



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:15 PM EDT

PDB ID : 2MEV / pdb_00002mev
Title : STRUCTURAL REFINEMENT AND ANALYSIS OF MENO VIRUS
Authors : Rossmann, M.G.
Deposited on : 1989-04-21
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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

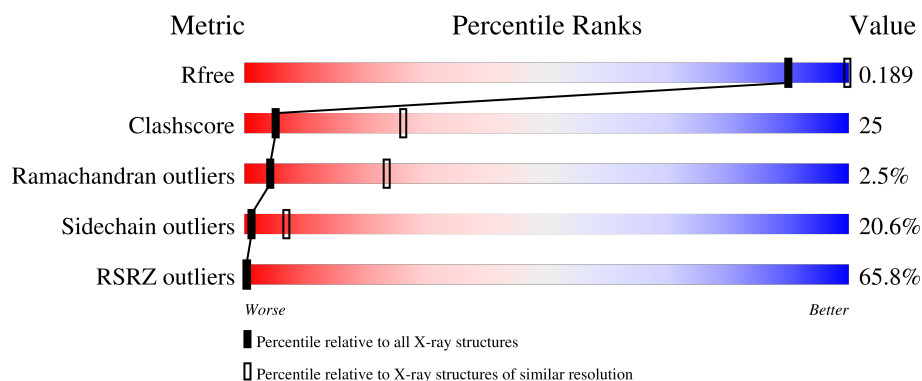
1 Overall quality at a glance

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))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	1	277	68% 34% 36% 18% 9% .
2	2	256	71% 37% 34% 17% 9% .
3	3	231	61% 42% 30% 20% 7%
4	4	70	26% 17% 33% 19% 14% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	2	257	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6507 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 MENO VIRUS COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	268	Total	C	N	O	S	0	0	0
			2091	1345	342	397	7			

- Molecule 2 is a protein called MENO VIRUS COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	249	Total	C	N	O	S	0	0	0
			1973	1247	349	372	5			

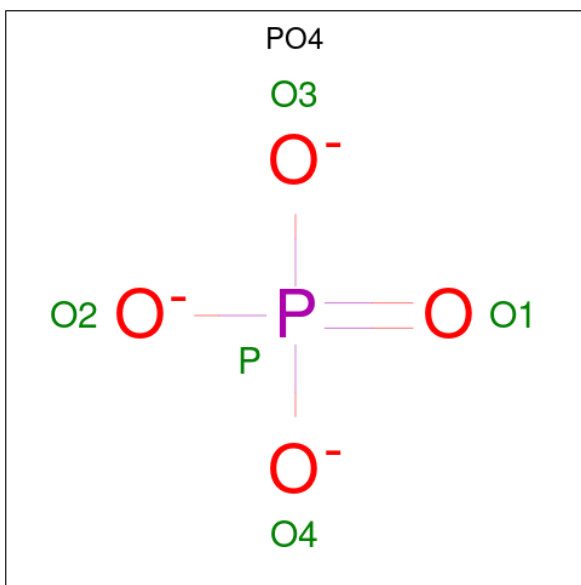
- Molecule 3 is a protein called MENO VIRUS COAT PROTEIN (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	231	Total	C	N	O	S	0	0	0
			1772	1153	283	326	10			

- Molecule 4 is a protein called MENO VIRUS COAT PROTEIN (SUBUNIT VP4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	58	Total	C	N	O	S	0	0	0
			433	270	71	91	1			

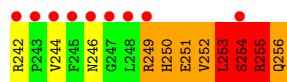
- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



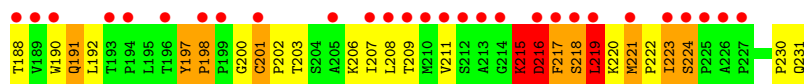
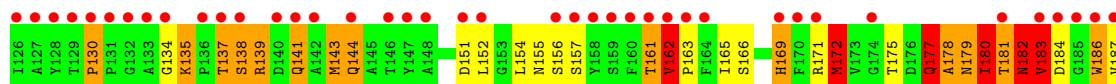
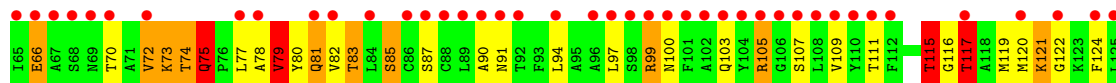
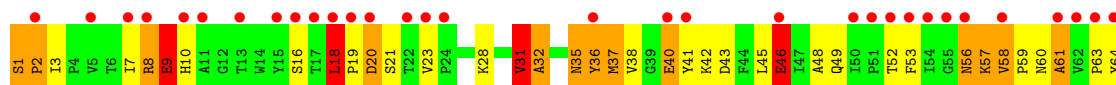
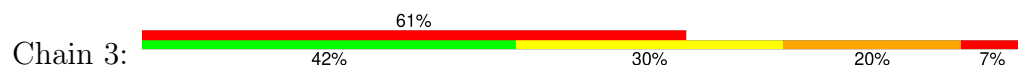
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	2	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

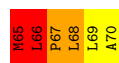
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	106	Total	O	0	0
			106	106		
6	2	69	Total	O	0	0
			69	69		
6	3	49	Total	O	0	0
			49	49		
6	4	9	Total	O	0	0
			9	9		



• Molecule 3: MENGO VIRUS COAT PROTEIN (SUBUNIT VP3)



• Molecule 4: MENGO VIRUS COAT PROTEIN (SUBUNIT VP4)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	441.42Å 427.31Å 421.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 10.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.00) 48.8 (10.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.61Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.221 , (Not available) 0.207 , 0.189	Depositor DCC
R_{free} test set	2516 reflections (0.25%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 162.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l 0.050 for -l,-k,-h 0.049 for -h,l,k 0.049 for l,h,k 0.049 for k,l,h	Xtriage
F_o, F_c correlation	0.07	EDS
Total number of atoms	6507	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	1.42	4/2159 (0.2%)	3.02	248/2952 (8.4%)
2	2	1.40	8/2028 (0.4%)	3.02	233/2776 (8.4%)
3	3	1.35	8/1829 (0.4%)	2.73	185/2512 (7.4%)
4	4	1.72	5/441 (1.1%)	4.11	101/600 (16.8%)
All	All	1.41	25/6457 (0.4%)	3.03	767/8840 (8.7%)

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	2	0	2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	20	GLY	N-CA	9.38	1.58	1.45
2	2	255	ARG	CA-C	7.89	1.63	1.53
1	1	211	THR	CB-OG1	7.74	1.56	1.43
3	3	180	ILE	CA-CB	7.16	1.64	1.54
1	1	67	ASN	N-CA	-6.12	1.38	1.46
3	3	181	THR	CA-CB	6.10	1.63	1.53
2	2	44	HIS	ND1-CE1	6.06	1.38	1.32
3	3	58	VAL	CA-C	5.99	1.59	1.52
4	4	47	THR	CB-OG1	5.97	1.53	1.43
4	4	21	ILE	CA-CB	5.78	1.60	1.54
3	3	57	LYS	C-N	-5.74	1.26	1.33
2	2	181	GLN	N-CA	5.71	1.53	1.46
1	1	260	THR	CA-CB	5.58	1.60	1.52
3	3	171	ARG	NE-CZ	5.51	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	47	THR	CA-CB	5.39	1.63	1.53
4	4	14	GLU	CA-C	5.33	1.59	1.52
2	2	255	ARG	CZ-NH2	5.32	1.40	1.33
3	3	58	VAL	N-CA	-5.29	1.40	1.46
2	2	32	ARG	NE-CZ	5.25	1.38	1.33
4	4	70	ALA	C-O	5.21	1.33	1.23
3	3	58	VAL	C-N	5.17	1.44	1.34
2	2	11	SER	CB-OG	5.16	1.52	1.42
3	3	216	ASP	CA-CB	5.14	1.61	1.53
1	1	265	ILE	C-O	5.12	1.30	1.24
2	2	254	SER	CA-C	5.09	1.59	1.52

