



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:29 PM UTC

PDB ID : 2BPA / pdb_00002bpa
Title : ATOMIC STRUCTURE OF SINGLE-STRANDED DNA BACTERIOPHAGE PHIX174 AND ITS FUNCTIONAL IMPLICATIONS
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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

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

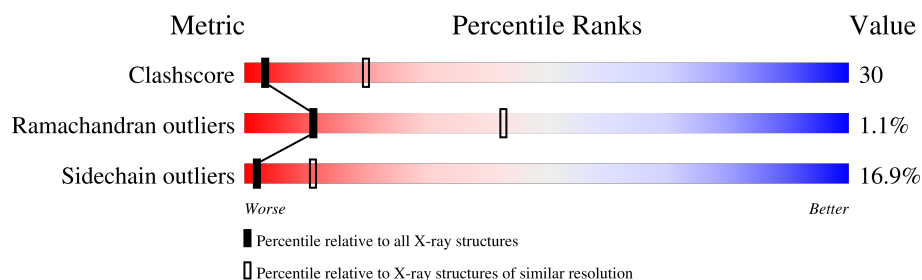
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 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	5	40% 40% 20%
2	1	426	38% 40% 18% .
3	2	175	36% 39% 17% 8%
4	3	37	11% 38% 19% 30% .

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	A	2	Total	O	0	0
			2	2		

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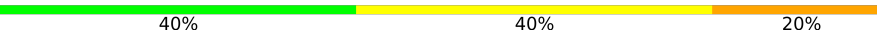
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1	129	Total 129	O 129	0	0
5	2	41	Total 41	O 41	0	0
5	3	6	Total 6	O 6	0	0

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.

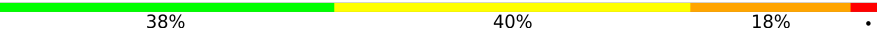
Note EDS was not executed.

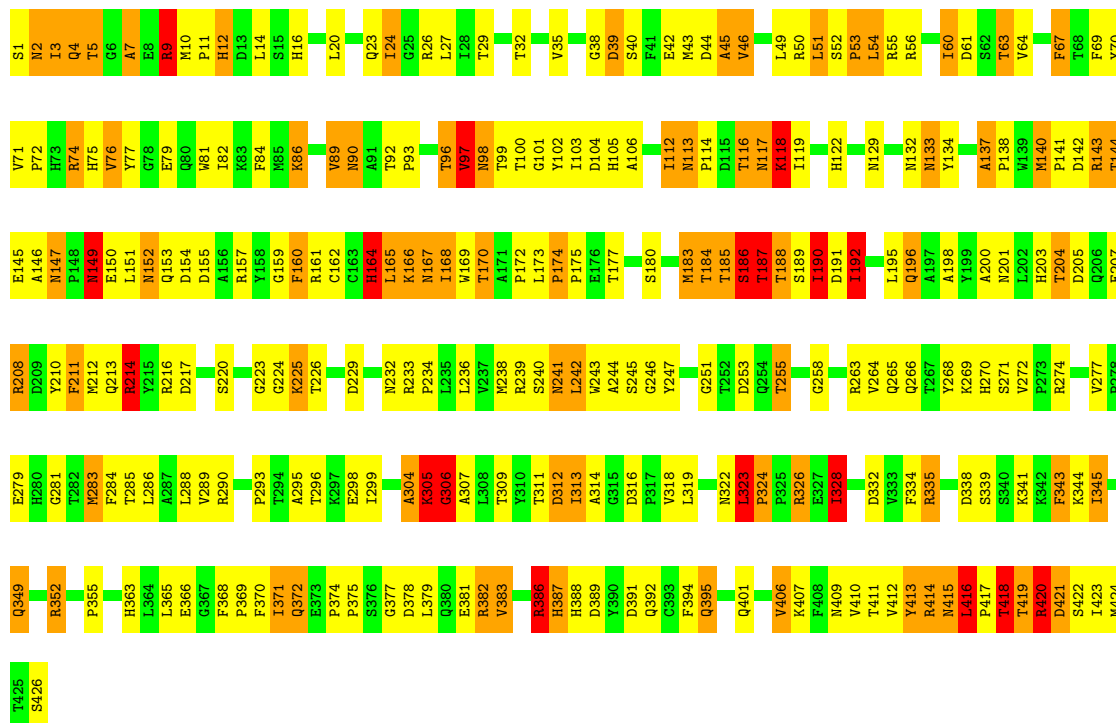
- Molecule 1: DNA (5'-D(*AP*AP*AP*AP*C)-3')

Chain A: 

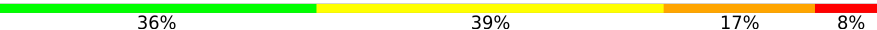


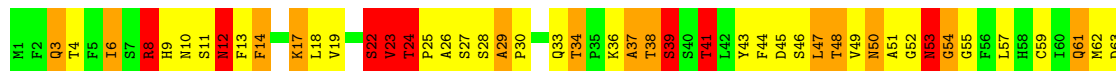
- Molecule 2: PROTEIN (SUBUNIT OF BACTERIOPHAGE PHIX174)

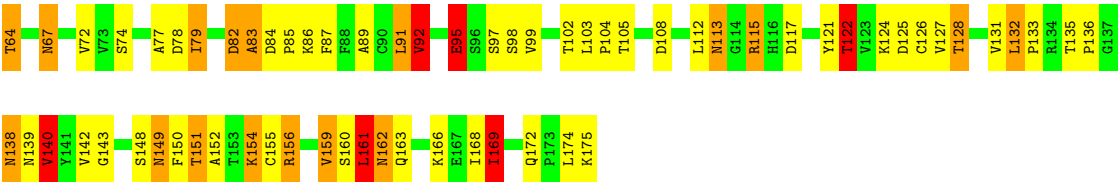
Chain 1: 



- Molecule 3: PROTEIN (SUBUNIT OF BACTERIOPHAGE PHIX174)

Chain 2: 





● Molecule 4: PROTEIN (SUBUNIT OF BACTERIOPHAGE PHIX174)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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	0.99	0/93	1.48	1/142 (0.7%)
2	1	1.81	39/3511 (1.1%)	2.51	256/4779 (5.4%)
3	2	1.83	10/1371 (0.7%)	2.44	95/1872 (5.1%)
4	3	2.71	23/289 (8.0%)	3.06	39/380 (10.3%)
All	All	1.87	72/5264 (1.4%)	2.51	391/7173 (5.5%)

