



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:15 PM UTC

PDB ID : 1MSC / pdb_00001msc
Title : CRYSTAL STRUCTURE OF MS2 COAT PROTEIN DIMER
Authors : Ni, C.-Z.; Kodandapani, R.; Ely, K.R.
Deposited on : 1995-04-28
Resolution : 2.00 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

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

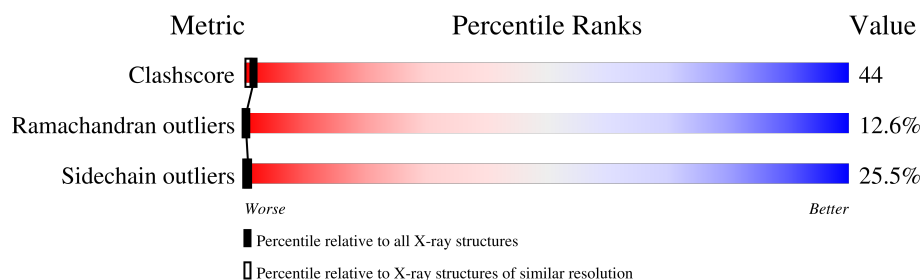
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 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	A	129	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1073 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 BACTERIOPHAGE MS2 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			962	601	167	190	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ARG	TRP	conflict	UNP P03612

- Molecule 2 is water.

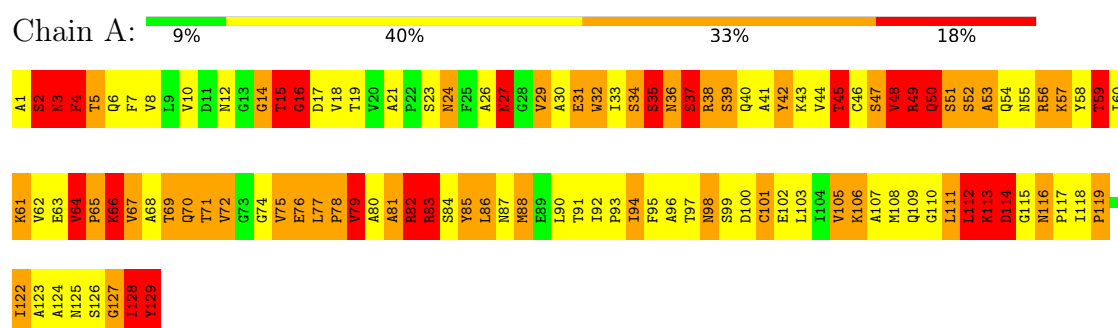
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	111	Total	O	0	0
			111	111		

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: BACTERIOPHAGE MS2 COAT PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	76.20Å 55.70Å 28.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	90.0 (8.00-2.00)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1073	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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	1.63	13/977 (1.3%)	3.67	206/1328 (15.5%)

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
1	A	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ILE	CA-CB	9.51	1.65	1.54
1	A	59	THR	CA-CB	8.59	1.65	1.53
1	A	64	VAL	N-CA	7.99	1.54	1.46
1	A	119	PRO	CA-C	7.55	1.63	1.52
1	A	31	GLU	C-O	7.18	1.32	1.23
1	A	45	THR	CB-OG1	6.13	1.53	1.43
1	A	119	PRO	N-CA	-5.82	1.40	1.47
1	A	7	PHE	C-O	5.79	1.31	1.23
1	A	101	CYS	C-N	-5.66	1.26	1.33
1	A	92	ILE	N-CA	5.43	1.53	1.46
1	A	58	TYR	CA-C	5.26	1.59	1.52
1	A	7	PHE	CA-C	5.13	1.59	1.52
1	A	57	LYS	CA-C	-5.02	1.47	1.52

