



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:48 PM UTC

PDB ID : 3TGL / pdb_00003tgl
Title : STRUCTURE AND MOLECULAR MODEL REFINEMENT OF RHIZOMUCOR MIEHEI TRIACYLGLYCERIDE LIPASE: A CASE STUDY OF THE USE OF SIMULATED ANNEALING IN PARTIAL MODEL REFINEMENT
Authors : Brady, L.; Brzozowski, A.M.; Derewenda, Z.S.; Dodson, E.J.; Dodson, G.G.; Tolley, S.P.; Turkenburg, J.P.; Christiansen, L.; Huge-Jensen, B.; Norskov, L.; Thim, L.
Deposited on : 1991-07-29
Resolution : 1.90 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

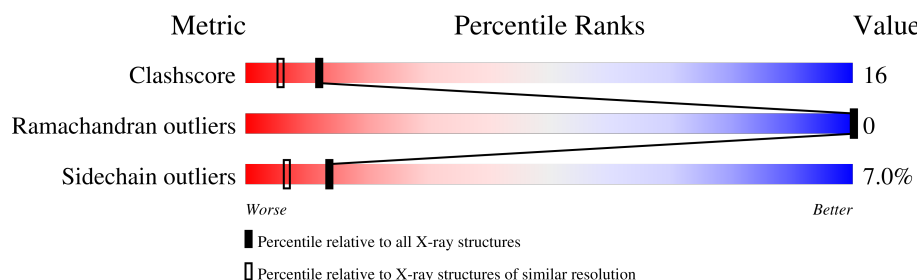
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	269	22% 58% 17% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2289 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 TRIACYL-GLYCEROL ACYLHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2059	1308	337	406	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ASN	ASP	conflict	UNP P19515
A	150	VAL	ALA	conflict	UNP P19515

- Molecule 2 is water.

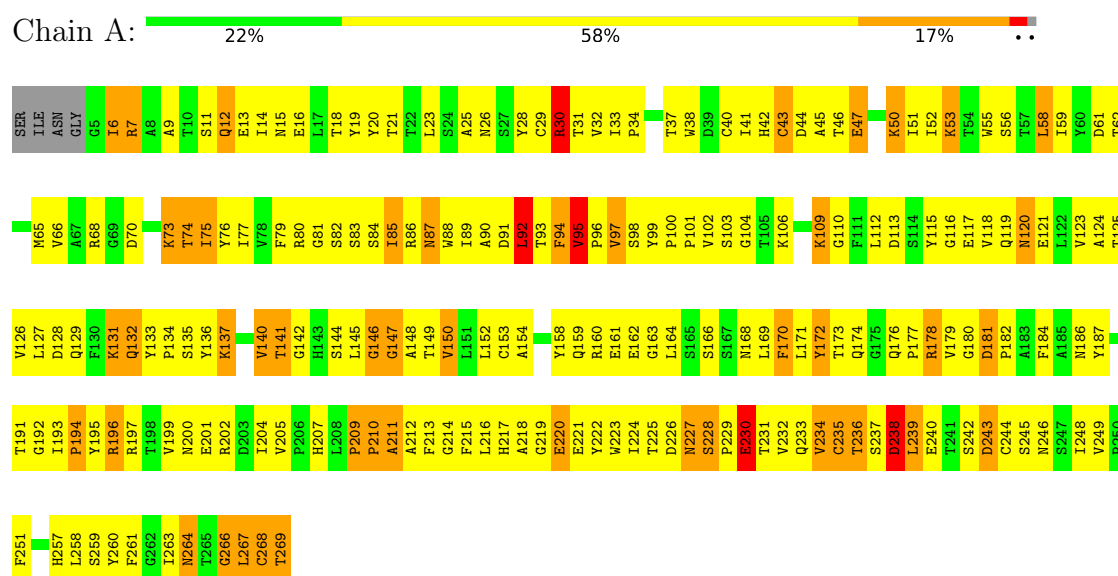
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	230	Total	O	0	0
			230	230		

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: TRIACYL-GLYCEROL ACYLHYDROLASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.60Å 75.00Å 55.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.50 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (7.50-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.129 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2289	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.27	3/2110 (0.1%)	3.70	457/2885 (15.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	GLY	N-CA	5.53	1.52	1.45
1	A	149	THR	CA-CB	5.17	1.61	1.53
1	A	244	CYS	N-CA	5.02	1.50	1.46

All (457) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	LEU	O-C-N	19.66	146.98	122.20
1	A	120	ASN	OD1-CG-ND2	18.37	140.97	122.60
1	A	267	LEU	CA-C-O	-16.80	101.03	119.34
1	A	44	ASP	CA-C-N	14.95	140.32	120.28
1	A	44	ASP	C-N-CA	14.95	140.32	120.28
1	A	137	LYS	CB-CA-C	13.89	134.14	109.83
1	A	160	ARG	NE-CZ-NH2	13.37	131.23	119.20
1	A	263	ILE	O-C-N	13.28	137.77	123.03
1	A	74	THR	O-C-N	13.13	139.22	123.33
1	A	15	ASN	CA-CB-CG	-12.95	99.65	112.60
1	A	110	GLY	O-C-N	-12.75	109.95	122.19
1	A	68	ARG	NE-CZ-NH1	12.51	134.01	121.50
1	A	192	GLY	O-C-N	-12.47	106.51	122.34
1	A	100	PRO	N-CA-C	12.30	125.70	110.70
1	A	85	ILE	O-C-N	12.24	133.74	121.87
1	A	43	CYS	CA-C-N	-12.18	102.73	120.28
1	A	43	CYS	C-N-CA	-12.18	102.73	120.28
1	A	25	ALA	O-C-N	12.03	134.46	122.07
1	A	70	ASP	CA-CB-CG	-11.98	100.62	112.60
1	A	85	ILE	CA-C-O	-11.94	108.53	120.95
1	A	181	ASP	CB-CG-OD1	11.93	145.83	118.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	CYS	O-C-N	11.83	139.70	122.43
1	A	132	GLN	CA-C-O	-11.82	105.84	119.79
1	A	87	ASN	CA-CB-CG	-11.58	101.02	112.60
1	A	85	ILE	CB-CA-C	11.57	127.76	112.14
1	A	227	ASN	CA-C-O	-11.55	106.35	119.05
1	A	268	CYS	O-C-N	11.52	136.84	122.55
1	A	162	GLU	O-C-N	11.50	137.17	122.22