All (767) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	267	MET	CA-C-N	28.35	172.73	121.70
1	1	267	MET	C-N-CA	28.35	172.73	121.70
4	4	64	ASN	CA-CB-CG	26.43	139.03	112.60
1	1	266	ASP	CA-CB-CG	24.89	137.49	112.60
2	2	10	LEU	CA-C-N	24.00	167.38	121.54
2	2	10	LEU	C-N-CA	24.00	167.38	121.54
3	3	180	ILE	CA-C-N	20.24	153.87	122.49
3	3	180	ILE	C-N-CA	20.24	153.87	122.49
1	1	66	PRO	CA-C-N	18.98	147.24	120.29
1	1	66	PRO	C-N-CA	18.98	147.24	120.29
1	1	263	ASP	CA-CB-CG	18.41	131.01	112.60
2	2	161	ARG	CD-NE-CZ	18.04	149.65	124.40
2	2	145	ARG	CD-NE-CZ	16.24	147.13	124.40
2	2	254	SER	CA-C-O	16.20	139.65	121.02
4	4	65	MET	CA-C-O	16.10	139.18	120.66
1	1	67	ASN	CA-CB-CG	-15.71	96.89	112.60
4	4	27	ASN	CA-CB-CG	-15.69	96.91	112.60
2	2	144	ASN	OD1-CG-ND2	15.12	137.72	122.60
2	2	186	ARG	CD-NE-CZ	15.09	145.52	124.40
1	1	154	PRO	CA-C-O	14.94	132.36	121.31
3	3	216	ASP	CA-CB-CG	-14.83	97.77	112.60
4	4	14	GLU	N-CA-CB	14.57	132.90	111.05
4	4	27	ASN	N-CA-C	14.21	128.05	111.71
2	2	253	LEU	O-C-N	14.07	141.30	122.59
1	1	266	ASP	CA-C-N	13.59	147.50	121.54
1	1	266	ASP	C-N-CA	13.59	147.50	121.54
4	4	63	SER	CA-CB-OG	13.57	138.25	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	223	THR	CA-CB-OG1	-13.52	89.33	109.60
2	2	9	ASN	CA-CB-CG	13.48	126.08	112.60
2	2	223	THR	CA-CB-CG2	13.34	133.17	110.50
2	2	254	SER	N-CA-CB	13.21	130.75	109.88
2	2	255	ARG	CA-C-N	13.13	145.34	121.70
2	2	255	ARG	C-N-CA	13.13	145.34	121.70
1	1	267	MET	CA-C-O	12.85	138.89	120.51
2	2	255	ARG	CA-C-O	12.80	135.30	120.70
2	2	144	ASN	CA-CB-CG	-12.73	99.87	112.60
2	2	255	ARG	N-CA-CB	12.64	131.82	110.46
2	2	9	ASN	OD1-CG-ND2	-12.58	110.02	122.60
2	2	71	THR	CA-CB-OG1	-12.45	90.93	109.60
3	3	99	ARG	CA-CB-CG	12.34	138.78	114.10
1	1	24	VAL	N-CA-CB	-12.34	90.87	111.23
3	3	144	GLN	OE1-CD-NE2	12.22	134.82	122.60
1	1	124	LYS	CA-CB-CG	12.13	138.36	114.10
4	4	60	ASN	CA-C-N	12.11	144.68	121.54
4	4	60	ASN	C-N-CA	12.11	144.68	121.54
1	1	213	ASP	CA-CB-CG	-12.03	100.57	112.60
2	2	139	VAL	N-CA-CB	-11.82	94.77	112.15
4	4	67	PRO	CA-C-N	11.74	138.39	121.02
4	4	67	PRO	C-N-CA	11.74	138.39	121.02
3	3	182	ASN	CB-CG-ND2	11.72	133.99	116.40
3	3	74	THR	CA-CB-OG1	-11.58	92.23	109.60
2	2	32	ARG	NE-CZ-NH2	11.45	129.51	119.20
4	4	65	MET	CA-C-N	11.41	149.65	121.80
4	4	65	MET	C-N-CA	11.41	149.65	121.80
2	2	32	ARG	CD-NE-CZ	-11.30	108.58	124.40
4	4	21	ILE	CA-C-O	11.16	133.63	121.36
1	1	188	VAL	N-CA-CB	-10.95	95.89	111.21
2	2	230	THR	CA-CB-OG1	-10.94	93.19	109.60
1	1	155	THR	CA-CB-OG1	-10.84	93.35	109.60
2	2	102	ARG	NE-CZ-NH2	-10.83	109.45	119.20
1	1	67	ASN	OD1-CG-ND2	10.77	133.37	122.60
3	3	181	THR	CA-C-O	10.69	132.04	119.32
2	2	160	ASN	CA-CB-CG	-10.67	101.93	112.60
1	1	267	MET	O-C-N	-10.67	108.40	122.59
2	2	138	ASP	CA-C-O	10.66	132.14	120.63
4	4	60	ASN	CA-CB-CG	10.64	123.24	112.60
4	4	63	SER	CA-C-N	10.59	137.89	122.21
4	4	63	SER	C-N-CA	10.59	137.89	122.21
1	1	87	GLN	OE1-CD-NE2	10.50	133.10	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	183	VAL	CB-CA-C	10.49	128.50	111.29
3	3	161	THR	CA-C-N	-10.46	115.06	122.59
3	3	161	THR	C-N-CA	-10.46	115.06	122.59
2	2	181	GLN	CB-CA-C	10.44	129.27	110.16
2	2	255	ARG	N-CA-C	-10.40	87.13	107.62
1	1	78	ASP	N-CA-CB	10.36	128.81	110.37
2	2	53	SER	N-CA-C	-10.33	92.40	109.24
1	1	190	TYR	N-CA-C	-10.31	91.43	108.34
1	1	211	THR	N-CA-CB	10.28	125.38	110.58
1	1	78	ASP	O-C-N	10.23	133.09	121.32
1	1	11	GLU	CA-CB-CG	10.21	134.53	114.10
2	2	22	THR	CA-CB-OG1	-10.18	94.33	109.60
4	4	59	VAL	CA-C-O	10.15	133.47	120.78
4	4	45	PRO	CA-C-N	10.15	134.90	120.28
4	4	45	PRO	C-N-CA	10.15	134.90	120.28
4	4	68	LEU	CA-C-N	10.15	135.21	120.90
4	4	68	LEU	C-N-CA	10.15	135.21	120.90
1	1	230	THR	CA-C-O	-10.12	108.14	118.97
2	2	144	ASN	N-CA-CB	-10.11	95.14	110.20
1	1	190	TYR	CB-CA-C	10.08	126.27	110.14
1	1	209	ASP	CA-CB-CG	10.03	122.63	112.60
1	1	207	ARG	CD-NE-CZ	10.00	138.40	124.40
4	4	23	ASN	OD1-CG-ND2	9.98	132.58	122.60
2	2	143	ASP	CA-C-O	9.96	132.31	121.16
1	1	87	GLN	CA-CB-CG	-9.91	94.28	114.10
3	3	60	ASN	OD1-CG-ND2	9.87	132.47	122.60
3	3	58	VAL	CB-CA-C	9.87	129.31	111.36
2	2	111	ARG	CD-NE-CZ	-9.86	110.59	124.40
2	2	22	THR	CA-C-O	-9.83	110.08	120.70
1	1	29	ASN	CA-CB-CG	-9.80	102.80	112.60
4	4	27	ASN	OD1-CG-ND2	9.71	132.31	122.60
3	3	58	VAL	N-CA-CB	-9.67	97.67	111.21
1	1	266	ASP	CA-C-O	9.66	134.33	120.51
3	3	183	VAL	CA-CB-CG2	9.59	126.70	110.40
3	3	219	LEU	CA-C-O	-9.57	109.95	121.06
2	2	20	GLY	O-C-N	9.56	135.12	122.70
2	2	101	ARG	NE-CZ-NH2	9.52	127.77	119.20
3	3	191	GLN	OE1-CD-NE2	9.52	132.12	122.60
2	2	19	ALA	CA-C-O	-9.50	108.94	119.40
2	2	230	THR	N-CA-C	9.50	125.18	113.50
2	2	81	ARG	CD-NE-CZ	-9.48	111.13	124.40
2	2	201	ALA	O-C-N	9.45	127.75	121.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	177	GLN	CB-CG-CD	9.43	128.63	112.60
4	4	54	LEU	CA-C-N	-9.42	110.25	122.77
4	4	54	LEU	C-N-CA	-9.42	110.25	122.77
3	3	3	ILE	N-CA-C	9.41	116.72	108.63
2	2	233	ASP	CA-CB-CG	9.29	121.89	112.60
2	2	10	LEU	N-CA-C	9.28	124.01	109.81
2	2	255	ARG	CD-NE-CZ	9.27	137.38	124.40
3	3	3	ILE	CB-CA-C	-9.24	102.34	110.94
1	1	13	THR	N-CA-CB	-9.24	96.92	110.87
4	4	14	GLU	N-CA-C	-9.22	95.70	109.81
1	1	263	ASP	CA-C-O	9.21	129.72	120.32
1	1	172	GLN	OE1-CD-NE2	9.20	131.80	122.60
2	2	72	SER	CA-C-O	9.17	130.58	119.49
2	2	127	LEU	CA-C-O	-9.15	110.50	120.30
1	1	32	LYS	N-CA-CB	9.14	123.87	110.06
1	1	67	ASN	N-CA-C	9.13	121.31	111.36
2	2	61	ARG	NE-CZ-NH1	9.10	130.60	121.50
3	3	32	ALA	O-C-N	9.06	129.69	121.35
1	1	155	THR	N-CA-C	9.05	123.63	112.23
4	4	14	GLU	O-C-N	8.98	135.79	122.94
1	1	151	PRO	O-C-N	8.94	133.29	123.01
2	2	50	ASP	CA-CB-CG	8.94	121.54	112.60
2	2	20	GLY	N-CA-C	-8.92	92.03	113.18
3	3	184	ASP	O-C-N	8.86	133.91	121.95
3	3	75	GLN	CB-CA-C	-8.84	98.85	110.34
4	4	70	ALA	CA-C-O	8.84	135.82	120.80
4	4	23	ASN	CA-CB-CG	-8.81	103.79	112.60
1	1	43	ILE	CA-C-O	-8.79	111.07	118.98
1	1	231	LYS	O-C-N	8.74	130.20	120.68
4	4	27	ASN	CB-CA-C	-8.68	94.58	110.63
1	1	250	PRO	O-C-N	8.66	133.75	123.01
1	1	165	LEU	CA-C-O	8.65	130.00	119.79
1	1	206	LYS	O-C-N	-8.63	111.01	122.23
4	4	54	LEU	N-CA-CB	-8.57	95.49	111.00
4	4	64	ASN	CA-C-O	8.55	133.90	122.44
1	1	181	SER	O-C-N	8.54	132.41	122.25
4	4	64	ASN	N-CA-C	-8.54	97.47	110.70
2	2	86	HIS	CA-CB-CG	-8.52	105.28	113.80
1	1	4	ASN	OD1-CG-ND2	-8.52	114.08	122.60
2	2	117	ASN	CA-CB-CG	8.45	121.05	112.60
1	1	167	GLU	CB-CG-CD	8.42	126.91	112.60
1	1	217	ALA	CA-C-O	8.40	126.55	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	10	LEU	O-C-N	-8.39	110.94	122.94
2	2	249	ARG	CD-NE-CZ	-8.39	112.65	124.40
3	3	40	GLU	CB-CG-CD	8.39	126.86	112.60
3	3	180	ILE	CA-C-O	8.33	131.19	120.78
1	1	213	ASP	O-C-N	8.30	133.62	122.59
3	3	56	ASN	OD1-CG-ND2	8.27	130.87	122.60
4	4	31	ASN	OD1-CG-ND2	8.26	130.86	122.60
3	3	182	ASN	OD1-CG-ND2	-8.26	114.34	122.60
1	1	169	ARG	CB-CG-CD	8.24	130.26	111.30
2	2	130	MET	CA-CB-CG	-8.24	97.61	114.10
1	1	15	ALA	CA-C-O	8.24	129.48	119.10
2	2	138	ASP	N-CA-C	8.21	121.27	111.33
1	1	211	THR	CA-C-O	8.21	132.34	122.41
2	2	8	GLU	CA-C-N	8.21	132.40	120.82
2	2	8	GLU	C-N-CA	8.21	132.40	120.82
2	2	22	THR	N-CA-CB	-8.20	96.57	110.83
2	2	59	VAL	CB-CA-C	8.19	118.27	111.06
1	1	264	LYS	O-C-N	8.16	130.93	123.26
2	2	120	GLN	OE1-CD-NE2	8.10	130.69	122.60
3	3	175	THR	CA-C-O	8.07	129.76	120.80
3	3	215	LYS	CA-C-N	8.06	131.08	120.28
3	3	215	LYS	C-N-CA	8.06	131.08	120.28
3	3	184	ASP	CA-C-O	-8.02	111.87	121.34
4	4	69	LEU	CA-C-O	8.00	129.94	121.15
2	2	143	ASP	CA-C-N	7.99	134.24	120.58
2	2	143	ASP	C-N-CA	7.99	134.24	120.58
2	2	189	THR	CA-CB-OG1	-7.98	97.63	109.60
1	1	92	ILE	CA-C-O	-7.97	111.60	120.84
2	2	113	GLN	CA-C-O	-7.97	110.48	120.20
2	2	144	ASN	N-CA-C	7.95	121.47	111.69
3	3	177	GLN	O-C-N	-7.95	112.02	122.59
3	3	162	VAL	O-C-N	7.94	128.48	121.57
1	1	29	ASN	O-C-N	7.94	131.80	122.19
4	4	27	ASN	O-C-N	7.94	131.51	122.22
3	3	183	VAL	N-CA-C	-7.94	92.83	109.34
3	3	74	THR	CA-C-N	7.93	134.00	122.66
3	3	74	THR	C-N-CA	7.93	134.00	122.66
2	2	251	GLU	O-C-N	7.90	132.53	122.89
3	3	49	GLN	OE1-CD-NE2	7.90	130.50	122.60
1	1	77	PHE	CA-CB-CG	-7.88	105.92	113.80
3	3	87	SER	N-CA-C	-7.87	102.94	112.54
2	2	246	ASN	OD1-CG-ND2	7.86	130.46	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	32	SER	N-CA-C	-7.84	100.42	110.53
2	2	145	ARG	NE-CZ-NH1	7.83	129.33	121.50
1	1	81	TYR	O-C-N	7.83	136.04	121.63
4	4	37	ALA	CA-C-N	-7.83	110.98	122.65
4	4	37	ALA	C-N-CA	-7.83	110.98	122.65
2	2	31	GLY	CA-C-O	-7.82	116.82	122.45
4	4	45	PRO	N-CA-C	-7.82	98.78	111.21
1	1	22	GLN	O-C-N	7.80	127.42	121.88
4	4	67	PRO	N-CA-C	-7.79	103.35	114.18
2	2	255	ARG	NE-CZ-NH1	7.78	129.28	121.50
3	3	172	MET	N-CA-CB	-7.78	98.09	109.83
3	3	182	ASN	O-C-N	7.77	132.92	122.59
1	1	99	GLU	CA-C-N	7.75	136.35	121.54
1	1	99	GLU	C-N-CA	7.75	136.35	121.54
2	2	230	THR	N-CA-CB	-7.74	99.15	110.53
2	2	32	ARG	NE-CZ-NH1	-7.73	113.77	121.50
2	2	246	ASN	CA-CB-CG	7.73	120.33	112.60
3	3	180	ILE	O-C-N	-7.73	112.91	122.57
2	2	72	SER	CA-CB-OG	-7.70	95.69	111.10
2	2	139	VAL	CB-CA-C	7.70	122.42	111.88
2	2	181	GLN	CA-CB-CG	7.69	129.47	114.10
2	2	120	GLN	CG-CD-OE1	-7.67	105.47	120.80
2	2	160	ASN	OD1-CG-ND2	7.67	130.26	122.60
3	3	177	GLN	CA-C-N	7.65	136.32	121.63
3	3	177	GLN	C-N-CA	7.65	136.32	121.63
3	3	154	LEU	N-CA-C	7.65	120.58	111.33
2	2	207	THR	CA-C-O	-7.65	112.72	120.90
3	3	74	THR	N-CA-CB	-7.64	98.46	110.46
3	3	20	ASP	CA-C-O	7.63	129.39	121.23
3	3	216	ASP	CB-CG-OD2	-7.61	100.90	118.40
1	1	102	GLU	CA-C-N	-7.60	109.87	120.74
1	1	102	GLU	C-N-CA	-7.60	109.87	120.74
1	1	198	PRO	CA-C-O	-7.59	113.11	121.23
1	1	156	THR	CA-C-O	-7.59	111.97	120.54
1	1	30	GLN	CA-C-O	-7.57	110.12	119.28
3	3	216	ASP	N-CA-C	7.56	119.52	111.28
3	3	155	ASN	CB-CG-ND2	-7.55	105.07	116.40
3	3	115	THR	CA-CB-OG1	-7.55	98.28	109.60
1	1	99	GLU	CB-CG-CD	7.54	125.42	112.60
3	3	156	SER	N-CA-C	7.54	119.58	111.36
2	2	253	LEU	CA-C-N	-7.53	109.26	122.07
2	2	253	LEU	C-N-CA	-7.53	109.26	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	62	PHE	CA-C-N	7.52	135.90	121.54
4	4	62	PHE	C-N-CA	7.52	135.90	121.54
2	2	16	GLN	CA-CB-CG	7.50	129.11	114.10
2	2	148	LYS	N-CA-C	-7.50	102.66	112.41
1	1	96	GLY	O-C-N	7.49	129.81	123.29
2	2	24	THR	CA-C-O	-7.49	112.77	120.71
2	2	10	LEU	CA-C-O	7.47	130.49	121.68
4	4	38	ASN	OD1-CG-ND2	7.46	130.06	122.60
2	2	38	THR	CB-CA-C	-7.46	93.66	110.07
2	2	249	ARG	NE-CZ-NH1	-7.46	114.04	121.50
1	1	245	MET	CA-C-O	-7.45	112.99	121.19
4	4	37	ALA	O-C-N	7.45	132.09	123.29
2	2	19	ALA	CA-C-N	-7.45	106.81	121.41
2	2	19	ALA	C-N-CA	-7.45	106.81	121.41
4	4	45	PRO	CA-C-O	7.44	130.19	121.56
2	2	43	GLU	CA-CB-CG	7.38	128.86	114.10
2	2	255	ARG	NE-CZ-NH2	-7.38	112.56	119.20
