



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:14 AM GMT

PDB ID : 2CAS  
Title : THE CANINE PARVOVIRUS EMPTY CAPSID STRUCTURE  
Authors : Wu, H.; Rossmann, M.G.  
Deposited on : 1993-08-24  
Resolution : 3.00 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

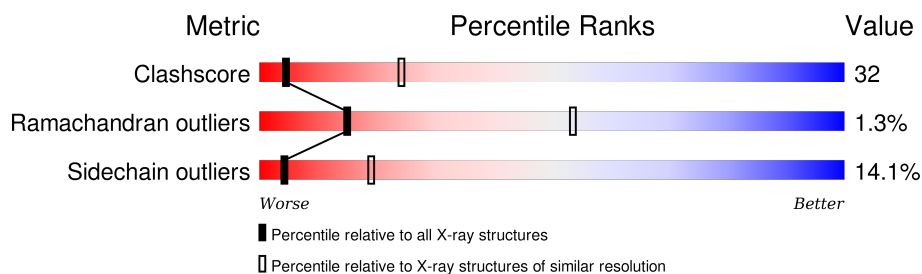
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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  $\geq 3$ , 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	A	548	<div>47% 37% 12% .</div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4434 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 CANINE PARVOVIRUS EMPTY CAPSID (STRAIN D) VIRAL PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4347	2760	742	829	16			

- Molecule 2 is water.

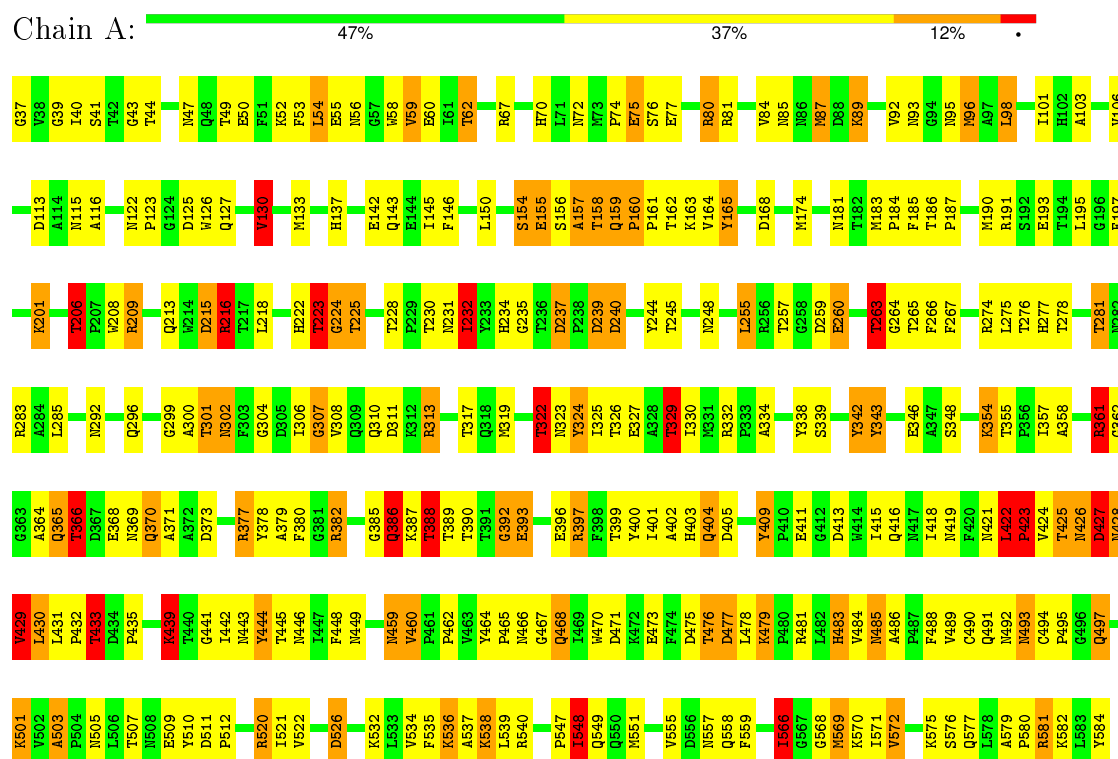
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	87	Total	O	0	0
			87	87		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: CANINE PARVOVIRUS EMPTY CAPSID (STRAIN D) VIRAL PROTEIN 2



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	254.50Å 254.50Å 795.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	0.211 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	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	A	1.17	10/4476 (0.2%)	2.23	188/6123 (3.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	509	GLU	CD-OE2	9.10	1.35	1.25
1	A	422	LEU	C-O	8.24	1.39	1.23
1	A	264	GLY	N-CA	8.15	1.58	1.46
1	A	307	GLY	N-CA	7.86	1.57	1.46
1	A	263	THR	C-O	7.45	1.37	1.23
1	A	306	ILE	C-O	6.87	1.36	1.23
1	A	423	PRO	N-CA	6.55	1.58	1.47
1	A	423	PRO	N-CD	-6.28	1.39	1.47
1	A	37	GLY	N-CA	5.73	1.54	1.46
1	A	274	ARG	NE-CZ	5.25	1.39	1.33

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ASP	CB-CG-OD2	26.52	142.17	118.30
1	A	405	ASP	CB-CG-OD1	21.22	137.40	118.30
1	A	237	ASP	CB-CG-OD2	19.44	135.80	118.30
1	A	81	ARG	NE-CZ-NH1	19.23	129.91	120.30
1	A	274	ARG	NE-CZ-NH2	-15.97	112.31	120.30
1	A	191	ARG	NE-CZ-NH2	15.84	128.22	120.30
1	A	427	ASP	CB-CG-OD2	-15.21	104.61	118.30
1	A	332	ARG	NE-CZ-NH1	14.30	127.45	120.30
1	A	240	ASP	CB-CG-OD1	-14.04	105.67	118.30
1	A	361	ARG	NE-CZ-NH1	13.56	127.08	120.30
1	A	274	ARG	CD-NE-CZ	-12.78	105.71	123.60
1	A	403	HIS	CA-CB-CG	12.60	135.02	113.60
1	A	80	ARG	NE-CZ-NH1	12.03	126.31	120.30
1	A	361	ARG	NE-CZ-NH2	-11.84	114.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ARG	CD-NE-CZ	10.95	138.94	123.60
1	A	274	ARG	NH1-CZ-NH2	10.75	131.22	119.40
1	A	306	ILE	CA-C-N	10.59	137.37	116.20
1	A	263	THR	CA-C-N	10.53	137.27	116.20
1	A	405	ASP	CA-CB-CG	10.44	136.37	113.40
1	A	113	ASP	CB-CG-OD1	10.12	127.41	118.30
1	A	165	TYR	CB-CG-CD1	-10.11	114.93	121.00
1	A	81	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	A	81	ARG	CD-NE-CZ	9.94	137.51	123.60
1	A	581	ARG	NE-CZ-NH1	-9.90	115.35	120.30
1	A	342	TYR	O-C-N	9.81	138.39	122.70
1	A	422	LEU	CA-C-N	9.77	144.45	117.10
1	A	413	ASP	CB-CG-OD2	9.64	126.98	118.30
1	A	165	TYR	CB-CG-CD2	9.60	126.76	121.00