1	A	268	CYS	CA-C-O	-11.43	108.58	121.84
1	A	86	ARG	CA-C-O	11.25	132.48	120.55
1	A	82	SER	CA-C-O	-11.20	108.87	121.19
1	A	210	PRO	O-C-N	11.18	137.09	122.89
1	A	249	VAL	N-CA-CB	-11.15	98.50	109.99
1	A	97	VAL	CA-C-O	-11.09	110.66	121.63
1	A	269	THR	CB-CA-C	11.08	133.49	109.10
1	A	161	GLU	CA-C-O	11.04	136.31	120.51
1	A	126	VAL	CA-C-O	-11.00	109.19	120.85
1	A	192	GLY	CA-C-O	10.89	131.20	119.00
1	A	68	ARG	NH1-CZ-NH2	-10.80	105.26	119.30
1	A	160	ARG	NH1-CZ-NH2	-10.70	105.39	119.30
1	A	264	ASN	OD1-CG-ND2	-10.54	112.06	122.60
1	A	94	PHE	CA-CB-CG	-10.42	103.38	113.80
1	A	62	THR	CA-CB-OG1	-10.32	94.12	109.60
1	A	196	ARG	NH1-CZ-NH2	-10.24	105.99	119.30
1	A	257	HIS	CE1-NE2-CD2	10.14	119.14	109.00
1	A	58	LEU	N-CA-C	10.04	122.30	111.36
1	A	261	PHE	CA-C-N	-10.03	105.14	122.09
1	A	261	PHE	C-N-CA	-10.03	105.14	122.09
1	A	94	PHE	CA-C-O	-9.89	109.65	120.43
1	A	113	ASP	CA-CB-CG	-9.84	102.76	112.60
1	A	263	ILE	CA-C-O	-9.78	110.10	120.57
1	A	13	GLU	O-C-N	-9.76	111.77	122.12
1	A	99	TYR	CA-C-N	-9.75	110.33	120.38
1	A	99	TYR	C-N-CA	-9.75	110.33	120.38
1	A	101	PRO	O-C-N	9.67	135.20	122.24
1	A	109	LYS	CA-C-O	9.67	131.25	120.90
1	A	230	GLU	CA-C-O	-9.65	109.60	120.70
1	A	90	ALA	O-C-N	-9.65	111.89	122.12
1	A	110	GLY	CA-C-N	9.61	133.94	120.29
1	A	110	GLY	C-N-CA	9.61	133.94	120.29
1	A	44	ASP	O-C-N	-9.56	111.03	122.22
1	A	186	ASN	CA-CB-CG	-9.50	103.10	112.60
1	A	162	GLU	CA-CB-CG	-9.47	95.16	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	TRP	CE2-CD2-CE3	-9.47	109.33	118.80
1	A	38	TRP	CG-CD2-CE3	9.45	143.35	133.90
1	A	92	LEU	O-C-N	-9.44	111.73	123.06
1	A	95	VAL	O-C-N	9.41	131.83	121.10
1	A	264	ASN	CA-CB-CG	-9.35	103.25	112.60
1	A	202	ARG	NE-CZ-NH1	-9.32	112.18	121.50
1	A	86	ARG	NE-CZ-NH1	-9.11	112.39	121.50
1	A	176	GLN	N-CA-CB	-9.08	97.33	110.14
1	A	25	ALA	CA-C-O	-9.02	111.36	120.82
1	A	207	HIS	CG-CD2-NE2	-8.98	98.22	107.20
1	A	218	ALA	N-CA-C	-8.96	96.10	109.81
1	A	7	ARG	CD-NE-CZ	-8.84	112.03	124.40
1	A	257	HIS	ND1-CE1-NE2	-8.81	99.59	108.40
1	A	56	SER	CA-CB-OG	-8.81	93.48	111.10
1	A	166	SER	CA-C-O	8.79	130.17	119.10
1	A	230	GLU	OE1-CD-OE2	8.74	143.88	122.90
1	A	180	GLY	CA-C-O	-8.67	111.86	121.31
1	A	99	TYR	O-C-N	8.66	129.32	121.35
1	A	168	ASN	OD1-CG-ND2	-8.63	113.97	122.60
1	A	245	SER	N-CA-C	8.61	122.77	111.75
1	A	216	LEU	CA-C-O	8.59	130.34	120.89
1	A	74	THR	CA-C-O	-8.58	110.30	120.60
1	A	180	GLY	O-C-N	8.53	131.24	123.73
1	A	81	GLY	O-C-N	-8.51	115.18	122.92
1	A	115	TYR	CA-C-O	8.49	129.74	120.82
1	A	55	TRP	CA-C-O	-8.47	111.23	121.06
1	A	251	PHE	N-CA-CB	-8.44	100.24	110.53
1	A	126	VAL	O-C-N	8.37	130.45	121.83
1	A	170	PHE	CA-CB-CG	-8.36	105.44	113.80
1	A	129	GLN	OE1-CD-NE2	-8.36	114.24	122.60
1	A	50	LYS	CA-CB-CG	-8.35	97.40	114.10
1	A	6	ILE	O-C-N	-8.32	114.22	123.20
1	A	119	GLN	OE1-CD-NE2	-8.31	114.29	122.60
1	A	196	ARG	CA-CB-CG	-8.31	97.48	114.10
1	A	97	VAL	N-CA-CB	-8.30	97.00	112.36
1	A	120	ASN	CA-CB-CG	-8.27	104.33	112.60
1	A	231	THR	CA-CB-OG1	-8.27	97.19	109.60
1	A	51	ILE	N-CA-CB	8.25	120.29	111.46
1	A	106	LYS	CA-C-N	8.25	135.72	122.68
