



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:47 AM GMT

PDB ID : 2BPA  
Title : ATOMIC STRUCTURE OF SINGLE-STRANDED DNA BACTERIO-  
PHAGE PHIX174 AND ITS FUNCTIONAL IMPLICATIONS  
Authors : McKenna, R.; Xia, D.; Willingmann, P.; Ilag, L.L.; Krishnaswamy, S.; Ross-  
mann, M.G.; Olson, N.H.; Baker, T.S.; Incardona, N.L.  
Deposited on : 1991-12-03  
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.

---

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

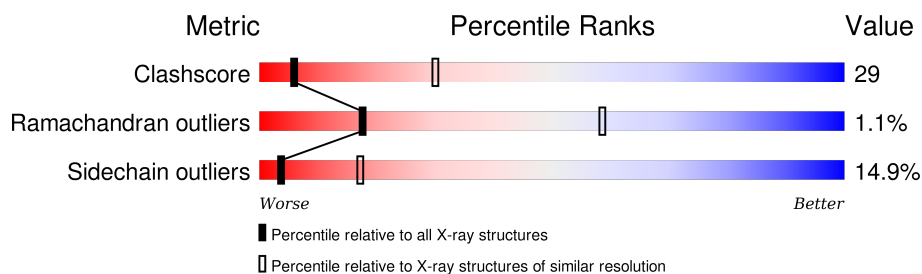
# 1 Overall quality at a glance

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	5	
2	1	426	
3	2	175	
4	3	37	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5298 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 DNA chain called DNA (5'-D(\*AP\*AP\*AP\*AP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	5	Total	C	N	O	P	0	0	1
			83	39	18	22	4			

- Molecule 2 is a protein called PROTEIN (SUBUNIT OF BACTERIOPHAGE PHIX174).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	426	Total	C	N	O	S	0	0	0
			3415	2173	590	638	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	216	ARG	HIS	CONFLICT	UNP P03641

- Molecule 3 is a protein called PROTEIN (SUBUNIT OF BACTERIOPHAGE PHIX174).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	175	Total	C	N	O	S	0	0	0
			1339	856	221	254	8			

- Molecule 4 is a protein called PROTEIN (SUBUNIT OF BACTERIOPHAGE PHIX174).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	3	36	Total	C	N	O	0	0	0
			283	177	64	42			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1	129	Total	O	0	0
			129	129		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2	41	Total 41	O 41	0	0
5	3	6	Total 6	O 6	0	0
5	A	2	Total 2	O 2	0	0

### 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.

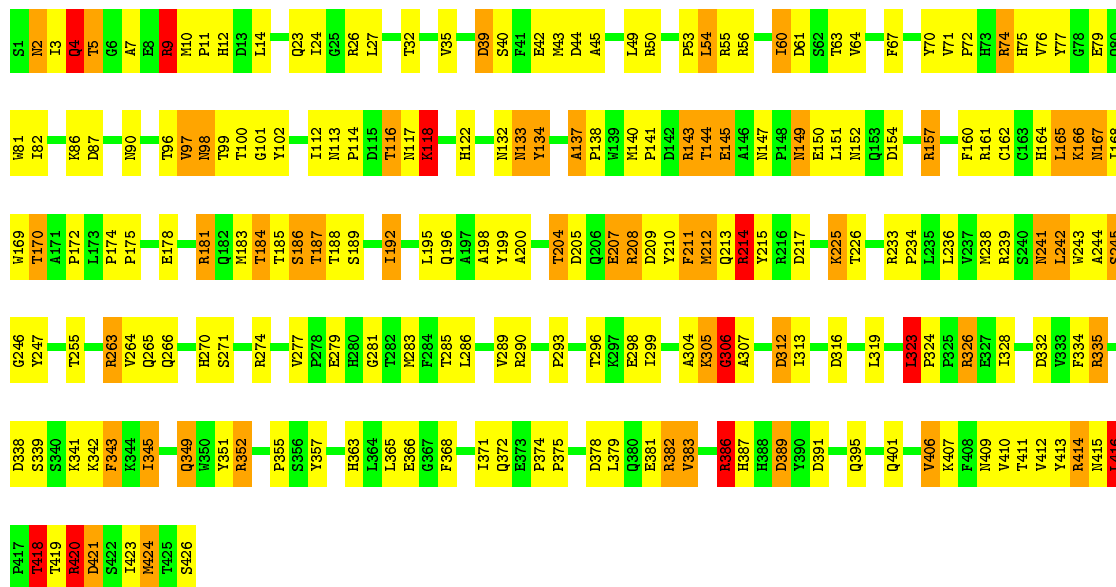
- Molecule 1: DNA (5'-D(\*AP\*AP\*AP\*AP\*C)-3')

Chain A: 



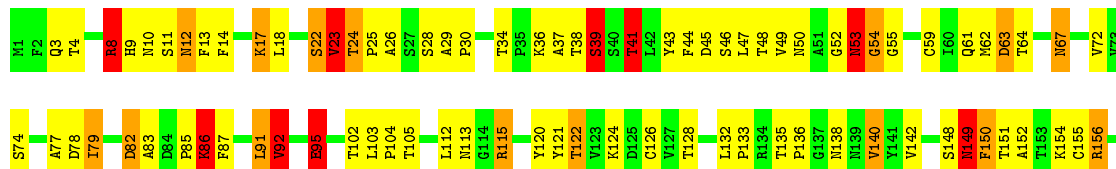
- Molecule 2: PROTEIN (SUBUNIT OF BACTERIOPHAGE PHIX174)

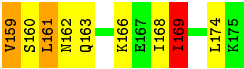
Chain 1: 



- Molecule 3: PROTEIN (SUBUNIT OF BACTERIOPHAGE PHIX174)

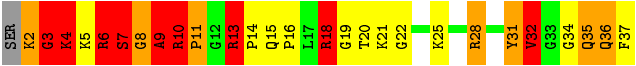
Chain 2: 





● Molecule 4: PROTEIN (SUBUNIT OF BACTERIOPHAGE PHIX174)

Chain 3: 24% 30% 19% 24% .



