



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 02:49 PM EDT

PDB ID : 3TGL
Title : STRUCTURE AND MOLECULAR MODEL REFINEMENT OF RHIZOMUCOR MIEHEI TRIACYLGLYCERIDE LIPASE: A CASE STUDY OF THE USE OF SIMULATED ANNEALING IN PARTIAL MODEL REFINEMENT
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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 : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

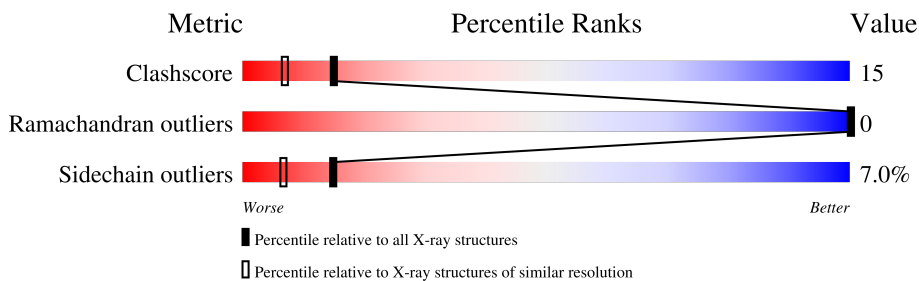
1 Overall quality at a glance i

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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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	 42% 41% 14% ..

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
			Total	C	N	O	S			
1	A	265	2059	1308	337	406	8	0	0	0

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		

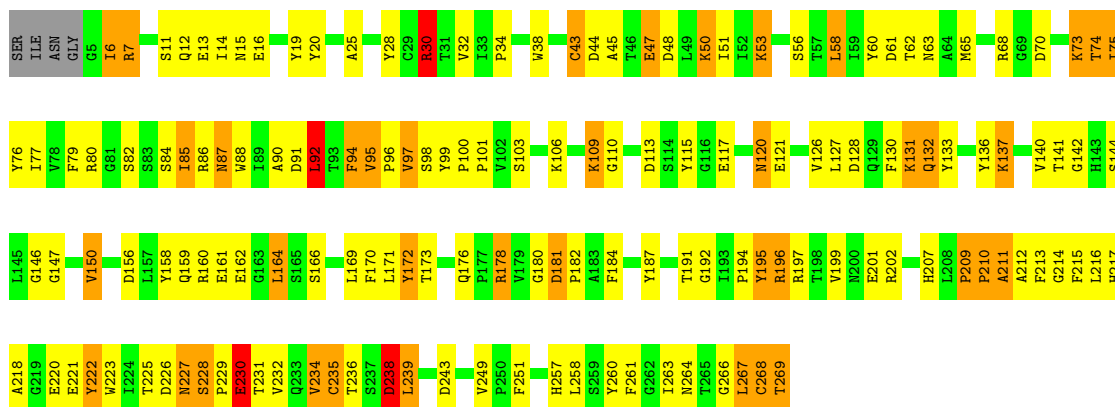
3 Residue-property plots

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

Chain A: 



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	1.00	0/2110	3.31	265/2885 (9.2%)

There are no bond length outliers.