1	A	106	LYS	C-N-CA	8.25	135.72	122.68
1	A	230	GLU	CG-CD-OE2	-8.23	99.47	118.40
1	A	207	HIS	CE1-NE2-CD2	8.22	117.22	109.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ASP	CA-C-O	-8.21	109.75	119.35
1	A	161	GLU	CB-CG-CD	-8.21	98.65	112.60
1	A	238	ASP	CB-CG-OD2	-8.20	99.54	118.40
1	A	45	ALA	O-C-N	-8.18	113.45	122.12
1	A	38	TRP	CD2-CE3-CZ3	8.15	129.20	118.60
1	A	213	PHE	CA-CB-CG	8.15	121.95	113.80
1	A	68	ARG	CG-CD-NE	-8.11	94.16	112.00
1	A	6	ILE	N-CA-CB	8.09	123.33	111.52
1	A	201	GLU	CG-CD-OE2	8.08	136.98	118.40
1	A	150	VAL	N-CA-CB	-8.01	99.65	110.54
1	A	53	LYS	N-CA-CB	-7.99	98.54	111.24
1	A	96	PRO	N-CA-CB	7.97	110.44	103.27
1	A	268	CYS	N-CA-C	-7.96	100.40	111.39
1	A	200	ASN	CA-C-O	7.89	129.36	120.84
1	A	257	HIS	CA-C-O	7.88	129.03	119.97
1	A	162	GLU	CB-CG-CD	7.86	125.97	112.60
1	A	65	MET	O-C-N	7.84	132.19	123.25
1	A	119	GLN	N-CA-C	7.84	124.22	111.37
1	A	146	GLY	CA-C-N	7.83	128.62	120.00
1	A	146	GLY	C-N-CA	7.83	128.62	120.00
1	A	187	TYR	CA-C-O	7.82	128.84	120.55
1	A	244	CYS	N-CA-C	-7.81	101.26	108.75
1	A	223	TRP	CA-C-O	-7.80	112.12	120.46
1	A	75	ILE	O-C-N	-7.78	114.00	123.10
1	A	219	GLY	CA-C-N	7.75	132.40	121.24
1	A	219	GLY	C-N-CA	7.75	132.40	121.24
1	A	223	TRP	CE3-CZ3-CH2	7.75	131.18	121.10
1	A	120	ASN	CA-C-O	7.74	129.58	121.07
1	A	106	LYS	CD-CE-NZ	7.73	136.63	111.90
1	A	225	THR	CA-CB-OG1	-7.72	98.02	109.60
1	A	11	SER	CA-CB-OG	-7.69	95.72	111.10
1	A	42	HIS	CA-CB-CG	-7.68	106.12	113.80
1	A	200	ASN	CA-CB-CG	-7.67	104.93	112.60
1	A	137	LYS	CB-CG-CD	-7.62	93.77	111.30
1	A	266	GLY	CA-C-O	-7.61	107.33	120.57
1	A	98	SER	CB-CA-C	-7.56	95.63	109.54
1	A	28	TYR	CG-CD1-CE1	-7.54	109.88	121.20
1	A	160	ARG	CA-C-O	-7.51	110.40	119.49
1	A	154	ALA	CA-C-O	-7.51	112.59	120.55
1	A	232	VAL	CA-C-N	7.50	133.06	122.72
1	A	232	VAL	C-N-CA	7.50	133.06	122.72
1	A	187	TYR	O-C-N	-7.47	114.20	122.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ASP	CA-CB-CG	-7.42	105.18	112.60
1	A	243	ASP	CA-C-N	-7.42	115.19	123.13
1	A	243	ASP	C-N-CA	-7.42	115.19	123.13
1	A	95	VAL	CB-CA-C	7.42	124.86	111.36
1	A	132	GLN	OE1-CD-NE2	7.42	130.02	122.60
1	A	45	ALA	CA-C-O	7.42	128.41	120.55
1	A	196	ARG	CD-NE-CZ	-7.42	114.02	124.40
1	A	213	PHE	N-CA-CB	-7.41	98.09	110.39
1	A	85	ILE	N-CA-CB	-7.38	100.50	110.54
1	A	30	ARG	CD-NE-CZ	7.37	134.71	124.40
1	A	225	THR	N-CA-C	-7.33	104.49	113.50
1	A	56	SER	N-CA-CB	7.33	124.89	111.11
1	A	159	GLN	N-CA-C	-7.33	103.37	111.36
1	A	99	TYR	CG-CD1-CE1	-7.32	110.22	121.20
1	A	221	GLU	CA-C-N	7.28	132.97	122.85
1	A	221	GLU	C-N-CA	7.28	132.97	122.85
1	A	226	ASP	CA-CB-CG	-7.28	105.32	112.60
1	A	269	THR	N-CA-C	-7.27	90.65	111.00
1	A	28	TYR	CD1-CG-CD2	7.23	128.94	118.10
1	A	184	PHE	CA-C-O	-7.20	112.79	120.42
1	A	163	GLY	N-CA-C	-7.18	105.58	114.92
1	A	244	CYS	CA-C-O	7.13	122.82	118.33
1	A	159	GLN	O-C-N	-7.11	114.05	122.15
1	A	196	ARG	NE-CZ-NH1	7.09	128.59	121.50
1	A	147	GLY	O-C-N	7.06	129.04	122.19
1	A	240	GLU	CA-C-O	-7.04	113.41	121.15
1	A	160	ARG	CA-C-N	7.01	134.93	121.54
1	A	160	ARG	C-N-CA	7.01	134.93	121.54
1	A	166	SER	CA-C-N	-7.00	109.05	122.06