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 (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	13	ARG	N-CA	8.89	1.58	1.45
4	3	18	ARG	C-O	8.82	1.35	1.23
4	3	7	SER	C-O	8.63	1.32	1.24
2	1	323	LEU	N-CA	8.17	1.54	1.45
4	3	19	GLY	N-CA	8.11	1.57	1.45
2	1	416	LEU	N-CA	8.10	1.52	1.45
3	2	54	GLY	N-CA	8.02	1.54	1.45
2	1	295	ALA	N-CA	7.96	1.55	1.45
4	3	8	GLY	N-CA	7.78	1.56	1.45
2	1	269	LYS	N-CA	7.45	1.55	1.46
4	3	11	PRO	C-O	7.45	1.33	1.24
2	1	386	ARG	N-CA	7.31	1.55	1.46
4	3	10	ARG	CD-NE	7.03	1.56	1.46
4	3	4	LYS	CA-CB	6.89	1.65	1.53
3	2	161	LEU	CA-C	6.83	1.60	1.52
2	1	103	ILE	C-O	6.79	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	168	ILE	CA-CB	6.67	1.62	1.53
4	3	4	LYS	C-N	6.60	1.42	1.33
2	1	224	GLY	N-CA	6.54	1.50	1.44
2	1	106	ALA	N-CA	6.48	1.53	1.46
3	2	6	ILE	C-O	6.42	1.30	1.24
4	3	12	GLY	C-O	6.37	1.31	1.24
4	3	13	ARG	CZ-NH2	6.37	1.41	1.33
3	2	41	THR	CB-OG1	6.33	1.53	1.43
2	1	52	SER	N-CA	6.32	1.55	1.45
2	1	96	THR	C-O	6.32	1.31	1.24
2	1	16	HIS	N-CA	6.30	1.54	1.46
2	1	159	GLY	N-CA	6.21	1.51	1.45
2	1	96	THR	CA-CB	6.20	1.62	1.53
4	3	36	GLN	N-CA	6.15	1.53	1.46
4	3	4	LYS	C-O	6.14	1.31	1.24
3	2	34	THR	N-CA	6.02	1.54	1.46
2	1	378	ASP	N-CA	6.01	1.53	1.45
2	1	173	LEU	C-O	5.99	1.31	1.23
2	1	116	THR	C-O	5.97	1.30	1.23
4	3	7	SER	N-CA	5.91	1.53	1.46
2	1	232	ASN	C-O	5.89	1.31	1.23
2	1	112	ILE	N-CA	5.87	1.53	1.46
4	3	13	ARG	NE-CZ	5.87	1.39	1.33
4	3	20	THR	CA-CB	5.75	1.62	1.53
2	1	192	ILE	CA-CB	5.62	1.61	1.54
2	1	96	THR	C-N	-5.60	1.26	1.34
4	3	20	THR	N-CA	5.58	1.52	1.46
3	2	143	GLY	N-CA	5.57	1.50	1.45
3	2	92	VAL	CA-C	5.56	1.59	1.52
2	1	344	LYS	N-CA	5.46	1.52	1.46
2	1	165	LEU	N-CA	5.43	1.52	1.46
2	1	140	MET	N-CA	5.43	1.53	1.45
2	1	343	PHE	CA-CB	-5.42	1.44	1.53
2	1	144	THR	CA-CB	5.35	1.60	1.53
4	3	10	ARG	CZ-NH2	5.33	1.40	1.33
4	3	16	PRO	C-O	5.32	1.29	1.23
2	1	413	TYR	N-CA	5.30	1.53	1.46
2	1	63	THR	N-CA	5.30	1.52	1.46
2	1	216	ARG	NE-CZ	5.26	1.38	1.33
4	3	24	ARG	NE-CZ	5.26	1.38	1.33
4	3	18	ARG	CZ-NH2	5.25	1.40	1.33
2	1	343	PHE	N-CA	5.22	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	386	ARG	NE-CZ	5.21	1.38	1.33
2	1	155	ASP	N-CA	5.19	1.52	1.46
2	1	45	ALA	N-CA	5.12	1.52	1.46
4	3	9	ALA	C-O	5.11	1.30	1.24
2	1	89	VAL	C-N	-5.10	1.27	1.33
2	1	2	ASN	CA-C	5.09	1.58	1.52
3	2	122	THR	N-CA	5.07	1.52	1.46
2	1	143	ARG	CZ-NH2	-5.05	1.26	1.33
2	1	191	ASP	CA-CB	-5.02	1.46	1.53
2	1	191	ASP	N-CA	5.02	1.52	1.46
2	1	370	PHE	C-N	-5.02	1.28	1.33
3	2	8	ARG	CZ-NH1	5.01	1.39	1.32
2	1	253	ASP	N-CA	5.01	1.51	1.45
4	3	3	GLY	C-O	5.00	1.30	1.23