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	VAL	CB-CA-C	18.39	130.05	110.37
1	A	53	ALA	CA-C-N	15.91	151.92	121.54
1	A	53	ALA	C-N-CA	15.91	151.92	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ILE	CB-CG1-CD1	15.70	146.77	113.80
1	A	36	ASN	CA-C-O	15.46	136.41	120.95
1	A	98	ASN	CA-CB-CG	-14.95	97.66	112.60
1	A	53	ALA	CA-C-O	14.88	141.80	120.51
1	A	37	SER	N-CA-C	14.14	130.49	113.23
1	A	106	LYS	CA-C-O	-13.69	106.60	120.70
1	A	53	ALA	O-C-N	-13.64	104.45	122.59
1	A	59	THR	CB-CA-C	12.65	131.41	110.79
1	A	125	ASN	OD1-CG-ND2	-11.89	110.71	122.60
1	A	125	ASN	CB-CG-ND2	11.68	133.91	116.40
1	A	94	ILE	CB-CA-C	11.36	126.92	112.04
1	A	82	ARG	CA-C-O	11.31	136.68	120.51
1	A	122	ILE	O-C-N	10.96	132.66	121.91
1	A	106	LYS	O-C-N	10.71	133.66	122.09
1	A	38	ARG	CD-NE-CZ	10.63	139.28	124.40
1	A	7	PHE	CA-CB-CG	10.47	124.27	113.80
1	A	49	ARG	CA-C-O	10.46	132.39	120.89
1	A	50	GLN	CB-CG-CD	10.22	129.97	112.60
1	A	35	SER	CA-C-N	10.15	137.40	121.56
1	A	35	SER	C-N-CA	10.15	137.40	121.56
1	A	5	THR	O-C-N	10.07	135.65	122.96
1	A	7	PHE	O-C-N	9.98	135.53	122.96
1	A	36	ASN	N-CA-C	9.79	124.71	110.42
1	A	12	ASN	OD1-CG-ND2	-9.73	112.87	122.60
1	A	4	PHE	CA-CB-CG	-9.68	104.12	113.80
1	A	67	VAL	CA-C-N	9.64	137.02	122.65
1	A	67	VAL	C-N-CA	9.64	137.02	122.65
1	A	35	SER	CA-C-O	9.53	134.13	120.51
1	A	18	VAL	CA-C-O	-9.33	110.59	120.57
1	A	36	ASN	CA-C-N	9.33	137.74	123.47
1	A	36	ASN	C-N-CA	9.33	137.74	123.47
1	A	49	ARG	NE-CZ-NH1	-9.26	112.24	121.50
1	A	45	THR	CA-CB-CG2	9.11	125.99	110.50
1	A	42	TYR	N-CA-CB	9.07	124.92	110.23
1	A	5	THR	CA-CB-CG2	9.02	125.83	110.50
1	A	99	SER	CB-CA-C	8.83	126.79	110.11
1	A	42	TYR	N-CA-C	-8.70	95.34	109.96
1	A	45	THR	CA-CB-OG1	-8.64	96.63	109.60
1	A	51	SER	CB-CA-C	8.64	127.62	110.42
1	A	83	ARG	CD-NE-CZ	8.53	136.35	124.40
1	A	37	SER	N-CA-CB	-8.49	98.96	112.63
1	A	67	VAL	CA-C-O	8.46	131.36	120.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	SER	N-CA-C	-8.38	95.22	108.63
1	A	62	VAL	CA-C-O	-8.31	111.55	120.36
1	A	19	THR	CA-C-O	-8.28	111.75	120.70
1	A	12	ASN	CB-CG-ND2	7.97	128.35	116.40
1	A	112	LEU	N-CA-C	7.95	123.95	113.30
1	A	52	SER	N-CA-CB	7.86	122.31	109.88
1	A	119	PRO	O-C-N	7.85	131.65	122.23
1	A	99	SER	N-CA-C	-7.78	101.64	112.45
1	A	114	ASP	CA-C-O	-7.75	109.43	120.51
1	A	91	THR	CA-C-O	-7.70	111.99	120.38
1	A	44	VAL	CA-CB-CG2	7.64	123.40	110.40
1	A	55	ASN	CA-C-N	7.61	135.12	122.87
1	A	55	ASN	C-N-CA	7.61	135.12	122.87
1	A	111	LEU	CA-C-O	7.57	128.68	120.20
1	A	55	ASN	CA-C-O	7.56	130.28	121.44
1	A	24	ASN	CA-C-O	7.55	129.49	121.33
1	A	94	ILE	N-CA-CB	-7.53	101.06	110.47
1	A	64	VAL	N-CA-CB	-7.40	103.70	111.61
1	A	29	VAL	O-C-N	7.37	131.90	122.77
1	A	5	THR	CA-C-O	-7.28	113.36	121.51
1	A	48	VAL	CA-CB-CG2	7.27	122.76	110.40
1	A	2	SER	CA-C-O	-7.22	110.18	120.51
1	A	102	GLU	O-C-N	7.21	129.88	122.09
1	A	32	TRP	CA-C-O	-7.21	113.01	121.16
1	A	110	GLY	CA-C-O	-7.19	112.85	120.90