1	A	166	SER	C-N-CA	-7.00	109.05	122.06
1	A	235	CYS	N-CA-C	-6.97	96.28	108.20
1	A	193	ILE	CA-C-O	-6.97	113.13	119.82
1	A	236	THR	CA-CB-OG1	-6.95	99.18	109.60
1	A	137	LYS	CA-C-N	6.95	132.56	123.11
1	A	137	LYS	C-N-CA	6.95	132.56	123.11
1	A	226	ASP	CB-CG-OD2	-6.94	102.43	118.40
1	A	269	THR	OG1-CB-CG2	-6.94	95.41	109.30
1	A	99	TYR	CD1-CG-CD2	6.92	128.48	118.10
1	A	213	PHE	CA-C-N	-6.91	111.20	122.40
1	A	213	PHE	C-N-CA	-6.91	111.20	122.40
1	A	211	ALA	CA-C-O	6.91	128.29	120.90
1	A	56	SER	N-CA-C	-6.90	93.09	107.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	PHE	O-C-N	6.89	134.14	122.21
1	A	150	VAL	CB-CA-C	6.89	121.44	112.14
1	A	30	ARG	O-C-N	-6.88	113.44	122.39
1	A	226	ASP	O-C-N	6.88	131.19	123.48
1	A	90	ALA	CA-C-O	6.86	128.04	120.63
1	A	81	GLY	CA-C-N	6.85	130.44	120.71
1	A	81	GLY	C-N-CA	6.85	130.44	120.71
1	A	95	VAL	CA-CB-CG1	6.83	122.02	110.40
1	A	196	ARG	NE-CZ-NH2	6.82	125.33	119.20
1	A	141	THR	O-C-N	-6.80	114.94	123.17
1	A	209	PRO	N-CA-CB	6.76	110.04	102.60
1	A	234	VAL	CA-CB-CG2	6.74	121.86	110.40
1	A	59	ILE	CA-C-N	-6.72	111.45	122.54
1	A	59	ILE	C-N-CA	-6.72	111.45	122.54
1	A	59	ILE	CB-CA-C	-6.72	103.48	111.94
1	A	207	HIS	ND1-CG-CD2	6.72	112.82	106.10
1	A	77	ILE	CA-CB-CG1	-6.71	98.99	110.40
1	A	21	THR	CA-CB-OG1	-6.71	99.54	109.60
1	A	229	PRO	N-CD-CG	-6.71	95.75	103.80
1	A	233	GLN	CA-C-O	6.69	127.72	120.43
1	A	100	PRO	O-C-N	6.69	129.35	121.46
1	A	26	ASN	CA-CB-CG	-6.67	105.93	112.60
1	A	83	SER	CA-C-N	6.66	133.63	123.04
1	A	83	SER	C-N-CA	6.66	133.63	123.04
1	A	120	ASN	CB-CG-OD1	-6.66	107.49	120.80
1	A	82	SER	O-C-N	6.64	131.04	122.87
1	A	257	HIS	CG-CD2-NE2	-6.64	100.56	107.20
1	A	163	GLY	CA-C-O	-6.62	111.65	119.07
1	A	103	SER	N-CA-CB	-6.60	99.86	109.83
1	A	32	VAL	O-C-N	-6.59	109.78	121.84
1	A	131	LYS	CA-CB-CG	6.57	127.23	114.10
1	A	195	TYR	N-CA-CB	-6.56	100.18	110.87
1	A	121	GLU	CA-C-N	-6.55	111.92	120.44
1	A	121	GLU	C-N-CA	-6.55	111.92	120.44
1	A	181	ASP	CA-CB-CG	-6.55	106.05	112.60
1	A	75	ILE	CA-C-O	6.54	127.53	120.53
1	A	52	ILE	CA-C-O	6.54	127.70	120.71
1	A	227	ASN	O-C-N	6.54	130.39	122.35
1	A	88	TRP	CA-C-O	6.53	127.47	120.55
1	A	140	VAL	CA-C-O	-6.53	113.56	120.48
1	A	32	VAL	CA-C-N	6.51	134.18	122.13
1	A	32	VAL	C-N-CA	6.51	134.18	122.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	GLN	CG-CD-NE2	6.51	126.17	116.40
1	A	249	VAL	CB-CA-C	6.50	117.37	111.00
1	A	243	ASP	CA-C-O	-6.50	111.45	119.18
1	A	75	ILE	N-CA-C	-6.50	98.38	107.80
1	A	140	VAL	CA-C-N	-6.48	111.71	122.21
1	A	140	VAL	C-N-CA	-6.48	111.71	122.21
1	A	181	ASP	OD1-CG-OD2	-6.47	107.36	122.90
1	A	174	GLN	O-C-N	-6.47	115.74	123.31
1	A	191	THR	CA-CB-OG1	-6.47	99.90	109.60
1	A	224	ILE	CA-C-O	6.46	128.77	120.95
1	A	84	SER	CA-C-O	6.45	134.74	122.23
1	A	99	TYR	N-CA-C	-6.44	100.28	109.24
1	A	248	ILE	CA-C-O	6.44	127.27	119.54
1	A	154	ALA	O-C-N	6.44	128.94	122.12
1	A	102	VAL	CA-C-O	6.43	126.61	120.31
1	A	73	LYS	CA-C-O	-6.42	114.40	121.84
1	A	109	LYS	CA-CB-CG	-6.42	101.27	114.10
1	A	197	ARG	N-CA-CB	-6.41	100.80	110.35
1	A	233	GLN	CB-CG-CD	-6.41	101.71	112.60
