36	123.48	120.30
3	3	25	VAL	CA-C-N	6.31	131.09	117.20
3	3	167	TYR	CB-CG-CD2	-6.30	117.22	121.00
2	2	43	VAL	N-CA-CB	-6.28	97.69	111.50
2	2	69	TRP	CE2-CD2-CG	-6.28	102.28	107.30
2	2	12	ASP	CA-CB-CG	6.24	127.14	113.40
3	3	169	TYR	CB-CG-CD1	6.24	124.75	121.00
2	2	129	LEU	CA-C-N	-6.24	103.47	117.20
3	3	151	LEU	CA-CB-CG	6.23	129.63	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	218	ARG	CA-CB-CG	6.23	127.11	113.40
1	1	174	THR	CA-CB-OG1	-6.22	95.94	109.00
4	4	29	GLN	N-CA-CB	-6.15	99.53	110.60
4	4	67	TRP	CB-CG-CD1	-6.14	119.02	127.00
2	2	30	VAL	CA-CB-CG1	6.13	120.10	110.90
3	3	5	VAL	CA-CB-CG2	-6.09	101.77	110.90
3	3	183	TRP	CG-CD2-CE3	6.07	139.36	133.90
2	2	78	CYS	CA-CB-SG	-6.05	103.11	114.00
3	3	183	TRP	CB-CG-CD1	-5.95	119.26	127.00
1	1	186	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	1	89	VAL	N-CA-CB	-5.89	98.54	111.50
2	2	177	TRP	CE2-CD2-CG	-5.87	102.60	107.30
1	1	206	VAL	N-CA-CB	-5.86	98.61	111.50
3	3	42	THR	OG1-CB-CG2	5.85	123.45	110.00
1	1	46	ASN	CB-CA-C	-5.82	98.75	110.40
3	3	56	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	1	130	TYR	CB-CG-CD2	-5.82	117.51	121.00
3	3	148	ASP	CB-CG-OD1	5.80	123.52	118.30
3	3	190	THR	N-CA-CB	5.78	121.27	110.30
1	1	157	ARG	CA-C-N	5.76	129.87	117.20
1	1	129	VAL	CA-CB-CG2	-5.75	102.28	110.90
1	1	33	SER	CA-CB-OG	-5.73	95.72	111.20
1	1	125	VAL	N-CA-CB	-5.72	98.90	111.50
3	3	5	VAL	N-CA-CB	-5.72	98.92	111.50
2	2	29	SER	CA-C-O	-5.70	108.14	120.10
2	2	54	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
3	3	147	TRP	CG-CD1-NE1	-5.66	104.44	110.10
2	2	56	VAL	N-CA-CB	-5.65	99.07	111.50
3	3	218	ARG	NE-CZ-NH1	5.65	123.12	120.30
2	2	13	ARG	N-CA-C	-5.62	95.83	111.00
3	3	64	VAL	CB-CA-C	5.61	122.06	111.40
3	3	183	TRP	CG-CD1-NE1	-5.57	104.53	110.10
4	4	22	ILE	CA-C-N	-5.56	104.98	117.20
3	3	42	THR	CA-CB-CG2	5.55	120.17	112.40
2	2	110	THR	CA-CB-CG2	5.53	120.15	112.40
1	1	88	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	1	120	THR	CA-CB-CG2	5.50	120.09	112.40
2	2	69	TRP	CD1-CG-CD2	5.49	110.69	106.30
3	3	176	GLU	N-CA-CB	-5.48	100.74	110.60
3	3	23	ASP	CB-CG-OD2	-5.45	113.39	118.30
3	3	23	ASP	CB-CG-OD1	5.45	123.21	118.30
2	2	113	GLY	N-CA-C	-5.45	99.48	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	115	THR	CA-CB-CG2	5.44	120.01	112.40
2	2	114	ASN	CB-CG-ND2	5.43	129.73	116.70
3	3	42	THR	CA-CB-OG1	-5.40	97.65	109.00
3	3	15	VAL	CG1-CB-CG2	-5.40	102.27	110.90
3	3	20	LYS	CB-CG-CD	-5.39	97.59	111.60
1	1	134	CYS	CA-CB-SG	5.38	123.69	114.00
1	1	25	GLN	CA-CB-CG	5.36	125.19	113.40
3	3	190	THR	CB-CA-C	-5.36	97.13	111.60
3	3	123	VAL	CG1-CB-CG2	5.35	119.47	110.90
2	2	13	ARG	NE-CZ-NH1	5.34	122.97	120.30
3	3	217	ALA	N-CA-CB	-5.34	102.63	110.10
3	3	219	ALA	CB-CA-C	-5.33	102.10	110.10
2	2	9	LEU	CA-CB-CG	5.33	127.55	115.30
3	3	154	LYS	CB-CG-CD	-5.32	97.76	111.60
3	3	218	ARG	CB-CG-CD	5.31	125.40	111.60
3	3	25	VAL	O-C-N	-5.28	114.25	122.70
2	2	100	TYR	CB-CG-CD2	-5.26	117.84	121.00
4	4	84	LEU	CA-C-N	-5.26	105.62	117.20
2	2	40	GLU	CA-CB-CG	-5.23	101.90	113.40
1	1	17	ASN	OD1-CG-ND2	-5.21	109.91	121.90
2	2	105	TRP	CG-CD2-CE3	5.20	138.58	133.90
2	2	18	ARG	CG-CD-NE	-5.19	100.91	111.80
2	2	51	LEU	CB-CG-CD2	-5.18	102.20	111.00
2	2	38	THR	N-CA-CB	-5.17	100.47	110.30
3	3	151	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	1	42	VAL	N-CA-CB	-5.15	100.17	111.50
2	2	177	TRP	CG-CD1-NE1	-5.15	104.95	110.10
2	2	12	ASP	CB-CG-OD1	5.11	122.90	118.30
3	3	178	THR	CA-CB-CG2	5.11	119.55	112.40
2	2	110	THR	N-CA-CB	-5.10	100.61	110.30
4	4	82	ALA	N-CA-C	-5.10	97.22	111.00
2	2	160	VAL	CB-CA-C	5.09	121.08	111.40
2	2	190	ASN	CA-C-N	5.09	128.39	117.20
3	3	178	THR	CA-CB-OG1	-5.07	98.35	109.00
3	3	116	ASP	CB-CG-OD1	5.07	122.86	118.30
1	1	178	TYR	CB-CG-CD2	5.05	124.03	121.00
2	2	29	SER	O-C-N	-5.03	114.65	122.70
1	1	88	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	1	85	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	1	182	ARG	CA-CB-CG	5.00	124.41	113.40