2	2	12	ASP	CA-CB-CG	7.37	119.97	112.60
2	2	111	ARG	CB-CG-CD	-7.35	94.39	111.30
3	3	216	ASP	N-CA-CB	-7.35	99.31	110.12
1	1	157	GLN	CA-C-O	-7.35	112.20	120.43
1	1	196	VAL	N-CA-CB	-7.34	97.68	111.62
2	2	113	GLN	CA-C-N	-7.34	113.64	123.10
2	2	113	GLN	C-N-CA	-7.34	113.64	123.10
1	1	82	ASP	CA-C-N	-7.33	111.17	122.60
1	1	82	ASP	C-N-CA	-7.33	111.17	122.60
2	2	207	THR	O-C-N	7.33	129.71	122.09
1	1	78	ASP	CA-CB-CG	-7.32	105.28	112.60
2	2	250	HIS	O-C-N	7.32	131.66	122.65
4	4	50	GLN	CA-CB-CG	-7.32	99.46	114.10
4	4	68	LEU	N-CA-CB	-7.31	97.95	109.51
3	3	186	TRP	N-CA-C	7.30	120.54	109.23
3	3	180	ILE	CA-CB-CG2	7.29	122.90	110.50
2	2	28	SER	CA-C-O	-7.29	114.89	121.67
1	1	137	GLY	CA-C-O	-7.27	111.90	122.52
1	1	76	GLN	OE1-CD-NE2	-7.26	115.34	122.60
2	2	59	VAL	N-CA-CB	-7.26	98.24	112.75
1	1	219	ASN	O-C-N	7.25	132.12	122.41
1	1	233	ASP	CB-CG-OD2	-7.24	101.75	118.40
1	1	260	THR	N-CA-CB	7.21	121.06	110.25
4	4	69	LEU	CA-C-N	7.20	134.66	121.70
4	4	69	LEU	C-N-CA	7.20	134.66	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	222	PRO	CA-C-O	7.20	129.39	120.97
1	1	87	GLN	CG-CD-NE2	-7.19	105.61	116.40
1	1	103	VAL	CB-CA-C	7.19	121.46	112.04
1	1	64	ALA	N-CA-C	-7.17	102.32	111.92
3	3	190	TRP	CA-C-O	-7.16	113.06	121.44
2	2	130	MET	CB-CA-C	7.15	122.80	109.71
4	4	64	ASN	CB-CA-C	7.15	122.78	111.91
2	2	102	ARG	CD-NE-CZ	-7.14	114.40	124.40
4	4	22	ASN	OD1-CG-ND2	7.14	129.74	122.60
1	1	3	GLU	OE1-CD-OE2	7.12	139.99	122.90
2	2	201	ALA	CA-C-O	-7.12	113.95	120.50
1	1	219	ASN	CA-C-O	-7.10	112.83	121.28
3	3	201	CYS	O-C-N	7.09	128.67	121.72
4	4	32	SER	CA-C-O	-7.09	113.79	121.94
1	1	182	ASN	CA-C-O	-7.08	110.38	120.51
2	2	8	GLU	O-C-N	-7.06	111.70	123.00
1	1	196	VAL	CB-CA-C	7.06	123.89	111.18
3	3	224	SER	CA-C-O	-7.04	113.10	119.86
3	3	169	HIS	O-C-N	7.04	130.46	122.22
3	3	139	ARG	CD-NE-CZ	-7.03	114.56	124.40
1	1	203	ASN	CA-C-O	-7.02	113.03	122.44
4	4	62	PHE	CA-CB-CG	7.01	120.81	113.80
1	1	255	PHE	CA-C-O	6.99	128.88	121.19
2	2	12	ASP	N-CA-C	-6.98	104.33	112.92
2	2	143	ASP	CA-CB-CG	-6.98	105.62	112.60
2	2	73	THR	CA-CB-OG1	-6.96	99.16	109.60
3	3	217	PHE	CA-C-O	6.94	128.83	120.92
1	1	110	GLN	OE1-CD-NE2	-6.94	115.66	122.60
1	1	46	PHE	CA-CB-CG	-6.93	106.87	113.80
3	3	137	THR	O-C-N	6.93	130.63	122.24
1	1	258	TRP	O-C-N	6.91	127.61	121.18
2	2	222	LEU	CA-C-N	6.91	133.92	122.73
2	2	222	LEU	C-N-CA	6.91	133.92	122.73
2	2	186	ARG	NE-CZ-NH1	6.91	128.41	121.50
3	3	23	VAL	N-CA-C	6.90	115.71	108.95
1	1	256	PHE	CA-C-N	6.89	127.27	119.83
1	1	256	PHE	C-N-CA	6.89	127.27	119.83
1	1	210	ASN	N-CA-CB	6.89	122.77	112.30
1	1	260	THR	N-CA-C	-6.88	101.91	111.81
2	2	189	THR	CA-CB-CG2	6.88	122.19	110.50
1	1	97	ASN	OD1-CG-ND2	6.86	129.46	122.60
3	3	8	ARG	CD-NE-CZ	-6.86	114.80	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	124	PHE	CA-C-O	-6.86	113.41	121.16
1	1	234	ILE	O-C-N	6.83	130.17	122.93
1	1	213	ASP	CB-CA-C	6.81	123.96	110.42
1	1	29	ASN	CB-CA-C	-6.79	98.96	110.64
4	4	55	LEU	CA-C-O	-6.78	113.10	120.36
1	1	207	ARG	NE-CZ-NH1	6.77	128.27	121.50
1	1	50	SER	CA-C-O	6.76	128.62	120.92
1	1	156	THR	O-C-N	6.75	130.91	123.22
2	2	244	VAL	N-CA-CB	-6.75	102.64	111.82
4	4	53	ASN	N-CA-C	-6.75	99.30	110.17
3	3	154	LEU	N-CA-CB	-6.73	99.96	110.06
1	1	128	GLU	CB-CG-CD	6.73	124.04	112.60
4	4	32	SER	CB-CA-C	6.69	124.25	110.40
3	3	60	ASN	CA-CB-CG	-6.69	105.91	112.60
4	4	38	ASN	CB-CA-C	6.69	120.71	109.48
3	3	66	GLU	CG-CD-OE2	-6.67	103.05	118.40
1	1	213	ASP	N-CA-C	-6.67	96.59	110.80
1	1	82	ASP	O-C-N	6.67	132.16	122.43
3	3	166	SER	N-CA-CB	-6.66	101.52	110.77
2	2	155	THR	CA-C-O	-6.64	113.63	120.54
1	1	14	ASP	N-CA-C	-6.63	99.52	108.86
3	3	137	THR	CA-C-O	-6.61	111.45	119.32
1	1	81	TYR	CA-CB-CG	-6.61	102.00	113.90
3	3	177	GLN	CB-CA-C	6.60	123.55	110.42
3	3	91	ASN	CA-CB-CG	-6.60	106.00	112.60
2	2	41	ASP	CA-C-O	-6.60	111.13	119.31
1	1	9	VAL	CB-CA-C	6.59	122.25	110.65
3	3	216	ASP	CA-C-N	6.59	130.11	120.82
3	3	216	ASP	C-N-CA	6.59	130.11	120.82
2	2	242	ARG	CA-CB-CG	-6.59	100.93	114.10
1	1	208	PHE	N-CA-CB	6.58	121.08	110.42
2	2	107	LYS	CA-C-O	-6.58	113.22	120.33
4	4	60	ASN	CA-C-O	6.58	129.93	120.51
2	2	102	ARG	NE-CZ-NH1	6.58	128.08	121.50
3	3	48	ALA	CA-C-O	6.58	127.61	119.05
3	3	217	PHE	CA-C-N	6.57	133.14	122.29
3	3	217	PHE	C-N-CA	6.57	133.14	122.29
1	1	185	SER	N-CA-CB	-6.57	99.37	111.13
4	4	68	LEU	CB-CA-C	6.57	119.62	110.16
2	2	184	ASN	CA-C-O	-6.56	113.34	120.36
4	4	21	ILE	CA-CB-CG2	6.56	121.65	110.50
2	2	138	ASP	CB-CA-C	-6.55	99.54	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	71	THR	N-CA-CB	-6.55	101.01	111.43
2	2	137	LEU	CA-C-N	6.55	129.35	120.38
2	2	137	LEU	C-N-CA	6.55	129.35	120.38
3	3	32	ALA	N-CA-CB	6.55	118.81	110.23
4	4	50	GLN	O-C-N	6.55	130.32	122.26
3	3	220	LYS	CA-CB-CG	6.53	127.16	114.10
1	1	211	THR	N-CA-C	-6.53	97.16	108.52
2	2	242	ARG	O-C-N	6.53	128.83	121.32
1	1	99	GLU	CA-C-O	6.52	129.84	120.51
2	2	155	THR	CA-C-N	-6.52	111.38	123.05
2	2	155	THR	C-N-CA	-6.52	111.38	123.05
1	1	88	ARG	N-CA-CB	6.52	119.90	110.06
2	2	39	VAL	N-CA-CB	-6.52	100.44	112.43
2	2	138	ASP	N-CA-CB	-6.52	100.29	110.06
1	1	98	GLU	CA-C-N	6.51	133.98	121.54
1	1	98	GLU	C-N-CA	6.51	133.98	121.54
1	1	39	ARG	CD-NE-CZ	-6.51	115.28	124.40
2	2	153	ASN	N-CA-C	6.49	120.80	113.02
2	2	71	THR	CA-C-O	6.48	129.10	121.58
4	4	15	GLY	O-C-N	6.48	130.63	122.85
1	1	169	ARG	CD-NE-CZ	-6.48	115.33	124.40
2	2	69	ASP	O-C-N	6.48	131.01	123.30
1	1	213	ASP	CA-C-O	-6.47	111.25	120.51
4	4	53	ASN	CA-CB-CG	-6.47	106.13	112.60
1	1	260	THR	CB-CA-C	-6.47	103.15	111.50
1	1	188	VAL	CA-C-N	6.47	127.93	119.84
1	1	188	VAL	C-N-CA	6.47	127.93	119.84
3	3	166	SER	N-CA-C	6.47	116.45	108.11
1	1	211	THR	CA-C-N	6.46	134.08	121.41
1	1	211	THR	C-N-CA	6.46	134.08	121.41
3	3	178	ALA	N-CA-CB	6.45	122.69	111.39
1	1	16	THR	CA-CB-OG1	-6.44	99.94	109.60
1	1	208	PHE	CA-CB-CG	-6.43	107.37	113.80
3	3	155	ASN	CA-C-N	6.42	129.41	120.29
3	3	155	ASN	C-N-CA	6.42	129.41	120.29
2	2	105	LEU	N-CA-C	6.37	119.79	109.40
4	4	70	ALA	N-CA-CB	-6.37	100.84	110.40
3	3	187	VAL	CA-C-O	-6.36	113.66	120.59
4	4	62	PHE	CA-C-O	6.36	129.61	120.51
2	2	38	THR	O-C-N	6.35	130.86	123.17
1	1	124	LYS	CA-C-O	-6.34	113.89	120.99
1	1	102	GLU	CA-C-O	-6.32	113.72	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	188	VAL	CB-CA-C	6.32	122.85	111.36
3	3	53	PHE	N-CA-C	6.31	119.80	109.76
3	3	141	GLN	OE1-CD-NE2	-6.31	116.29	122.60
1	1	131	LEU	N-CA-CB	-6.30	100.14	110.42
3	3	70	THR	O-C-N	6.30	131.19	123.44
1	1	205	HIS	CA-CB-CG	-6.29	107.51	113.80
2	2	53	SER	N-CA-CB	6.29	120.69	110.43
3	3	46	GLU	CG-CD-OE1	6.28	132.84	118.40
2	2	128	VAL	CA-C-O	-6.28	113.81	120.53
3	3	75	GLN	N-CA-CB	-6.27	99.77	110.43
3	3	182	ASN	CA-CB-CG	6.27	118.87	112.60
3	3	230	PRO	CA-C-O	6.27	128.35	118.89
3	3	2	PRO	N-CA-C	-6.27	101.35	111.19
4	4	34	ASP	O-C-N	-6.26	115.71	123.04
1	1	172	GLN	CB-CG-CD	6.26	123.24	112.60
2	2	226	THR	CA-C-O	-6.25	113.79	120.92
3	3	218	SER	N-CA-CB	-6.25	99.90	111.53
2	2	188	ASN	OD1-CG-ND2	-6.25	116.35	122.60
3	3	190	TRP	CA-C-N	-6.25	112.84	122.09
3	3	190	TRP	C-N-CA	-6.25	112.84	122.09
2	2	65	PHE	CA-CB-CG	-6.25	107.55	113.80
2	2	163	GLY	O-C-N	6.25	128.02	121.77
3	3	75	GLN	N-CA-C	6.25	122.79	108.93
3	3	117	THR	CA-CB-OG1	-6.24	100.24	109.60
1	1	259	PRO	O-C-N	6.24	131.06	122.64
3	3	207	ILE	CA-C-N	6.23	129.72	120.87
3	3	207	ILE	C-N-CA	6.23	129.72	120.87
1	1	190	TYR	CA-C-O	-6.23	113.64	120.24
1	1	197	LEU	N-CA-CB	-6.22	99.84	110.11
1	1	239	TYR	CA-C-O	-6.22	114.08	121.11
1	1	241	ARG	NE-CZ-NH1	6.21	127.72	121.50
1	1	108	THR	CA-CB-OG1	-6.21	100.28	109.60
2	2	138	ASP	CA-CB-CG	-6.21	106.39	112.60
3	3	175	THR	CA-CB-OG1	-6.21	100.28	109.60
3	3	180	ILE	N-CA-CB	-6.20	101.01	111.23
2	2	130	MET	CG-SD-CE	-6.19	87.27	100.90
2	2	27	GLN	CA-CB-CG	-6.19	101.72	114.10
1	1	32	LYS	CB-CA-C	-6.18	99.08	109.53
2	2	252	VAL	O-C-N	6.18	130.30	122.57
1	1	259	PRO	N-CA-CB	6.18	109.74	103.25
2	2	70	TRP	CA-C-O	6.18	126.97	120.36
2	2	66	LYS	CA-C-O	-6.17	113.82	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	59	PRO	O-C-N	6.17	130.49	123.03
2	2	224	TYR	CA-CB-CG	-6.17	102.80	113.90
2	2	60	GLU	CB-CG-CD	6.16	123.08	112.60
1	1	265	ILE	CB-CA-C	6.16	121.39	111.29
1	1	208	PHE	N-CA-C	-6.15	105.75	113.20
2	2	27	GLN	OE1-CD-NE2	6.15	128.75	122.60
1	1	152	THR	CA-C-O	-6.15	114.19	121.32
3	3	73	LYS	CA-C-O	6.14	126.83	119.10
3	3	78	ALA	O-C-N	6.14	130.35	123.48
1	1	67	ASN	N-CA-CB	-6.13	101.08	110.16
1	1	231	LYS	CA-C-O	-6.13	114.07	120.38
1	1	138	ALA	O-C-N	6.12	130.34	122.81
3	3	111	THR	CA-C-O	-6.11	113.72	120.38
1	1	10	THR	CA-CB-CG2	6.10	120.87	110.50
3	3	179	ASN	N-CA-C	6.08	120.99	112.72
2	2	13	ARG	CA-CB-CG	-6.08	101.94	114.10
3	3	192	LEU	N-CA-C	-6.08	103.29	112.04
3	3	94	LEU	O-C-N	6.07	128.32	122.07
4	4	54	LEU	O-C-N	6.05	130.65	123.27
3	3	74	THR	CA-C-O	6.04	126.37	119.18
1	1	251	ARG	O-C-N	6.04	126.68	121.54
3	3	70	THR	CA-C-N	-6.04	113.75	123.23
3	3	70	THR	C-N-CA	-6.04	113.75	123.23
2	2	242	ARG	CB-CA-C	-6.03	105.75	111.00
3	3	7	ILE	CA-CB-CG1	-6.03	100.15	110.40
2	2	188	ASN	CA-C-O	6.03	128.57	121.58
1	1	41	SER	O-C-N	6.03	126.16	121.88
1	1	155	THR	OG1-CB-CG2	6.02	121.35	109.30
4	4	41	GLY	O-C-N	6.02	128.93	122.60
1	1	63	LYS	O-C-N	6.02	130.60	122.59
2	2	114	VAL	CB-CA-C	6.02	119.96	110.81
4	4	45	PRO	O-C-N	-6.02	115.55	123.01
4	4	36	SER	CB-CA-C	6.01	121.59	109.38
4	4	63	SER	N-CA-CB	6.01	120.64	110.49
1	1	53	LEU	O-C-N	6.01	130.48	122.43
1	1	18	ASP	CA-C-O	-6.00	112.58	119.60
2	2	169	HIS	ND1-CE1-NE2	6.00	114.40	108.40
1	1	54	GLU	N-CA-C	5.99	119.83	111.56
1	1	208	PHE	O-C-N	5.99	131.25	122.39
2	2	81	ARG	CG-CD-NE	5.98	125.15	112.00
2	2	227	GLY	N-CA-C	-5.98	107.15	114.92
1	1	155	THR	N-CA-CB	-5.97	101.10	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	191	GLN	CA-C-O	-5.97	114.05	120.92
2	2	55	LYS	CB-CA-C	-5.97	103.08	111.80
1	1	64	ALA	CA-C-N	5.96	130.49	123.16
1	1	64	ALA	C-N-CA	5.96	130.49	123.16
3	3	80	TYR	CA-C-N	-5.96	111.88	122.07
3	3	80	TYR	C-N-CA	-5.96	111.88	122.07
1	1	107	LYS	O-C-N	5.96	131.04	122.28
1	1	9	VAL	N-CA-CB	-5.95	101.15	111.63
3	3	79	VAL	N-CA-CB	5.95	120.79	111.99
2	2	191	VAL	CB-CA-C	5.93	119.65	110.28
2	2	112	VAL	N-CA-CB	-5.93	99.64	111.91
2	2	38	THR	CA-CB-OG1	-5.93	100.71	109.60
1	1	167	GLU	CA-C-O	-5.92	114.20	121.06
1	1	167	GLU	CG-CD-OE2	5.90	131.98	118.40
3	3	9	GLU	CA-CB-CG	5.90	125.90	114.10
2	2	72	SER	O-C-N	-5.89	114.73	122.39
2	2	165	PHE	CA-C-O	-5.88	114.99	121.28
1	1	67	ASN	CB-CA-C	-5.88	100.86	110.85
3	3	105	ARG	NH1-CZ-NH2	-5.87	111.68	119.30
1	1	219	ASN	CA-C-N	-5.86	114.44	123.17
1	1	219	ASN	C-N-CA	-5.86	114.44	123.17
1	1	3	GLU	CG-CD-OE1	-5.86	104.93	118.40