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASP	CB-CG-OD1	30.59	145.83	118.30
1	A	68	ARG	NE-CZ-NH1	27.41	134.01	120.30
1	A	160	ARG	NE-CZ-NH2	21.86	131.23	120.30
1	A	238	ASP	CB-CG-OD2	-20.85	99.54	118.30
1	A	226	ASP	CB-CG-OD2	-17.63	102.43	118.30
1	A	230	GLU	OE1-CD-OE2	17.15	143.88	123.30
1	A	196	ARG	NE-CZ-NH1	16.57	128.59	120.30
1	A	202	ARG	NE-CZ-NH1	-16.23	112.18	120.30
1	A	86	ARG	NE-CZ-NH1	-15.83	112.39	120.30
1	A	70	ASP	CB-CG-OD1	15.82	132.54	118.30
1	A	28	TYR	CB-CG-CD2	-15.67	111.60	121.00
1	A	267	LEU	O-C-N	15.17	146.98	122.70
1	A	28	TYR	CG-CD1-CE1	-14.27	109.88	121.30
1	A	172	TYR	CB-CG-CD1	-14.12	112.53	121.00
1	A	99	TYR	CG-CD1-CE1	-13.85	110.22	121.30
1	A	44	ASP	CB-CG-OD1	13.71	130.64	118.30
1	A	30	ARG	NE-CZ-NH1	13.39	126.99	120.30
1	A	68	ARG	NH1-CZ-NH2	-12.86	105.26	119.40
1	A	181	ASP	CB-CG-OD2	-12.77	106.81	118.30
1	A	160	ARG	NH1-CZ-NH2	-12.73	105.39	119.40
1	A	196	ARG	NH1-CZ-NH2	-12.19	105.99	119.40
1	A	137	LYS	CB-CA-C	11.87	134.14	110.40
1	A	115	TYR	CG-CD2-CE2	-11.87	111.81	121.30
1	A	19	TYR	CG-CD2-CE2	-11.68	111.96	121.30
1	A	19	TYR	CZ-CE2-CD2	11.67	130.30	119.80
1	A	19	TYR	CG-CD1-CE1	11.17	130.24	121.30
1	A	215	PHE	CB-CG-CD1	11.01	128.51	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	TYR	CB-CG-CD1	-10.92	114.45	121.00
1	A	106	LYS	CD-CE-NZ	10.84	136.63	111.70
1	A	70	ASP	CB-CG-OD2	-10.73	108.64	118.30
1	A	115	TYR	CZ-CE2-CD2	10.73	129.45	119.80
1	A	187	TYR	CD1-CE1-CZ	-10.72	110.15	119.80
1	A	239	LEU	CB-CG-CD1	-10.65	92.89	111.00
1	A	43	CYS	O-C-N	10.62	139.70	122.70
1	A	213	PHE	CB-CG-CD2	-10.58	113.39	120.80
1	A	130	PHE	CB-CG-CD2	10.52	128.16	120.80
1	A	38	TRP	CG-CD2-CE3	10.49	143.35	133.90
1	A	187	TYR	CB-CG-CD2	-10.35	114.79	121.00
1	A	260	TYR	CG-CD2-CE2	10.33	129.57	121.30
1	A	74	THR	O-C-N	10.33	139.22	122.70
1	A	260	TYR	CZ-CE2-CD2	-10.22	110.61	119.80
1	A	128	ASP	CB-CG-OD1	-10.19	109.12	118.30
1	A	192	GLY	O-C-N	-10.12	106.51	122.70
1	A	121	GLU	OE1-CD-OE2	10.12	135.44	123.30
1	A	196	ARG	NE-CZ-NH2	10.07	125.33	120.30
1	A	28	TYR	CD1-CG-CD2	10.04	128.94	117.90
1	A	136	TYR	CG-CD2-CE2	9.86	129.19	121.30
1	A	113	ASP	CB-CG-OD2	-9.70	109.57	118.30
1	A	99	TYR	CD1-CG-CD2	9.62	128.48	117.90
1	A	56	SER	N-CA-CB	9.59	124.89	110.50
1	A	48	ASP	CB-CG-OD1	9.56	126.91	118.30
1	A	76	TYR	CB-CG-CD2	-9.50	115.30	121.00
1	A	230	GLU	CG-CD-OE2	-9.42	99.47	118.30
1	A	263	ILE	O-C-N	9.42	137.77	122.70
1	A	7	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	A	201	GLU	CG-CD-OE2	9.34	136.98	118.30