1	A	66	LYS	O-C-N	-7.12	113.12	122.59
1	A	17	ASP	CA-C-O	-7.10	114.03	121.55
1	A	128	ILE	CB-CG1-CD1	7.09	128.70	113.80
1	A	113	LYS	CA-CB-CG	7.03	128.17	114.10
1	A	18	VAL	CA-CB-CG2	-7.00	98.49	110.40
1	A	88	MET	CA-CB-CG	6.98	128.06	114.10
1	A	6	GLN	CA-C-O	-6.97	113.36	121.16
1	A	4	PHE	N-CA-C	-6.96	101.77	111.52
1	A	39	SER	N-CA-C	-6.95	104.38	112.86
1	A	59	THR	CA-C-O	6.95	127.89	120.46
1	A	30	ALA	CB-CA-C	-6.93	98.44	109.80
1	A	63	GLU	CA-C-O	-6.93	112.89	120.30
1	A	93	PRO	N-CA-CB	6.92	109.77	103.34
1	A	82	ARG	CA-C-N	6.87	133.98	121.06
1	A	82	ARG	C-N-CA	6.87	133.98	121.06
1	A	93	PRO	CA-C-N	6.80	130.12	120.53
1	A	93	PRO	C-N-CA	6.80	130.12	120.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ASN	O-C-N	-6.80	115.50	123.11
1	A	109	GLN	OE1-CD-NE2	-6.79	115.81	122.60
1	A	51	SER	CA-C-O	-6.78	110.81	120.51
1	A	39	SER	CA-C-O	6.76	128.30	120.32
1	A	14	GLY	CA-C-O	-6.76	115.00	121.49
1	A	18	VAL	O-C-N	6.76	130.53	123.03
1	A	96	ALA	CB-CA-C	6.72	119.92	109.84
1	A	91	THR	O-C-N	6.71	131.21	123.29
1	A	119	PRO	N-CA-CB	6.70	110.70	103.33
1	A	109	GLN	CA-C-N	6.62	127.16	119.94
1	A	109	GLN	C-N-CA	6.62	127.16	119.94
1	A	82	ARG	CB-CA-C	6.62	123.59	110.42
1	A	95	PHE	CA-CB-CG	6.62	120.42	113.80
1	A	58	TYR	CB-CG-CD2	-6.60	110.90	120.80
1	A	56	ARG	CD-NE-CZ	-6.59	115.17	124.40
1	A	111	LEU	CA-C-N	6.54	132.62	122.49
1	A	111	LEU	C-N-CA	6.54	132.62	122.49
1	A	21	ALA	N-CA-CB	-6.53	98.01	110.42
1	A	108	MET	CA-C-O	6.49	127.64	120.82
1	A	107	ALA	N-CA-C	-6.48	104.21	111.28
1	A	30	ALA	N-CA-CB	6.46	120.81	110.16
1	A	34	SER	CA-C-O	-6.45	112.88	121.46
1	A	56	ARG	CA-C-O	-6.36	113.97	121.16
1	A	92	ILE	CA-CB-CG2	6.36	121.31	110.50
1	A	110	GLY	CA-C-N	6.34	129.64	120.38
1	A	110	GLY	C-N-CA	6.34	129.64	120.38
1	A	64	VAL	CA-C-N	6.28	125.90	119.56
1	A	64	VAL	C-N-CA	6.28	125.90	119.56
1	A	101	CYS	CA-C-N	6.26	128.96	120.44
1	A	101	CYS	C-N-CA	6.26	128.96	120.44
1	A	31	GLU	CG-CD-OE1	-6.22	104.10	118.40
1	A	90	LEU	CA-C-N	-6.20	114.44	123.00
1	A	90	LEU	C-N-CA	-6.20	114.44	123.00
1	A	18	VAL	N-CA-CB	6.18	118.41	110.99
1	A	122	ILE	CA-C-N	-6.15	111.43	120.28
1	A	122	ILE	C-N-CA	-6.15	111.43	120.28
1	A	114	ASP	CB-CG-OD2	6.14	132.53	118.40
1	A	87	ASN	CA-C-N	-6.10	114.08	122.93
1	A	87	ASN	C-N-CA	-6.10	114.08	122.93
1	A	108	MET	N-CA-C	6.10	117.59	111.07
1	A	27	ASN	CA-CB-CG	6.09	118.69	112.60
1	A	31	GLU	CA-CB-CG	5.99	126.08	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	GLN	CA-C-N	5.99	131.99	122.59
1	A	54	GLN	C-N-CA	5.99	131.99	122.59
1	A	116	ASN	CA-CB-CG	5.96	118.56	112.60
1	A	31	GLU	N-CA-CB	-5.93	100.26	111.00
1	A	46	CYS	O-C-N	5.93	131.46	123.34
1	A	79	VAL	N-CA-CB	5.93	121.01	111.23
1	A	16	GLY	CA-C-N	5.92	129.70	120.75
1	A	16	GLY	C-N-CA	5.92	129.70	120.75
1	A	119	PRO	CA-C-O	-5.92	110.63	119.86
1	A	8	VAL	O-C-N	5.86	130.04	122.77
1	A	60	ILE	N-CA-CB	-5.85	103.29	111.25
1	A	46	CYS	CA-C-O	-5.85	112.09	120.11