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	7	0
All	All	5142	0	5003	75	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 7.

All (75) 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
2:2:115:GLN:H	2:2:115:GLN:NE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	4:4:65:ASN:O	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HG21	3:3:2:ILE:HD13	1.76	0.42
1:1:159:LEU:HA	1:1:159:LEU:HD12	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

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%)	17	35
2	2	208/218 (95%)	195 (94%)	11 (5%)	2 (1%)	18	37
3	3	218/220 (99%)	211 (97%)	5 (2%)	2 (1%)	20	40
4	4	42/85 (49%)	35 (83%)	5 (12%)	2 (5%)	2	3
All	All	650/736 (88%)	617 (95%)	25 (4%)	8 (1%)	15	32

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%)	135 (85%)	24 (15%)	3	5
2	2	183/191 (96%)	157 (86%)	26 (14%)	4	6
3	3	176/176 (100%)	145 (82%)	31 (18%)	2	3
4	4	37/67 (55%)	30 (81%)	7 (19%)	2	2
All	All	555/617 (90%)	467 (84%)	88 (16%)	3	5

All (88) 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	50	ILE
1	1	53	LEU
1	1	65	LEU
1	1	70	THR
1	1	89	VAL
1	1	98	LEU
1	1	101	THR
1	1	111	PRO

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Mol	Chain	Res	Type
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
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	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
2	2	77	ARG
2	2	83	LEU
2	2	94	LEU
2	2	102	ARG
2	2	110	THR
2	2	114	ASN
2	2	115	GLN
2	2	130	CYS
2	2	153	ASN
2	2	160	VAL
2	2	161	PRO
2	2	172	LYS
2	2	189	VAL
3	3	5	VAL
3	3	14	LEU
3	3	17	THR
3	3	29	VAL
3	3	34	ARG
3	3	44	LEU

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Mol	Chain	Res	Type
3	3	56	ARG
3	3	64	VAL
3	3	67	LYS
3	3	68	THR
3	3	69	ASP
3	3	72	ARG
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	151	LEU
3	3	162	LEU
3	3	168	THR
3	3	174	VAL
3	3	178	THR
3	3	190	THR
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
4	4	80	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	49	ASN
1	1	55	GLN
1	1	103	ASN
2	2	65	HIS
2	2	114	ASN
2	2	115	GLN

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Mol	Chain	Res	Type
2	2	149	ASN
2	2	153	ASN
2	2	157	HIS
2	2	166	ASN
3	3	43	ASN
3	3	100	GLN
3	3	152	ASN
4	4	17	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 carbohydrates 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.