1	A	113	ASP	CB-CG-OD1	9.23	126.61	118.30
1	A	201	GLU	OE1-CD-OE2	-9.09	112.40	123.30
1	A	267	LEU	CA-C-O	-9.08	101.03	120.10
1	A	223	TRP	CE3-CZ3-CH2	9.07	131.18	121.20
1	A	99	TYR	CB-CG-CD2	-9.06	115.57	121.00
1	A	210	PRO	O-C-N	8.99	137.09	122.70
1	A	258	LEU	CB-CG-CD2	-8.92	95.84	111.00
1	A	268	CYS	O-C-N	8.84	136.84	122.70
1	A	99	TYR	CZ-CE2-CD2	-8.59	112.07	119.80
1	A	80	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	A	144	SER	N-CA-CB	-8.47	97.80	110.50
1	A	99	TYR	CB-CG-CD1	-8.41	115.95	121.00
1	A	61	ASP	CB-CG-OD1	8.40	125.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ARG	CG-CD-NE	-8.40	94.16	111.80
1	A	181	ASP	OD1-CG-OD2	-8.39	107.36	123.30
1	A	178	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	A	120	ASN	OD1-CG-ND2	8.29	140.97	121.90
1	A	162	GLU	CA-CB-CG	-8.29	95.16	113.40
1	A	7	ARG	CD-NE-CZ	-8.27	112.03	123.60
1	A	162	GLU	O-C-N	8.22	137.17	123.20
1	A	261	PHE	C-N-CA	-8.17	105.14	122.30
1	A	269	THR	CB-CA-C	8.11	133.49	111.60
1	A	199	VAL	CG1-CB-CG2	8.10	123.86	110.90
1	A	85	ILE	CB-CA-C	8.08	127.76	111.60
1	A	32	VAL	O-C-N	-8.07	109.78	122.70
1	A	58	LEU	CB-CG-CD2	-8.04	97.34	111.00
1	A	215	PHE	CG-CD2-CE2	8.01	129.61	120.80
1	A	38	TRP	CD2-CE3-CZ3	8.00	129.20	118.80
1	A	110	GLY	O-C-N	-7.97	109.95	122.70
1	A	30	ARG	CD-NE-CZ	7.94	134.71	123.60
1	A	101	PRO	O-C-N	7.81	135.20	122.70
1	A	38	TRP	CE2-CD2-CE3	-7.81	109.33	118.70
1	A	133	TYR	CG-CD2-CE2	-7.75	115.10	121.30
1	A	161	GLU	CA-C-O	7.72	136.31	120.10
1	A	130	PHE	CB-CG-CD1	-7.71	115.40	120.80
1	A	98	SER	CB-CA-C	-7.62	95.63	110.10
1	A	187	TYR	CG-CD2-CE2	-7.60	115.22	121.30
1	A	43	CYS	C-N-CA	-7.59	102.73	121.70
1	A	269	THR	N-CA-C	-7.54	90.65	111.00
1	A	238	ASP	CB-CG-OD1	7.52	125.07	118.30
1	A	48	ASP	CB-CG-OD2	-7.46	111.58	118.30
1	A	44	ASP	C-N-CA	7.45	140.32	121.70
1	A	95	VAL	CA-CB-CG1	7.41	122.02	110.90
1	A	176	GLN	N-CA-CB	-7.37	97.33	110.60
1	A	266	GLY	CA-C-O	-7.37	107.33	120.60
1	A	218	ALA	N-CA-CB	7.37	120.42	110.10
1	A	25	ALA	O-C-N	7.35	134.46	122.70
1	A	234	VAL	CA-CB-CG2	7.31	121.86	110.90
1	A	43	CYS	CA-C-N	-7.30	101.15	117.20
1	A	19	TYR	CD1-CE1-CZ	-7.29	113.23	119.80
1	A	44	ASP	O-C-N	-7.29	111.03	122.70
1	A	86	ARG	NH1-CZ-NH2	7.28	127.41	119.40
1	A	50	LYS	CA-CB-CG	-7.27	97.40	113.40
1	A	187	TYR	CG-CD1-CE1	7.27	127.11	121.30
1	A	196	ARG	CA-CB-CG	-7.24	97.48	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	TYR	CB-CG-CD1	7.20	125.32	121.00
1	A	103	SER	N-CA-CB	-7.09	99.86	110.50
1	A	158	TYR	CG-CD2-CE2	-7.09	115.62	121.30