1	A	67	ARG	NE-CZ-NH2	9.52	125.06	120.30
1	A	425	THR	CA-CB-OG1	-9.42	89.21	109.00
1	A	311	ASP	CB-CG-OD1	9.33	126.69	118.30
1	A	477	ASP	CB-CG-OD2	9.24	126.62	118.30
1	A	540	ARG	CD-NE-CZ	-9.14	110.80	123.60
1	A	405	ASP	CB-CG-OD2	-8.96	110.23	118.30
1	A	388	THR	CA-CB-CG2	8.67	124.54	112.40
1	A	113	ASP	CB-CG-OD2	-8.62	110.54	118.30
1	A	566	ILE	CA-CB-CG2	8.54	127.98	110.90
1	A	548	ILE	CA-CB-CG2	8.49	127.88	110.90
1	A	125	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	A	168	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	A	422	LEU	N-CA-C	8.35	133.54	111.00
1	A	206	THR	N-CA-CB	8.18	125.85	110.30
1	A	397	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	A	75	GLU	CG-CD-OE1	8.04	134.38	118.30
1	A	548	ILE	CA-CB-CG1	-7.95	95.90	111.00
1	A	526	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	A	75	GLU	CG-CD-OE2	-7.90	102.50	118.30
1	A	540	ARG	NE-CZ-NH1	-7.75	116.43	120.30
1	A	274	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	A	237	ASP	N-CA-CB	7.67	124.41	110.60
1	A	216	ARG	CA-CB-CG	7.63	130.20	113.40
1	A	492	ASN	CA-CB-CG	-7.58	96.72	113.40
1	A	423	PRO	CB-CA-C	7.51	130.79	112.00
1	A	237	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	A	377	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	A	96	MET	CA-CB-CG	-7.43	100.67	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	TYR	CA-C-N	-7.28	101.17	117.20
1	A	263	THR	N-CA-CB	-7.25	96.52	110.30
1	A	409	TYR	CB-CG-CD1	-7.24	116.66	121.00
1	A	481	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	433	THR	CA-CB-OG1	-7.15	93.98	109.00
1	A	422	LEU	CA-C-O	-7.12	105.16	120.10
1	A	209	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	A	460	VAL	N-CA-CB	-7.11	95.85	111.50
1	A	386	GLN	CG-CD-OE1	7.05	135.69	121.60
1	A	584	TYR	CB-CG-CD2	7.02	125.21	121.00
1	A	566	ILE	CA-CB-CG1	-6.97	97.77	111.00
1	A	306	ILE	C-N-CA	-6.89	107.84	122.30
1	A	75	GLU	CA-CB-CG	6.88	128.54	113.40
1	A	72	ASN	CB-CG-OD1	-6.85	107.90	121.60
1	A	41	SER	N-CA-CB	6.81	120.72	110.50
1	A	510	TYR	CB-CG-CD2	6.78	125.06	121.00
1	A	481	ARG	CD-NE-CZ	-6.76	114.13	123.60
1	A	477	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	A	409	TYR	CB-CG-CD2	6.67	125.00	121.00
1	A	338	TYR	CB-CG-CD2	6.66	125.00	121.00
1	A	67	ARG	CD-NE-CZ	-6.66	114.28	123.60
1	A	223	THR	CA-CB-OG1	-6.62	95.09	109.00
1	A	397	ARG	CD-NE-CZ	-6.62	114.33	123.60
1	A	404	GLN	CA-C-O	-6.57	106.31	120.10
1	A	240	ASP	CB-CA-C	6.56	123.51	110.40
1	A	429	VAL	O-C-N	6.55	133.17	122.70
1	A	60	GLU	CG-CD-OE2	-6.52	105.26	118.30
1	A	313	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	80	ARG	NH1-CZ-NH2	-6.43	112.33	119.40
1	A	50	GLU	CG-CD-OE2	6.40	131.09	118.30
1	A	306	ILE	O-C-N	-6.39	112.34	123.20
1	A	366	THR	CA-CB-CG2	-6.37	103.48	112.40
1	A	520	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	168	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	460	VAL	CA-CB-CG1	6.30	120.35	110.90
1	A	263	THR	O-C-N	-6.29	112.51	123.20
1	A	365	GLN	C-N-CA	-6.28	105.99	121.70
1	A	569	MET	N-CA-CB	6.28	121.90	110.60