3	3	155	ASN	OD1-CG-ND2	5.86	128.46	122.60
1	1	181	SER	N-CA-C	-5.85	105.33	112.88
2	2	45	PRO	CB-CA-C	5.85	118.53	111.46
1	1	84	LEU	CA-C-O	-5.84	114.49	121.56
2	2	149	ASP	CA-C-O	5.84	127.11	120.80
1	1	191	ASN	O-C-N	5.84	129.26	122.19
2	2	73	THR	N-CA-CB	-5.84	100.88	110.40
1	1	22	GLN	CA-C-O	-5.83	114.28	120.28
1	1	30	GLN	CG-CD-NE2	5.83	125.14	116.40
4	4	52	SER	N-CA-C	5.82	117.37	108.52
1	1	191	ASN	CB-CG-ND2	-5.81	107.68	116.40
2	2	158	GLN	CA-C-N	5.79	130.53	120.68
2	2	158	GLN	C-N-CA	5.79	130.53	120.68
4	4	16	ASN	O-C-N	5.78	129.08	122.55
3	3	156	SER	CA-C-O	-5.78	114.30	120.42
3	3	209	THR	CA-CB-OG1	-5.78	100.94	109.60
1	1	84	LEU	O-C-N	5.77	130.55	123.10
1	1	250	PRO	N-CA-CB	5.77	108.37	103.35
1	1	67	ASN	CB-CG-ND2	-5.76	107.75	116.40
3	3	122	GLY	CA-C-O	-5.75	116.00	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	165	ILE	O-C-N	5.75	130.41	122.88
2	2	246	ASN	O-C-N	5.75	129.80	123.25
2	2	197	TYR	CA-C-O	-5.75	114.05	120.54
1	1	62	ASN	CA-C-N	-5.74	110.58	121.54
1	1	62	ASN	C-N-CA	-5.74	110.58	121.54
4	4	33	ILE	CA-C-O	-5.74	113.94	120.66
2	2	29	THR	OG1-CB-CG2	5.74	120.78	109.30
1	1	207	ARG	CG-CD-NE	5.74	124.62	112.00
3	3	201	CYS	N-CA-CB	-5.74	99.52	110.42
4	4	59	VAL	O-C-N	-5.72	115.41	122.57
4	4	33	ILE	N-CA-CB	-5.72	104.46	111.67
1	1	253	THR	CA-CB-OG1	-5.70	101.05	109.60
2	2	44	HIS	CB-CA-C	-5.70	100.09	109.27
1	1	87	GLN	N-CA-CB	-5.68	101.66	111.55
2	2	44	HIS	CA-CB-CG	-5.67	108.13	113.80
1	1	52	SER	N-CA-CB	-5.67	100.98	110.39
1	1	29	ASN	CA-C-O	-5.66	112.80	119.48
1	1	216	ILE	N-CA-C	5.66	116.09	108.17
2	2	103	HIS	CA-CB-CG	-5.66	108.14	113.80
4	4	13	SER	CA-C-N	-5.66	112.90	123.03
4	4	13	SER	C-N-CA	-5.66	112.90	123.03
1	1	114	PHE	CA-CB-CG	5.64	119.44	113.80
4	4	44	PRO	N-CA-C	-5.64	103.82	110.70
2	2	256	GLN	CB-CG-CD	5.63	122.18	112.60
1	1	98	GLU	CA-CB-CG	-5.62	102.86	114.10
2	2	135	PRO	CB-CA-C	5.62	117.68	111.56
1	1	87	GLN	N-CA-C	5.61	118.22	109.52
1	1	180	THR	CA-CB-OG1	5.61	118.01	109.60
2	2	168	ASP	O-C-N	5.61	129.42	122.19
3	3	117	THR	N-CA-CB	-5.60	102.35	110.36
3	3	116	GLY	O-C-N	-5.60	118.34	122.71
3	3	130	PRO	N-CA-CB	5.60	108.51	103.08
1	1	244	ASN	CA-C-O	-5.59	115.78	122.27
2	2	77	PHE	CA-CB-CG	-5.59	108.21	113.80
2	2	170	GLN	OE1-CD-NE2	-5.58	117.02	122.60
2	2	35	GLY	CA-C-O	-5.57	116.51	121.41
3	3	40	GLU	CA-CB-CG	5.57	125.25	114.10
2	2	18	THR	CA-C-O	-5.57	114.25	120.54
1	1	246	ARG	CG-CD-NE	5.57	124.25	112.00
2	2	204	SER	N-CA-C	5.57	118.48	109.40
1	1	64	ALA	O-C-N	5.56	129.81	122.47
1	1	185	SER	CA-C-O	-5.56	113.93	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	243	LYS	CG-CD-CE	5.56	124.09	111.30
1	1	242	TYR	CA-CB-CG	-5.56	103.89	113.90
1	1	189	PRO	N-CA-CB	5.56	109.08	103.25
2	2	12	ASP	N-CA-CB	5.56	118.67	110.56
1	1	30	GLN	CB-CA-C	5.56	120.01	110.01
2	2	73	THR	N-CA-C	5.55	119.78	112.89
1	1	63	LYS	CA-C-N	-5.55	114.25	122.35
1	1	63	LYS	C-N-CA	-5.55	114.25	122.35
3	3	38	VAL	CB-CA-C	-5.55	102.81	110.91
4	4	35	LEU	CA-C-N	-5.54	112.84	122.37
4	4	35	LEU	C-N-CA	-5.54	112.84	122.37
2	2	21	ASN	N-CA-C	-5.54	104.95	112.26
3	3	31	VAL	N-CA-CB	-5.54	102.10	111.23
2	2	72	SER	N-CA-CB	-5.53	100.92	110.32
1	1	77	PHE	CA-C-O	-5.52	112.61	120.51
3	3	201	CYS	CA-C-O	-5.52	113.55	120.23
3	3	180	ILE	CB-CA-C	5.52	120.34	111.29
3	3	134	GLY	CA-C-O	-5.52	116.85	122.59
3	3	135	LYS	CB-CA-C	5.51	117.38	109.11
3	3	182	ASN	CA-C-N	-5.51	112.05	121.97
3	3	182	ASN	C-N-CA	-5.51	112.05	121.97
1	1	104	PHE	CA-CB-CG	-5.51	108.29	113.80
4	4	28	GLN	N-CA-C	-5.51	105.81	112.54
1	1	193	PRO	N-CA-C	-5.51	107.26	114.03
3	3	184	ASP	CA-C-N	-5.51	113.01	122.21
3	3	184	ASP	C-N-CA	-5.51	113.01	122.21
3	3	141	GLN	CB-CG-CD	-5.50	103.25	112.60
2	2	40	HIS	CA-CB-CG	-5.50	108.30	113.80
4	4	30	GLN	CA-CB-CG	-5.50	103.11	114.10
2	2	78	GLU	N-CA-C	-5.49	101.52	110.20
1	1	97	ASN	CA-CB-CG	-5.49	107.11	112.60
2	2	202	PRO	CA-C-N	5.49	130.87	121.87
2	2	202	PRO	C-N-CA	5.49	130.87	121.87
3	3	56	ASN	O-C-N	5.49	130.18	123.21
4	4	63	SER	CA-C-O	5.48	128.35	120.51
1	1	19	PHE	CA-CB-CG	-5.48	108.32	113.80
3	3	61	ALA	O-C-N	5.48	129.66	122.97
3	3	116	GLY	CA-C-N	5.48	130.95	120.97
3	3	116	GLY	C-N-CA	5.48	130.95	120.97
1	1	30	GLN	N-CA-C	-5.48	106.37	113.16
1	1	207	ARG	NH1-CZ-NH2	-5.48	112.18	119.30
3	3	80	TYR	CA-C-O	-5.48	114.41	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	12	ASN	N-CA-CB	5.47	119.55	110.52
2	2	17	ASP	CA-C-O	-5.47	113.36	120.25
3	3	79	VAL	CB-CA-C	5.46	117.55	110.12
1	1	82	ASP	N-CA-C	-5.46	106.58	113.18
1	1	133	PRO	N-CA-CB	5.46	108.17	103.31
3	3	35	ASN	CA-C-O	-5.45	111.97	119.12
2	2	86	HIS	CA-C-O	-5.45	114.81	120.92
1	1	153	LYS	N-CA-CB	-5.45	102.38	110.99
1	1	181	SER	CA-CB-OG	-5.45	100.21	111.10
2	2	249	ARG	NE-CZ-NH2	5.44	124.10	119.20
3	3	36	TYR	CA-C-N	5.44	128.97	120.75
3	3	36	TYR	C-N-CA	5.44	128.97	120.75
1	1	11	GLU	CA-C-O	-5.43	115.04	120.96
4	4	28	GLN	O-C-N	5.43	129.71	122.43
1	1	150	THR	CB-CA-C	5.42	120.86	110.17
1	1	29	ASN	OD1-CG-ND2	5.41	128.00	122.60
2	2	181	GLN	N-CA-C	-5.41	100.22	108.76
2	2	175	TRP	CA-C-O	-5.40	113.24	119.61
3	3	200	GLY	CA-C-O	5.40	125.71	119.13
1	1	172	GLN	CA-C-N	5.39	130.50	123.06
1	1	172	GLN	C-N-CA	5.39	130.50	123.06
2	2	51	THR	CA-CB-OG1	-5.39	101.51	109.60
2	2	160	ASN	CA-C-N	5.39	127.95	120.29
2	2	160	ASN	C-N-CA	5.39	127.95	120.29
3	3	20	ASP	CA-CB-CG	5.39	117.99	112.60
1	1	126	ASP	CA-C-O	-5.39	115.04	121.56
2	2	81	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	2	209	HIS	CA-CB-CG	5.39	119.19	113.80
1	1	126	ASP	N-CA-C	-5.38	101.79	110.14
1	1	167	GLU	CA-CB-CG	5.38	124.86	114.10
1	1	10	THR	CA-C-O	-5.38	114.55	120.30
1	1	22	GLN	OE1-CD-NE2	-5.37	117.23	122.60
3	3	151	ASP	CB-CG-OD1	5.37	130.75	118.40
3	3	175	THR	N-CA-CB	5.36	119.36	110.52
3	3	197	TYR	CA-CB-CG	-5.36	104.26	113.90
2	2	120	GLN	CB-CG-CD	-5.35	103.50	112.60
3	3	105	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	1	254	VAL	O-C-N	5.35	129.03	122.72
3	3	115	THR	N-CA-CB	-5.34	102.17	110.98
1	1	151	PRO	CA-C-O	-5.34	115.52	121.23
2	2	226	THR	O-C-N	5.33	129.56	122.95
4	4	50	GLN	OE1-CD-NE2	5.33	127.93	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	233	ASP	O-C-N	5.33	129.41	122.42
2	2	109	GLY	N-CA-C	-5.33	102.40	112.10
4	4	51	PHE	O-C-N	5.33	129.30	123.01
1	1	102	GLU	N-CA-C	5.33	117.92	109.50
3	3	85	SER	CB-CA-C	-5.32	100.62	109.55
2	2	213	THR	O-C-N	5.30	129.74	123.27
2	2	183	LEU	CB-CA-C	5.30	120.42	111.41
1	1	201	TRP	O-C-N	5.30	129.42	123.27
2	2	71	THR	N-CA-C	5.30	117.46	109.41
2	2	88	LEU	N-CA-CB	-5.30	102.83	110.56
1	1	77	PHE	N-CA-CB	5.29	119.44	110.49
1	1	78	ASP	N-CA-C	-5.29	98.12	109.81
2	2	43	GLU	N-CA-CB	-5.29	102.25	110.29
3	3	184	ASP	N-CA-CB	-5.29	103.61	111.43
1	1	128	GLU	CA-C-O	-5.28	114.71	120.36
3	3	9	GLU	CB-CG-CD	5.28	121.57	112.60
1	1	26	LEU	CA-C-O	5.26	124.59	119.22
2	2	180	HIS	N-CA-C	5.26	116.00	108.74
4	4	65	MET	N-CA-C	5.26	118.02	109.24
3	3	138	SER	CA-C-O	-5.25	115.66	121.33
1	1	244	ASN	N-CA-CB	5.25	119.69	111.71
2	2	163	GLY	CA-C-O	-5.25	114.02	121.52
3	3	154	LEU	CB-CA-C	-5.25	101.76	110.68
1	1	243	LYS	CA-C-N	5.25	130.27	122.82
1	1	243	LYS	C-N-CA	5.25	130.27	122.82
2	2	188	ASN	N-CA-C	5.24	117.38	109.41
1	1	79	PRO	O-C-N	5.23	129.25	122.24
2	2	94	GLY	O-C-N	5.23	128.79	122.67
2	2	172	PHE	CA-CB-CG	-5.22	108.58	113.80
3	3	45	LEU	O-C-N	5.22	129.18	122.39
3	3	85	SER	CA-CB-OG	-5.22	100.66	111.10
3	3	103	GLN	CA-C-O	-5.21	115.51	121.40
1	1	132	SER	CA-C-O	-5.21	114.98	120.09
1	1	146	CYS	O-C-N	5.21	127.75	121.60
1	1	51	GLY	CA-C-O	-5.20	113.51	119.80
1	1	182	ASN	OD1-CG-ND2	5.20	127.80	122.60
3	3	121	LYS	CA-CB-CG	-5.20	103.71	114.10
1	1	161	GLU	N-CA-CB	-5.19	104.27	112.63
3	3	23	VAL	N-CA-CB	-5.19	105.25	110.08
4	4	38	ASN	CA-C-N	5.19	131.45	121.54
4	4	38	ASN	C-N-CA	5.19	131.45	121.54
2	2	12	ASP	CA-C-N	5.19	130.38	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	12	ASP	C-N-CA	5.19	130.38	122.23
3	3	83	THR	CB-CA-C	5.18	118.61	109.80
3	3	78	ALA	CA-C-O	-5.18	115.19	120.89
4	4	31	ASN	N-CA-C	5.18	117.15	109.69
2	2	239	GLN	CB-CG-CD	5.17	121.40	112.60
1	1	60	PHE	CA-C-O	-5.17	114.96	120.75
2	2	9	ASN	CB-CA-C	5.16	117.95	109.90
2	2	192	ASP	CA-CB-CG	5.16	117.76	112.60
2	2	30	VAL	CA-C-O	-5.16	114.33	120.78
1	1	124	LYS	N-CA-C	-5.15	100.90	108.99
3	3	28	LYS	CG-CD-CE	5.15	123.15	111.30
3	3	41	TYR	CA-C-N	-5.15	114.10	121.98
3	3	41	TYR	C-N-CA	-5.15	114.10	121.98
4	4	19	VAL	CA-C-N	5.15	128.79	120.55
4	4	19	VAL	C-N-CA	5.15	128.79	120.55
3	3	124	PHE	CA-CB-CG	-5.15	108.65	113.80
2	2	159	THR	OG1-CB-CG2	5.14	119.59	109.30
3	3	37	MET	CA-C-O	-5.14	116.10	121.55
2	2	10	LEU	CA-CB-CG	-5.14	98.31	116.30
3	3	74	THR	N-CA-C	5.14	119.55	113.28
3	3	117	THR	OG1-CB-CG2	5.13	119.57	109.30
2	2	161	ARG	NE-CZ-NH1	5.13	126.63	121.50
2	2	16	GLN	CG-CD-NE2	5.13	124.09	116.40
4	4	21	ILE	CA-CB-CG1	-5.13	101.68	110.40
2	2	186	ARG	CB-CG-CD	-5.13	99.51	111.30
2	2	200	ILE	CA-CB-CG2	5.12	119.21	110.50
1	1	205	HIS	O-C-N	5.12	128.55	122.20
3	3	18	LEU	N-CA-C	5.12	115.87	109.57
2	2	78	GLU	N-CA-CB	5.11	117.78	110.06
2	2	244	VAL	CB-CA-C	5.11	117.31	110.42
3	3	52	THR	CB-CA-C	5.10	119.83	110.24
3	3	82	VAL	O-C-N	5.10	126.24	121.96
2	2	237	SER	CA-C-O	-5.10	114.85	120.30
1	1	262	GLY	O-C-N	5.09	129.32	122.70
2	2	145	ARG	NH1-CZ-NH2	-5.08	112.69	119.30
3	3	42	LYS	CA-CB-CG	-5.08	103.94	114.10
1	1	51	GLY	O-C-N	5.08	127.39	122.41
4	4	20	ILE	CA-CB-CG2	5.08	119.13	110.50
3	3	161	THR	CA-C-O	-5.07	114.90	120.43
1	1	247	VAL	CA-C-O	-5.07	115.40	121.28
3	3	49	GLN	CG-CD-OE1	-5.07	110.66	120.80
2	2	152	PRO	N-CA-CB	-5.07	97.03	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	97	GLY	CA-C-O	5.06	126.27	121.05
3	3	100	ASN	OD1-CG-ND2	-5.06	117.54	122.60
3	3	183	VAL	CA-C-N	-5.06	114.70	123.25
3	3	183	VAL	C-N-CA	-5.06	114.70	123.25
2	2	194	GLU	O-C-N	5.06	129.33	123.41
4	4	19	VAL	CB-CA-C	5.06	118.11	110.98
2	2	256	GLN	CA-CB-CG	-5.05	104.00	114.10
1	1	182	ASN	CB-CG-OD1	-5.05	110.71	120.80
1	1	185	SER	CA-CB-OG	-5.05	101.01	111.10
1	1	241	ARG	NH1-CZ-NH2	-5.05	112.74	119.30
3	3	138	SER	O-C-N	5.04	129.00	123.25
3	3	42	LYS	O-C-N	5.04	127.38	122.19
3	3	21	SER	N-CA-C	5.04	117.89	110.59
1	1	89	LEU	N-CA-CB	-5.03	103.20	110.70
1	1	68	SER	CA-C-O	-5.03	115.72	121.40
4	4	28	GLN	OE1-CD-NE2	5.03	127.63	122.60
4	4	39	ALA	N-CA-CB	-5.03	102.00	110.49
2	2	98	ALA	CA-C-O	-5.02	115.22	120.55
2	2	8	GLU	CA-C-O	5.02	129.34	120.80
2	2	75	LYS	CA-CB-CG	-5.02	104.06	114.10
4	4	22	ASN	N-CA-C	-5.02	102.96	110.23
1	1	81	TYR	CB-CA-C	-5.01	101.64	112.12
2	2	79	TYR	N-CA-C	5.01	115.93	108.86
1	1	96	GLY	CA-C-O	-5.01	116.01	121.77
2	2	104	TYR	N-CA-CB	-5.01	102.74	110.16
4	4	47	THR	N-CA-CB	-5.01	102.06	111.13