1	A	66	VAL	N-CA-CB	6.40	120.24	111.41
1	A	242	SER	O-C-N	6.38	129.99	122.34
1	A	201	GLU	CB-CG-CD	6.38	123.44	112.60
1	A	118	VAL	O-C-N	6.37	128.47	122.23
1	A	226	ASP	CA-C-N	-6.36	112.15	122.26
1	A	226	ASP	C-N-CA	-6.36	112.15	122.26
1	A	73	LYS	CA-CB-CG	-6.35	101.41	114.10
1	A	186	ASN	CA-C-N	-6.33	111.79	120.28
1	A	186	ASN	C-N-CA	-6.33	111.79	120.28
1	A	116	GLY	CA-C-N	6.33	128.76	120.28
1	A	116	GLY	C-N-CA	6.33	128.76	120.28
1	A	194	PRO	O-C-N	-6.32	116.09	122.98
1	A	32	VAL	N-CA-C	-6.31	105.58	111.45
1	A	200	ASN	O-C-N	-6.29	115.13	122.87
1	A	118	VAL	N-CA-CB	-6.29	101.10	111.98
1	A	124	ALA	O-C-N	-6.28	115.46	122.12
1	A	148	ALA	CA-C-O	-6.26	114.25	120.70
1	A	115	TYR	CG-CD2-CE2	-6.26	111.81	121.20
1	A	218	ALA	N-CA-CB	6.25	120.42	111.05
1	A	174	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	A	86	ARG	NH1-CZ-NH2	6.24	127.41	119.30
1	A	117	GLU	O-C-N	-6.22	115.52	122.12
1	A	73	LYS	CB-CA-C	-6.21	103.07	111.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ILE	N-CA-CB	6.20	119.28	111.46
1	A	104	GLY	CA-C-O	-6.20	112.11	119.06
1	A	82	SER	N-CA-C	6.16	119.17	110.23
1	A	19	TYR	CG-CD2-CE2	-6.16	111.96	121.20
1	A	70	ASP	CB-CG-OD1	6.15	132.54	118.40
1	A	28	TYR	CB-CG-CD2	-6.14	111.60	120.80
1	A	149	THR	CA-CB-OG1	-6.13	100.40	109.60
1	A	152	LEU	O-C-N	-6.12	115.63	122.12
1	A	85	ILE	CB-CG1-CD1	-6.11	100.96	113.80
1	A	137	LYS	N-CA-CB	-6.11	100.69	110.46
1	A	91	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	23	LEU	N-CA-C	-6.09	104.55	111.07
1	A	103	SER	CA-CB-OG	-6.05	98.99	111.10
1	A	117	GLU	CA-C-O	-6.04	114.14	120.55
1	A	217	HIS	CB-CA-C	-6.04	99.17	109.51
1	A	269	THR	CA-CB-OG1	6.03	118.64	109.60
1	A	19	TYR	CG-CD1-CE1	6.02	130.24	121.20
1	A	259	SER	CA-C-O	-6.01	112.09	120.21
1	A	97	VAL	CA-CB-CG1	5.98	120.56	110.40
1	A	162	GLU	CA-C-O	-5.97	112.72	119.95
1	A	125	THR	CA-CB-OG1	-5.96	100.66	109.60
1	A	32	VAL	CA-C-O	5.96	128.10	120.83
1	A	93	THR	CA-CB-OG1	-5.96	100.67	109.60
1	A	158	TYR	CA-C-N	5.96	128.75	120.29
1	A	158	TYR	C-N-CA	5.96	128.75	120.29
1	A	81	GLY	N-CA-C	-5.95	101.20	112.27
1	A	19	TYR	CZ-CE2-CD2	5.95	130.30	119.60
1	A	199	VAL	CG1-CB-CG2	5.94	123.86	110.80
1	A	239	LEU	CB-CG-CD1	-5.94	92.89	110.70
1	A	80	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	A	197	ARG	CA-C-O	-5.93	114.75	120.92
1	A	243	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	51	ILE	CA-CB-CG1	-5.93	100.32	110.40
1	A	197	ARG	CB-CA-C	5.93	121.38	111.30
1	A	76	TYR	O-C-N	5.92	130.12	123.19
1	A	92	LEU	CA-C-O	5.92	127.41	120.96
1	A	137	LYS	CA-C-O	-5.91	114.75	121.72
1	A	28	TYR	O-C-N	-5.90	113.66	122.39
1	A	160	ARG	CD-NE-CZ	5.88	132.64	124.40
1	A	117	GLU	CA-C-N	5.87	129.88	121.55
1	A	117	GLU	C-N-CA	5.87	129.88	121.55
1	A	230	GLU	CA-CB-CG	-5.86	102.39	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	GLU	N-CA-C	5.85	123.27	110.80
1	A	181	ASP	N-CA-CB	-5.85	102.52	109.59
1	A	129	GLN	CA-C-N	-5.84	111.43	120.31
1	A	129	GLN	C-N-CA	-5.84	111.43	120.31
1	A	58	LEU	N-CA-CB	-5.84	101.52	110.16
1	A	238	ASP	CA-CB-CG	-5.84	106.76	112.60