1	A	510	TYR	CB-CG-CD1	-6.27	117.24	121.00
1	A	216	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	399	THR	N-CA-CB	6.22	122.11	110.30
1	A	342	TYR	C-N-CA	6.20	137.19	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ASN	N-CA-CB	-6.15	99.53	110.60
1	A	311	ASP	CB-CG-OD2	-6.13	112.79	118.30
1	A	559	PHE	CB-CG-CD1	-6.11	116.52	120.80
1	A	260	GLU	OE1-CD-OE2	6.11	130.63	123.30
1	A	388	THR	CA-CB-OG1	-6.10	96.20	109.00
1	A	155	GLU	CG-CD-OE1	-6.03	106.24	118.30
1	A	358	ALA	CA-C-N	6.03	130.46	117.20
1	A	301	THR	O-C-N	6.01	132.31	122.70
1	A	195	LEU	CB-CA-C	5.99	121.57	110.20
1	A	379	ALA	N-CA-CB	5.97	118.46	110.10
1	A	216	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	160	PRO	N-CA-C	-5.90	96.76	112.10
1	A	405	ASP	CB-CA-C	5.88	122.17	110.40
1	A	428	ASN	CB-CG-OD1	-5.88	109.83	121.60
1	A	343	TYR	O-C-N	5.87	132.09	122.70
1	A	240	ASP	OD1-CG-OD2	-5.86	112.16	123.30
1	A	72	ASN	CA-CB-CG	-5.84	100.56	113.40
1	A	224	GLY	C-N-CA	5.81	136.23	121.70
1	A	416	GLN	CB-CA-C	5.81	122.02	110.40
1	A	421	ASN	CA-CB-CG	-5.79	100.66	113.40
1	A	422	LEU	O-C-N	-5.79	110.09	121.10
1	A	430	LEU	CB-CA-C	5.77	121.16	110.20
1	A	405	ASP	OD1-CG-OD2	-5.76	112.35	123.30
1	A	421	ASN	OD1-CG-ND2	5.76	135.14	121.90
1	A	400	TYR	CB-CG-CD1	5.75	124.45	121.00
1	A	422	LEU	N-CA-CB	-5.74	98.92	110.40
1	A	304	GLY	N-CA-C	-5.73	98.78	113.10
1	A	419	ASN	CB-CA-C	5.72	121.84	110.40
1	A	429	VAL	CB-CA-C	-5.70	100.58	111.40
1	A	572	VAL	N-CA-CB	-5.70	98.97	111.50
1	A	512	PRO	C-N-CA	-5.68	107.49	121.70
1	A	483	HIS	CA-CB-CG	5.68	123.25	113.60
1	A	324	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	A	329	THR	CA-CB-OG1	-5.65	97.13	109.00
1	A	191	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	142	GLU	CA-CB-CG	5.61	125.74	113.40
1	A	237	ASP	OD1-CG-OD2	-5.60	112.66	123.30
1	A	225	THR	N-CA-C	-5.58	95.94	111.00
1	A	72	ASN	OD1-CG-ND2	5.57	134.72	121.90
1	A	103	ALA	N-CA-CB	5.57	117.89	110.10
1	A	125	ASP	OD1-CG-OD2	5.56	133.86	123.30
1	A	348	SER	N-CA-CB	5.52	118.78	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ALA	CB-CA-C	5.52	118.38	110.10
1	A	503	ALA	CB-CA-C	5.51	118.36	110.10
1	A	511	ASP	O-C-N	5.51	131.56	121.10
1	A	223	THR	C-N-CA	-5.50	110.75	122.30
1	A	475	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	511	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	419	ASN	CA-CB-CG	-5.47	101.36	113.40
1	A	322	THR	O-C-N	5.43	131.39	122.70
1	A	206	THR	CB-CA-C	-5.43	96.95	111.60
1	A	392	GLY	O-C-N	5.41	131.35	122.70
1	A	87	MET	N-CA-CB	-5.40	100.88	110.60
1	A	225	THR	N-CA-CB	5.39	120.55	110.30
1	A	400	TYR	CB-CG-CD2	-5.39	117.76	121.00
1	A	380	PHE	C-N-CA	5.39	133.61	122.30
1	A	186	THR	CA-CB-CG2	5.38	119.94	112.40
1	A	547	PRO	C-N-CA	5.36	135.11	121.70
1	A	322	THR	N-CA-CB	5.35	120.47	110.30
1	A	142	GLU	N-CA-CB	5.35	120.23	110.60
1	A	313	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	215	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	142	GLU	OE1-CD-OE2	5.33	129.70	123.30
1	A	263	THR	C-N-CA	-5.33	111.12	122.30