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	255	ARG	Sidechain
2	2	81	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	1	2091	0	2010	108	0
2	2	1973	0	1900	104	0
3	3	1772	0	1760	91	0
4	4	433	0	405	32	0
5	2	5	0	0	0	0
6	1	106	0	0	0	0
6	2	69	0	0	3	0
6	3	49	0	0	0	0
6	4	9	0	0	0	0
All	All	6507	0	6075	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 25.

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)
2:2:10:LEU:O	2:2:13:ARG:HB2	1.38	1.19
2:2:101:ARG:HD3	2:2:255:ARG:HB2	1.36	1.05
4:4:60:ASN:HD21	4:4:65:MET:HE1	1.22	1.04
3:3:179:ASN:HB3	3:3:183:VAL:HG13	1.39	1.04
1:1:14:ASP:OD2	1:1:16:THR:HB	1.58	1.03
1:1:32:LYS:HE2	4:4:13:SER:HB2	1.41	1.02
1:1:70:ILE:H	1:1:76:GLN:HE22	1.03	0.99
2:2:22:THR:HG21	2:2:62:TYR:H	1.23	0.98
4:4:46:LYS:H	4:4:46:LYS:HD2	1.26	0.97
4:4:21:ILE:HG23	4:4:22:ASN:O	1.72	0.90
2:2:10:LEU:O	2:2:13:ARG:CB	2.19	0.90
2:2:252:VAL:O	2:2:253:LEU:HB2	1.70	0.90
2:2:14:VAL:HG22	2:2:27:GLN:HG2	1.53	0.89
2:2:19:ALA:HB1	2:2:61:ARG:HA	1.53	0.89
2:2:255:ARG:HD2	2:2:255:ARG:C	2.00	0.87
2:2:19:ALA:HB3	2:2:22:THR:CG2	2.05	0.86
3:3:179:ASN:CB	3:3:183:VAL:HG13	2.06	0.86
2:2:19:ALA:HB3	2:2:22:THR:HG22	1.58	0.85
1:1:49:LYS:HG2	1:1:50:SER:N	1.89	0.84
3:3:197:TYR:CZ	3:3:203:THR:HG22	2.13	0.83
1:1:265:ILE:HG23	1:1:266:ASP:H	1.44	0.83
1:1:206:LYS:N	1:1:206:LYS:HD2	1.93	0.83
1:1:207:ARG:CD	3:3:180:ILE:HD13	2.11	0.81
2:2:181:GLN:HG2	2:2:191:VAL:HG22	1.60	0.81
2:2:10:LEU:HG	2:2:11:SER:N	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:61:ALA:O	4:4:62:PHE:HB3	1.77	0.80
3:3:177:GLN:HG2	3:3:178:ALA:H	1.47	0.80
3:3:143:MET:O	3:3:143:MET:HG2	1.83	0.79
1:1:95:ASN:HB2	1:1:105:PRO:O	1.83	0.79
2:2:101:ARG:HD3	2:2:255:ARG:CB	2.11	0.78
1:1:207:ARG:NE	3:3:180:ILE:HD13	2.00	0.77
3:3:79:VAL:HB	3:3:188:THR:HG22	1.65	0.77
2:2:72:SER:HB2	6:2:321:HOH:O	1.83	0.77
4:4:65:MET:HA	4:4:67:PRO:CD	2.15	0.77
2:2:249:ARG:HG3	2:2:249:ARG:HH11	1.48	0.76
3:3:75:GLN:CA	3:3:75:GLN:HE21	1.98	0.76
2:2:181:GLN:CG	2:2:191:VAL:HG22	2.16	0.75
2:2:252:VAL:O	2:2:253:LEU:CB	2.35	0.75
3:3:117:THR:HG22	3:3:120:MET:H	1.50	0.74
2:2:10:LEU:HG	2:2:11:SER:HB2	1.69	0.74
2:2:186:ARG:NH1	2:2:187:THR:OG1	2.20	0.74
2:2:22:THR:HG21	2:2:62:TYR:N	2.03	0.73
1:1:79:PRO:HG3	1:1:107:LYS:HB3	1.69	0.73
4:4:46:LYS:HD2	4:4:46:LYS:N	2.02	0.73
4:4:60:ASN:ND2	4:4:65:MET:HE1	2.01	0.73
1:1:209:ASP:CG	1:1:211:THR:HG23	2.14	0.72
3:3:31:VAL:HG13	3:3:32:ALA:N	2.04	0.71
2:2:19:ALA:CB	2:2:61:ARG:HA	2.22	0.70
3:3:117:THR:HG23	3:3:119:MET:H	1.57	0.70
3:3:18:LEU:HD22	3:3:19:PRO:HD2	1.74	0.70
2:2:158:GLN:NE2	2:2:158:GLN:HA	2.07	0.69
1:1:3:GLU:HG3	1:1:4:ASN:N	2.06	0.69
2:2:59:VAL:HG22	2:2:96:PHE:HA	1.75	0.69
1:1:63:LYS:H	1:1:65:CYS:HB2	1.56	0.69
2:2:101:ARG:O	2:2:252:VAL:HG23	1.92	0.69
2:2:10:LEU:CG	2:2:11:SER:N	2.55	0.69
3:3:75:GLN:CA	3:3:75:GLN:NE2	2.56	0.68
4:4:59:VAL:HG22	4:4:60:ASN:H	1.57	0.68
1:1:205:HIS:CE1	1:1:210:ASN:HB3	2.29	0.68
4:4:65:MET:HA	4:4:67:PRO:HD2	1.75	0.68
1:1:208:PHE:HE1	3:3:182:ASN:CB	2.08	0.67
2:2:71:THR:CG2	2:2:73:THR:HB	2.24	0.67
3:3:75:GLN:NE2	3:3:75:GLN:HA	2.10	0.67
3:3:117:THR:HG22	3:3:120:MET:N	2.09	0.67
2:2:10:LEU:HG	2:2:11:SER:CB	2.25	0.66
4:4:65:MET:HA	4:4:67:PRO:HD3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:71:THR:HG23	2:2:73:THR:H	1.61	0.65
2:2:249:ARG:HH11	2:2:249:ARG:CG	2.04	0.65
1:1:205:HIS:NE2	1:1:212:GLY:HA2	2.12	0.64
4:4:66:LEU:N	4:4:67:PRO:CD	2.61	0.64
2:2:87:VAL:HG12	2:2:88:LEU:HD13	1.78	0.64
4:4:60:ASN:HD21	4:4:65:MET:CE	2.04	0.64
1:1:208:PHE:CE1	3:3:182:ASN:HA	2.34	0.63
3:3:179:ASN:O	3:3:182:ASN:HB2	1.99	0.63
3:3:137:THR:H	3:3:141:GLN:NE2	1.96	0.63
1:1:205:HIS:ND1	1:1:210:ASN:HA	2.14	0.62
2:2:81:ARG:HD3	2:2:143:ASP:OD1	1.99	0.62
2:2:255:ARG:HD2	2:2:255:ARG:O	2.00	0.62
2:2:249:ARG:HG3	2:2:249:ARG:NH1	2.12	0.62
2:2:39:VAL:HG22	2:2:194:GLU:OE2	2.00	0.62
3:3:105:ARG:HH12	3:3:169:HIS:CD2	2.18	0.62
1:1:39:ARG:C	1:1:241:ARG:HG3	2.25	0.61
2:2:9:ASN:HB3	2:2:27:GLN:O	2.01	0.61
1:1:91:GLU:OE1	2:2:156:ARG:HB2	2.01	0.61
1:1:205:HIS:CD2	1:1:212:GLY:HA2	2.35	0.61
1:1:96:GLY:O	2:2:162:LYS:HG2	2.01	0.60
1:1:135:THR:HB	1:1:234:ILE:HG12	1.83	0.60
2:2:44:HIS:HB3	6:2:270:HOH:O	2.01	0.60
3:3:180:ILE:CG2	3:3:181:THR:HG23	2.32	0.60
1:1:149:GLY:HA3	3:3:172:MET:HE2	1.83	0.60
2:2:255:ARG:HH11	2:2:255:ARG:HB3	1.66	0.60
1:1:96:GLY:HA3	1:1:101:SER:HB3	1.83	0.60
2:2:158:GLN:HA	2:2:158:GLN:HE21	1.67	0.60
1:1:81:TYR:HB3	1:1:84:LEU:HB2	1.84	0.59
1:1:181:SER:HB2	3:3:9:GLU:O	2.02	0.59
3:3:56:ASN:O	3:3:61:ALA:HA	2.02	0.59
3:3:43:ASP:O	3:3:46:GLU:HB2	2.01	0.59
2:2:249:ARG:CG	2:2:249:ARG:NH1	2.59	0.59
1:1:32:LYS:CE	4:4:13:SER:HB2	2.27	0.59
2:2:253:LEU:O	2:2:255:ARG:N	2.35	0.59
4:4:46:LYS:H	4:4:46:LYS:CD	2.06	0.59
2:2:82:ILE:HG12	2:2:142:MET:HG3	1.85	0.59
2:2:255:ARG:HB3	2:2:255:ARG:NH1	2.17	0.58
1:1:265:ILE:O	1:1:266:ASP:HB2	2.02	0.58
1:1:207:ARG:NH1	3:3:182:ASN:OD1	2.36	0.58
2:2:19:ALA:HB3	2:2:22:THR:HG21	1.85	0.58
3:3:179:ASN:CB	3:3:183:VAL:CG1	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:63:LYS:O	1:1:64:ALA:HB3	2.03	0.57
1:1:71:LEU:HD21	1:1:225:LEU:HD22	1.85	0.57
3:3:72:VAL:HB	3:3:75:GLN:HB2	1.87	0.57
1:1:265:ILE:CG2	1:1:266:ASP:H	2.16	0.56
1:1:98:GLU:O	1:1:101:SER:N	2.38	0.56
1:1:7:LYS:HE3	1:1:9:VAL:O	2.05	0.56
1:1:61:SER:HA	1:1:66:PRO:HA	1.87	0.56
1:1:230:THR:O	1:1:232:PRO:HD3	2.06	0.56
2:2:10:LEU:HG	2:2:11:SER:CA	2.36	0.56
2:2:251:GLU:HG2	2:2:253:LEU:H	1.70	0.56
1:1:24:VAL:HG13	1:1:24:VAL:O	2.05	0.56
3:3:107:SER:H	3:3:216:ASP:HB3	1.70	0.56
3:3:182:ASN:O	3:3:183:VAL:HG23	2.06	0.56
2:2:202:PRO:HG3	3:3:169:HIS:CE1	2.40	0.56
3:3:105:ARG:HH12	3:3:169:HIS:HD2	1.51	0.56
2:2:71:THR:HG22	2:2:73:THR:HB	1.87	0.55
1:1:210:ASN:O	1:1:212:GLY:N	2.38	0.55
1:1:49:LYS:HG2	1:1:50:SER:H	1.66	0.55
1:1:207:ARG:CD	3:3:180:ILE:CD1	2.84	0.55
1:1:77:PHE:CZ	1:1:82:ASP:HA	2.42	0.55
3:3:182:ASN:O	3:3:183:VAL:CG2	2.55	0.55
2:2:159:THR:O	2:2:161:ARG:N	2.40	0.54
3:3:215:LYS:HB2	4:4:44:PRO:HG3	1.89	0.54
4:4:60:ASN:CG	4:4:61:ALA:H	2.14	0.54
1:1:208:PHE:HE1	3:3:182:ASN:HA	1.72	0.54
1:1:206:LYS:N	1:1:206:LYS:CD	2.69	0.54
3:3:75:GLN:HE21	3:3:75:GLN:HA	1.66	0.53
1:1:122:TYR:HB3	1:1:196:VAL:HG13	1.91	0.53
3:3:177:GLN:HG2	3:3:178:ALA:N	2.19	0.53
1:1:169:ARG:HD2	3:3:223:ILE:O	2.09	0.53
1:1:60:PHE:O	1:1:67:ASN:HB2	2.09	0.53
1:1:96:GLY:HA3	1:1:101:SER:CB	2.38	0.53
3:3:217:PHE:HE2	3:3:219:LEU:HD22	1.74	0.53
1:1:185:SER:HB2	3:3:10:HIS:HB3	1.91	0.53
1:1:148:THR:H	1:1:191:ASN:ND2	2.07	0.53
3:3:180:ILE:HG23	3:3:181:THR:HG23	1.90	0.53
2:2:9:ASN:HB2	2:2:27:GLN:HB3	1.89	0.53
1:1:202:TYR:CG	1:1:217:ALA:HB2	2.43	0.52
4:4:66:LEU:H	4:4:67:PRO:CD	2.22	0.52
3:3:197:TYR:CE2	3:3:203:THR:HG22	2.44	0.52
2:2:16:GLN:HE21	2:2:25:ASN:HD21	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:81:GLN:NE2	3:3:183:VAL:HG21	2.25	0.52
3:3:83:THR:C	3:3:85:SER:H	2.18	0.52
3:3:180:ILE:CG2	3:3:182:ASN:ND2	2.73	0.52
2:2:10:LEU:HD12	2:2:11:SER:N	2.25	0.51
1:1:210:ASN:C	1:1:212:GLY:N	2.68	0.51
3:3:31:VAL:CG1	3:3:32:ALA:N	2.67	0.51
4:4:65:MET:CA	4:4:67:PRO:HD3	2.40	0.51
2:2:79:TYR:C	2:2:79:TYR:CD2	2.88	0.51
2:2:181:GLN:HG3	2:2:191:VAL:HG22	1.93	0.51
1:1:248:PHE:N	1:1:248:PHE:CD2	2.77	0.51
4:4:67:PRO:CD	4:4:68:LEU:H	2.23	0.51
1:1:98:GLU:H	1:1:101:SER:HB2	1.76	0.50
1:1:61:SER:HB3	1:1:82:ASP:O	2.11	0.50
3:3:8:ARG:NH1	3:3:9:GLU:OE1	2.45	0.50
1:1:208:PHE:HE1	3:3:182:ASN:CA	2.23	0.50
2:2:189:THR:HG22	2:2:190:THR:HG23	1.93	0.50
4:4:66:LEU:N	4:4:67:PRO:HD3	2.26	0.50
2:2:26:THR:HB	2:2:190:THR:HG21	1.93	0.50
2:2:71:THR:CG2	2:2:73:THR:H	2.24	0.49
3:3:117:THR:CG2	3:3:119:MET:HB2	2.42	0.49
2:2:10:LEU:CD1	2:2:11:SER:N	2.76	0.49
1:1:207:ARG:HD2	3:3:180:ILE:CD1	2.42	0.49
1:1:205:HIS:CE1	1:1:210:ASN:CB	2.95	0.49
1:1:77:PHE:HD1	1:1:77:PHE:HA	1.52	0.49
2:2:249:ARG:HB3	3:3:130:PRO:HD2	1.95	0.49
3:3:135:LYS:HB3	3:3:186:TRP:CE2	2.48	0.49
1:1:205:HIS:ND1	1:1:210:ASN:OD1	2.43	0.49
2:2:19:ALA:CB	2:2:22:THR:HG22	2.37	0.48
2:2:253:LEU:C	2:2:255:ARG:N	2.70	0.48
2:2:88:LEU:O	2:2:93:GLY:HA3	2.13	0.48
2:2:181:GLN:HE21	2:2:191:VAL:HA	1.79	0.48
3:3:37:MET:HE2	3:3:37:MET:HA	1.95	0.48
1:1:252:PRO:HB3	2:2:174:GLN:HB2	1.96	0.48
1:1:24:VAL:O	1:1:24:VAL:CG1	2.61	0.48
1:1:128:GLU:HB3	1:1:241:ARG:HB3	1.96	0.48
4:4:21:ILE:CG2	4:4:22:ASN:O	2.54	0.48
2:2:181:GLN:NE2	2:2:192:ASP:H	2.11	0.48
2:2:35:GLY:C	2:2:37:GLY:H	2.21	0.48
2:2:33:LEU:HD13	2:2:33:LEU:C	2.39	0.47
2:2:38:THR:HG22	2:2:39:VAL:H	1.79	0.47
4:4:63:SER:OG	4:4:65:MET:HE3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:182:ASN:C	3:3:183:VAL:O	2.52	0.47
2:2:183:LEU:C	2:2:183:LEU:HD23	2.38	0.47
3:3:182:ASN:C	3:3:183:VAL:CG2	2.88	0.47
4:4:14:GLU:N	4:4:14:GLU:OE1	2.47	0.47
1:1:207:ARG:HB3	3:3:182:ASN:HD21	1.80	0.47
3:3:115:THR:HB	3:3:206:LYS:O	2.15	0.47
1:1:81:TYR:CD2	1:1:84:LEU:HD12	2.49	0.46
2:2:79:TYR:CE2	2:2:81:ARG:HD2	2.51	0.46
2:2:130:MET:HG3	2:2:214:LEU:HA	1.96	0.46
1:1:1:GLY:N	1:1:18:ASP:OD2	2.49	0.46
1:1:243:LYS:HD2	1:1:243:LYS:HA	1.48	0.46
3:3:117:THR:CG2	3:3:120:MET:HG3	2.45	0.46
1:1:142:LEU:HD21	1:1:166:SER:HB2	1.98	0.46
2:2:38:THR:HG22	2:2:39:VAL:N	2.30	0.46
2:2:74:GLN:HB3	2:2:218:VAL:HG21	1.98	0.46
3:3:197:TYR:HB2	3:3:198:PRO:HD2	1.97	0.46
2:2:144:ASN:HD22	2:2:144:ASN:HA	1.20	0.46
3:3:1:SER:N	3:3:2:PRO:CD	2.79	0.46
3:3:201:CYS:HA	3:3:202:PRO:HD3	1.86	0.46
1:1:94:GLY:HA3	2:2:162:LYS:HB2	1.97	0.46
1:1:208:PHE:HE1	3:3:182:ASN:CG	2.22	0.46
3:3:36:TYR:CE1	3:3:37:MET:CE	2.98	0.45
4:4:21:ILE:HA	4:4:21:ILE:HD12	1.19	0.45
1:1:191:ASN:HA	3:3:221:MET:HE1	1.99	0.45
1:1:224:THR:HG22	1:1:225:LEU:N	2.31	0.45
1:1:75:PRO:HA	1:1:110:GLN:HB3	1.99	0.45
1:1:98:GLU:O	1:1:98:GLU:HG3	2.16	0.45
1:1:148:THR:H	1:1:191:ASN:HD22	1.63	0.45
1:1:206:LYS:HE2	1:1:216:ILE:O	2.17	0.45
1:1:256:PHE:HA	1:1:257:PRO:HD3	1.63	0.45
1:1:207:ARG:HD3	3:3:182:ASN:OD1	2.17	0.45
3:3:36:TYR:CE1	3:3:37:MET:HE3	2.52	0.45
3:3:64:TYR:CZ	3:3:206:LYS:HD3	2.52	0.45
3:3:179:ASN:HB3	3:3:183:VAL:CG1	2.27	0.45
3:3:180:ILE:HG22	3:3:181:THR:HG23	1.97	0.45
1:1:98:GLU:HA	2:2:161:ARG:HG2	1.99	0.45
2:2:162:LYS:HE3	2:2:162:LYS:HA	1.99	0.45
3:3:179:ASN:HB2	3:3:183:VAL:CG1	2.47	0.44
2:2:10:LEU:O	2:2:13:ARG:CA	2.64	0.44
1:1:81:TYR:N	1:1:81:TYR:CD1	2.84	0.44
2:2:59:VAL:HG22	2:2:96:PHE:CA	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:253:LEU:HD13	2:2:253:LEU:HA	1.73	0.44
3:3:144:GLN:NE2	3:3:144:GLN:CA	2.81	0.44
1:1:231:LYS:HB3	1:1:234:ILE:HD13	1.99	0.44
2:2:20:GLY:H	2:2:22:THR:HB	1.81	0.44
3:3:139:ARG:HH11	3:3:139:ARG:HD3	1.51	0.44
1:1:46:PHE:CD1	1:1:46:PHE:N	2.85	0.44
2:2:35:GLY:C	2:2:37:GLY:N	2.76	0.44
3:3:8:ARG:HH11	3:3:8:ARG:HD2	1.60	0.44
1:1:205:HIS:HD1	1:1:210:ASN:HA	1.82	0.44
1:1:231:LYS:HD2	1:1:231:LYS:HA	1.63	0.44
2:2:105:LEU:HD13	2:2:203:THR:HG21	2.00	0.44
1:1:4:ASN:O	1:1:7:LYS:HE2	2.18	0.44
1:1:77:PHE:O	1:1:78:ASP:CB	2.61	0.44
2:2:22:THR:HG23	2:2:62:TYR:HB2	2.00	0.44
2:2:122:HIS:CE1	2:2:228:ALA:HB1	2.52	0.44
1:1:217:ALA:HA	1:1:218:PRO:HD2	1.67	0.44
3:3:107:SER:HB3	3:3:161:THR:CG2	2.48	0.43
3:3:162:VAL:HA	3:3:163:PRO:HD3	1.82	0.43
1:1:3:GLU:HG3	1:1:4:ASN:H	1.80	0.43
1:1:205:HIS:C	1:1:206:LYS:HD2	2.43	0.43
2:2:28:SER:OG	2:2:189:THR:HB	2.18	0.43
1:1:38:ASP:OD2	1:1:241:ARG:HD3	2.18	0.43
1:1:96:GLY:CA	1:1:101:SER:HB3	2.48	0.43
1:1:107:LYS:HD3	1:1:107:LYS:HA	1.79	0.43
1:1:131:LEU:HD12	1:1:238:VAL:HG22	2.00	0.43
2:2:130:MET:HE3	2:2:130:MET:HB2	1.39	0.43
1:1:67:ASN:HD22	1:1:67:ASN:HA	0.88	0.43
2:2:16:GLN:HB2	2:2:25:ASN:ND2	2.33	0.43
2:2:156:ARG:HD3	6:2:305:HOH:O	2.18	0.43
1:1:34:ALA:O	1:1:38:ASP:HB2	2.18	0.43
3:3:117:THR:HG22	3:3:120:MET:HG3	2.01	0.43
3:3:180:ILE:HG22	3:3:182:ASN:ND2	2.33	0.43
2:2:86:HIS:H	2:2:86:HIS:CD2	2.36	0.42
4:4:53:ASN:HD22	4:4:53:ASN:HA	1.35	0.42
1:1:208:PHE:CE1	3:3:182:ASN:CB	2.96	0.42
2:2:9:ASN:CB	2:2:27:GLN:O	2.67	0.42
2:2:82:ILE:HG23	2:2:87:VAL:HG21	2.01	0.42
2:2:253:LEU:HB3	2:2:254:SER:H	1.19	0.42
2:2:10:LEU:HD12	2:2:10:LEU:C	2.38	0.42
3:3:83:THR:C	3:3:85:SER:N	2.78	0.42
1:1:49:LYS:CG	1:1:50:SER:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:205:HIS:CD2	1:1:214:LEU:HD23	2.55	0.42
2:2:224:TYR:CD1	2:2:224:TYR:C	2.96	0.42
3:3:19:PRO:HB3	4:4:29:TYR:CD2	2.55	0.42
3:3:197:TYR:CZ	3:3:203:THR:CG2	2.96	0.42
2:2:151:LEU:HA	2:2:152:PRO:HA	1.92	0.42
2:2:158:GLN:NE2	2:2:158:GLN:CA	2.80	0.42
3:3:58:VAL:HA	3:3:59:PRO:HA	1.94	0.42
1:1:14:ASP:C	1:1:16:THR:H	2.27	0.42
1:1:172:GLN:O	3:3:16:SER:HB3	2.20	0.42
1:1:207:ARG:HD3	3:3:180:ILE:HD13	1.97	0.42
3:3:217:PHE:CE2	3:3:219:LEU:HD22	2.53	0.42
1:1:85:ARG:O	1:1:85:ARG:HG2	2.20	0.41
3:3:109:VAL:O	3:3:211:VAL:HA	2.19	0.41
2:2:111:ARG:NH1	2:2:194:GLU:OE1	2.53	0.41
2:2:249:ARG:NH1	2:2:250:HIS:O	2.54	0.41
3:3:35:ASN:H	3:3:35:ASN:HD22	1.68	0.41
1:1:153:LYS:C	1:1:155:THR:H	2.28	0.41
2:2:39:VAL:HG22	2:2:194:GLU:CD	2.45	0.41
3:3:18:LEU:HD13	3:3:20:ASP:HB3	2.01	0.41
1:1:169:ARG:HD2	1:1:169:ARG:HH11	1.43	0.41
4:4:30:GLN:O	4:4:30:GLN:HG3	2.21	0.41
4:4:59:VAL:HG22	4:4:60:ASN:N	2.32	0.41
1:1:99:GLU:HB2	1:1:100:THR:HG23	2.03	0.41
3:3:73:LYS:O	3:3:138:SER:HA	2.20	0.40
1:1:48:VAL:HG12	1:1:232:PRO:HA	2.02	0.40
2:2:160:ASN:HD22	2:2:160:ASN:HA	1.39	0.40
4:4:65:MET:HE3	4:4:65:MET:HB3	1.81	0.40
4:4:66:LEU:H	4:4:67:PRO:HD2	1.85	0.40
1:1:207:ARG:HB2	1:1:209:ASP:OD1	2.22	0.40
2:2:40:HIS:HB3	2:2:241:VAL:HG12	2.04	0.40
2:2:201:ALA:HB1	2:2:202:PRO:HD2	2.02	0.40
1:1:191:ASN:OD1	1:1:191:ASN:N	2.53	0.40
4:4:14:GLU:OE1	4:4:14:GLU:CA	2.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	266/277 (96%)	238 (90%)	20 (8%)	8 (3%)	3	19
2	2	247/256 (96%)	227 (92%)	17 (7%)	3 (1%)	10	40
3	3	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	5	26
4	4	56/70 (80%)	46 (82%)	6 (11%)	4 (7%)	1	4
All	All	798/834 (96%)	719 (90%)	59 (7%)	20 (2%)	4	23