All (391) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	39	ASP	CA-CB-CG	19.73	132.34	112.60
2	1	116	THR	CA-C-O	-17.98	101.42	121.19
2	1	416	LEU	CB-CA-C	16.33	134.05	109.22
2	1	214	ARG	NE-CZ-NH2	16.28	133.85	119.20
2	1	312	ASP	CA-CB-CG	14.75	127.35	112.60
2	1	208	ARG	NE-CZ-NH2	14.74	132.47	119.20
2	1	421	ASP	N-CA-C	-14.45	95.53	111.28
2	1	144	THR	N-CA-CB	-14.27	90.31	111.43
4	3	32	VAL	N-CA-CB	-14.26	93.63	112.16
2	1	241	ASN	OD1-CG-ND2	13.72	136.32	122.60
2	1	241	ASN	CA-CB-CG	-13.08	99.52	112.60
2	1	44	ASP	CA-CB-CG	-12.85	99.75	112.60
2	1	56	ARG	NE-CZ-NH2	-12.23	108.20	119.20
2	1	147	ASN	O-C-N	12.05	130.44	121.88
2	1	192	ILE	CA-CB-CG2	11.75	130.48	110.50
2	1	378	ASP	CA-CB-CG	-11.57	101.03	112.60
2	1	409	ASN	OD1-CG-ND2	11.52	134.12	122.60
3	2	8	ARG	CD-NE-CZ	-11.25	108.65	124.40
2	1	9	ARG	NE-CZ-NH2	-10.80	109.48	119.20
2	1	56	ARG	NH1-CZ-NH2	10.59	133.07	119.30
4	3	36	GLN	CA-C-O	-10.51	107.38	120.20
3	2	139	ASN	OD1-CG-ND2	10.30	132.90	122.60
2	1	352	ARG	NE-CZ-NH1	10.15	131.65	121.50
3	2	24	THR	CB-CA-C	10.14	124.33	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	149	ASN	CA-CB-CG	-10.13	102.47	112.60
2	1	143	ARG	NE-CZ-NH1	-9.96	111.54	121.50
3	2	168	ILE	CA-C-O	-9.95	109.53	120.48
2	1	214	ARG	NH1-CZ-NH2	-9.81	106.54	119.30
2	1	323	LEU	CA-C-O	-9.69	110.68	120.66
3	2	138	ASN	OD1-CG-ND2	9.54	132.14	122.60
2	1	205	ASP	CA-CB-CG	-9.44	103.16	112.60
2	1	213	GLN	OE1-CD-NE2	9.44	132.04	122.60
3	2	113	ASN	CA-CB-CG	-9.43	103.17	112.60
1	A	1	DA	P-O3'-C3'	9.32	134.19	120.20
2	1	217	ASP	CA-CB-CG	-9.15	103.45	112.60
4	3	4	LYS	CA-C-N	-9.02	108.53	121.42
4	3	4	LYS	C-N-CA	-9.02	108.53	121.42
2	1	189	SER	O-C-N	8.85	132.88	123.42
2	1	90	ASN	CA-CB-CG	-8.84	103.76	112.60
2	1	133	ASN	CA-C-O	-8.84	109.08	119.15
2	1	143	ARG	CD-NE-CZ	-8.76	112.14	124.40
2	1	409	ASN	CA-CB-CG	-8.68	103.92	112.60
2	1	378	ASP	CB-CA-C	8.61	128.97	110.19
2	1	117	ASN	CA-CB-CG	8.55	121.15	112.60
2	1	104	ASP	CA-CB-CG	-8.50	104.10	112.60
2	1	407	LYS	N-CA-CB	8.49	124.06	110.65
4	3	7	SER	O-C-N	-8.47	113.57	122.30
2	1	314	ALA	N-CA-C	8.42	122.81	112.54
3	2	138	ASN	N-CA-C	8.42	120.76	110.41
2	1	133	ASN	OD1-CG-ND2	8.37	130.97	122.60
4	3	18	ARG	CA-C-O	-8.35	110.82	121.17
4	3	28	ARG	CD-NE-CZ	-8.34	112.73	124.40
3	2	159	VAL	CB-CA-C	8.29	121.40	110.12
3	2	128	THR	CB-CA-C	8.26	123.35	109.80
3	2	10	ASN	CB-CG-ND2	8.24	128.76	116.40
2	1	322	ASN	CA-C-O	-8.20	110.27	119.78
4	3	13	ARG	N-CA-C	-8.18	99.00	110.29
2	1	116	THR	O-C-N	-8.16	112.84	122.87
2	1	307	ALA	CA-C-O	-8.15	112.23	121.19
3	2	50	ASN	CA-C-O	-8.12	112.14	121.47
3	2	53	ASN	CB-CA-C	8.02	124.82	111.51
2	1	323	LEU	O-C-N	7.99	128.14	121.35
2	1	184	THR	CA-CB-OG1	-7.97	97.65	109.60
3	2	61	GLN	CA-C-O	-7.90	111.58	120.43
3	2	169	ILE	CA-CB-CG2	7.88	123.89	110.50
2	1	7	ALA	CA-C-N	-7.85	112.16	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	7	ALA	C-N-CA	-7.85	112.16	123.00
2	1	411	THR	CA-CB-OG1	-7.81	97.89	109.60
2	1	386	ARG	CB-CA-C	7.79	123.28	110.74
2	1	406	VAL	O-C-N	7.79	131.69	123.04
4	3	7	SER	N-CA-CB	-7.74	97.88	111.42
3	2	84	ASP	O-C-N	7.73	128.66	120.85
2	1	284	PHE	CA-CB-CG	7.72	121.52	113.80
2	1	296	THR	CA-CB-CG2	7.68	123.56	110.50
2	1	3	ILE	N-CA-CB	-7.67	102.70	112.60
2	1	119	ILE	O-C-N	7.64	128.37	121.57
2	1	274	ARG	CD-NE-CZ	-7.63	113.72	124.40
3	2	155	CYS	CA-C-N	7.61	135.06	122.73
3	2	155	CYS	C-N-CA	7.61	135.06	122.73
2	1	105	HIS	CA-CB-CG	-7.61	106.19	113.80
2	1	335	ARG	N-CA-CB	7.53	121.81	110.22
4	3	20	THR	N-CA-CB	-7.49	100.22	110.56
2	1	313	ILE	N-CA-C	7.47	119.50	111.58
2	1	386	ARG	CD-NE-CZ	-7.46	113.96	124.40
2	1	84	PHE	CA-CB-CG	7.43	121.23	113.80
2	1	118	LYS	O-C-N	7.43	131.73	123.33
2	1	426	SER	CA-C-O	-7.43	108.17	120.80
2	1	4	GLN	CA-CB-CG	7.39	128.89	114.10
2	1	116	THR	CA-C-N	-7.35	112.04	122.41
2	1	116	THR	C-N-CA	-7.35	112.04	122.41
2	1	316	ASP	CA-CB-CG	-7.23	105.37	112.60
3	2	23	VAL	O-C-N	7.22	131.23	123.00
4	3	13	ARG	CB-CA-C	7.20	119.23	108.86
2	1	9	ARG	NH1-CZ-NH2	7.20	128.65	119.30
3	2	168	ILE	N-CA-CB	-7.18	102.85	111.90
2	1	352	ARG	CD-NE-CZ	7.14	134.40	124.40