1	A	209	ARG	CD-NE-CZ	5.29	131.01	123.60
1	A	468	GLN	CA-CB-CG	5.29	125.04	113.40
1	A	459	ASN	CB-CG-OD1	-5.26	111.07	121.60
1	A	278	THR	CA-CB-CG2	5.26	119.77	112.40
1	A	257	THR	CA-CB-OG1	-5.22	98.03	109.00
1	A	130	VAL	N-CA-CB	-5.22	100.01	111.50
1	A	232	ILE	CB-CA-C	-5.22	101.16	111.60
1	A	281	THR	CA-CB-OG1	-5.22	98.05	109.00
1	A	244	TYR	CB-CA-C	-5.20	100.00	110.40
1	A	371	ALA	C-N-CA	5.19	134.69	121.70
1	A	382	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	404	GLN	O-C-N	5.17	130.97	122.70
1	A	115	ASN	CA-CB-CG	5.16	124.76	113.40
1	A	60	GLU	CG-CD-OE1	5.15	128.61	118.30
1	A	413	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	A	322	THR	CB-CA-C	-5.15	97.70	111.60
1	A	263	THR	OG1-CB-CG2	5.15	121.84	110.00
1	A	327	GLU	OE1-CD-OE2	5.12	129.44	123.30
1	A	385	GLY	CA-C-O	-5.12	111.39	120.60
1	A	427	ASP	OD1-CG-OD2	5.11	133.00	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	LYS	CB-CA-C	5.10	120.60	110.40
1	A	285	LEU	CA-C-O	-5.08	109.43	120.10
1	A	157	ALA	CB-CA-C	5.08	117.71	110.10
1	A	201	LYS	CA-CB-CG	5.08	124.57	113.40
1	A	423	PRO	N-CA-C	-5.07	98.91	112.10
1	A	425	THR	N-CA-CB	-5.07	100.67	110.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4347	0	4143	275	0
2	A	87	0	0	9	0
All	All	4434	0	4143	275	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 32.

All (275) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ARG:NE	1:A:366:THR:CG2	1.93	1.31
1:A:366:THR:HB	1:A:370:GLN:O	1.28	1.30
1:A:361:ARG:CZ	1:A:366:THR:HG21	1.68	1.21
1:A:361:ARG:NE	1:A:366:THR:HG21	1.56	1.19
1:A:366:THR:HG22	1:A:370:GLN:CG	1.73	1.18
1:A:159:GLN:O	1:A:161:PRO:HD3	1.45	1.13
1:A:366:THR:CG2	1:A:370:GLN:HG3	1.78	1.12
1:A:422:LEU:O	1:A:424:VAL:N	1.84	1.10
1:A:156:SER:HB3	1:A:162:THR:HG23	1.30	1.10
1:A:361:ARG:CZ	1:A:366:THR:CG2	2.29	1.08
1:A:370:GLN:HE21	1:A:370:GLN:HA	1.13	1.06
1:A:159:GLN:HB2	1:A:160:PRO:HD3	1.10	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:THR:HA	1:A:370:GLN:HB3	1.09	1.06
1:A:122:ASN:HB2	1:A:123:PRO:HD2	1.39	1.01
1:A:366:THR:CA	1:A:370:GLN:HB3	1.90	1.01
1:A:159:GLN:HB2	1:A:160:PRO:CD	1.89	1.01
1:A:366:THR:HG22	1:A:370:GLN:HG3	0.95	0.93
1:A:361:ARG:NH2	1:A:370:GLN:OE1	2.00	0.93
1:A:361:ARG:NE	1:A:366:THR:HG23	1.78	0.93
1:A:389:THR:HG21	1:A:566:ILE:HG22	1.50	0.93
1:A:85:ASN:HA	1:A:101:ILE:HG12	1.49	0.93
1:A:361:ARG:CD	1:A:366:THR:CG2	2.50	0.90
1:A:159:GLN:CB	1:A:160:PRO:HD3	2.02	0.88
1:A:370:GLN:NE2	1:A:370:GLN:HA	1.88	0.88
1:A:361:ARG:NH2	1:A:409:TYR:HE1	1.72	0.88
1:A:361:ARG:HA	2:A:784:HOH:O	1.74	0.88
1:A:292:ASN:HD22	1:A:307:GLY:H	1.17	0.87
1:A:361:ARG:CD	1:A:366:THR:HG23	2.05	0.86
1:A:388:THR:HG22	1:A:568:GLY:HA2	1.54	0.86
1:A:185:PHE:CE2	1:A:187:PRO:HG3	2.10	0.86
1:A:93:ASN:HD22	1:A:225:THR:HB	1.40	0.86
1:A:158:THR:HG23	1:A:159:GLN:H	1.39	0.85
1:A:158:THR:HG22	1:A:160:PRO:HD2	1.57	0.85
1:A:361:ARG:NH2	1:A:409:TYR:CE1	2.44	0.85
1:A:53:PHE:CD1	1:A:59:VAL:CG1	2.60	0.85
1:A:266:PHE:HZ	1:A:493:ASN:O	1.58	0.85
1:A:302:ASN:HD22	1:A:302:ASN:N	1.75	0.84