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	77	PHE
1	1	99	GLU
1	1	266	ASP
2	2	11	SER
2	2	253	LEU
3	3	183	VAL
4	4	66	LEU
1	1	265	ILE
3	3	90	ALA
3	3	177	GLN
4	4	59	VAL
4	4	62	PHE
4	4	63	SER
1	1	189	PRO
1	1	78	ASP
3	3	180	ILE
1	1	176	ALA
1	1	249	CYS
2	2	160	ASN
3	3	221	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	233/240 (97%)	185 (79%)	48 (21%)	1	7
2	2	217/224 (97%)	176 (81%)	41 (19%)	1	9
3	3	195/195 (100%)	158 (81%)	37 (19%)	1	8
4	4	48/59 (81%)	31 (65%)	17 (35%)	0	1
All	All	693/718 (96%)	550 (79%)	143 (21%)	1	7

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	2	VAL
1	1	9	VAL
1	1	10	THR
1	1	12	ASN
1	1	16	THR
1	1	22	GLN
1	1	24	VAL
1	1	48	VAL
1	1	60	PHE
1	1	67	ASN
1	1	77	PHE
1	1	83	GLN
1	1	85	ARG
1	1	89	LEU
1	1	99	GLU
1	1	103	VAL
1	1	110	GLN
1	1	116	LEU
1	1	124	LYS
1	1	131	LEU
1	1	153	LYS
1	1	155	THR
1	1	158	VAL
1	1	161	GLU