2	1	332	ASP	CA-CB-CG	-7.14	105.46	112.60
2	1	232	ASN	CA-C-O	-7.14	113.56	121.84
3	2	95	GLU	CB-CG-CD	7.13	124.72	112.60
2	1	67	PHE	CA-CB-CG	7.11	120.91	113.80
2	1	406	VAL	CB-CA-C	-7.10	99.75	110.55
3	2	14	PHE	CA-C-O	-7.10	113.03	120.70
2	1	418	THR	CA-CB-OG1	-7.09	98.96	109.60
2	1	208	ARG	NH1-CZ-NH2	-7.09	110.09	119.30
2	1	168	ILE	N-CA-C	-7.03	103.92	110.53
2	1	343	PHE	CA-CB-CG	7.03	120.83	113.80
2	1	54	LEU	CB-CA-C	7.01	121.36	109.80
3	2	82	ASP	CA-CB-CG	-7.00	105.60	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	18	ARG	CD-NE-CZ	7.00	134.21	124.40
4	3	5	LYS	CA-C-O	7.00	129.03	121.05
2	1	395	GLN	N-CA-C	-6.98	100.66	110.50
2	1	307	ALA	O-C-N	6.97	131.45	122.87
2	1	213	GLN	CA-CB-CG	-6.95	100.20	114.10
2	1	420	ARG	O-C-N	6.90	129.93	122.34
2	1	98	ASN	N-CA-C	6.89	120.17	109.07
2	1	369	PRO	CA-C-O	-6.88	113.58	121.97
2	1	382	ARG	NE-CZ-NH1	-6.82	114.68	121.50
4	3	6	ARG	CA-CB-CG	-6.81	100.48	114.10
2	1	371	ILE	CA-C-O	-6.81	112.39	120.76
2	1	60	ILE	CB-CA-C	-6.80	99.53	110.28
3	2	41	THR	CA-CB-CG2	6.80	122.06	110.50
2	1	63	THR	CA-CB-OG1	-6.76	99.46	109.60
2	1	323	LEU	CB-CA-C	6.76	119.42	109.08
3	2	10	ASN	CA-CB-CG	6.69	119.29	112.60
4	3	4	LYS	CA-C-O	6.69	130.07	120.51
2	1	274	ARG	CA-C-O	-6.68	113.86	121.07
2	1	76	VAL	CA-C-O	-6.67	113.05	120.46
2	1	381	GLU	CA-C-O	-6.67	112.30	119.97
4	3	6	ARG	CG-CD-NE	-6.67	97.33	112.00
2	1	46	VAL	CB-CA-C	6.66	119.18	110.12
2	1	192	ILE	CA-CB-CG1	-6.65	99.09	110.40
2	1	188	THR	CA-CB-OG1	-6.65	99.63	109.60
2	1	304	ALA	CA-C-O	-6.62	111.36	119.18
4	3	3	GLY	O-C-N	6.61	131.30	122.70
2	1	60	ILE	N-CA-C	6.60	117.81	108.17
2	1	161	ARG	NE-CZ-NH1	-6.56	114.94	121.50
3	2	59	CYS	CB-CA-C	-6.56	97.91	109.71
2	1	74	ARG	NE-CZ-NH2	6.55	125.09	119.20
2	1	268	TYR	CA-C-N	-6.55	111.51	121.86
2	1	268	TYR	C-N-CA	-6.55	111.51	121.86
2	1	180	SER	O-C-N	6.55	130.13	123.26
2	1	214	ARG	CD-NE-CZ	-6.55	115.23	124.40
2	1	418	THR	N-CA-CB	-6.54	100.43	110.04
4	3	11	PRO	O-C-N	6.53	131.46	122.64
2	1	420	ARG	N-CA-CB	-6.53	102.22	110.90
2	1	166	LYS	O-C-N	6.52	130.89	122.87
2	1	161	ARG	CD-NE-CZ	-6.51	115.28	124.40
2	1	174	PRO	CB-CA-C	6.49	118.83	110.92
2	1	418	THR	OG1-CB-CG2	6.48	122.25	109.30
2	1	55	ARG	NE-CZ-NH2	6.46	125.01	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	223	GLY	CA-C-N	-6.45	114.97	122.77
2	1	223	GLY	C-N-CA	-6.45	114.97	122.77
2	1	409	ASN	CA-C-N	-6.44	114.04	122.99
2	1	409	ASN	C-N-CA	-6.44	114.04	122.99
2	1	165	LEU	CB-CA-C	6.44	120.66	109.65
3	2	8	ARG	CA-C-O	-6.43	111.75	119.27
3	2	23	VAL	CA-C-N	-6.42	112.66	122.42
3	2	23	VAL	C-N-CA	-6.42	112.66	122.42
2	1	140	MET	N-CA-CB	6.42	118.64	109.78
3	2	149	ASN	N-CA-CB	6.39	119.89	110.49
2	1	271	SER	CA-C-O	6.37	127.12	120.30
2	1	96	THR	CA-C-O	-6.36	113.72	120.40
4	3	12	GLY	CA-C-O	6.35	127.59	121.49
2	1	240	SER	CA-C-O	6.33	127.54	120.70
2	1	187	THR	N-CA-C	6.33	118.18	111.28
3	2	54	GLY	N-CA-C	-6.30	101.91	111.42
3	2	91	LEU	N-CA-C	-6.29	99.47	109.59
3	2	127	VAL	CA-C-N	-6.28	113.34	122.19
3	2	127	VAL	C-N-CA	-6.28	113.34	122.19
2	1	106	ALA	CA-C-O	6.27	125.54	119.08
2	1	271	SER	CB-CA-C	-6.25	99.79	110.16
3	2	10	ASN	OD1-CG-ND2	-6.24	116.36	122.60
2	1	394	PHE	N-CA-C	6.24	119.81	110.14
2	1	419	THR	CA-C-N	-6.24	112.45	122.24
2	1	419	THR	C-N-CA	-6.24	112.45	122.24
2	1	366	GLU	CB-CG-CD	6.23	123.19	112.60
2	1	9	ARG	CG-CD-NE	-6.23	98.30	112.00
2	1	29	THR	CA-C-O	-6.22	113.60	120.69
2	1	112	ILE	CB-CA-C	6.22	119.73	111.21
2	1	165	LEU	N-CA-C	-6.21	101.09	110.28
3	2	117	ASP	CA-CB-CG	-6.20	106.40	112.60
2	1	251	GLY	N-CA-C	-6.19	103.70	112.37
2	1	191	ASP	CA-C-N	6.19	129.26	120.53
2	1	191	ASP	C-N-CA	6.19	129.26	120.53
3	2	38	THR	CA-C-O	6.19	125.64	118.77
2	1	142	ASP	CA-CB-CG	-6.18	106.42	112.60
4	3	3	GLY	CA-C-N	-6.16	109.77	121.54
4	3	3	GLY	C-N-CA	-6.16	109.77	121.54
3	2	162	ASN	CA-CB-CG	-6.15	106.45	112.60
3	2	172	GLN	O-C-N	6.14	126.91	121.32
3	2	132	LEU	CB-CA-C	6.14	118.01	108.61
2	1	151	LEU	N-CA-C	6.14	120.08	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	258	GLY	N-CA-C	-6.14	106.30	114.95