1	A	95	VAL	CB-CA-C	7.09	124.86	111.40
1	A	62	THR	CA-CB-OG1	-7.08	94.12	109.00
1	A	120	ASN	CB-CG-OD1	-7.06	107.49	121.60
1	A	218	ALA	CB-CA-C	-7.04	99.54	110.10
1	A	84	SER	CA-C-O	6.97	134.74	120.10
1	A	213	PHE	N-CA-CB	-6.95	98.09	110.60
1	A	85	ILE	O-C-N	6.90	133.74	122.70
1	A	92	LEU	O-C-N	-6.86	111.73	122.70
1	A	137	LYS	CB-CG-CD	-6.86	93.77	111.60
1	A	196	ARG	CD-NE-CZ	-6.85	114.02	123.60
1	A	16	GLU	OE1-CD-OE2	6.84	131.51	123.30
1	A	13	GLU	O-C-N	-6.83	111.77	122.70
1	A	132	GLN	CA-C-O	-6.79	105.84	120.10
1	A	90	ALA	O-C-N	-6.75	111.89	122.70
1	A	187	TYR	CB-CG-CD1	6.72	125.03	121.00
1	A	53	LYS	N-CA-CB	-6.70	98.54	110.60
1	A	110	GLY	CA-C-N	6.70	131.94	117.20
1	A	260	TYR	CG-CD1-CE1	-6.69	115.95	121.30
1	A	38	TRP	CD1-NE1-CE2	6.68	115.01	109.00
1	A	222	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	A	56	SER	N-CA-C	-6.63	93.09	111.00
1	A	97	VAL	N-CA-CB	-6.59	97.00	111.50
1	A	212	ALA	CB-CA-C	-6.58	100.22	110.10
1	A	30	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	56	SER	CA-CB-OG	-6.56	93.48	111.20
1	A	61	ASP	OD1-CG-OD2	-6.55	110.86	123.30
1	A	227	ASN	CA-C-O	-6.55	106.35	120.10
1	A	60	TYR	CD1-CE1-CZ	-6.51	113.94	119.80
1	A	202	ARG	NH1-CZ-NH2	6.50	126.56	119.40
1	A	158	TYR	CD1-CG-CD2	6.48	125.03	117.90
1	A	160	ARG	CD-NE-CZ	6.45	132.64	123.60
1	A	128	ASP	OD1-CG-OD2	6.45	135.54	123.30
1	A	136	TYR	CZ-CE2-CD2	-6.45	114.00	119.80
1	A	172	TYR	CG-CD2-CE2	-6.45	116.14	121.30
1	A	97	VAL	CA-CB-CG1	6.44	120.56	110.90
1	A	261	PHE	O-C-N	6.43	134.14	123.20
1	A	238	ASP	OD1-CG-OD2	6.36	135.39	123.30
1	A	44	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	A	269	THR	OG1-CB-CG2	-6.34	95.41	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ILE	CA-CB-CG1	-6.32	98.99	111.00
1	A	131	LYS	CA-CB-CG	6.29	127.23	113.40
1	A	15	ASN	CA-CB-CG	-6.25	99.65	113.40
1	A	211	ALA	CB-CA-C	6.24	119.46	110.10
1	A	121	GLU	CG-CD-OE2	-6.20	105.89	118.30
1	A	58	LEU	CB-CG-CD1	6.17	121.49	111.00
1	A	223	TRP	CZ3-CH2-CZ2	-6.17	114.20	121.60
1	A	86	ARG	CA-C-N	-6.11	103.75	117.20
1	A	228	SER	N-CA-CB	6.10	119.65	110.50
1	A	222	TYR	CB-CG-CD1	6.05	124.63	121.00
1	A	28	TYR	CG-CD2-CE2	-6.04	116.47	121.30
1	A	159	GLN	CA-C-N	6.03	130.46	117.20
1	A	226	ASP	OD1-CG-OD2	5.99	134.69	123.30
1	A	117	GLU	CA-C-N	5.96	130.32	117.20
1	A	160	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	96	PRO	N-CA-CB	5.95	110.44	103.30
1	A	47	GLU	OE1-CD-OE2	-5.93	116.19	123.30
1	A	65	MET	O-C-N	5.93	132.19	122.70
1	A	28	TYR	CD1-CE1-CZ	5.91	125.12	119.80