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	305.58Å 360.78Å 299.46Å 90.00° 92.89° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.209 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5298	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.74	0/93	1.80	2/142 (1.4%)
2	1	1.39	3/3511 (0.1%)	2.17	125/4779 (2.6%)
3	2	1.38	3/1371 (0.2%)	1.95	31/1872 (1.7%)
4	3	2.24	11/289 (3.8%)	2.57	24/380 (6.3%)
All	All	1.45	17/5264 (0.3%)	2.13	182/7173 (2.5%)

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
2	1	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	19	GLY	N-CA	7.39	1.57	1.46
4	3	8	GLY	N-CA	7.07	1.56	1.46
2	1	178	GLU	CD-OE2	-6.82	1.18	1.25
4	3	13	ARG	CZ-NH2	6.68	1.41	1.33
4	3	18	ARG	C-O	6.49	1.35	1.23
4	3	13	ARG	N-CA	6.16	1.58	1.46
4	3	10	ARG	CD-NE	5.67	1.56	1.46
4	3	10	ARG	CZ-NH2	5.64	1.40	1.33
2	1	245	SER	CB-OG	5.60	1.49	1.42
2	1	366	GLU	CD-OE2	5.59	1.31	1.25
4	3	18	ARG	CZ-NH2	5.56	1.40	1.33
3	2	54	GLY	N-CA	5.54	1.54	1.46
3	2	41	THR	CB-OG1	5.31	1.53	1.43
4	3	7	SER	CA-CB	5.20	1.60	1.52
4	3	11	PRO	C-O	5.20	1.33	1.23
3	2	8	ARG	CZ-NH1	5.17	1.39	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	4	LYS	CA-CB	5.07	1.65	1.53