3	2	138	ASN	O-C-N	6.12	130.12	122.65
2	1	142	ASP	CA-C-O	-6.11	115.15	121.87
3	2	122	THR	CB-CA-C	6.11	121.44	109.35
3	2	24	THR	CA-C-O	6.10	125.35	119.62
3	2	92	VAL	CB-CA-C	-6.09	101.54	110.62
2	1	388	HIS	CA-C-O	-6.09	111.89	119.38
2	1	210	TYR	N-CA-C	6.09	119.18	111.69
2	1	372	GLN	N-CA-C	6.08	117.99	111.36
3	2	19	VAL	CA-C-N	6.08	132.04	120.97
3	2	19	VAL	C-N-CA	6.08	132.04	120.97
2	1	185	THR	CA-CB-OG1	-6.08	100.49	109.60
2	1	183	MET	N-CA-CB	6.06	120.11	110.65
2	1	391	ASP	CA-C-O	-6.06	114.42	120.90
2	1	241	ASN	CB-CG-OD1	-6.05	108.70	120.80
3	2	156	ARG	N-CA-CB	-6.02	100.10	111.00
4	3	29	LEU	CA-C-O	-6.01	112.44	119.24
2	1	242	LEU	CA-CB-CG	6.01	137.35	116.30
2	1	183	MET	N-CA-C	-5.99	98.65	108.41
4	3	18	ARG	CA-C-N	-5.97	109.70	121.41
4	3	18	ARG	C-N-CA	-5.97	109.70	121.41
2	1	144	THR	CA-CB-OG1	-5.97	100.64	109.60
2	1	38	GLY	CA-C-N	-5.96	111.89	122.74
2	1	38	GLY	C-N-CA	-5.96	111.89	122.74
2	1	255	THR	N-CA-CB	-5.94	101.17	110.44
4	3	9	ALA	N-CA-CB	-5.92	100.49	110.49
3	2	138	ASN	N-CA-CB	-5.91	102.28	110.38
2	1	143	ARG	NH1-CZ-NH2	5.91	126.98	119.30
2	1	305	LYS	O-C-N	-5.88	115.72	123.13
2	1	24	ILE	N-CA-C	5.88	116.52	110.82
3	2	33	GLN	CA-C-N	-5.85	112.69	120.65
3	2	33	GLN	C-N-CA	-5.85	112.69	120.65
3	2	169	ILE	CA-CB-CG1	-5.85	100.45	110.40
3	2	169	ILE	CB-CG1-CD1	-5.85	101.52	113.80
2	1	97	VAL	O-C-N	-5.85	117.50	122.65
2	1	112	ILE	CA-CB-CG1	-5.84	100.46	110.40
2	1	146	ALA	CA-C-O	-5.84	112.89	119.79
3	2	22	SER	CA-CB-OG	-5.84	99.41	111.10
2	1	232	ASN	CB-CA-C	-5.84	103.59	111.89
4	3	13	ARG	N-CA-CB	5.84	117.09	110.03
2	1	137	ALA	N-CA-C	-5.82	102.43	109.83
2	1	51	LEU	CB-CA-C	5.82	119.39	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	53	PRO	CA-C-N	-5.81	112.17	122.74
2	1	53	PRO	C-N-CA	-5.81	112.17	122.74
4	3	35	GLN	CB-CA-C	5.81	119.35	109.53
3	2	168	ILE	CA-CB-CG1	-5.77	100.59	110.40
2	1	164	HIS	CA-CB-CG	-5.77	108.03	113.80
2	1	53	PRO	CB-CA-C	5.77	118.91	111.64
2	1	103	ILE	CA-C-O	-5.76	115.07	121.17
2	1	117	ASN	N-CA-CB	5.75	118.94	110.49
2	1	420	ARG	NE-CZ-NH1	-5.75	115.75	121.50
2	1	283	MET	CA-CB-CG	5.75	125.60	114.10
2	1	306	GLY	N-CA-C	5.74	126.79	113.18
2	1	203	HIS	O-C-N	5.74	127.98	122.07
3	2	140	VAL	CB-CA-C	5.72	119.95	111.31
3	2	51	ALA	N-CA-C	-5.72	102.18	110.24
3	2	8	ARG	NE-CZ-NH2	-5.71	114.06	119.20
3	2	64	THR	CA-CB-OG1	-5.71	101.04	109.60
2	1	113	ASN	O-C-N	5.70	126.48	121.18
2	1	152	ASN	N-CA-CB	5.70	118.19	110.38
2	1	116	THR	N-CA-C	-5.69	101.97	110.23
3	2	175	LYS	CA-C-O	-5.69	111.13	120.80
4	3	13	ARG	CB-CG-CD	-5.68	98.24	111.30
2	1	422	SER	CA-C-O	-5.68	114.53	120.55
2	1	3	ILE	CB-CA-C	5.67	118.97	111.19
2	1	153	GLN	OE1-CD-NE2	5.65	128.25	122.60
3	2	115	ARG	NE-CZ-NH2	5.64	124.28	119.20
3	2	39	SER	CB-CA-C	5.62	119.98	109.86
3	2	108	ASP	CA-C-O	-5.62	114.89	121.46
3	2	125	ASP	N-CA-CB	-5.61	102.53	111.62
4	3	4	LYS	N-CA-CB	-5.61	101.01	110.49
3	2	50	ASN	O-C-N	5.60	129.29	122.96
2	1	232	ASN	CA-CB-CG	-5.60	107.00	112.60
2	1	213	GLN	CA-C-O	5.59	126.24	119.31
2	1	283	MET	N-CA-CB	-5.58	101.20	110.47
2	1	217	ASP	OD1-CG-OD2	5.57	136.28	122.90
3	2	83	ALA	CA-C-O	-5.57	115.11	121.68
3	2	78	ASP	CA-C-O	-5.57	114.32	120.33
2	1	328	ILE	N-CA-CB	-5.56	105.43	112.60
4	3	7	SER	CA-C-N	-5.54	110.54	121.41
4	3	7	SER	C-N-CA	-5.54	110.54	121.41
3	2	95	GLU	CA-CB-CG	5.54	125.19	114.10
4	3	6	ARG	N-CA-CB	-5.54	101.38	110.41
3	2	48	THR	CB-CA-C	5.53	119.25	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	51	LEU	O-C-N	-5.52	116.79	123.03
4	3	19	GLY	CA-C-N	-5.52	113.49	122.65
4	3	19	GLY	C-N-CA	-5.52	113.49	122.65
2	1	387	HIS	N-CA-CB	5.51	118.70	110.22
3	2	12	ASN	CB-CG-ND2	5.50	124.65	116.40
2	1	96	THR	CA-C-N	5.49	128.81	120.13
2	1	96	THR	C-N-CA	5.49	128.81	120.13
2	1	387	HIS	ND1-CE1-NE2	-5.49	102.91	108.40
2	1	98	ASN	CB-CA-C	-5.48	100.23	109.72
2	1	288	LEU	CA-C-O	-5.48	113.52	120.20
3	2	48	THR	CA-C-O	5.47	126.34	120.32
2	1	352	ARG	NE-CZ-NH2	-5.47	114.28	119.20
2	1	414	ARG	NE-CZ-NH2	-5.45	114.29	119.20
2	1	20	LEU	N-CA-C	5.45	118.59	110.14
2	1	89	VAL	CA-C-N	-5.45	113.96	122.73
2	1	89	VAL	C-N-CA	-5.45	113.96	122.73