1	A	47	SER	CA-C-O	5.81	128.24	121.44
1	A	49	ARG	NH1-CZ-NH2	5.80	126.83	119.30
1	A	62	VAL	CA-CB-CG2	5.78	120.23	110.40
1	A	65	PRO	CB-CA-C	-5.77	103.26	111.68
1	A	129	TYR	CB-CA-C	5.74	121.01	110.10
1	A	94	ILE	CA-CB-CG2	5.72	120.23	110.50
1	A	87	ASN	CB-CA-C	5.66	119.89	111.17
1	A	14	GLY	O-C-N	5.64	129.57	123.87
1	A	8	VAL	CA-C-N	-5.63	112.78	120.44
1	A	8	VAL	C-N-CA	-5.63	112.78	120.44
1	A	66	LYS	CA-C-N	5.63	132.10	121.97
1	A	66	LYS	C-N-CA	5.63	132.10	121.97
1	A	98	ASN	O-C-N	5.62	130.21	122.46
1	A	114	ASP	CA-CB-CG	-5.62	106.98	112.60
1	A	59	THR	O-C-N	-5.60	116.07	123.13
1	A	4	PHE	N-CA-CB	5.60	120.42	111.91
1	A	101	CYS	CA-CB-SG	-5.58	101.56	114.40
1	A	31	GLU	CG-CD-OE2	5.57	131.20	118.40
1	A	100	ASP	CA-C-O	5.57	126.32	120.42
1	A	50	GLN	N-CA-C	-5.56	100.74	109.25
1	A	93	PRO	O-C-N	-5.55	116.43	123.10
1	A	62	VAL	CA-C-N	-5.55	115.18	123.00
1	A	62	VAL	C-N-CA	-5.55	115.18	123.00
1	A	126	SER	N-CA-C	5.54	118.72	109.96
1	A	71	THR	OG1-CB-CG2	5.54	120.38	109.30
1	A	5	THR	N-CA-CB	5.54	120.59	111.62
1	A	17	ASP	CA-C-N	-5.52	115.98	122.93
1	A	17	ASP	C-N-CA	-5.52	115.98	122.93
1	A	97	THR	CA-C-O	-5.52	115.70	121.99
1	A	29	VAL	CA-C-O	-5.50	114.04	120.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	VAL	CB-CA-C	-5.50	104.27	111.25
1	A	61	LYS	CB-CG-CD	-5.49	98.69	111.30
1	A	52	SER	O-C-N	5.48	129.93	122.48
1	A	55	ASN	CB-CG-ND2	-5.43	108.26	116.40
1	A	6	GLN	CB-CG-CD	5.43	121.83	112.60
1	A	17	ASP	CA-CB-CG	-5.41	107.19	112.60
1	A	122	ILE	CB-CA-C	-5.41	105.05	111.97
1	A	35	SER	CA-CB-OG	5.41	121.91	111.10
1	A	124	ALA	N-CA-CB	-5.40	102.18	110.44
1	A	58	TYR	CB-CG-CD1	5.40	128.90	120.80
1	A	55	ASN	CB-CA-C	-5.39	98.74	109.79
1	A	27	ASN	N-CA-C	5.38	122.26	110.80
1	A	3	ASN	N-CA-C	5.36	122.21	110.80
1	A	49	ARG	CD-NE-CZ	-5.32	116.95	124.40
1	A	127	GLY	O-C-N	-5.32	116.42	122.91
1	A	24	ASN	N-CA-CB	-5.30	102.80	111.66
1	A	114	ASP	N-CA-C	5.30	122.08	110.80
1	A	17	ASP	N-CA-CB	-5.28	102.27	110.04
1	A	112	LEU	CA-C-N	5.26	128.18	120.71
1	A	112	LEU	C-N-CA	5.26	128.18	120.71
1	A	48	VAL	CA-CB-CG1	-5.26	101.46	110.40
1	A	49	ARG	CA-C-N	5.25	129.34	121.72
1	A	49	ARG	C-N-CA	5.25	129.34	121.72
1	A	32	TRP	CA-CB-CG	5.24	123.56	113.60
1	A	62	VAL	O-C-N	5.23	128.85	123.20
1	A	103	LEU	N-CA-CB	5.22	117.72	109.94
1	A	59	THR	CA-CB-OG1	-5.22	101.77	109.60
1	A	109	GLN	CG-CD-NE2	5.21	124.21	116.40
1	A	64	VAL	N-CA-C	-5.20	102.22	107.89
1	A	29	VAL	CA-CB-CG1	-5.16	101.63	110.40
1	A	55	ASN	OD1-CG-ND2	5.10	127.70	122.60
1	A	66	LYS	CB-CA-C	5.06	120.48	110.42
1	A	105	VAL	CA-CB-CG1	5.04	118.96	110.40
1	A	38	ARG	NE-CZ-NH1	5.03	126.53	121.50
1	A	85	TYR	CA-CB-CG	5.03	122.95	113.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	VAL	Mainchain
1	A	49	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	56	ARG	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	A	962	0	966	84	27
2	A	111	0	0	27	25
All	All	1073	0	966	84	29