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	214	ARG	NE-CZ-NH2	27.10	133.85	120.30
2	1	208	ARG	NE-CZ-NH2	24.34	132.47	120.30
2	1	56	ARG	NE-CZ-NH2	-24.21	108.20	120.30
2	1	352	ARG	NE-CZ-NH1	22.71	131.65	120.30
2	1	9	ARG	NE-CZ-NH2	-21.64	109.48	120.30
2	1	143	ARG	NE-CZ-NH1	-17.52	111.54	120.30
2	1	116	THR	CA-C-N	12.97	145.73	117.20
2	1	416	LEU	CB-CA-C	12.55	134.05	110.20
3	2	8	ARG	NE-CZ-NH2	-12.48	114.06	120.30
2	1	56	ARG	NH1-CZ-NH2	12.43	133.07	119.40
1	A	1	DA	P-O3'-C3'	12.07	134.19	119.70
2	1	352	ARG	NE-CZ-NH2	-12.04	114.28	120.30
2	1	414	ARG	NE-CZ-NH2	-12.01	114.29	120.30
2	1	214	ARG	NH1-CZ-NH2	-11.69	106.54	119.40
2	1	382	ARG	NE-CZ-NH1	-11.24	114.68	120.30
2	1	161	ARG	NE-CZ-NH1	-10.72	114.94	120.30
3	2	8	ARG	CD-NE-CZ	-10.68	108.65	123.60
2	1	144	THR	N-CA-CB	-10.52	90.31	110.30
2	1	192	ILE	CA-CB-CG2	9.79	130.48	110.90
2	1	74	ARG	NE-CZ-NH2	9.59	125.09	120.30
2	1	242	LEU	CA-CB-CG	9.59	137.35	115.30
2	1	55	ARG	NE-CZ-NH2	9.43	125.01	120.30
2	1	44	ASP	CB-CG-OD1	-9.39	109.85	118.30
2	1	209	ASP	CB-CG-OD2	9.39	126.75	118.30
2	1	378	ASP	CB-CA-C	9.28	128.97	110.40
4	3	6	ARG	NE-CZ-NH1	9.28	124.94	120.30
2	1	420	ARG	NE-CZ-NH1	-9.10	115.75	120.30
2	1	116	THR	CA-C-O	-8.90	101.42	120.10
2	1	39	ASP	CA-CB-CG	8.61	132.34	113.40
2	1	181	ARG	NE-CZ-NH1	8.48	124.54	120.30
2	1	208	ARG	NH1-CZ-NH2	-8.46	110.09	119.40
2	1	181	ARG	NE-CZ-NH2	-8.42	116.09	120.30
4	3	7	SER	N-CA-CB	-8.41	97.88	110.50
2	1	9	ARG	NH1-CZ-NH2	8.41	128.65	119.40
4	3	13	ARG	NE-CZ-NH2	-8.20	116.20	120.30
2	1	143	ARG	CD-NE-CZ	-8.18	112.14	123.60
4	3	32	VAL	N-CA-CB	-8.12	93.63	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	217	ASP	CB-CG-OD1	-8.08	111.03	118.30
2	1	296	THR	CA-CB-CG2	7.97	123.56	112.40
2	1	351	TYR	CB-CG-CD2	7.97	125.78	121.00
3	2	115	ARG	NE-CZ-NH2	7.95	124.28	120.30
4	3	28	ARG	CD-NE-CZ	-7.76	112.73	123.60
2	1	352	ARG	CD-NE-CZ	7.71	134.40	123.60
2	1	332	ASP	CB-CG-OD2	7.68	125.21	118.30
4	3	18	ARG	CD-NE-CZ	7.58	134.21	123.60
3	2	78	ASP	CB-CG-OD1	-7.55	111.51	118.30
2	1	290	ARG	NE-CZ-NH2	7.51	124.06	120.30
2	1	407	LYS	N-CA-CB	7.48	124.06	110.60
2	1	326	ARG	NE-CZ-NH2	7.41	124.00	120.30
4	3	6	ARG	NE-CZ-NH2	-7.26	116.67	120.30
2	1	74	ARG	NE-CZ-NH1	-7.24	116.68	120.30
2	1	283	MET	CA-CB-CG	7.23	125.60	113.30
3	2	53	ASN	CB-CA-C	7.21	124.82	110.40
2	1	178	GLU	OE1-CD-OE2	-7.19	114.67	123.30
2	1	389	ASP	CB-CG-OD2	-7.13	111.88	118.30
2	1	274	ARG	CD-NE-CZ	-7.05	113.72	123.60
2	1	4	GLN	CA-CB-CG	7.04	128.89	113.40
2	1	134	TYR	CB-CG-CD2	-7.01	116.79	121.00
2	1	205	ASP	CB-CG-OD1	-7.00	112.00	118.30
2	1	381	GLU	OE1-CD-OE2	6.93	131.62	123.30
3	2	41	THR	CA-CB-CG2	6.90	122.06	112.40
2	1	143	ARG	NH1-CZ-NH2	6.89	126.98	119.40
4	3	6	ARG	CG-CD-NE	-6.89	97.33	111.80
2	1	386	ARG	CD-NE-CZ	-6.88	113.96	123.60
3	2	120	TYR	CB-CG-CD2	-6.88	116.88	121.00
4	3	9	ALA	N-CA-CB	-6.87	100.49	110.10
2	1	217	ASP	OD1-CG-OD2	6.83	136.28	123.30
2	1	209	ASP	CB-CG-OD1	-6.77	112.20	118.30
3	2	78	ASP	CB-CG-OD2	6.74	124.36	118.30
2	1	263	ARG	NE-CZ-NH2	6.68	123.64	120.30
2	1	335	ARG	NE-CZ-NH2	6.68	123.64	120.30
2	1	157	ARG	NE-CZ-NH2	6.68	123.64	120.30
2	1	55	ARG	NH1-CZ-NH2	-6.52	112.23	119.40
3	2	91	LEU	CA-CB-CG	6.51	130.27	115.30
3	2	169	ILE	CA-CB-CG2	6.50	123.89	110.90
3	2	120	TYR	CB-CG-CD1	6.49	124.89	121.00
2	1	241	ASN	CB-CG-OD1	-6.45	108.70	121.60
2	1	386	ARG	CB-CA-C	6.44	123.28	110.40
2	1	9	ARG	CG-CD-NE	-6.43	98.30	111.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	189	SER	O-C-N	6.37	132.88	122.70
2	1	332	ASP	CB-CG-OD1	-6.35	112.58	118.30
2	1	312	ASP	CA-CB-CG	6.34	127.35	113.40
2	1	217	ASP	CB-CG-OD2	-6.33	112.60	118.30
2	1	241	ASN	CA-CB-CG	-6.31	99.52	113.40
2	1	208	ARG	NE-CZ-NH1	-6.30	117.15	120.30
2	1	241	ASN	OD1-CG-ND2	6.27	136.32	121.90
2	1	357	TYR	CG-CD1-CE1	6.27	126.31	121.30
2	1	192	ILE	CA-CB-CG1	-6.27	99.09	111.00
3	2	59	CYS	CB-CA-C	-6.25	97.91	110.40
2	1	335	ARG	N-CA-CB	6.23	121.81	110.60
2	1	44	ASP	CA-CB-CG	-6.21	99.75	113.40
2	1	39	ASP	CB-CG-OD1	6.18	123.87	118.30
2	1	116	THR	O-C-N	-6.17	112.84	122.70
2	1	151	LEU	CA-CB-CG	6.13	129.40	115.30