1:A:365:GLN:O	1:A:370:GLN:CB	2.25	0.84
1:A:366:THR:HA	1:A:370:GLN:CB	2.03	0.84
1:A:364:ALA:HB3	1:A:365:GLN:NE2	1.93	0.82
1:A:362:GLY:HA2	1:A:366:THR:OG1	1.80	0.82
1:A:485:ASN:HD22	1:A:485:ASN:H	1.27	0.82
1:A:193:GLU:OE1	1:A:206:THR:HG21	1.78	0.82
1:A:156:SER:HB3	1:A:162:THR:CG2	2.09	0.81
1:A:158:THR:CG2	1:A:159:GLN:H	1.94	0.81
1:A:388:THR:HB	1:A:569:MET:H	1.46	0.81
1:A:435:PRO:HB3	1:A:439:LYS:O	1.81	0.81
1:A:158:THR:CG2	1:A:159:GLN:N	2.44	0.80
1:A:324:TYR:O	1:A:329:THR:HG21	1.82	0.79
1:A:53:PHE:CD1	1:A:59:VAL:HG12	2.18	0.78
1:A:422:LEU:O	1:A:423:PRO:C	2.20	0.76
1:A:478:LEU:N	1:A:478:LEU:HD23	2.00	0.76
1:A:389:THR:HG23	1:A:568:GLY:HA2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLU:OE1	1:A:393:GLU:HA	1.86	0.75
1:A:158:THR:H	1:A:161:PRO:HA	1.50	0.75
1:A:361:ARG:HH21	1:A:409:TYR:HE1	1.34	0.75
1:A:471:ASP:OD2	1:A:483:HIS:HD2	1.67	0.75
1:A:443:ASN:H	1:A:446:ASN:ND2	1.85	0.75
1:A:89:LYS:HD2	1:A:98:LEU:HD12	1.70	0.73
1:A:174:MET:HE3	1:A:501:LYS:HZ2	1.53	0.73
1:A:156:SER:O	1:A:158:THR:N	2.21	0.73
1:A:361:ARG:CD	1:A:366:THR:HG21	2.14	0.72
1:A:127:GLN:HG3	1:A:551:MET:HG2	1.71	0.72
1:A:292:ASN:HD22	1:A:307:GLY:N	1.87	0.72
1:A:382:ARG:NH2	1:A:390:THR:O	2.19	0.72
1:A:84:VAL:O	1:A:101:ILE:HA	1.91	0.71
1:A:266:PHE:CD1	1:A:495:PRO:HG3	2.26	0.70
1:A:322:THR:HG22	1:A:324:TYR:H	1.56	0.70
1:A:377:ARG:NH2	1:A:397:ARG:HD2	2.07	0.70
1:A:361:ARG:HD2	1:A:366:THR:HG23	1.72	0.70
1:A:156:SER:N	1:A:162:THR:O	2.25	0.69
1:A:361:ARG:HE	1:A:366:THR:CG2	2.04	0.69
1:A:174:MET:CE	1:A:503:ALA:HA	2.22	0.69
1:A:74:PRO:HB2	1:A:76:SER:O	1.91	0.69
1:A:266:PHE:HZ	1:A:493:ASN:C	1.96	0.68
1:A:389:THR:CG2	1:A:566:ILE:HG22	2.23	0.68
1:A:424:VAL:HG22	1:A:429:VAL:HG22	1.74	0.68
1:A:281:THR:HG22	1:A:283:ARG:H	1.58	0.67
1:A:401:ILE:O	1:A:575:LYS:HE2	1.95	0.66
1:A:216:ARG:NH2	1:A:231:ASN:OD1	2.20	0.66
1:A:319:MET:CE	1:A:329:THR:OG1	2.45	0.65
1:A:465:PRO:HD2	1:A:466:ASN:ND2	2.11	0.65
1:A:507:THR:HG22	1:A:521:ILE:HG13	1.78	0.65
1:A:174:MET:HE3	1:A:501:LYS:NZ	2.10	0.65
1:A:459:ASN:ND2	1:A:460:VAL:H	1.95	0.65
1:A:310:GLN:HA	1:A:313:ARG:HD2	1.78	0.64
1:A:158:THR:CG2	1:A:160:PRO:HD2	2.27	0.64
1:A:53:PHE:CE1	1:A:59:VAL:HG11	2.33	0.64
1:A:362:GLY:CA	1:A:366:THR:OG1	2.46	0.64
1:A:431:LEU:C	1:A:433:THR:H	2.00	0.64
1:A:396:GLU:HG3	1:A:397:ARG:N	2.12	0.64
1:A:386:GLN:HB2	1:A:396:GLU:HB2	1.79	0.64
1:A:361:ARG:NH2	1:A:370:GLN:CD	2.52	0.64
1:A:174:MET:HE2	1:A:503:ALA:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLN:O	1:A:161:PRO:CD	2.35	0.63
1:A:346:GLU:OE2	1:A:355:THR:OG1	2.16	0.63
1:A:74:PRO:O	1:A:520:ARG:NH2	2.28	0.62
1:A:361:ARG:NH2	1:A:370:GLN:CG	2.63	0.62
1:A:302:ASN:ND2	1:A:302:ASN:N	2.48	0.62
1:A:237:ASP:OD1	1:A:239:ASP:N	2.33	0.61
1:A:425:THR:O	1:A:427:ASP:N	2.33	0.61
1:A:240:ASP:OD2	2:A:816:HOH:O	2.16	0.61
1:A:158:THR:HG22	1:A:159:GLN:N	2.16	0.61
1:A:361:ARG:CZ	1:A:366:THR:HG22	2.26	0.60
1:A:570:LYS:HD3	1:A:572:VAL:HG23	1.84	0.60
1:A:365:GLN:O	1:A:370:GLN:HB2	2.00	0.60
1:A:266:PHE:CZ	1:A:493:ASN:O	2.48	0.60