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 44.

All (84) 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:3:ASN:ND2	1:A:4:PHE:H	1.62	0.97
1:A:66:LYS:C	1:A:68:ALA:H	1.69	0.93
1:A:70:GLN:HB2	1:A:78:PRO:HG3	1.55	0.87
1:A:3:ASN:HD22	1:A:4:PHE:H	1.16	0.87
1:A:40:GLN:HG3	2:A:306:HOH:O	1.73	0.86
1:A:114:ASP:O	2:A:309:HOH:O	1.98	0.80
1:A:45:THR:HG22	2:A:253:HOH:O	1.81	0.80
1:A:66:LYS:HB3	1:A:68:ALA:HB3	1.64	0.79
1:A:69:THR:HG21	1:A:81:ALA:HA	1.66	0.78
1:A:112:LEU:HD21	2:A:291:HOH:O	1.84	0.76
1:A:80:ALA:O	1:A:82:ARG:N	2.20	0.75
1:A:122:ILE:HD12	2:A:293:HOH:O	1.85	0.75
1:A:36:ASN:HB2	2:A:284:HOH:O	1.91	0.71
1:A:3:ASN:HD22	1:A:4:PHE:N	1.87	0.70
1:A:81:ALA:HB3	1:A:83:ARG:HG3	1.73	0.70
1:A:86:LEU:HD11	1:A:88:MET:HE2	1.73	0.69
1:A:69:THR:HG22	1:A:78:PRO:HB3	1.72	0.69
1:A:71:THR:HG23	2:A:329:HOH:O	1.92	0.68
1:A:34:SER:O	1:A:36:ASN:N	2.28	0.66
1:A:69:THR:CG2	1:A:78:PRO:HB3	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASN:HD21	1:A:26:ALA:HB2	1.61	0.65
1:A:70:GLN:NE2	2:A:329:HOH:O	2.29	0.65
1:A:27:ASN:C	1:A:29:VAL:H	2.06	0.64
1:A:34:SER:O	1:A:36:ASN:HB3	1.98	0.64
1:A:40:GLN:O	1:A:65:PRO:HB3	1.99	0.63
1:A:64:VAL:HG13	1:A:84:SER:HB2	1.81	0.63
1:A:3:ASN:ND2	1:A:32:TRP:HZ2	1.96	0.62
1:A:77:LEU:H	1:A:77:LEU:HD22	1.66	0.59
1:A:76:GLU:O	1:A:78:PRO:HD3	2.03	0.58
1:A:24:ASN:ND2	1:A:26:ALA:HB2	2.18	0.58
1:A:45:THR:HB	1:A:61:LYS:HB2	1.84	0.58
1:A:85:TYR:HB2	2:A:256:HOH:O	2.02	0.58
1:A:50:GLN:HG2	2:A:202:HOH:O	2.03	0.58
1:A:118:ILE:HG22	2:A:293:HOH:O	2.02	0.58
1:A:118:ILE:HG21	2:A:343:HOH:O	2.03	0.57
1:A:113:LYS:HE3	1:A:116:ASN:HD21	1.70	0.57
1:A:66:LYS:C	1:A:68:ALA:N	2.50	0.56
1:A:38:ARG:C	1:A:40:GLN:N	2.64	0.55
1:A:3:ASN:ND2	1:A:4:PHE:N	2.44	0.55
1:A:37:SER:H	1:A:41:ALA:HB2	1.71	0.55