2	1	406	VAL	CB-CA-C	-6.13	99.75	111.40
3	2	39	SER	N-CA-CB	-6.08	101.37	110.50
4	3	36	GLN	CA-C-O	-6.06	107.38	120.10
2	1	343	PHE	CB-CG-CD2	-6.05	116.56	120.80
2	1	60	ILE	CB-CA-C	-6.03	99.53	111.60
2	1	54	LEU	CB-CG-CD1	-6.03	100.75	111.00
2	1	424	MET	CG-SD-CE	6.03	109.84	100.20
2	1	213	GLN	CA-CB-CG	-6.00	100.20	113.40
4	3	18	ARG	C-N-CA	-6.00	109.70	122.30
2	1	214	ARG	CD-NE-CZ	-5.98	115.23	123.60
2	1	421	ASP	CB-CG-OD1	-5.94	112.95	118.30
2	1	161	ARG	CD-NE-CZ	-5.94	115.28	123.60
3	2	8	ARG	NH1-CZ-NH2	5.92	125.91	119.40
3	2	53	ASN	N-CA-CB	-5.92	99.95	110.60
2	1	54	LEU	CB-CA-C	5.88	121.36	110.20
4	3	6	ARG	CA-CB-CG	-5.87	100.48	113.40
2	1	274	ARG	NE-CZ-NH2	-5.85	117.38	120.30
3	2	86	LYS	CD-CE-NZ	-5.83	98.28	111.70
3	2	156	ARG	N-CA-CB	-5.83	100.10	110.60
4	3	31	TYR	CB-CG-CD2	5.76	124.46	121.00
2	1	421	ASP	N-CA-C	-5.73	95.53	111.00
4	3	31	TYR	CB-CG-CD1	-5.71	117.58	121.00
2	1	426	SER	CA-C-O	-5.68	108.17	120.10
4	3	7	SER	O-C-N	-5.66	113.57	123.20
2	1	118	LYS	O-C-N	5.64	131.73	122.70
3	2	82	ASP	CB-CG-OD1	-5.64	113.22	118.30
2	1	207	GLU	OE1-CD-OE2	5.64	130.07	123.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	63	ASP	CB-CG-OD1	5.62	123.36	118.30
2	1	378	ASP	CA-CB-CG	-5.62	101.03	113.40
2	1	406	VAL	O-C-N	5.62	131.69	122.70
4	3	18	ARG	NE-CZ-NH1	5.61	123.10	120.30
4	3	7	SER	C-N-CA	-5.60	110.54	122.30
2	1	212	MET	CG-SD-CE	-5.58	91.26	100.20
3	2	169	ILE	CA-CB-CG1	-5.55	100.45	111.00
2	1	112	ILE	CA-CB-CG1	-5.55	100.46	111.00
2	1	323	LEU	CB-CG-CD2	-5.55	101.57	111.00
2	1	32	THR	N-CA-CB	5.53	120.81	110.30
2	1	215	TYR	CB-CG-CD1	-5.52	117.69	121.00
2	1	165	LEU	CB-CA-C	5.50	120.66	110.20
3	2	168	ILE	CA-CB-CG1	-5.48	100.59	111.00
2	1	306	GLY	N-CA-C	5.47	126.79	113.10
2	1	307	ALA	O-C-N	5.47	131.45	122.70
2	1	386	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	1	271	SER	CB-CA-C	-5.43	99.79	110.10
2	1	5	THR	C-N-CA	-5.42	110.91	122.30
2	1	184	THR	CA-CB-OG1	-5.40	97.65	109.00
2	1	416	LEU	CB-CG-CD2	-5.37	101.87	111.00
4	3	3	GLY	O-C-N	5.37	131.30	122.70
2	1	70	TYR	CB-CG-CD1	5.36	124.22	121.00
3	2	95	GLU	CA-CB-CG	5.36	125.19	113.40
2	1	316	ASP	CB-CG-OD1	-5.35	113.48	118.30
3	2	155	CYS	C-N-CA	5.34	135.06	121.70
3	2	23	VAL	O-C-N	5.33	131.23	122.70
2	1	418	THR	OG1-CB-CG2	5.33	122.25	110.00
4	3	4	LYS	N-CA-CB	-5.33	101.01	110.60
4	3	28	ARG	NE-CZ-NH1	-5.32	117.64	120.30
2	1	409	ASN	OD1-CG-ND2	5.32	134.12	121.90
2	1	145	GLU	CG-CD-OE1	5.31	128.91	118.30
4	3	20	THR	N-CA-CB	-5.30	100.22	110.30
2	1	411	THR	CA-CB-OG1	-5.29	97.89	109.00
2	1	183	MET	N-CA-CB	5.28	120.11	110.60
4	3	4	LYS	C-N-CA	-5.27	108.53	121.70
2	1	178	GLU	CG-CD-OE2	5.27	128.84	118.30
3	2	159	VAL	CB-CA-C	5.26	121.40	111.40
2	1	199	TYR	CB-CG-CD1	5.26	124.16	121.00
2	1	283	MET	CG-SD-CE	-5.25	91.79	100.20
2	1	133	ASN	CA-C-O	-5.25	109.08	120.10
2	1	137	ALA	CB-CA-C	5.24	117.96	110.10
3	2	150	PHE	CB-CG-CD1	-5.24	117.13	120.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	391	ASP	CB-CG-OD1	-5.23	113.59	118.30
2	1	283	MET	N-CA-CB	-5.22	101.20	110.60
3	2	39	SER	CB-CA-C	5.20	119.98	110.10
2	1	418	THR	N-CA-CB	-5.20	100.43	110.30
3	2	92	VAL	CB-CA-C	-5.19	101.54	111.40
3	2	149	ASN	N-CA-CB	5.16	119.89	110.60
4	3	13	ARG	CB-CG-CD	-5.14	98.24	111.60
2	1	210	TYR	CB-CG-CD2	-5.13	117.92	121.00
2	1	166	LYS	O-C-N	5.12	130.89	122.70
4	3	6	ARG	N-CA-CB	-5.12	101.38	110.60
2	1	70	TYR	CB-CG-CD2	-5.09	117.94	121.00
2	1	98	ASN	CB-CA-C	-5.08	100.23	110.40
2	1	342	LYS	CD-CE-NZ	-5.08	100.02	111.70
1	A	2	DA	C8-N9-C4	-5.06	103.78	105.80
2	1	98	ASN	CB-CG-OD1	-5.04	111.53	121.60
3	2	168	ILE	CA-C-O	-5.03	109.53	120.10
2	1	87	ASP	CB-CG-OD2	-5.03	113.77	118.30
3	2	10	ASN	CB-CG-ND2	5.03	128.76	116.70
2	1	241	ASN	N-CA-CB	-5.00	101.59	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	386	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	83	0	45	13	0
2	1	3415	0	3305	186	0
3	2	1339	0	1322	72	0
4	3	283	0	305	35	0
5	1	129	0	0	12	0
5	2	41	0	0	1	0
5	3	6	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	2	0
All	All	5298	0	4977	289	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 29.