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Mol	Chain	Res	Type
1	1	167	GLU
1	1	169	ARG
1	1	172	GLN
1	1	175	SER
1	1	185	SER
1	1	188	VAL
1	1	190	TYR
1	1	191	ASN
1	1	196	VAL
1	1	197	LEU
1	1	206	LYS
1	1	207	ARG
1	1	208	PHE
1	1	213	ASP
1	1	225	LEU
1	1	233	ASP
1	1	241	ARG
1	1	243	LYS
1	1	251	ARG
1	1	261	SER
1	1	264	LYS
1	1	265	ILE
1	1	267	MET
1	1	268	THR
2	2	8	GLU
2	2	9	ASN
2	2	11	SER
2	2	16	GLN
2	2	22	THR
2	2	27	GLN
2	2	29	THR
2	2	38	THR
2	2	39	VAL
2	2	57	LEU
2	2	59	VAL
2	2	71	THR
2	2	72	SER
2	2	75	LYS
2	2	81	ARG
2	2	87	VAL
2	2	88	LEU
2	2	114	VAL

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Mol	Chain	Res	Type
2	2	117	ASN
2	2	120	GLN
2	2	137	LEU
2	2	144	ASN
2	2	145	ARG
2	2	148	LYS
2	2	156	ARG
2	2	158	GLN
2	2	159	THR
2	2	161	ARG
2	2	181	GLN
2	2	186	ARG
2	2	189	THR
2	2	191	VAL
2	2	207	THR
2	2	223	THR
2	2	230	THR
2	2	231	SER
2	2	239	GLN
2	2	253	LEU
2	2	254	SER
2	2	255	ARG
2	2	256	GLN
3	3	1	SER
3	3	9	GLU
3	3	18	LEU
3	3	31	VAL
3	3	40	GLU
3	3	46	GLU
3	3	57	LYS
3	3	63	PRO
3	3	66	GLU
3	3	72	VAL
3	3	74	THR
3	3	75	GLN
3	3	77	LEU
3	3	79	VAL
3	3	81	GLN
3	3	97	LEU
3	3	99	ARG
3	3	115	THR
3	3	117	THR

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Mol	Chain	Res	Type
3	3	121	LYS
3	3	143	MET
3	3	152	LEU
3	3	157	SER
3	3	162	VAL
3	3	172	MET
3	3	177	GLN
3	3	182	ASN
3	3	191	GLN
3	3	198	PRO
3	3	208	LEU
3	3	215	LYS
3	3	216	ASP
3	3	218	SER
3	3	219	LEU
3	3	223	ILE
3	3	224	SER
3	3	231	GLN
4	4	13	SER
4	4	14	GLU
4	4	19	VAL
4	4	20	ILE
4	4	21	ILE
4	4	22	ASN
4	4	30	GLN
4	4	34	ASP
4	4	35	LEU
4	4	38	ASN
4	4	46	LYS
4	4	47	THR
4	4	54	LEU
4	4	56	SER
4	4	62	PHE
4	4	65	MET
4	4	66	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	29	ASN
1	1	67	ASN
1	1	76	GLN

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Mol	Chain	Res	Type
1	1	83	GLN
1	1	97	ASN
1	1	157	GLN
1	1	172	GLN
1	1	244	ASN
2	2	25	ASN
2	2	144	ASN
2	2	158	GLN
2	2	160	ASN
2	2	171	ASN
2	2	181	GLN
2	2	184	ASN
2	2	208	GLN
2	2	250	HIS
3	3	35	ASN
3	3	56	ASN
3	3	75	GLN
3	3	81	GLN
3	3	103	GLN
3	3	141	GLN
3	3	144	GLN
3	3	169	HIS
4	4	16	ASN
4	4	27	ASN
4	4	50	GLN
4	4	53	ASN
4	4	60	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PO4	2	257	-	4,4,4	2.95	4 (100%)	6,6,6	0.31	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	257	PO4	P-O2	-3.17	1.45	1.54
5	2	257	PO4	P-O3	-3.15	1.45	1.54
5	2	257	PO4	P-O4	-3.14	1.45	1.54
5	2	257	PO4	P-O1	-2.22	1.45	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	268/277 (96%)	2.86	189 (70%) 0 0	2, 9, 57, 77	0
2	2	249/256 (97%)	3.05	181 (72%) 0 0	2, 7, 44, 62	0
3	3	231/231 (100%)	2.66	142 (61%) 0 0	2, 7, 40, 82	0
4	4	58/70 (82%)	1.63	18 (31%) 1 1	13, 38, 60, 61	0
All	All	806/834 (96%)	2.77	530 (65%) 0 0	2, 8, 52, 82	0

All (530) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	2	33	LEU	9.2
3	3	151	ASP	8.8
1	1	118	SER	8.7
2	2	48	CYS	8.5
2	2	90	GLY	8.3
3	3	65	ILE	8.1
3	3	194	PRO	8.1
2	2	135	PRO	7.7
2	2	217	ALA	7.5
3	3	212	SER	7.4
2	2	246	ASN	7.4
3	3	217	PHE	7.3
2	2	176	THR	7.1
2	2	240	PRO	7.0
2	2	36	TYR	6.9
2	2	58	ALA	6.9
1	1	74	GLY	6.8
4	4	19	VAL	6.8
4	4	16	ASN	6.7
1	1	69	VAL	6.7
1	1	75	PRO	6.7