1	A	147	GLY	CA-C-O	-5.83	114.47	120.66
1	A	62	THR	CA-C-N	5.83	131.22	123.05
1	A	62	THR	C-N-CA	5.83	131.22	123.05
1	A	131	LYS	CG-CD-CE	5.83	124.72	111.30
1	A	79	PHE	N-CA-CB	5.81	119.69	110.57
1	A	92	LEU	N-CA-C	5.79	118.75	110.24
1	A	53	LYS	CB-CA-C	-5.76	100.72	109.99
1	A	29	CYS	O-C-N	5.75	130.10	123.02
1	A	33	ILE	N-CA-CB	5.74	119.25	111.21
1	A	100	PRO	CA-C-O	-5.73	112.25	120.56
1	A	261	PHE	CA-C-O	-5.73	113.70	120.81
1	A	124	ALA	CA-C-O	5.73	126.63	120.55
1	A	82	SER	CA-CB-OG	-5.73	99.64	111.10
1	A	227	ASN	CA-C-N	-5.72	107.84	121.80
1	A	227	ASN	C-N-CA	-5.72	107.84	121.80
1	A	158	TYR	N-CA-CB	-5.71	101.72	110.12
1	A	258	LEU	N-CA-C	5.71	120.11	113.20
1	A	210	PRO	CA-C-N	5.70	128.24	120.54
1	A	210	PRO	C-N-CA	5.70	128.24	120.54
1	A	133	TYR	CA-C-N	5.69	125.37	119.56
1	A	133	TYR	C-N-CA	5.69	125.37	119.56
1	A	218	ALA	CB-CA-C	-5.69	99.54	110.24
1	A	220	GLU	CA-C-O	5.69	127.18	120.58
1	A	120	ASN	CA-C-N	-5.67	112.24	120.29
1	A	120	ASN	C-N-CA	-5.67	112.24	120.29
1	A	193	ILE	O-C-N	5.66	127.82	120.75
1	A	47	GLU	CB-CG-CD	-5.63	103.02	112.60
1	A	212	ALA	CB-CA-C	-5.63	100.22	110.63
1	A	62	THR	N-CA-CB	5.62	119.03	109.87
1	A	127	LEU	CA-C-O	5.62	126.43	119.97
1	A	223	TRP	CZ3-CH2-CZ2	-5.62	114.20	121.50
1	A	166	SER	CA-CB-OG	-5.59	99.93	111.10
1	A	229	PRO	CA-C-O	5.59	133.61	120.20
1	A	202	ARG	NH1-CZ-NH2	5.58	126.56	119.30
1	A	260	TYR	CG-CD2-CE2	5.58	129.57	121.20
1	A	79	PHE	CA-CB-CG	-5.58	108.22	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLY	O-C-N	-5.54	115.49	122.70
1	A	145	LEU	CA-C-N	5.54	127.06	120.14
1	A	145	LEU	C-N-CA	5.54	127.06	120.14
1	A	123	VAL	CA-C-O	-5.53	115.20	120.95
1	A	41	ILE	CA-C-N	-5.52	113.49	122.65
1	A	41	ILE	C-N-CA	-5.52	113.49	122.65
1	A	172	TYR	CB-CG-CD1	-5.51	112.53	120.80
1	A	170	PHE	CA-C-O	-5.51	114.75	120.70
1	A	201	GLU	CA-CB-CG	-5.50	103.10	114.10
1	A	30	ARG	NE-CZ-NH1	5.49	126.99	121.50
1	A	131	LYS	N-CA-C	-5.49	105.29	111.28
1	A	53	LYS	CA-C-O	5.49	126.90	120.75
1	A	224	ILE	N-CA-C	-5.49	101.59	108.84
1	A	204	ILE	CB-CG1-CD1	-5.48	102.29	113.80
1	A	227	ASN	CA-CB-CG	-5.48	107.12	112.60
1	A	115	TYR	CZ-CE2-CD2	5.47	129.45	119.60
1	A	123	VAL	CA-C-N	-5.47	112.95	120.28
1	A	123	VAL	C-N-CA	-5.47	112.95	120.28
1	A	30	ARG	CG-CD-NE	5.46	124.02	112.00
1	A	20	TYR	CA-CB-CG	-5.46	104.07	113.90
1	A	14	ILE	CA-CB-CG1	-5.45	101.14	110.40
1	A	121	GLU	CG-CD-OE2	-5.44	105.89	118.40
1	A	141	THR	CA-C-O	5.44	127.54	121.40
1	A	153	CYS	CA-C-O	5.43	126.53	120.82
1	A	134	PRO	O-C-N	5.43	129.51	122.24
1	A	223	TRP	N-CA-CB	-5.42	101.46	110.47
1	A	259	SER	CA-CB-OG	-5.41	100.27	111.10
1	A	239	LEU	CA-C-O	5.41	128.10	121.56
1	A	211	ALA	CB-CA-C	5.41	119.46	110.81
1	A	179	VAL	CA-C-O	-5.40	115.22	120.30
1	A	15	ASN	N-CA-CB	5.40	117.84	110.01
1	A	177	PRO	O-C-N	5.38	129.70	123.14
1	A	19	TYR	CA-CB-CG	-5.38	104.22	113.90
1	A	153	CYS	O-C-N	-5.37	116.54	122.07
1	A	232	VAL	CA-CB-CG2	5.37	119.53	110.40
1	A	74	THR	CA-C-N	-5.36	116.16	123.12
1	A	74	THR	C-N-CA	-5.36	116.16	123.12
1	A	85	ILE	N-CA-C	5.36	116.08	110.62
1	A	89	ILE	N-CA-C	5.35	115.56	110.42