All (289) 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)
3:2:41:THR:HG21	5:2:199:HOH:O	1.40	1.22
2:1:167:ASN:HB2	2:1:170:THR:HB	1.15	1.14
4:3:9:ALA:O	4:3:11:PRO:HD3	1.51	1.11
2:1:363:HIS:O	2:1:372:GLN:OE1	1.71	1.06
3:2:39:SER:HB2	3:2:162:ASN:HD22	1.13	1.05
1:A:2:DA:OP2	1:A:2:DA:H4'	1.50	1.04
2:1:24:ILE:O	2:1:289:VAL:O	1.76	1.02
4:3:4:LYS:HE2	4:3:5:LYS:H	1.23	1.02
1:A:1:DA:N7	5:A:44:HOH:O	1.94	1.01
4:3:6:ARG:H	4:3:6:ARG:CD	1.65	1.00
1:A:1:DA:OP1	2:1:211:PHE:CE2	2.15	1.00
2:1:90:ASN:HB2	5:1:532:HOH:O	1.58	1.00
2:1:61:ASP:OD2	4:3:18:ARG:HD2	1.62	0.99
2:1:165:LEU:O	2:1:170:THR:HG21	1.63	0.98
3:2:37:ALA:O	3:2:61:GLN:O	1.82	0.98
1:A:2:DA:C5'	4:3:28:ARG:HB3	1.95	0.97
3:2:103:LEU:HD12	3:2:104:PRO:HD2	1.47	0.96
2:1:244:ALA:HA	2:1:266:GLN:HG2	1.47	0.96
2:1:132:ASN:HD21	2:1:143:ARG:H	1.13	0.96
2:1:245:SER:H	2:1:266:GLN:HE21	1.10	0.93
3:2:12:ASN:HD22	3:2:13:PHE:N	1.67	0.93
4:3:4:LYS:HE2	4:3:5:LYS:N	1.83	0.93
2:1:323:LEU:N	2:1:323:LEU:CD2	2.32	0.93
3:2:67:ASN:C	3:2:67:ASN:HD22	1.72	0.93
2:1:265:GLN:HB2	5:1:435:HOH:O	1.70	0.91
2:1:149:ASN:HD22	2:1:149:ASN:C	1.74	0.90
3:2:63:ASP:H	3:2:163:GLN:HE22	1.17	0.90
2:1:98:ASN:H	2:1:147:ASN:HD22	0.92	0.90
2:1:323:LEU:N	2:1:323:LEU:HD22	1.90	0.87
3:2:53:ASN:HB2	3:2:149:ASN:HD21	1.40	0.86
2:1:167:ASN:HB2	2:1:170:THR:CB	2.04	0.86
4:3:6:ARG:H	4:3:6:ARG:HD3	1.39	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:53:ASN:HB2	3:2:149:ASN:ND2	1.92	0.84
1:A:2:DA:H5"	4:3:28:ARG:HB3	1.57	0.84
2:1:143:ARG:NH1	2:1:145:GLU:OE2	2.11	0.84
2:1:167:ASN:H	2:1:170:THR:HG22	1.44	0.82
2:1:77:TYR:OH	2:1:122:HIS:HD2	1.62	0.82
3:2:39:SER:CB	3:2:162:ASN:HD22	1.93	0.82
2:1:132:ASN:ND2	2:1:143:ARG:H	1.78	0.81
2:1:418:THR:HG22	2:1:421:ASP:H	1.44	0.81
3:2:24:THR:HB	3:2:50:ASN:HB2	1.63	0.81
2:1:167:ASN:CB	2:1:170:THR:HB	2.06	0.80
1:A:1:DA:OP2	2:1:207:GLU:OE2	2.02	0.78
2:1:238:MET:HE3	2:1:239:ARG:H	1.47	0.78
3:2:169:ILE:HD13	3:2:169:ILE:H	1.49	0.78
2:1:167:ASN:N	2:1:170:THR:HG22	1.99	0.77
2:1:98:ASN:N	2:1:147:ASN:HD22	1.76	0.77
2:1:42:GLU:OE2	2:1:413:TYR:HE1	1.67	0.77
2:1:98:ASN:H	2:1:147:ASN:ND2	1.78	0.77
2:1:323:LEU:H	2:1:323:LEU:CD2	1.97	0.76
4:3:6:ARG:N	4:3:6:ARG:CD	2.47	0.76
3:2:83:ALA:O	3:2:85:PRO:HD3	1.86	0.76
2:1:7:ALA:HB3	2:1:415:ASN:OD1	1.87	0.75
2:1:245:SER:N	2:1:266:GLN:HE21	1.84	0.74
2:1:132:ASN:HD21	2:1:143:ARG:N	1.86	0.74
2:1:319:LEU:O	2:1:323:LEU:HD22	1.88	0.74
2:1:138:PRO:HD2	4:3:32:VAL:HG13	1.69	0.74
2:1:175:PRO:HG3	2:1:379:LEU:HD23	1.69	0.73
3:2:39:SER:HB2	3:2:162:ASN:ND2	1.98	0.73
2:1:323:LEU:HD23	2:1:323:LEU:H	1.52	0.73
4:3:2:LYS:HG2	4:3:3:GLY:N	2.03	0.72
4:3:6:ARG:O	4:3:6:ARG:HG2	1.89	0.72
3:2:169:ILE:HD13	3:2:169:ILE:N	2.03	0.72
2:1:238:MET:CE	2:1:239:ARG:H	2.02	0.72
2:1:9:ARG:N	5:1:436:HOH:O	2.18	0.72
3:2:48:THR:HG22	3:2:154:LYS:HE3	1.73	0.70
2:1:172:PRO:HG3	2:1:379:LEU:HD11	1.74	0.70
2:1:76:VAL:HG11	2:1:122:HIS:HA	1.73	0.70
2:1:418:THR:HG23	2:1:420:ARG:H	1.57	0.70
4:3:9:ALA:O	4:3:11:PRO:CD	2.36	0.69
2:1:77:TYR:OH	2:1:122:HIS:CD2	2.44	0.69
2:1:196:GLN:NE2	2:1:196:GLN:HA	2.07	0.69
1:A:2:DA:H5"	4:3:28:ARG:CB	2.24	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:323:LEU:HD23	2:1:323:LEU:N	2.06	0.67
3:2:22:SER:HA	3:2:48:THR:O	1.95	0.67
3:2:67:ASN:C	3:2:67:ASN:ND2	2.46	0.66
2:1:166:LYS:HA	2:1:170:THR:HG22	1.76	0.66
2:1:323:LEU:HB2	2:1:324:PRO:HD2	1.78	0.66
2:1:96:THR:HG21	2:1:118:LYS:HD3	1.78	0.66
2:1:82:ILE:O	2:1:86:LYS:HG3	1.96	0.66
2:1:420:ARG:HA	2:1:423:ILE:HG12	1.77	0.66
2:1:305:LYS:HD3	2:1:305:LYS:O	1.96	0.66
3:2:63:ASP:H	3:2:163:GLN:NE2	1.90	0.65
1:A:1:DA:C8	5:A:44:HOH:O	2.44	0.65
2:1:319:LEU:O	2:1:323:LEU:CD2	2.45	0.65
2:1:63:THR:HB	2:1:243:TRP:CZ3	2.32	0.64
1:A:2:DA:H5'	4:3:28:ARG:HB3	1.79	0.64
1:A:2:DA:C2'	1:A:3:DA:OP2	2.46	0.64
2:1:175:PRO:HG3	2:1:379:LEU:CD2	2.28	0.63
2:1:96:THR:CG2	2:1:118:LYS:HD3	2.29	0.63
2:1:187:THR:CG2	2:1:188:THR:HG23	2.29	0.63
3:2:82:ASP:OD1	3:2:156:ARG:NH2	2.32	0.62
2:1:45:ALA:HB3	2:1:270:HIS:HB3	1.81	0.62
2:1:149:ASN:ND2	2:1:149:ASN:C	2.49	0.62
2:1:26:ARG:HH11	2:1:387:HIS:CD2	2.17	0.62
2:1:246:GLY:HA3	2:1:263:ARG:O	1.99	0.62
3:2:135:THR:HG23	3:2:136:PRO:HD2	1.82	0.62
2:1:26:ARG:HH11	2:1:387:HIS:HD2	1.48	0.61