1:A:54:LEU:HD13	1:A:54:LEU:N	2.15	0.60
1:A:365:GLN:O	1:A:370:GLN:HG2	2.02	0.60
1:A:322:THR:HG22	1:A:323:ASN:N	2.16	0.60
1:A:54:LEU:N	1:A:54:LEU:CD1	2.63	0.60
1:A:58:TRP:CZ2	1:A:538:LYS:HD2	2.37	0.60
1:A:156:SER:O	1:A:162:THR:HG22	2.02	0.59
1:A:39:GLY:O	1:A:40:ILE:HD13	2.02	0.59
1:A:477:ASP:C	1:A:478:LEU:HD23	2.23	0.59
1:A:317:THR:HG22	1:A:330:ILE:HA	1.84	0.59
1:A:174:MET:CE	1:A:501:LYS:NZ	2.64	0.59
1:A:223:THR:HG22	2:A:820:HOH:O	2.03	0.59
1:A:389:THR:HG23	1:A:568:GLY:CA	2.32	0.59
1:A:143:GLN:O	1:A:263:THR:HB	2.03	0.58
1:A:476:THR:CG2	1:A:478:LEU:O	2.50	0.58
1:A:378:TYR:O	1:A:397:ARG:HA	2.04	0.58
1:A:424:VAL:CG2	1:A:429:VAL:HG22	2.34	0.58
1:A:308:VAL:HG12	1:A:313:ARG:HG3	1.85	0.58
1:A:85:ASN:HA	1:A:101:ILE:CG1	2.30	0.57
1:A:59:VAL:HG23	1:A:537:ALA:HB3	1.86	0.57
1:A:471:ASP:OD2	1:A:483:HIS:CD2	2.55	0.57
1:A:364:ALA:HB3	1:A:365:GLN:HE22	1.65	0.57
1:A:365:GLN:O	1:A:370:GLN:CG	2.53	0.56
1:A:319:MET:HE1	1:A:329:THR:OG1	2.04	0.56
1:A:310:GLN:HG2	1:A:313:ARG:NH1	2.20	0.56
1:A:122:ASN:HB2	1:A:123:PRO:CD	2.25	0.56
1:A:183:MET:HE2	1:A:208:TRP:CH2	2.41	0.56
1:A:53:PHE:CE1	1:A:59:VAL:CG1	2.89	0.56
1:A:230:THR:HB	1:A:232:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:PRO:HD2	1:A:576:SER:OG	2.07	0.55
1:A:361:ARG:NH2	1:A:370:GLN:HG3	2.21	0.55
1:A:361:ARG:CG	1:A:366:THR:HG21	2.36	0.55
1:A:93:ASN:ND2	1:A:225:THR:HB	2.16	0.55
1:A:388:THR:CG2	1:A:569:MET:H	2.20	0.55
1:A:377:ARG:HH21	1:A:397:ARG:HD2	1.72	0.55
1:A:299:GLY:C	1:A:301:THR:H	2.11	0.54
1:A:276:THR:C	1:A:577:GLN:HB3	2.26	0.54
1:A:174:MET:HE1	1:A:503:ALA:HA	1.88	0.54
1:A:361:ARG:NH2	1:A:366:THR:HG22	2.23	0.54
1:A:62:THR:HB	1:A:534:VAL:HG22	1.90	0.54
1:A:443:ASN:H	1:A:446:ASN:HD21	1.56	0.53
1:A:52:LYS:HG2	1:A:52:LYS:O	2.07	0.53
1:A:52:LYS:O	1:A:54:LEU:HD13	2.09	0.53
1:A:570:LYS:CD	1:A:572:VAL:HG23	2.38	0.53
1:A:281:THR:HG22	1:A:283:ARG:HB2	1.91	0.53
1:A:393:GLU:CA	1:A:393:GLU:OE1	2.56	0.52
1:A:174:MET:CE	1:A:501:LYS:HZ3	2.22	0.52
1:A:354:LYS:NZ	1:A:373:ASP:OD1	2.41	0.52
1:A:213:GLN:HG3	1:A:240:ASP:HB3	1.91	0.52
1:A:382:ARG:HG3	1:A:386:GLN:HG2	1.90	0.52
1:A:465:PRO:HD2	1:A:466:ASN:HD22	1.74	0.52
1:A:460:VAL:HG21	1:A:484:VAL:HA	1.91	0.52
1:A:158:THR:N	1:A:161:PRO:HA	2.23	0.52
1:A:485:ASN:H	1:A:485:ASN:ND2	2.03	0.52
1:A:483:HIS:HB3	1:A:485:ASN:ND2	2.25	0.52
1:A:339:SER:O	1:A:449:ASN:HA	2.10	0.52
1:A:154:SER:OG	1:A:164:VAL:HG13	2.09	0.51
1:A:322:THR:HG22	1:A:323:ASN:H	1.75	0.51
1:A:343:TYR:HE1	1:A:373:ASP:HB2	1.76	0.51
1:A:361:ARG:NH2	1:A:409:TYR:CD1	2.78	0.51
1:A:435:PRO:CB	1:A:439:LYS:O	2.57	0.51
1:A:299:GLY:O	1:A:301:THR:N	2.43	0.51
1:A:364:ALA:CB	1:A:365:GLN:NE2	2.71	0.51
1:A:58:TRP:CE2	1:A:538:LYS:HD2	2.45	0.51
1:A:245:THR:OG1	1:A:248:ASN:HB2	2.11	0.51
1:A:232:ILE:HB	1:A:234:HIS:CD2	2.46	0.51
1:A:122:ASN:CB	1:A:123:PRO:CD	2.88	0.50
1:A:319:MET:HE3	1:A:329:THR:OG1	2.11	0.50
1:A:361:ARG:HG3	1:A:362:GLY:N	2.26	0.50
1:A:431:LEU:C	1:A:433:THR:N	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:MET:HB3	1:A:184:PRO:HD2	1.94	0.50