1:A:66:LYS:O	1:A:68:ALA:N	2.40	0.55
1:A:35:SER:HB3	2:A:306:HOH:O	2.07	0.54
1:A:65:PRO:HA	1:A:83:ARG:NH1	2.22	0.54
1:A:69:THR:CG2	1:A:81:ALA:HA	2.37	0.54
1:A:111:LEU:HD22	2:A:287:HOH:O	2.07	0.54
1:A:48:VAL:HG22	2:A:279:HOH:O	2.07	0.54
1:A:52:SER:HB3	2:A:320:HOH:O	2.07	0.54
1:A:66:LYS:CB	1:A:68:ALA:HB3	2.36	0.53
1:A:1:ALA:HB2	2:A:225:HOH:O	2.09	0.52
1:A:3:ASN:HD21	1:A:32:TRP:HZ2	1.56	0.52
1:A:50:GLN:CD	1:A:50:GLN:H	2.16	0.52
1:A:119:PRO:HA	2:A:293:HOH:O	2.10	0.52
1:A:1:ALA:HB3	2:A:231:HOH:O	2.09	0.51
1:A:69:THR:O	1:A:70:GLN:HB3	2.10	0.51
1:A:115:GLY:O	2:A:316:HOH:O	2.19	0.50
1:A:38:ARG:C	1:A:40:GLN:H	2.16	0.50
1:A:38:ARG:HB2	2:A:295:HOH:O	2.11	0.49
1:A:78:PRO:O	1:A:79:VAL:HG13	2.11	0.49
1:A:45:THR:HG21	1:A:61:LYS:HD2	1.94	0.49
1:A:27:ASN:C	1:A:29:VAL:N	2.69	0.48
1:A:37:SER:N	1:A:41:ALA:HB2	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:NH1	2:A:295:HOH:O	2.40	0.48
1:A:86:LEU:CD1	1:A:88:MET:HE2	2.41	0.48
1:A:16:GLY:N	2:A:233:HOH:O	2.46	0.47
1:A:23:SER:HB3	1:A:33:ILE:HG12	1.97	0.47
1:A:49:ARG:O	1:A:57:LYS:N	2.45	0.47
1:A:47:SER:OG	1:A:59:THR:HG23	2.15	0.47
1:A:76:GLU:HB3	1:A:77:LEU:HD13	1.97	0.47
1:A:74:GLY:O	1:A:75:VAL:C	2.57	0.47
1:A:14:GLY:O	1:A:15:THR:C	2.57	0.46
1:A:14:GLY:O	1:A:16:GLY:N	2.49	0.46
1:A:128:ILE:O	1:A:129:TYR:CB	2.64	0.46
1:A:98:ASN:HA	1:A:101:CYS:HB2	1.98	0.46
1:A:98:ASN:HA	1:A:98:ASN:HD22	1.62	0.45
1:A:51:SER:O	1:A:53:ALA:N	2.49	0.44
1:A:64:VAL:O	1:A:83:ARG:HB3	2.18	0.43
1:A:40:GLN:HG2	2:A:303:HOH:O	2.16	0.43
1:A:40:GLN:HB3	1:A:41:ALA:H	1.53	0.43
1:A:111:LEU:HG	2:A:343:HOH:O	2.20	0.42
1:A:66:LYS:HE3	1:A:82:ARG:O	2.19	0.41
1:A:66:LYS:HB3	1:A:68:ALA:CB	2.41	0.41
1:A:70:GLN:HB3	2:A:329:HOH:O	2.21	0.41
1:A:2:SER:O	1:A:3:ASN:HB3	2.21	0.41
1:A:16:GLY:HA3	2:A:233:HOH:O	2.22	0.40