2:1:43:MET:CE	2:1:270:HIS:HD2	2.13	0.61
2:1:166:LYS:HA	2:1:170:THR:CG2	2.31	0.60
4:3:8:GLY:O	4:3:10:ARG:N	2.33	0.60
3:2:17:LYS:HD2	3:2:43:TYR:OH	2.01	0.60
2:1:187:THR:HG23	2:1:188:THR:HG23	1.83	0.59
2:1:375:PRO:HB2	2:1:382:ARG:HG2	1.83	0.59
2:1:326:ARG:O	2:1:345:ILE:HG22	2.03	0.59
3:2:53:ASN:CB	3:2:149:ASN:ND2	2.64	0.59
2:1:335:ARG:O	2:1:335:ARG:HG2	2.03	0.59
3:2:23:VAL:HG22	3:2:47:LEU:HD11	1.85	0.58
1:A:2:DA:H2''	1:A:3:DA:OP2	2.02	0.58
2:1:96:THR:O	2:1:96:THR:HG23	2.04	0.58
2:1:140:MET:HB3	2:1:141:PRO:HD2	1.84	0.58
2:1:338:ASP:HB3	2:1:341:LYS:HG2	1.84	0.58
2:1:352:ARG:HD3	5:1:443:HOH:O	2.03	0.58
3:2:64:THR:HG21	3:2:133:PRO:HD3	1.85	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:72:VAL:HG13	3:2:126:CYS:HB2	1.86	0.58
2:1:77:TYR:HB2	2:1:81:TRP:HB2	1.86	0.58
2:1:365:LEU:HD23	2:1:368:PHE:HE2	1.69	0.57
2:1:379:LEU:O	2:1:383:VAL:HG13	2.04	0.57
2:1:10:MET:O	2:1:12:HIS:HD2	1.87	0.57
2:1:122:HIS:HE1	5:1:496:HOH:O	1.87	0.57
2:1:72:PRO:O	2:1:75:HIS:HB2	2.05	0.57
3:2:82:ASP:CG	3:2:156:ARG:HH22	2.08	0.56
4:3:8:GLY:C	4:3:10:ARG:H	2.07	0.56
2:1:100:THR:HG22	2:1:102:TYR:CD2	2.41	0.56
2:1:71:VAL:HG22	2:1:234:PRO:HB3	1.87	0.56
2:1:418:THR:HG22	2:1:421:ASP:N	2.20	0.56
2:1:365:LEU:HD23	2:1:368:PHE:CE2	2.41	0.55
2:1:3:ILE:HD12	2:1:5:THR:HG23	1.87	0.55
2:1:419:THR:CG2	2:1:419:THR:O	2.55	0.55
1:A:1:DA:OP1	2:1:211:PHE:CZ	2.58	0.55
3:2:63:ASP:N	3:2:163:GLN:HE22	1.96	0.55
3:2:24:THR:HB	3:2:50:ASN:CB	2.35	0.55
3:2:22:SER:HB3	3:2:48:THR:OG1	2.06	0.54
2:1:167:ASN:HB2	2:1:170:THR:CG2	2.37	0.54
2:1:419:THR:HG22	2:1:419:THR:O	2.08	0.54
2:1:99:THR:OG1	2:1:117:ASN:HB3	2.06	0.54
2:1:138:PRO:HD2	4:3:32:VAL:CG1	2.38	0.54
2:1:134:TYR:HB3	4:3:37:PHE:CD2	2.43	0.54
3:2:64:THR:HG22	3:2:132:LEU:HD23	1.90	0.53
2:1:14:LEU:HD12	2:1:412:VAL:CG2	2.38	0.53
2:1:149:ASN:HD22	2:1:150:GLU:N	2.05	0.53
2:1:238:MET:HG3	2:1:239:ARG:N	2.22	0.53
2:1:167:ASN:HB3	2:1:170:THR:H	1.73	0.53
2:1:298:GLU:OE2	2:1:355:PRO:HB3	2.09	0.53
4:3:4:LYS:CE	4:3:5:LYS:N	2.65	0.53
2:1:100:THR:CG2	2:1:102:TYR:CD2	2.92	0.53
2:1:349:GLN:NE2	2:1:349:GLN:HA	2.25	0.52
2:1:64:VAL:O	2:1:241:ASN:HA	2.10	0.52
2:1:186:SER:OG	2:1:187:THR:N	2.43	0.52
2:1:3:ILE:CD1	2:1:5:THR:HG22	2.40	0.52
3:2:12:ASN:HD22	3:2:13:PHE:H	1.50	0.52
4:3:7:SER:C	4:3:9:ALA:H	2.12	0.51
1:A:2:DA:O5'	4:3:31:TYR:OH	2.25	0.51
3:2:12:ASN:ND2	3:2:14:PHE:H	2.09	0.51
3:2:12:ASN:HD22	3:2:12:ASN:C	2.12	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:26:ALA:C	3:2:54:GLY:HA3	2.30	0.51
3:2:95:GLU:HB2	3:2:138:ASN:HB3	1.92	0.51
3:2:49:VAL:O	3:2:152:ALA:HA	2.11	0.51
3:2:45:ASP:OD1	3:2:45:ASP:C	2.45	0.51
3:2:156:ARG:NH1	3:2:156:ARG:HG3	2.24	0.51
2:1:208:ARG:HA	2:1:212:MET:HE2	1.93	0.51
3:2:67:ASN:O	3:2:67:ASN:ND2	2.43	0.50
3:2:79:ILE:HG12	3:2:121:TYR:HB3	1.94	0.50
2:1:11:PRO:HB3	2:1:413:TYR:CE2	2.47	0.50
4:3:21:LYS:CE	4:3:25:LYS:HE3	2.41	0.50
2:1:214:ARG:HD2	5:1:502:HOH:O	2.11	0.50
3:2:74:SER:HA	3:2:126:CYS:HA	1.93	0.50
2:1:238:MET:CE	2:1:239:ARG:O	2.59	0.50
2:1:3:ILE:CD1	2:1:5:THR:CG2	2.90	0.50
2:1:74:ARG:HH11	2:1:74:ARG:HG2	1.77	0.50
2:1:133:ASN:C	2:1:214:ARG:HH21	2.15	0.50
3:2:77:ALA:O	3:2:122:THR:HA	2.10	0.49
3:2:92:VAL:O	3:2:142:VAL:HA	2.12	0.49
2:1:50:ARG:HA	2:1:264:VAL:O	2.11	0.49
2:1:50:ARG:NH1	2:1:265:GLN:OE1	2.45	0.49
2:1:208:ARG:HG2	2:1:212:MET:CE	2.42	0.49
2:1:137:ALA:HA	4:3:36:GLN:HG3	1.93	0.49
2:1:208:ARG:HG2	2:1:212:MET:HE1	1.95	0.49
2:1:154:ASP:OD1	2:1:157:ARG:NH2	2.45	0.49
2:1:168:ILE:HD11	2:1:345:ILE:HD11	1.94	0.48
2:1:9:ARG:HG2	2:1:9:ARG:O	2.14	0.48
2:1:164:HIS:CD2	2:1:293:PRO:HB3	2.47	0.48
2:1:265:GLN:CG	5:1:435:HOH:O	2.61	0.48
3:2:38:THR:HG23	3:2:163:GLN:HB3	1.96	0.48
4:3:21:LYS:HE3	4:3:25:LYS:HE3	1.95	0.48
2:1:299:ILE:HG21	2:1:304:ALA:HB2	1.94	0.48
3:2:25:PRO:HD2	3:2:50:ASN:O	2.13	0.48
2:1:238:MET:HE2	2:1:239:ARG:O	2.13	0.48
3:2:37:ALA:HA	3:2:61:GLN:HB3	1.95	0.48
3:2:169:ILE:HG23	3:2:169:ILE:HD12	1.48	0.48
3:2:48:THR:CG2	3:2:154:LYS:HE3	2.44	0.47
2:1:334:PHE:CD1	2:1:374:PRO:HB3	2.49	0.47
3:2:41:THR:HB	3:2:160:SER:OG	2.14	0.47
2:1:247:TYR:CE1	2:1:263:ARG:HD3	2.49	0.47
2:1:97:VAL:HG22	2:1:147:ASN:HA	1.96	0.47