1	A	207	HIS	ND1-CE1-NE2	-5.35	103.05	108.40
1	A	246	ASN	N-CA-C	-5.35	106.02	112.54
1	A	101	PRO	CA-C-N	-5.34	115.73	123.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	PRO	C-N-CA	-5.34	115.73	123.11
1	A	178	ARG	O-C-N	-5.34	116.37	122.89
1	A	135	SER	CA-C-N	-5.33	110.13	121.32
1	A	135	SER	C-N-CA	-5.33	110.13	121.32
1	A	44	ASP	CB-CG-OD1	5.32	130.64	118.40
1	A	136	TYR	CG-CD2-CE2	5.32	129.19	121.20
1	A	205	VAL	CA-C-N	5.31	125.03	119.82
1	A	205	VAL	C-N-CA	5.31	125.03	119.82
1	A	51	ILE	O-C-N	-5.31	116.69	122.64
1	A	191	THR	CA-C-N	-5.31	111.27	121.78
1	A	191	THR	C-N-CA	-5.31	111.27	121.78
1	A	103	SER	O-C-N	-5.30	116.35	122.87
1	A	120	ASN	N-CA-C	5.28	117.46	111.02
1	A	243	ASP	N-CA-C	5.27	119.71	113.28
1	A	128	ASP	OD1-CG-OD2	5.27	135.54	122.90
1	A	9	ALA	CA-C-O	5.25	127.51	121.47
1	A	187	TYR	CD1-CE1-CZ	-5.25	110.15	119.60
1	A	243	ASP	O-C-N	5.25	129.86	122.41
1	A	40	CYS	CA-C-O	5.24	126.84	121.23
1	A	215	PHE	CG-CD2-CE2	5.24	129.61	120.70
1	A	97	VAL	CA-C-N	-5.24	112.72	120.94
1	A	97	VAL	C-N-CA	-5.24	112.72	120.94
1	A	236	THR	CB-CA-C	5.24	120.86	110.17
1	A	16	GLU	CB-CG-CD	-5.22	103.72	112.60
1	A	121	GLU	OE1-CD-OE2	5.22	135.44	122.90
1	A	228	SER	N-CA-CB	5.22	119.65	110.37
1	A	213	PHE	N-CA-C	5.21	118.89	112.54
1	A	238	ASP	OD1-CG-OD2	5.21	135.39	122.90
1	A	16	GLU	N-CA-CB	-5.20	102.53	110.07
1	A	12	GLN	CB-CG-CD	5.19	121.42	112.60
1	A	137	LYS	CA-CB-CG	-5.18	103.74	114.10
1	A	37	THR	CA-C-O	5.18	127.31	121.51
1	A	68	ARG	CD-NE-CZ	-5.17	117.16	124.40
1	A	101	PRO	N-CD-CG	-5.17	95.45	103.20
1	A	125	THR	O-C-N	-5.16	116.65	122.12
1	A	18	THR	N-CA-C	-5.16	105.74	111.36
1	A	53	LYS	CB-CG-CD	-5.15	99.45	111.30
1	A	144	SER	N-CA-CB	-5.14	97.80	110.71
1	A	232	VAL	CA-C-O	-5.14	114.91	120.36
1	A	101	PRO	CA-C-O	-5.14	111.84	119.18
1	A	231	THR	CA-C-O	-5.13	114.63	120.32
1	A	237	SER	CA-C-O	-5.13	115.55	121.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	THR	CA-CB-CG2	5.12	119.20	110.50
1	A	46	THR	N-CA-CB	-5.12	102.54	110.98
1	A	13	GLU	CB-CA-C	-5.11	102.31	110.79
1	A	125	THR	CA-CB-CG2	5.10	119.17	110.50
1	A	84	SER	N-CA-CB	-5.10	103.84	111.64
1	A	159	GLN	N-CA-CB	5.09	117.69	110.16
1	A	176	GLN	N-CA-C	5.08	116.23	109.93
1	A	204	ILE	N-CA-C	5.07	119.14	112.04
1	A	230	GLU	CB-CG-CD	-5.05	104.01	112.60
1	A	112	LEU	N-CA-CB	-5.05	102.70	110.12
1	A	181	ASP	CB-CG-OD2	-5.04	106.81	118.40
1	A	88	TRP	CE3-CZ3-CH2	5.03	127.64	121.10
1	A	160	ARG	N-CA-CB	5.03	118.88	110.32
1	A	102	VAL	CB-CA-C	5.02	116.71	110.73
1	A	61	ASP	OD1-CG-OD2	-5.02	110.86	122.90
1	A	41	ILE	CA-CB-CG1	-5.01	101.89	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2059	0	1981	63	0
2	A	230	0	0	12	1
All	All	2289	0	1981	63	1

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 16.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLN:HG2	2:A:449:HOH:O	1.37	1.18
1:A:147:GLY:O	1:A:150:VAL:HG12	1.54	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASP:OD1	2:A:432:HOH:O	1.70	1.06
1:A:140:VAL:HG12	1:A:150:VAL:HG22	1.43	0.97
1:A:211:ALA:HA	2:A:381:HOH:O	1.68	0.94