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Mol	Chain	Res	Type	RSRZ
3	3	54	ILE	6.6
3	3	136	PRO	6.6
1	1	45	ALA	6.5
2	2	215	VAL	6.5
3	3	211	VAL	6.5
2	2	136	THR	6.4
2	2	131	ALA	6.3
3	3	55	GLY	6.3
3	3	162	VAL	6.3
2	2	47	SER	6.3
2	2	67	VAL	6.3
2	2	201	ALA	6.1
1	1	229	GLY	6.1
3	3	221	MET	6.0
1	1	201	TRP	6.0
2	2	37	GLY	6.0
1	1	146	CYS	6.0
1	1	217	ALA	6.0
1	1	228	ALA	5.9
2	2	42	GLY	5.9
2	2	127	LEU	5.9
1	1	132	SER	5.8
2	2	195	VAL	5.8
1	1	170	THR	5.8
2	2	96	PHE	5.8
1	1	68	SER	5.8
3	3	214	GLY	5.8
1	1	120	PHE	5.7
1	1	188	VAL	5.7
1	1	200	VAL	5.7
2	2	142	MET	5.7
2	2	194	GLU	5.6
2	2	128	VAL	5.6
3	3	78	ALA	5.6
2	2	117	ASN	5.5
1	1	221	ASP	5.5
2	2	15	SER	5.5
2	2	155	THR	5.5
1	1	195	SER	5.5
2	2	191	VAL	5.4
3	3	64	TYR	5.4
1	1	43	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
3	3	89	LEU	5.3
1	1	129	VAL	5.3
1	1	125	CYS	5.2
1	1	222	PHE	5.2
1	1	121	VAL	5.2
2	2	168	ASP	5.2
1	1	249	CYS	5.2
3	3	216	ASP	5.1
1	1	122	TYR	5.1
2	2	125	SER	5.1
2	2	171	ASN	5.1
1	1	227	PHE	5.0
2	2	29	THR	5.0
1	1	126	ASP	5.0
1	1	48	VAL	5.0
1	1	252	PRO	4.9
3	3	110	TYR	4.9
1	1	240	LEU	4.9
3	3	126	ILE	4.9
1	1	226	PHE	4.9
3	3	218	SER	4.9
2	2	109	GLY	4.9
1	1	198	PRO	4.9
1	1	245	MET	4.9
4	4	32	SER	4.9
3	3	88	CYS	4.9
3	3	224	SER	4.8
3	3	127	ALA	4.8
2	2	28	SER	4.8
1	1	47	ALA	4.8
1	1	154	PRO	4.8
2	2	188	ASN	4.7
3	3	120	MET	4.7
2	2	180	HIS	4.7
2	2	200	ILE	4.7
1	1	44	GLY	4.7
1	1	76	GLN	4.7
2	2	223	THR	4.7
1	1	123	TYR	4.7
1	1	173	VAL	4.6
1	1	157	GLN	4.6
1	1	176	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
2	2	209	HIS	4.6
1	1	203	ASN	4.6
2	2	50	ASP	4.5
2	2	178	TYR	4.5
1	1	131	LEU	4.5
1	1	186	PHE	4.5
2	2	243	PRO	4.4
2	2	89	SER	4.4
2	2	236	ALA	4.4
1	1	150	THR	4.4
3	3	131	PRO	4.4
3	3	227	PRO	4.4
2	2	193	LEU	4.3
2	2	237	SER	4.3
1	1	46	PHE	4.3
1	1	167	GLU	4.3
2	2	247	GLY	4.3
2	2	129	PHE	4.3
2	2	123	ALA	4.3
1	1	8	GLY	4.3
2	2	163	GLY	4.3
4	4	44	PRO	4.3
3	3	188	THR	4.2
1	1	185	SER	4.2
2	2	88	LEU	4.2
1	1	134	HIS	4.2
3	3	100	ASN	4.2
4	4	31	ASN	4.2
3	3	111	THR	4.2
2	2	134	TYR	4.2
1	1	113	SER	4.2
3	3	77	LEU	4.2
2	2	213	THR	4.2
3	3	209	THR	4.2
3	3	102	ALA	4.1
1	1	204	GLY	4.1
2	2	94	GLY	4.1
1	1	165	LEU	4.1
2	2	105	LEU	4.1
1	1	5	ALA	4.1
3	3	164	PHE	4.1
1	1	62	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
2	2	169	HIS	4.1
1	1	38	ASP	4.1
1	1	220	SER	4.1
2	2	132	PRO	4.0
2	2	97	GLY	4.0
3	3	109	VAL	4.0
2	2	199	ASN	4.0
3	3	53	PHE	4.0
1	1	110	GLN	4.0
2	2	76	PRO	4.0
1	1	238	VAL	4.0
2	2	20	GLY	4.0
2	2	130	MET	4.0
1	1	162	VAL	4.0
3	3	112	PHE	4.0
1	1	29	ASN	4.0
1	1	237	THR	4.0
3	3	187	VAL	3.9
1	1	87	GLN	3.9
1	1	239	TYR	3.9
2	2	40	HIS	3.9
2	2	214	LEU	3.9
2	2	248	LEU	3.9
4	4	26	SER	3.9
1	1	115	CYS	3.9
2	2	141	ALA	3.9
1	1	145	TRP	3.9
2	2	220	ALA	3.8
1	1	65	CYS	3.8
1	1	184	ILE	3.8
3	3	101	PHE	3.8
1	1	244	ASN	3.8
1	1	9	VAL	3.8
3	3	67	ALA	3.8
3	3	184	ASP	3.8
3	3	207	ILE	3.7
4	4	27	ASN	3.7
2	2	56	ILE	3.7
1	1	86	PRO	3.7
1	1	248	PHE	3.7
1	1	7	LYS	3.7
2	2	79	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
3	3	97	LEU	3.7
1	1	190	TYR	3.7
3	3	92	THR	3.7
1	1	219	ASN	3.7
1	1	250	PRO	3.6
1	1	192	SER	3.6
3	3	158	TYR	3.6
3	3	22	THR	3.6
3	3	129	THR	3.6
3	3	201	CYS	3.6
3	3	147	TYR	3.6
3	3	193	THR	3.6
4	4	40	THR	3.6
1	1	140	GLY	3.6
3	3	2	PRO	3.6
2	2	218	VAL	3.6
2	2	244	VAL	3.6
3	3	226	ALA	3.6
3	3	94	LEU	3.6
2	2	181	GLN	3.6
2	2	173	TRP	3.6
3	3	130	PRO	3.6
1	1	187	VAL	3.6
2	2	104	TYR	3.6
3	3	128	TYR	3.6
2	2	212	TRP	3.6
2	2	62	TYR	3.6
3	3	152	LEU	3.6
1	1	148	THR	3.6
2	2	53	SER	3.6
2	2	204	SER	3.6
1	1	58	ALA	3.5
3	3	142	ALA	3.5
1	1	107	LYS	3.5
2	2	235	THR	3.5
2	2	110	TRP	3.5
1	1	6	GLU	3.5
2	2	80	ILE	3.5
3	3	205	ALA	3.5
1	1	242	TYR	3.5
1	1	108	THR	3.5
2	2	208	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
2	2	175	TRP	3.5
3	3	190	TRP	3.5
2	2	111	ARG	3.5
3	3	69	ASN	3.5
2	2	34	VAL	3.5
3	3	161	THR	3.4
3	3	82	VAL	3.4
3	3	63	PRO	3.4
3	3	86	CYS	3.4
1	1	142	LEU	3.4
1	1	194	LEU	3.4
1	1	241	ARG	3.4
1	1	156	THR	3.4
1	1	50	SER	3.4
1	1	127	LEU	3.4
1	1	30	GLN	3.4
1	1	71	LEU	3.3
1	1	199	ALA	3.3
3	3	189	VAL	3.3
3	3	40	GLU	3.3
3	3	156	SER	3.3
3	3	15	TYR	3.3
1	1	59	PRO	3.3
1	1	191	ASN	3.3
2	2	126	LEU	3.3
2	2	238	ILE	3.3
3	3	185	GLY	3.3
3	3	198	PRO	3.3
2	2	108	THR	3.3
2	2	189	THR	3.3
1	1	141	LEU	3.3
2	2	46	ALA	3.3
2	2	211	SER	3.3
1	1	232	PRO	3.3
3	3	99	ARG	3.3
2	2	84	LEU	3.3
3	3	52	THR	3.3
3	3	223	ILE	3.3
2	2	179	PRO	3.2
1	1	33	VAL	3.2
1	1	72	THR	3.2
1	1	82	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	1	205	HIS	3.2
2	2	139	VAL	3.2
3	3	108	LEU	3.2
3	3	107	SER	3.2
3	3	117	THR	3.2
1	1	139	HIS	3.2
1	1	152	THR	3.2
3	3	210	MET	3.2
1	1	128	GLU	3.2
3	3	58	VAL	3.2
3	3	11	ALA	3.2
2	2	92	ASP	3.1
2	2	233	ASP	3.1
1	1	51	GLY	3.1
1	1	147	PRO	3.1
1	1	171	PRO	3.1
1	1	111	ASP	3.1
1	1	158	VAL	3.1
1	1	3	GLU	3.1
3	3	163	PRO	3.1
4	4	48	TYR	3.1
2	2	166	ALA	3.1
1	1	149	GLY	3.1
1	1	253	THR	3.1
1	1	88	ARG	3.1
2	2	114	VAL	3.1
3	3	171	ARG	3.1
3	3	170	PHE	3.1
2	2	68	ASN	3.1
1	1	225	LEU	3.1
2	2	35	GLY	3.1
2	2	13	ARG	3.1
2	2	32	ARG	3.1
3	3	68	SER	3.1
3	3	103	GLN	3.0
2	2	107	LYS	3.0
1	1	193	PRO	3.0
3	3	36	TYR	3.0
3	3	61	ALA	3.0
4	4	35	LEU	3.0
3	3	13	THR	3.0
2	2	146	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
3	3	169	HIS	3.0
1	1	182	ASN	3.0
2	2	95	VAL	3.0
2	2	172	PHE	3.0
3	3	66	GLU	3.0
3	3	18	LEU	3.0
3	3	98	SER	3.0
2	2	44	HIS	3.0
2	2	113	GLN	3.0
3	3	174	GLY	3.0
1	1	77	PHE	3.0
2	2	77	PHE	3.0
2	2	182	PHE	3.0
1	1	55	SER	3.0
2	2	197	TYR	3.0
2	2	143	ASP	3.0
2	2	30	VAL	3.0
3	3	196	THR	3.0
1	1	202	TYR	2.9
2	2	41	ASP	2.9
2	2	192	ASP	2.9
1	1	4	ASN	2.9
2	2	144	ASN	2.9
1	1	155	THR	2.9
3	3	146	THR	2.9
2	2	19	ALA	2.9
1	1	40	SER	2.9
3	3	160	PHE	2.9
2	2	232	LEU	2.9
2	2	202	PRO	2.9
2	2	38	THR	2.9
2	2	54	GLU	2.9
3	3	134	GLY	2.9
3	3	159	SER	2.9
1	1	66	PRO	2.9
3	3	90	ALA	2.9
3	3	225	PRO	2.8
2	2	186	ARG	2.8
3	3	106	GLY	2.8
1	1	234	ILE	2.8
2	2	63	TYR	2.8
1	1	251	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	1	89	LEU	2.8
2	2	147	SER	2.8
1	1	169	ARG	2.8
1	1	247	VAL	2.8
4	4	47	THR	2.8
2	2	151	LEU	2.8
2	2	153	ASN	2.8
2	2	100	LEU	2.8
2	2	187	THR	2.8
3	3	70	THR	2.8
3	3	133	ALA	2.8
3	3	5	VAL	2.8
2	2	157	THR	2.8
3	3	20	ASP	2.7
2	2	249	ARG	2.7
2	2	174	GLN	2.7
1	1	175	SER	2.7
2	2	150	ASN	2.7
3	3	91	ASN	2.7
1	1	24	VAL	2.7
1	1	90	THR	2.7
2	2	14	VAL	2.7
1	1	73	PRO	2.7
3	3	132	GLY	2.7
3	3	186	TRP	2.7
3	3	96	ALA	2.7
1	1	42	PRO	2.7
2	2	45	PRO	2.7
4	4	56	SER	2.7
2	2	86	HIS	2.7
1	1	53	LEU	2.6
1	1	144	ARG	2.6
1	1	137	GLY	2.6
2	2	183	LEU	2.6
1	1	52	SER	2.6
1	1	164	SER	2.6
3	3	138	SER	2.6
1	1	83	GLN	2.6
2	2	99	THR	2.6
3	3	137	THR	2.6
2	2	116	CYS	2.6
1	1	112	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	2	224	TYR	2.6
3	3	87	SER	2.6
2	2	27	GLN	2.6
1	1	54	GLU	2.6
2	2	106	VAL	2.6
3	3	84	LEU	2.6
1	1	91	GLU	2.6
4	4	14	GLU	2.6
1	1	254	VAL	2.6
2	2	198	VAL	2.6
2	2	66	LYS	2.6
3	3	50	ILE	2.5
2	2	65	PHE	2.5
3	3	124	PHE	2.5
3	3	10	HIS	2.5
1	1	119	PRO	2.5
1	1	214	LEU	2.5
2	2	210	ALA	2.5
2	2	245	PHE	2.5
3	3	41	TYR	2.5
1	1	166	SER	2.5
2	2	229	SER	2.5
1	1	243	LYS	2.5
2	2	149	ASP	2.5
3	3	56	ASN	2.5
3	3	148	ALA	2.5
3	3	17	THR	2.5
1	1	104	PHE	2.5
3	3	144	GLN	2.5
2	2	184	ASN	2.5
3	3	7	ILE	2.5
2	2	254	SER	2.5
3	3	140	ASP	2.5
3	3	24	PRO	2.5
3	3	51	PRO	2.5
2	2	103	HIS	2.5
1	1	70	ILE	2.4
1	1	181	SER	2.4
3	3	46	GLU	2.4
2	2	160	ASN	2.4
1	1	130	THR	2.4
2	2	207	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	1	151	PRO	2.4
3	3	141	GLN	2.4
2	2	167	MET	2.4
4	4	51	PHE	2.4
1	1	210	ASN	2.4
2	2	112	VAL	2.4
3	3	23	VAL	2.4
3	3	122	GLY	2.4
1	1	109	LYS	2.4
2	2	177	LEU	2.4
1	1	211	THR	2.4
2	2	22	THR	2.4
3	3	199	PRO	2.4
2	2	170	GLN	2.4
1	1	27	PRO	2.4
2	2	26	THR	2.4
2	2	85	PRO	2.4
1	1	213	ASP	2.4
1	1	223	GLY	2.3
2	2	203	THR	2.3
1	1	95	ASN	2.3
1	1	153	LYS	2.3
1	1	39	ARG	2.3
4	4	37	ALA	2.3
2	2	205	SER	2.3
3	3	219	LEU	2.3
1	1	92	ILE	2.3
2	2	82	ILE	2.3
2	2	234	ILE	2.3
1	1	80	ALA	2.3
2	2	24	THR	2.3
3	3	208	LEU	2.3
2	2	206	TRP	2.3
2	2	121	PHE	2.3
1	1	78	ASP	2.3
2	2	242	ARG	2.3
1	1	258	TRP	2.3
1	1	208	PHE	2.3
1	1	180	THR	2.2
1	1	61	SER	2.2
4	4	28	GLN	2.2
3	3	157	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	3	62	VAL	2.2
3	3	81	GLN	2.2
1	1	67	ASN	2.2
2	2	25	ASN	2.2
2	2	133	GLU	2.2
1	1	177	GLY	2.2
1	1	218	PRO	2.2
2	2	221	PRO	2.2
2	2	162	LYS	2.2
1	1	135	THR	2.2
1	1	12	ASN	2.2
1	1	15	ALA	2.2
1	1	96	GLY	2.2
1	1	105	PRO	2.2
2	2	17	ASP	2.2
1	1	57	PHE	2.2
2	2	98	ALA	2.1
3	3	16	SER	2.1
1	1	168	GLY	2.1
1	1	215	GLY	2.1
3	3	8	ARG	2.1
3	3	105	ARG	2.1
1	1	209	ASP	2.1
3	3	104	TYR	2.1
2	2	78	GLU	2.1
2	2	91	GLU	2.1
1	1	114	PHE	2.1
1	1	37	TYR	2.1
1	1	36	PHE	2.1
2	2	9	ASN	2.1
2	2	185	LEU	2.1
4	4	20	ILE	2.1
3	3	181	THR	2.1
2	2	87	VAL	2.1
1	1	85	ARG	2.1
1	1	34	ALA	2.1
3	3	19	PRO	2.1
2	2	148	LYS	2.0
3	3	213	ALA	2.0
4	4	49	GLY	2.0
3	3	72	VAL	2.0
3	3	183	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	1	116	LEU	2.0
3	3	125	LEU	2.0
2	2	196	PRO	2.0
1	1	196	VAL	2.0
1	1	246	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	2	257	5/5	0.89	0.25	43,56,64,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.