2:1:195:LEU:O	2:1:198:ALA:HB3	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:39:SER:HA	3:2:161:LEU:O	2.15	0.47
4:3:7:SER:C	4:3:9:ALA:N	2.68	0.47
3:2:45:ASP:OD1	3:2:46:SER:N	2.48	0.47
2:1:35:VAL:CG2	2:1:277:VAL:HG11	2.45	0.47
3:2:53:ASN:HD22	3:2:53:ASN:C	2.18	0.46
2:1:265:GLN:CB	5:1:435:HOH:O	2.47	0.46
2:1:23:GLN:OE1	2:1:401:GLN:HG3	2.16	0.46
4:3:8:GLY:C	4:3:10:ARG:N	2.68	0.46
2:1:2:ASN:HD22	2:1:3:ILE:H	1.63	0.46
2:1:192:ILE:HA	2:1:192:ILE:HD13	1.28	0.46
2:1:27:LEU:HB2	2:1:162:CYS:SG	2.56	0.46
2:1:418:THR:CG2	2:1:420:ARG:H	2.25	0.45
3:2:87:PHE:HB3	3:2:148:SER:HB2	1.98	0.45
2:1:96:THR:O	2:1:96:THR:CG2	2.65	0.45
2:1:200:ALA:O	2:1:204:THR:HG23	2.15	0.45
2:1:116:THR:HG23	2:1:116:THR:H	1.49	0.45
2:1:244:ALA:HA	2:1:266:GLN:CG	2.32	0.45
3:2:151:THR:O	3:2:152:ALA:C	2.54	0.45
3:2:169:ILE:H	3:2:169:ILE:CD1	2.24	0.44
4:3:4:LYS:HE2	4:3:4:LYS:HB3	1.38	0.44
4:3:35:GLN:HA	5:3:40:HOH:O	2.17	0.44
2:1:98:ASN:O	2:1:147:ASN:HB3	2.17	0.44
2:1:185:THR:HG23	2:1:186:SER:O	2.17	0.44
3:2:72:VAL:CG1	3:2:126:CYS:HB2	2.47	0.44
2:1:246:GLY:HA3	2:1:264:VAL:HA	2.00	0.44
3:2:87:PHE:CB	3:2:148:SER:HB2	2.48	0.44
2:1:67:PHE:CE1	2:1:239:ARG:HD2	2.53	0.44
2:1:43:MET:HE3	2:1:270:HIS:HD2	1.82	0.44
2:1:233:ARG:HA	2:1:234:PRO:HD3	1.90	0.44
3:2:8:ARG:HD2	3:2:8:ARG:HH11	1.41	0.44
2:1:174:PRO:HA	2:1:175:PRO:HD3	1.79	0.43
2:1:82:ILE:O	2:1:86:LYS:CG	2.65	0.43
2:1:305:LYS:O	2:1:306:GLY:O	2.36	0.43
2:1:63:THR:HB	2:1:243:TRP:CH2	2.52	0.43
2:1:415:ASN:OD1	2:1:415:ASN:O	2.36	0.43
2:1:3:ILE:HD11	2:1:5:THR:HG22	2.01	0.43
3:2:52:GLY:O	3:2:150:PHE:N	2.51	0.43
2:1:42:GLU:OE2	2:1:413:TYR:CE1	2.58	0.43
2:1:187:THR:HG22	2:1:188:THR:HG23	1.99	0.43
3:2:86:LYS:HZ2	3:2:86:LYS:HG2	1.40	0.43
2:1:386:ARG:HD3	2:1:389:ASP:OD1	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:39:ASP:HB3	5:1:448:HOH:O	2.18	0.43
2:1:61:ASP:OD1	4:3:16:PRO:HB2	2.18	0.43
2:1:43:MET:CE	2:1:270:HIS:CD2	3.00	0.43
2:1:371:ILE:HD13	2:1:371:ILE:HG21	1.87	0.43
2:1:9:ARG:CG	2:1:9:ARG:O	2.63	0.43
2:1:35:VAL:HG22	2:1:281:GLY:O	2.17	0.43
3:2:62:MET:HA	3:2:62:MET:CE	2.49	0.43
3:2:113:ASN:ND2	3:2:113:ASN:C	2.70	0.43
2:1:90:ASN:CB	5:1:532:HOH:O	2.40	0.43
2:1:328:ILE:O	2:1:343:PHE:N	2.50	0.43
2:1:225:LYS:HB3	2:1:225:LYS:HE3	1.70	0.42
3:2:30:PRO:HD2	3:2:55:GLY:O	2.18	0.42
2:1:10:MET:O	2:1:12:HIS:CD2	2.70	0.42
2:1:167:ASN:CB	2:1:170:THR:H	2.32	0.42
4:3:5:LYS:HA	4:3:6:ARG:HD3	2.02	0.42
2:1:90:ASN:N	5:1:532:HOH:O	2.46	0.42
2:1:286:LEU:HD12	2:1:286:LEU:N	2.35	0.42
3:2:29:ALA:O	3:2:102:THR:HA	2.20	0.42
2:1:113:ASN:HA	2:1:114:PRO:HD3	1.86	0.42
2:1:26:ARG:HD2	2:1:26:ARG:HH11	1.68	0.42
2:1:169:TRP:CZ3	2:1:375:PRO:CG	3.03	0.42
2:1:74:ARG:CZ	2:1:74:ARG:HB3	2.50	0.42
2:1:169:TRP:CZ3	2:1:375:PRO:HG2	2.54	0.42
2:1:416:LEU:C	2:1:416:LEU:HD23	2.40	0.42
3:2:18:LEU:HB3	3:2:44:PHE:HB3	2.02	0.42
2:1:238:MET:CG	2:1:239:ARG:N	2.82	0.42
2:1:138:PRO:HG2	4:3:34:GLY:N	2.35	0.42
2:1:175:PRO:CG	2:1:379:LEU:HD23	2.46	0.42
2:1:74:ARG:NH1	2:1:74:ARG:CG	2.80	0.42
2:1:349:GLN:HG2	5:1:475:HOH:O	2.19	0.41
2:1:26:ARG:HA	2:1:160:PHE:O	2.20	0.41
2:1:165:LEU:O	2:1:170:THR:CG2	2.52	0.41
2:1:12:HIS:CE1	2:1:416:LEU:CD2	3.04	0.41
2:1:74:ARG:HG2	2:1:74:ARG:NH1	2.34	0.41
3:2:62:MET:CG	3:2:140:VAL:HG22	2.50	0.41
2:1:305:LYS:HB2	2:1:305:LYS:HE2	1.70	0.41
3:2:9:HIS:HB3	3:2:124:LYS:HG3	2.02	0.41
2:1:420:ARG:O	2:1:424:MET:HB2	2.21	0.41
2:1:134:TYR:HB3	4:3:37:PHE:CE2	2.55	0.41
3:2:62:MET:HG2	3:2:140:VAL:HG22	2.02	0.41
2:1:328:ILE:HG22	2:1:343:PHE:O	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:53:PRO:HG2	2:1:395:GLN:HB2	2.02	0.41
2:1:138:PRO:CD	4:3:32:VAL:CG1	2.99	0.40
2:1:196:GLN:NE2	2:1:196:GLN:CA	2.76	0.40
2:1:4:GLN:HE21	2:1:4:GLN:HB3	1.71	0.40
3:2:3:GLN:HG3	3:2:4:THR:O	2.21	0.40
2:1:35:VAL:HB	2:1:277:VAL:HG11	2.03	0.40
2:1:204:THR:O	2:1:208:ARG:HG3	2.20	0.40
4:3:13:ARG:HA	4:3:14:PRO:HD3	1.88	0.40
2:1:67:PHE:O	2:1:285:THR:HA	2.22	0.40
3:2:29:ALA:HA	3:2:30:PRO:HD2	1.83	0.40
3:2:112:LEU:HA	3:2:112:LEU:HD23	1.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	424/426 (100%)	406 (96%)	16 (4%)	2 (0%)	34	76
3	2	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
4	3	34/37 (92%)	24 (71%)	5 (15%)	5 (15%)	0	1
All	All	631/638 (99%)	595 (94%)	29 (5%)	7 (1%)	17	58