1:A:145:ILE:O	1:A:260:GLU:HG2	2.11	0.50
1:A:470:TRP:HA	1:A:488:PHE:O	2.11	0.49
1:A:365:GLN:O	1:A:370:GLN:HB3	2.00	0.49
1:A:579:ALA:HB1	1:A:580:PRO:HD2	1.93	0.49
1:A:77:GLU:OE1	1:A:520:ARG:NH1	2.45	0.49
1:A:215:ASP:N	1:A:235:GLY:O	2.43	0.49
1:A:476:THR:O	1:A:479:LYS:HE2	2.12	0.49
1:A:183:MET:CE	1:A:208:TRP:CH2	2.96	0.49
1:A:158:THR:HB	1:A:162:THR:HG22	1.95	0.49
1:A:557:ASN:OD1	1:A:558:GLN:N	2.46	0.48
1:A:292:ASN:ND2	1:A:307:GLY:H	1.97	0.48
1:A:326:THR:H	1:A:329:THR:CG2	2.26	0.48
1:A:361:ARG:HE	1:A:366:THR:HG23	1.66	0.48
1:A:185:PHE:HA	1:A:497:GLN:NE2	2.28	0.48
1:A:95:ASN:O	1:A:98:LEU:HB2	2.13	0.47
1:A:365:GLN:C	1:A:370:GLN:HG2	2.35	0.47
1:A:409:TYR:CE2	1:A:411:GLU:HB2	2.49	0.47
1:A:411:GLU:N	1:A:411:GLU:OE1	2.47	0.47
1:A:126:TRP:O	1:A:130:VAL:HB	2.13	0.47
1:A:361:ARG:HH11	1:A:361:ARG:HG2	1.79	0.47
1:A:425:THR:O	1:A:428:ASN:N	2.48	0.47
1:A:43:GLY:HA3	1:A:146:PHE:CD2	2.50	0.47
1:A:137:HIS:O	1:A:535:PHE:HA	2.15	0.46
1:A:368:GLU:HA	2:A:793:HOH:O	2.15	0.46
1:A:571:ILE:HA	2:A:731:HOH:O	2.14	0.46
1:A:92:VAL:O	1:A:95:ASN:HB2	2.16	0.46
1:A:441:GLY:O	1:A:442:ILE:HD13	2.15	0.46
1:A:425:THR:O	1:A:426:ASN:C	2.53	0.46
1:A:158:THR:HG22	1:A:160:PRO:CD	2.39	0.46
1:A:183:MET:CE	1:A:208:TRP:HH2	2.29	0.46
1:A:80:ARG:HB2	1:A:106:VAL:HB	1.98	0.45
1:A:133:MET:SD	1:A:539:LEU:HD23	2.57	0.45
1:A:197:PHE:CD1	1:A:197:PHE:N	2.83	0.45
1:A:213:GLN:HG3	1:A:240:ASP:CB	2.47	0.45
1:A:468:GLN:HG2	1:A:486:ALA:HB2	1.99	0.45
1:A:183:MET:HE2	1:A:208:TRP:CZ3	2.53	0.44
1:A:370:GLN:OE1	1:A:409:TYR:HE1	2.00	0.44
1:A:122:ASN:CB	1:A:123:PRO:HD2	2.16	0.44
1:A:566:ILE:HD12	1:A:566:ILE:HA	1.56	0.44
1:A:432:PRO:HA	1:A:443:ASN:HD22	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:VAL:HG11	1:A:431:LEU:HD21	1.99	0.44
1:A:443:ASN:ND2	1:A:445:THR:H	2.15	0.44
1:A:266:PHE:CZ	1:A:493:ASN:C	2.84	0.44
1:A:222:HIS:CE1	1:A:224:GLY:O	2.71	0.44
1:A:548:ILE:HD12	1:A:548:ILE:HA	1.15	0.43
1:A:59:VAL:CG2	1:A:537:ALA:HB3	2.48	0.43
1:A:296:GLN:HA	1:A:296:GLN:OE1	2.11	0.43
1:A:365:GLN:CD	1:A:365:GLN:N	2.72	0.43
1:A:322:THR:CG2	1:A:324:TYR:H	2.29	0.43
1:A:326:THR:H	1:A:329:THR:HB	1.83	0.43
1:A:155:GLU:HA	1:A:163:LYS:HA	2.00	0.43
1:A:266:PHE:CZ	1:A:494:CYS:HA	2.54	0.43
1:A:485:ASN:HD22	1:A:485:ASN:N	2.04	0.43
1:A:361:ARG:CG	1:A:362:GLY:N	2.79	0.43
1:A:354:LYS:CE	1:A:355:THR:O	2.67	0.43
1:A:325:ILE:HA	1:A:329:THR:CG2	2.49	0.43
1:A:382:ARG:NH2	1:A:392:GLY:O	2.48	0.43
1:A:74:PRO:HD2	1:A:520:ARG:NH1	2.34	0.43
1:A:255:LEU:HB3	1:A:259:ASP:HB2	2.01	0.43
1:A:265:THR:HG21	1:A:267:PHE:CZ	2.54	0.43
1:A:536:LYS:HB2	1:A:536:LYS:HE3	1.41	0.43
1:A:174:MET:CG	1:A:503:ALA:HB2	2.47	0.43
1:A:183:MET:HE3	1:A:208:TRP:HH2	1.84	0.43
1:A:70:HIS:CD2	1:A:526:ASP:OD1	2.72	0.43
1:A:388:THR:HB	1:A:569:MET:O	2.17	0.42
1:A:397:ARG:HH11	1:A:397:ARG:HD3	1.46	0.42
1:A:266:PHE:CZ	1:A:494:CYS:CA	3.02	0.42
1:A:430:LEU:HA	1:A:430:LEU:HD12	1.95	0.42
1:A:325:ILE:HA	1:A:329:THR:HG22	2.01	0.42
1:A:126:TRP:NE1	1:A:130:VAL:HG21	2.35	0.42
1:A:232:ILE:HB	1:A:234:HIS:NE2	2.35	0.42