2	1	45	ALA	CA-C-N	-5.44	114.37	122.70
2	1	45	ALA	C-N-CA	-5.44	114.37	122.70
2	1	137	ALA	CB-CA-C	5.44	117.96	109.42
2	1	55	ARG	NH1-CZ-NH2	-5.44	112.23	119.30
2	1	56	ARG	CD-NE-CZ	-5.44	116.79	124.40
2	1	192	ILE	CB-CG1-CD1	-5.43	102.39	113.80
3	2	39	SER	N-CA-CB	-5.43	101.37	110.99
3	2	29	ALA	CA-C-O	5.43	127.60	120.16
2	1	392	GLN	CA-CB-CG	-5.43	103.24	114.10
2	1	160	PHE	CA-CB-CG	5.42	119.22	113.80
2	1	39	ASP	CB-CA-C	5.40	118.71	109.80
2	1	290	ARG	NE-CZ-NH2	5.40	124.06	119.20
2	1	187	THR	CA-C-N	-5.40	111.34	121.81
2	1	187	THR	C-N-CA	-5.40	111.34	121.81
2	1	324	PRO	N-CA-C	5.39	117.28	110.70
4	3	24	ARG	O-C-N	5.39	129.58	123.27
2	1	60	ILE	CA-C-O	-5.39	114.56	120.43
2	1	241	ASN	CA-C-O	-5.38	114.47	120.66
3	2	89	ALA	CA-C-O	-5.38	115.05	121.56
2	1	63	THR	CB-CA-C	5.37	118.51	109.48
3	2	168	ILE	N-CA-C	5.37	115.82	107.28
2	1	322	ASN	OD1-CG-ND2	-5.36	117.24	122.60
2	1	5	THR	CA-C-N	-5.36	110.91	121.41
2	1	5	THR	C-N-CA	-5.36	110.91	121.41
2	1	220	SER	O-C-N	5.36	128.49	122.22
2	1	311	THR	N-CA-CB	5.35	117.99	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	32	THR	N-CA-CB	5.35	120.81	111.13
2	1	60	ILE	CB-CG1-CD1	-5.34	102.58	113.80
2	1	89	VAL	N-CA-C	5.34	116.71	110.62
2	1	326	ARG	NE-CZ-NH2	5.34	124.00	119.20
2	1	421	ASP	CA-C-O	5.34	126.21	120.55
2	1	3	ILE	O-C-N	5.33	128.57	122.97
4	3	12	GLY	O-C-N	-5.33	118.49	123.87
2	1	272	VAL	O-C-N	5.30	124.71	121.37
3	2	53	ASN	N-CA-CB	-5.29	99.95	110.64
2	1	416	LEU	N-CA-C	-5.28	99.89	109.09
3	2	8	ARG	N-CA-CB	5.28	118.68	110.44
3	2	37	ALA	O-C-N	-5.27	115.18	122.30
3	2	86	LYS	CA-CB-CG	-5.27	103.56	114.10
3	2	34	THR	CB-CA-C	5.27	117.89	109.62
2	1	422	SER	CA-C-N	-5.26	114.26	122.09
2	1	422	SER	C-N-CA	-5.26	114.26	122.09
2	1	93	PRO	CA-C-O	-5.25	115.47	121.56
2	1	12	HIS	CA-CB-CG	-5.25	108.55	113.80
2	1	183	MET	CA-C-N	-5.25	114.11	121.72
2	1	183	MET	C-N-CA	-5.25	114.11	121.72
3	2	166	LYS	CA-C-N	-5.25	113.34	122.64
3	2	166	LYS	C-N-CA	-5.25	113.34	122.64
3	2	139	ASN	CA-C-N	-5.25	114.19	122.64
3	2	139	ASN	C-N-CA	-5.25	114.19	122.64
3	2	47	LEU	CA-C-N	-5.24	115.71	123.05
3	2	47	LEU	C-N-CA	-5.24	115.71	123.05
4	3	37	PHE	CA-CB-CG	-5.24	108.56	113.80
3	2	117	ASP	O-C-N	5.24	129.32	123.40
2	1	269	LYS	CB-CA-C	5.22	117.86	110.24
2	1	74	ARG	O-C-N	5.21	127.64	122.12
3	2	3	GLN	OE1-CD-NE2	-5.21	117.39	122.60
2	1	241	ASN	N-CA-CB	-5.20	101.59	111.00
2	1	98	ASN	O-C-N	5.19	129.42	123.29
2	1	186	SER	CA-CB-OG	-5.17	100.75	111.10
3	2	92	VAL	O-C-N	5.17	128.76	123.18
2	1	415	ASN	OD1-CG-ND2	-5.17	117.43	122.60
2	1	417	PRO	CA-C-N	5.17	128.55	120.75
2	1	417	PRO	C-N-CA	5.17	128.55	120.75
2	1	69	PHE	CA-CB-CG	5.16	118.96	113.80
2	1	186	SER	CA-C-O	-5.15	115.59	121.82
2	1	413	TYR	CB-CA-C	5.15	120.27	111.68
2	1	129	ASN	O-C-N	5.14	127.57	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	144	THR	O-C-N	-5.14	115.01	121.95
3	2	27	SER	N-CA-C	-5.11	105.71	111.28
3	2	95	GLU	N-CA-CB	5.11	119.47	111.20
2	1	142	ASP	O-C-N	5.10	128.72	122.75
2	1	190	ILE	N-CA-C	-5.10	100.55	108.86
2	1	144	THR	OG1-CB-CG2	5.10	119.50	109.30
2	1	180	SER	CA-C-O	-5.10	115.98	121.38
3	2	131	VAL	CA-C-O	-5.10	113.11	119.43
2	1	309	THR	O-C-N	-5.10	116.72	122.68
3	2	8	ARG	NH1-CZ-NH2	5.09	125.91	119.30
3	2	37	ALA	CA-C-N	-5.09	114.25	122.24
3	2	37	ALA	C-N-CA	-5.09	114.25	122.24
2	1	201	ASN	CB-CG-ND2	5.08	124.03	116.40
4	3	2	LYS	CA-C-N	5.07	131.35	121.41
4	3	2	LYS	C-N-CA	5.07	131.35	121.41
2	1	229	ASP	CA-C-O	-5.07	113.81	119.79
2	1	177	THR	CA-CB-OG1	-5.07	102.00	109.60
2	1	417	PRO	CA-C-O	5.06	128.28	121.95
2	1	92	THR	CA-C-O	-5.06	114.79	120.25
2	1	343	PHE	CB-CA-C	5.06	119.42	110.16
3	2	97	SER	CA-CB-OG	-5.05	101.00	111.10
2	1	143	ARG	N-CA-C	-5.05	100.94	108.96
2	1	52	SER	N-CA-C	-5.03	102.96	110.20
2	1	283	MET	CB-CA-C	5.02	118.97	110.79
2	1	149	ASN	CA-CB-CG	-5.01	107.59	112.60
2	1	377	GLY	CA-C-N	-5.01	111.64	121.06
2	1	377	GLY	C-N-CA	-5.01	111.64	121.06
2	1	174	PRO	CA-C-N	5.01	126.10	119.84
2	1	174	PRO	C-N-CA	5.01	126.10	119.84
2	1	189	SER	N-CA-C	-5.01	101.13	108.79
2	1	344	LYS	O-C-N	5.00	128.92	123.27