All (29) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:333:HOH:O	2:A:333:HOH:O[2_665]	1.16	1.04
1:A:3:ASN:CB	2:A:242:HOH:O[2_665]	1.25	0.95
1:A:123:ALA:C	2:A:301:HOH:O[2_665]	1.32	0.88
1:A:86:LEU:CG	2:A:285:HOH:O[2_665]	1.37	0.83
1:A:123:ALA:O	2:A:301:HOH:O[2_665]	1.39	0.81
1:A:82:ARG:NH2	2:A:288:HOH:O[3_546]	1.41	0.79
1:A:3:ASN:CA	2:A:242:HOH:O[2_665]	1.47	0.73
1:A:4:PHE:N	2:A:242:HOH:O[2_665]	1.53	0.67
1:A:2:SER:OG	1:A:127:GLY:O[2_665]	1.54	0.66
1:A:5:THR:OG1	2:A:308:HOH:O[2_665]	1.57	0.63
1:A:3:ASN:C	2:A:242:HOH:O[2_665]	1.58	0.62
1:A:86:LEU:CD2	2:A:285:HOH:O[2_665]	1.66	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:THR:CA	2:A:308:HOH:O[2_665]	1.72	0.48
1:A:3:ASN:CG	2:A:242:HOH:O[2_665]	1.75	0.45
1:A:5:THR:O	2:A:308:HOH:O[2_665]	1.80	0.40
1:A:5:THR:C	2:A:308:HOH:O[2_665]	1.81	0.39
1:A:3:ASN:ND2	2:A:242:HOH:O[2_665]	1.89	0.31
1:A:10:VAL:CG1	1:A:106:LYS:NZ[2_665]	1.90	0.30
1:A:5:THR:N	2:A:308:HOH:O[2_665]	1.91	0.29
1:A:3:ASN:CG	1:A:117:PRO:CB[2_665]	1.94	0.26
1:A:123:ALA:CA	2:A:301:HOH:O[2_665]	1.98	0.22
2:A:206:HOH:O	2:A:307:HOH:O[2_665]	2.06	0.14
1:A:82:ARG:CZ	2:A:288:HOH:O[3_546]	2.08	0.12
1:A:5:THR:CB	2:A:308:HOH:O[2_665]	2.09	0.11
1:A:123:ALA:CB	2:A:301:HOH:O[2_665]	2.09	0.11
1:A:85:TYR:CD2	2:A:340:HOH:O[1_554]	2.13	0.07
1:A:114:ASP:OD1	2:A:312:HOH:O[2_665]	2.13	0.07
1:A:86:LEU:CD1	2:A:285:HOH:O[2_665]	2.14	0.06
1:A:75:VAL:N	1:A:127:GLY:N[3_546]	2.19	0.01

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	A	127/129 (98%)	96 (76%)	15 (12%)	16 (13%)	0 0

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	75	VAL
1	A	79	VAL
1	A	81	ALA
1	A	82	ARG
1	A	2	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	15	THR
1	A	16	GLY
1	A	35	SER
1	A	69	THR
1	A	72	VAL
1	A	76	GLU
1	A	27	ASN
1	A	66	LYS
1	A	78	PRO
1	A	67	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	106/106 (100%)	79 (74%)	27 (26%)	0 0

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	15	THR
1	A	31	GLU
1	A	35	SER
1	A	37	SER
1	A	39	SER
1	A	42	TYR
1	A	43	LYS
1	A	45	THR
1	A	48	VAL
1	A	49	ARG
1	A	50	GLN
1	A	59	THR
1	A	64	VAL
1	A	66	LYS
1	A	70	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	72	VAL
1	A	77	LEU
1	A	82	ARG
1	A	83	ARG
1	A	86	LEU
1	A	94	ILE
1	A	112	LEU
1	A	113	LYS
1	A	114	ASP
1	A	128	ILE
1	A	129	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	24	ASN
1	A	27	ASN
1	A	50	GLN
1	A	55	ASN
1	A	98	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.