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	306	GLY
4	3	3	GLY
4	3	4	LYS
4	3	22	GLY
2	1	101	GLY
4	3	9	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	3	10	ARG

### 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	
2	1	372/372 (100%)	329 (88%)	43 (12%)	7	27
3	2	153/153 (100%)	123 (80%)	30 (20%)	1	9
4	3	26/27 (96%)	17 (65%)	9 (35%)	0	1
All	All	551/552 (100%)	469 (85%)	82 (15%)	4	17

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	2	ASN
2	1	4	GLN
2	1	9	ARG
2	1	40	SER
2	1	49	LEU
2	1	54	LEU
2	1	60	ILE
2	1	79	GLU
2	1	97	VAL
2	1	118	LYS
2	1	144	THR
2	1	149	ASN
2	1	152	ASN
2	1	167	ASN
2	1	170	THR
2	1	181	ARG
2	1	184	THR
2	1	186	SER
2	1	187	THR
2	1	204	THR
2	1	211	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	1	214	ARG
2	1	225	LYS
2	1	226	THR
2	1	236	LEU
2	1	242	LEU
2	1	255	THR
2	1	279	GLU
2	1	305	LYS
2	1	312	ASP
2	1	313	ILE
2	1	323	LEU
2	1	339	SER
2	1	345	ILE
2	1	349	GLN
2	1	383	VAL
2	1	386	ARG
2	1	406	VAL
2	1	410	VAL
2	1	414	ARG
2	1	416	LEU
2	1	418	THR
2	1	420	ARG
3	2	8	ARG
3	2	11	SER
3	2	12	ASN
3	2	17	LYS
3	2	22	SER
3	2	23	VAL
3	2	24	THR
3	2	28	SER
3	2	34	THR
3	2	36	LYS
3	2	39	SER
3	2	41	THR
3	2	53	ASN
3	2	67	ASN
3	2	79	ILE
3	2	86	LYS
3	2	91	LEU
3	2	92	VAL
3	2	95	GLU
3	2	105	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	2	115	ARG
3	2	122	THR
3	2	128	THR
3	2	140	VAL
3	2	149	ASN
3	2	159	VAL
3	2	161	LEU
3	2	166	LYS
3	2	169	ILE
3	2	174	LEU
4	3	2	LYS
4	3	4	LYS
4	3	6	ARG
4	3	7	SER
4	3	13	ARG
4	3	15	GLN
4	3	18	ARG
4	3	32	VAL
4	3	35	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	2	ASN
2	1	4	GLN
2	1	12	HIS
2	1	16	HIS
2	1	105	HIS
2	1	117	ASN
2	1	122	HIS
2	1	125	GLN
2	1	129	ASN
2	1	132	ASN
2	1	147	ASN
2	1	149	ASN
2	1	153	GLN
2	1	164	HIS
2	1	167	ASN
2	1	182	GLN
2	1	196	GLN
2	1	266	GLN
2	1	300	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	1	303	ASN
2	1	349	GLN
2	1	372	GLN
2	1	387	HIS
2	1	392	GLN
2	1	398	GLN
2	1	405	GLN
3	2	9	HIS
3	2	12	ASN
3	2	53	ASN
3	2	67	ASN
3	2	70	ASN
3	2	113	ASN
3	2	149	ASN
3	2	162	ASN
3	2	163	GLN
4	3	15	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no 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 ⓘ

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 will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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