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	198	0
3	2	1339	0	1323	75	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
5	A	2	0	0	2	0
All	All	5298	0	4978	304	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 30.

All (304) 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
2:1:238:MET:HE3	2:1:239:ARG:H	1.19	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
2:1:244:ALA:HA	2:1:266:GLN:HG2	1.47	0.96
3:2:103:LEU:HD12	3:2:104:PRO:HD2	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:132:ASN:HD21	2:1:143:ARG:H	1.13	0.96
2:1:149:ASN:C	2:1:149:ASN:HD22	1.74	0.94
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
2:1:323:LEU:CD2	2:1:323:LEU:N	2.32	0.93
4:3:4:LYS:HE2	4:3:5:LYS:N	1.83	0.93
3:2:67:ASN:C	3:2:67:ASN:HD22	1.72	0.92
2:1:265:GLN:HB2	5:1:435:HOH:O	1.70	0.91
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
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
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
2:1:42:GLU:OE2	2:1:413:TYR:HE1	1.67	0.77
2:1:98:ASN:N	2:1:147:ASN:HD22	1.76	0.77
2:1:98:ASN:H	2:1:147:ASN:ND2	1.78	0.77
2:1:323:LEU:CD2	2:1:323:LEU:H	1.97	0.76
4:3:6:ARG:CD	4:3:6:ARG:N	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
2:1:137:ALA:CB	2:1:140:MET:HE3	2.17	0.74
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
2:1:238:MET:HE3	2:1:239:ARG:N	1.99	0.74
2:1:138:PRO:HD2	4:3:32:VAL:HG13	1.69	0.74
2:1:319:LEU:O	2:1:323:LEU:HD22	1.88	0.74
2:1:175:PRO:HG3	2:1:379:LEU:HD23	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:39:SER:HB2	3:2:162:ASN:ND2	1.98	0.73
2:1:323:LEU:H	2:1:323:LEU:HD23	1.52	0.73
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
2:1:9:ARG:N	5:1:436:HOH:O	2.18	0.72
2:1:137:ALA:HB3	2:1:140:MET:HE3	1.72	0.71
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
4:3:2:LYS:HG2	4:3:3:GLY:N	2.03	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
2:1:238:MET:CE	2:1:239:ARG:H	2.02	0.69
1:A:2:DA:H5''	4:3:28:ARG:CB	2.24	0.68
2:1:323:LEU:N	2:1:323:LEU:HD23	2.06	0.67
3:2:22:SER:HA	3:2:48:THR:O	1.95	0.67
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
2:1:82:ILE:O	2:1:86:LYS:HG3	1.96	0.66
2:1:96:THR:HG21	2:1:118:LYS:HD3	1.78	0.66
2:1:420:ARG:HA	2:1:423:ILE:HG12	1.77	0.66
2:1:305:LYS:O	2:1:305:LYS:HD3	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
2:1:43:MET:HE1	2:1:270:HIS:HD2	1.61	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
2:1:70:TYR:CD1	2:1:283:MET:HE1	2.33	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
2:1:96:THR:CG2	2:1:118:LYS:HD3	2.29	0.63
2:1:175:PRO:HG3	2:1:379:LEU:CD2	2.28	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
3:2:82:ASP:CG	3:2:156:ARG:HH22	2.08	0.62
2:1:45:ALA:HB3	2:1:270:HIS:HB3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:26:ARG:HH11	2:1:387:HIS:HD2	1.48	0.61
2:1:183:MET:HE2	2:1:190:ILE:CD1	2.30	0.61
4:3:8:GLY:C	4:3:10:ARG:H	2.07	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
3:2:62:MET:HE2	3:2:62:MET:HA	1.83	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:HG23	2:1:96:THR:O	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
3:2:67:ASN:C	3:2:67:ASN:ND2	2.46	0.58
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
2:1:183:MET:HE2	2:1:190:ILE:HD12	1.86	0.58
2:1:365:LEU:HD23	2:1:368:PHE:HE2	1.69	0.57
2:1:10:MET:O	2:1:12:HIS:HD2	1.87	0.57
2:1:379:LEU:O	2:1:383:VAL:HG13	2.04	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
3:2:22:SER:HB3	3:2:48:THR:HG1	1.70	0.56
2:1:70:TYR:HD1	2:1:283:MET:HE1	1.70	0.56
4:3:7:SER:C	4:3:9:ALA:H	2.12	0.56
2:1:71:VAL:HG22	2:1:234:PRO:HB3	1.87	0.56
2:1:100:THR:HG22	2:1:102:TYR:CD2	2.41	0.56
3:2:12:ASN:HD22	3:2:12:ASN:C	2.12	0.56
2:1:418:THR:HG22	2:1:421:ASP:N	2.20	0.56
3:2:26:ALA:C	3:2:54:GLY:HA3	2.30	0.55
2:1:3:ILE:HD12	2:1:5:THR:HG23	1.87	0.55
2:1:149:ASN:C	2:1:149:ASN:ND2	2.49	0.55
2:1:365:LEU:HD23	2:1:368:PHE:CE2	2.41	0.55
3:2:45:ASP:OD1	3:2:45:ASP:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:419:THR:O	2:1:419:THR:CG2	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
1:A:2:DA:O5'	4:3:31:TYR:OH	2.25	0.55
3:2:24:THR:HB	3:2:50:ASN:CB	2.35	0.55
2:1:133:ASN:C	2:1:214:ARG:HH21	2.15	0.54
3:2:22:SER:HB3	3:2:48:THR:OG1	2.06	0.54
2:1:99:THR:OG1	2:1:117:ASN:HB3	2.06	0.54
2:1:167:ASN:HB2	2:1:170:THR:CG2	2.37	0.54
2:1:419:THR:O	2:1:419:THR:HG22	2.08	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
2:1:14:LEU:HD12	2:1:412:VAL:CG2	2.38	0.53
3:2:64:THR:HG22	3:2:132:LEU:HD23	1.90	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
2:1:137:ALA:HB2	2:1:140:MET:HE3	1.90	0.52
2:1:64:VAL:O	2:1:241:ASN:HA	2.10	0.52
2:1:349:GLN:HA	2:1:349:GLN:NE2	2.25	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
3:2:12:ASN:ND2	3:2:14:PHE:H	2.09	0.51
3:2:95:GLU:HB2	3:2:138:ASN:HB3	1.92	0.51
4:3:7:SER:C	4:3:9:ALA:N	2.68	0.51
3:2:49:VAL:O	3:2:152:ALA:HA	2.11	0.51
3:2:156:ARG:NH1	3:2:156:ARG:HG3	2.24	0.51
3:2:67:ASN:ND2	3:2:67:ASN:O	2.43	0.50
2:1:238:MET:HE3	2:1:239:ARG:O	2.11	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
2:1:214:ARG:HD2	5:1:502:HOH:O	2.11	0.50
3:2:53:ASN:HD22	3:2:53:ASN:C	2.18	0.50
4:3:21:LYS:CE	4:3:25:LYS:HE3	2.41	0.50
3:2:74:SER:HA	3:2:126:CYS:HA	1.93	0.50
2:1:3:ILE:CD1	2:1:5:THR:CG2	2.90	0.50
2:1:74:ARG:HG2	2:1:74:ARG:HH11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:238:MET:CE	2:1:239:ARG:O	2.59	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
3:2:151:THR:O	3:2:152:ALA:C	2.54	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
2:1:137:ALA:HA	4:3:36:GLN:HG3	1.93	0.49
2:1:208:ARG:HG2	2:1:212:MET:CE	2.42	0.49
2:1:43:MET:HE1	2:1:270:HIS:CD2	2.46	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:O	2:1:9:ARG:HG2	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
2:1:299:ILE:HG21	2:1:304:ALA:HB2	1.94	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
3:2:25:PRO:HD2	3:2:50:ASN:O	2.13	0.48
3:2:37:ALA:HA	3:2:61:GLN:HB3	1.95	0.48
3:2:169:ILE:HD12	3:2:169:ILE:HG23	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
2:1:97: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
2:1:247:TYR:CE1	2:1:263:ARG:HD3	2.49	0.47
3:2:39:SER:HA	3:2:161:LEU:O	2.15	0.47
3:2:62:MET:HE2	3:2:62:MET:CA	2.45	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
2:1:416:LEU:HD23	2:1:416:LEU:C	2.40	0.47
2:1:265:GLN:CB	5:1:435:HOH:O	2.47	0.46
3:2:113:ASN:C	3:2:113:ASN:ND2	2.70	0.46
2:1:23:GLN:OE1	2:1:401:GLN:HG3	2.16	0.46
2:1:208:ARG:HG2	2:1:212:MET:HE1	1.98	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:CG2	2:1:96:THR:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:200:ALA:O	2:1:204:THR:HG23	2.15	0.45
4:3:8:GLY:C	4:3:10:ARG:N	2.68	0.45
2:1:116:THR:H	2:1:116:THR:HG23	1.49	0.45
2:1:244:ALA:HA	2:1:266:GLN:CG	2.32	0.45
2:1:35:VAL:HG11	2:1:283:MET:HE3	1.99	0.44
2:1:183:MET:HE2	2:1:190:ILE:HD11	1.98	0.44
3:2:169:ILE:H	3:2:169:ILE:CD1	2.24	0.44
2:1:212:MET:HB2	2:1:212:MET:HE3	1.41	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
3:2:12:ASN:C	3:2:12:ASN:ND2	2.74	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
2:1:233:ARG:HA	2:1:234:PRO:HD3	1.90	0.44
3:2:8:ARG:HH11	3:2:8:ARG:HD2	1.41	0.44
2:1:82:ILE:O	2:1:86:LYS:CG	2.65	0.43
2:1:174:PRO:HA	2:1:175:PRO:HD3	1.79	0.43
2:1:63:THR:HB	2:1:243:TRP:CH2	2.52	0.43
2:1:305:LYS:O	2:1:306:GLY:O	2.36	0.43
2:1:3:ILE:HD11	2:1:5:THR:HG22	2.01	0.43
2:1:415:ASN:OD1	2:1:415:ASN:O	2.36	0.43
3:2:52:GLY:O	3:2:150:PHE:N	2.51	0.43
2:1:39:ASP:HB3	5:1:448:HOH:O	2.18	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
2:1:386:ARG:HD3	2:1:389:ASP:OD1	2.18	0.43
2:1:43:MET:CE	2:1:270:HIS:CD2	3.00	0.43
2:1:61:ASP:OD1	4:3:16:PRO:HB2	2.18	0.43
2:1:371:ILE:HD13	2:1:371:ILE:HG21	1.87	0.43
2:1:35:VAL:HG22	2:1:281:GLY:O	2.17	0.43
2:1:9:ARG:O	2:1:9:ARG:CG	2.63	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:HE3	2:1:225:LYS:HB3	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
3:2:98:SER:O	3:2:99:VAL:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:90:ASN:N	5:1:532:HOH:O	2.46	0.42
2:1:167:ASN:CB	2:1:170:THR:H	2.32	0.42
2:1:286:LEU:N	2:1:286:LEU:HD12	2.35	0.42
4:3:5:LYS:HA	4:3:6:ARG:HD3	2.02	0.42
2:1:113:ASN:HA	2:1:114:PRO:HD3	1.86	0.42
3:2:29:ALA:O	3:2:102:THR:HA	2.20	0.42
2:1:26:ARG:HH11	2:1:26:ARG:HD2	1.68	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:CG	3.03	0.42
2:1:169:TRP:CZ3	2:1:375:PRO:HG2	2.54	0.42
3:2:18:LEU:HB3	3:2:44:PHE:HB3	2.02	0.42
2:1:74:ARG:NH1	2:1:74:ARG:CG	2.80	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
2:1:238:MET:CG	2:1:239:ARG:N	2.82	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
2:1:12: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
2:1:165:LEU:O	2:1:170:THR:CG2	2.52	0.41
2:1:208:ARG:HA	2:1:212:MET:HE2	2.02	0.41
3:2:62:MET:CG	3:2:140:VAL:HG22	2.50	0.41
2:1:305:LYS:HE2	2:1:305:LYS:HB2	1.70	0.41
3:2:9:HIS:HB3	3:2:124:LYS:HG3	2.02	0.41
2:1:134:TYR:HB3	4:3:37:PHE:CE2	2.55	0.41
2:1:420:ARG:O	2:1:424:MET:HB2	2.21	0.41
2:1:53:PRO:HG2	2:1:395:GLN:HB2	2.02	0.41
2:1:328:ILE:HG22	2:1:343:PHE:O	2.21	0.41
3:2:62:MET:HG2	3:2:140:VAL:HG22	2.02	0.41
2:1:138:PRO:CD	4:3:32:VAL:CG1	2.99	0.40
2:1:4:GLN:HE21	2:1:4:GLN:HB3	1.71	0.40
2:1:196:GLN:NE2	2:1:196:GLN:CA	2.76	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:HD23	3:2:112:LEU:HA	1.89	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	
2	1	424/426 (100%)	406 (96%)	16 (4%)	2 (0%)	24	60
3	2	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
4	3	34/37 (92%)	24 (71%)	5 (15%)	5 (15%)	0	0
All	All	631/638 (99%)	595 (94%)	29 (5%)	7 (1%)	11	43