1:A:201:LYS:HG2	2:A:759:HOH:O	2.19	0.42
1:A:74:PRO:HD2	1:A:520:ARG:HH12	1.84	0.42
1:A:432:PRO:HA	1:A:443:ASN:ND2	2.35	0.42
1:A:133:MET:HB2	1:A:275:LEU:HD12	2.02	0.42
1:A:216:ARG:CZ	1:A:218:LEU:HB2	2.50	0.42
1:A:137:HIS:HA	2:A:761:HOH:O	2.20	0.42
1:A:464:TYR:HA	1:A:465:PRO:HA	1.86	0.42
1:A:277:HIS:O	1:A:580:PRO:HA	2.19	0.42
1:A:409:TYR:CD2	1:A:411:GLU:HB2	2.55	0.41
1:A:43:GLY:HA3	1:A:146:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:O	1:A:56:ASN:HB2	2.19	0.41
1:A:299:GLY:C	1:A:301:THR:N	2.74	0.41
1:A:361:ARG:CG	1:A:366:THR:CG2	2.98	0.41
1:A:471:ASP:O	1:A:489:VAL:HA	2.19	0.41
1:A:174:MET:HG2	1:A:503:ALA:HB2	2.03	0.41
1:A:53:PHE:HD1	1:A:59:VAL:CG1	2.26	0.41
1:A:163:LYS:HE2	1:A:165:TYR:OH	2.21	0.41
1:A:266:PHE:CE1	1:A:495:PRO:HD3	2.56	0.41
1:A:302:ASN:H	1:A:302:ASN:HD22	1.61	0.41
1:A:476:THR:HG23	1:A:478:LEU:O	2.19	0.41
1:A:580:PRO:HD3	2:A:803:HOH:O	2.20	0.41
1:A:415:ILE:HG12	1:A:444:TYR:CZ	2.56	0.41
1:A:116:ALA:HA	1:A:467:GLY:O	2.21	0.41
1:A:156:SER:CB	1:A:162:THR:HG23	2.22	0.40
1:A:326:THR:OG1	1:A:329:THR:HB	2.21	0.40
1:A:325:ILE:HD13	1:A:325:ILE:HG21	1.73	0.40
1:A:522:VAL:HB	2:A:824:HOH:O	2.22	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	A	546/548 (100%)	509 (93%)	30 (6%)	7 (1%)	15 53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
1	A	300	ALA
1	A	426	ASN
1	A	402	ALA

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Mol	Chain	Res	Type
1	A	87	MET
1	A	159	GLN
1	A	423	PRO

### 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	A	476/476 (100%)	409 (86%)	67 (14%)	4 19

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	47	ASN
1	A	49	THR
1	A	54	LEU
1	A	59	VAL
1	A	62	THR
1	A	75	GLU
1	A	89	LYS
1	A	96	MET
1	A	98	LEU
1	A	130	VAL
1	A	150	LEU
1	A	154	SER
1	A	158	THR
1	A	181	ASN
1	A	190	MET
1	A	206	THR
1	A	209	ARG
1	A	216	ARG
1	A	223	THR
1	A	228	THR
1	A	232	ILE
1	A	239	ASP

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Mol	Chain	Res	Type
1	A	255	LEU
1	A	263	THR
1	A	302	ASN
1	A	322	THR
1	A	329	THR
1	A	342	TYR
1	A	354	LYS
1	A	357	ILE
1	A	361	ARG
1	A	366	THR
1	A	369	ASN
1	A	370	GLN
1	A	386	GLN
1	A	387	LYS
1	A	388	THR
1	A	393	GLU
1	A	404	GLN
1	A	418	ILE
1	A	422	LEU
1	A	427	ASP
1	A	429	VAL
1	A	433	THR
1	A	439	LYS
1	A	444	TYR
1	A	448	PHE
1	A	473	GLU
1	A	476	THR
1	A	479	LYS
1	A	485	ASN
1	A	490	CYS
1	A	491	GLN
1	A	493	ASN
1	A	497	GLN
1	A	501	LYS
1	A	505	ASN
1	A	532	LYS
1	A	536	LYS
1	A	538	LYS
1	A	548	ILE
1	A	549	GLN
1	A	555	VAL
1	A	566	ILE

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Mol	Chain	Res	Type
1	A	581	ARG
1	A	582	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	93	ASN
1	A	104	GLN
1	A	159	GLN
1	A	181	ASN
1	A	234	HIS
1	A	292	ASN
1	A	302	ASN
1	A	309	GLN
1	A	350	GLN
1	A	365	GLN
1	A	384	HIS
1	A	386	GLN
1	A	419	ASN
1	A	443	ASN
1	A	446	ASN
1	A	459	ASN
1	A	466	ASN
1	A	468	GLN
1	A	483	HIS
1	A	485	ASN
1	A	491	GLN
1	A	493	ASN
1	A	497	GLN
1	A	505	ASN
1	A	560	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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.