1:A:141:THR:C	1:A:150:VAL:HG21	1.99	0.88
1:A:140:VAL:HG12	1:A:150:VAL:CG2	2.07	0.84
1:A:85:ILE:HG22	2:A:482:HOH:O	1.79	0.82
1:A:50:LYS:HD2	2:A:404:HOH:O	1.82	0.78
1:A:146:GLY:O	1:A:150:VAL:HB	1.86	0.76
1:A:92:LEU:HD13	1:A:94:PHE:CE1	2.24	0.72
1:A:150:VAL:CG1	1:A:173:THR:HG22	2.20	0.71
1:A:47:GLU:CG	2:A:373:HOH:O	2.39	0.70
1:A:47:GLU:HG2	2:A:373:HOH:O	1.94	0.67
1:A:196:ARG:HD3	2:A:462:HOH:O	1.95	0.67
1:A:147:GLY:C	1:A:150:VAL:HG12	2.18	0.67
1:A:95:VAL:HG22	1:A:109:LYS:HB3	1.77	0.66
1:A:47:GLU:CD	2:A:373:HOH:O	2.40	0.64
1:A:264:ASN:HD21	1:A:267:LEU:CD1	2.11	0.64
1:A:92:LEU:HD13	1:A:94:PHE:CZ	2.34	0.62
1:A:150:VAL:HG11	1:A:173:THR:HG22	1.84	0.59
1:A:147:GLY:HA2	1:A:150:VAL:CG1	2.33	0.59
1:A:150:VAL:HG13	1:A:171:LEU:HD11	1.85	0.58
1:A:181:ASP:HB2	1:A:182:PRO:CD	2.34	0.57
1:A:43:CYS:O	1:A:47:GLU:HB3	2.05	0.57
1:A:6:ILE:HD11	1:A:243:ASP:CB	2.35	0.56
1:A:6:ILE:HD13	1:A:235:CYS:SG	2.48	0.54
1:A:141:THR:HA	1:A:172:TYR:O	2.08	0.53
1:A:264:ASN:HD21	1:A:267:LEU:HD13	1.72	0.52
1:A:147:GLY:HA2	1:A:150:VAL:HG11	1.91	0.51
1:A:268:CYS:SG	1:A:268:CYS:O	2.69	0.51
1:A:150:VAL:HG13	1:A:173:THR:HG22	1.94	0.49
1:A:264:ASN:HD21	1:A:267:LEU:HD12	1.76	0.48
1:A:220:GLU:OE2	1:A:236:THR:HA	2.14	0.48
1:A:170:PHE:N	1:A:170:PHE:CD1	2.82	0.48
1:A:209:PRO:CB	1:A:210:PRO:HD2	2.43	0.47
1:A:178:ARG:HB2	1:A:209:PRO:HD2	1.97	0.47
1:A:147:GLY:CA	1:A:150:VAL:HG12	2.46	0.46
1:A:50:LYS:CD	2:A:404:HOH:O	2.54	0.46
1:A:147:GLY:HA2	1:A:150:VAL:HG12	1.98	0.45
1:A:6:ILE:CD1	1:A:235:CYS:SG	3.04	0.45
1:A:30:ARG:HG2	1:A:30:ARG:HH11	1.80	0.45
1:A:142:GLY:N	1:A:150:VAL:HG21	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.78	0.45
1:A:182:PRO:HD3	1:A:214:GLY:O	2.17	0.45
1:A:196:ARG:HG2	1:A:222:TYR:CE1	2.52	0.44
1:A:6:ILE:HD11	1:A:243:ASP:HB3	1.98	0.44
1:A:181:ASP:CB	1:A:182:PRO:CD	2.95	0.44
1:A:227:ASN:ND2	1:A:230:GLU:OE2	2.41	0.44
1:A:34:PRO:HB3	2:A:278:HOH:O	2.16	0.44
1:A:181:ASP:HB2	1:A:182:PRO:HD2	2.00	0.44
1:A:30:ARG:NH2	2:A:396:HOH:O	2.51	0.43
1:A:239:LEU:HD23	1:A:239:LEU:HA	1.91	0.42
1:A:6:ILE:HD11	1:A:243:ASP:HB2	2.01	0.42
1:A:74:THR:HG22	1:A:75:ILE:N	2.34	0.42
1:A:169:LEU:O	1:A:194:PRO:HD2	2.20	0.42
1:A:209:PRO:O	1:A:210:PRO:C	2.60	0.41
1:A:222:TYR:CD2	1:A:234:VAL:HG22	2.55	0.41
1:A:30:ARG:HA	1:A:30:ARG:HD3	1.67	0.41
1:A:85:ILE:HD13	1:A:85:ILE:HG21	1.75	0.41
1:A:266:GLY:C	1:A:267:LEU:HG	2.45	0.41
1:A:7:ARG:HH11	1:A:7:ARG:HD2	1.67	0.41
1:A:95:VAL:HG22	1:A:109:LYS:CB	2.47	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:327:HOH:O	2:A:378:HOH:O[3_556]	1.93	0.27

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/269 (98%)	254 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	230/233 (99%)	214 (93%)	16 (7%)	14 7

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	30	ARG
1	A	53	LYS
1	A	58	LEU
1	A	73	LYS
1	A	87	ASN
1	A	92	LEU
1	A	95	VAL
1	A	97	VAL
1	A	120	ASN
1	A	131	LYS
1	A	137	LYS
1	A	228	SER
1	A	230	GLU
1	A	238	ASP
1	A	269	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	87	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.