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
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%)	321 (86%)	51 (14%)	3	17
3	2	153/153 (100%)	122 (80%)	31 (20%)	1	7
4	3	26/27 (96%)	15 (58%)	11 (42%)	0	0
All	All	551/552 (100%)	458 (83%)	93 (17%)	2	11

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	1	SER
2	1	9	ARG
2	1	40	SER
2	1	46	VAL
2	1	49	LEU
2	1	51	LEU
2	1	54	LEU
2	1	60	ILE
2	1	79	GLU
2	1	86	LYS
2	1	89	VAL
2	1	97	VAL
2	1	112	ILE
2	1	118	LYS
2	1	144	THR
2	1	149	ASN
2	1	152	ASN
2	1	164	HIS
2	1	167	ASN
2	1	170	THR
2	1	184	THR
2	1	186	SER
2	1	187	THR
2	1	190	ILE
2	1	192	ILE
2	1	196	GLN
2	1	204	THR
2	1	211	PHE
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	318	VAL
2	1	323	LEU
2	1	328	ILE
2	1	339	SER

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Mol	Chain	Res	Type
2	1	345	ILE
2	1	349	GLN
2	1	383	VAL
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	6	ILE
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	57	LEU
3	2	67	ASN
3	2	79	ILE
3	2	91	LEU
3	2	92	VAL
3	2	95	GLU
3	2	105	THR
3	2	115	ARG
3	2	122	THR
3	2	128	THR
3	2	140	VAL
3	2	151	THR
3	2	154	LYS
3	2	159	VAL
3	2	161	LEU
3	2	169	ILE
3	2	174	LEU
4	3	2	LYS
4	3	4	LYS

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Mol	Chain	Res	Type
4	3	6	ARG
4	3	7	SER
4	3	13	ARG
4	3	15	GLN
4	3	17	LEU
4	3	18	ARG
4	3	23	LYS
4	3	32	VAL
4	3	35	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) 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	73	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	167	ASN
2	1	182	GLN
2	1	196	GLN
2	1	206	GLN
2	1	266	GLN
2	1	300	GLN
2	1	303	ASN
2	1	322	ASN
2	1	349	GLN
2	1	387	HIS
2	1	392	GLN
2	1	398	GLN
3	2	9	HIS
3	2	12	ASN
3	2	53	ASN
3	2	67	ASN

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Mol	Chain	Res	Type
3	2	113	ASN
3	2	149	ASN
3	2	162	ASN
3	2	163	GLN
4	3	15	GLN
4	3	36	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 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.