1	A	249	VAL	N-CA-CB	-5.91	98.50	111.50
1	A	86	ARG	CA-C-O	5.89	132.48	120.10
1	A	192	GLY	CA-C-O	5.89	131.20	120.60
1	A	88	TRP	CE3-CZ3-CH2	5.86	127.64	121.20
1	A	14	ILE	CG1-CB-CG2	5.84	124.26	111.40
1	A	30	ARG	CG-CD-NE	5.82	124.02	111.80
1	A	127	LEU	CB-CG-CD2	5.82	120.89	111.00
1	A	70	ASP	CA-CB-CG	-5.81	100.62	113.40
1	A	268	CYS	CA-CB-SG	5.80	124.45	114.00
1	A	19	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	A	195	TYR	N-CA-CB	-5.79	100.18	110.60
1	A	30	ARG	O-C-N	-5.79	113.44	122.70
1	A	45	ALA	O-C-N	-5.78	113.45	122.70
1	A	221	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	A	207	HIS	CG-CD2-NE2	-5.78	98.22	109.20
1	A	161	GLU	CA-C-N	-5.76	104.52	117.20
1	A	161	GLU	CB-CG-CD	-5.76	98.65	114.20
1	A	251	PHE	N-CA-CB	-5.76	100.24	110.60
1	A	232	VAL	CA-CB-CG2	5.75	119.53	110.90
1	A	20	TYR	CD1-CE1-CZ	-5.75	114.62	119.80
1	A	11	SER	CA-CB-OG	-5.73	95.72	111.20
1	A	74	THR	CA-CB-CG2	-5.71	104.41	112.40
1	A	222	TYR	CD1-CE1-CZ	5.70	124.93	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	LEU	CA-C-N	-5.67	104.72	117.20
1	A	28	TYR	O-C-N	-5.65	113.66	122.70
1	A	95	VAL	O-C-N	5.65	131.83	121.10
1	A	87	ASN	CA-CB-CG	-5.63	101.02	113.40
1	A	231	THR	CA-CB-OG1	-5.62	97.19	109.00
1	A	51	ILE	CA-CB-CG1	-5.62	100.32	111.00
1	A	209	PRO	N-CA-CB	5.62	110.04	103.30
1	A	217	HIS	CB-CA-C	-5.61	99.17	110.40
1	A	106	LYS	C-N-CA	5.61	135.72	121.70
1	A	166	SER	N-CA-CB	-5.60	102.09	110.50
1	A	229	PRO	CA-C-O	5.59	133.61	120.20
1	A	7	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	91	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	227	ASN	C-N-CA	-5.54	107.84	121.70
1	A	38	TRP	CG-CD1-NE1	-5.53	104.57	110.10
1	A	215	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	A	218	ALA	N-CA-C	-5.52	96.10	111.00
1	A	109	LYS	CA-CB-CG	-5.51	101.27	113.40
1	A	85	ILE	CA-C-O	-5.51	108.53	120.10
1	A	137	LYS	N-CA-CB	-5.51	100.69	110.60
1	A	61	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	197	ARG	CB-CA-C	5.49	121.38	110.40
1	A	268	CYS	CA-C-O	-5.49	108.58	120.10
1	A	235	CYS	N-CA-C	-5.45	96.28	111.00
1	A	73	LYS	CA-CB-CG	-5.45	101.41	113.40
1	A	6	ILE	N-CA-CB	5.45	123.33	110.80
1	A	197	ARG	N-CA-CB	-5.44	100.80	110.60
1	A	75	ILE	O-C-N	-5.43	114.00	122.70
1	A	164	LEU	CA-CB-CG	-5.43	102.82	115.30
1	A	159	GLN	O-C-N	-5.41	114.05	122.70
1	A	115	TYR	CD1-CE1-CZ	-5.40	114.94	119.80
1	A	150	VAL	N-CA-CB	-5.38	99.65	111.50
1	A	184	PHE	CG-CD1-CE1	5.37	126.71	120.80
1	A	172	TYR	CD1-CG-CD2	5.35	123.79	117.90
1	A	82	SER	CA-C-O	-5.35	108.87	120.10
1	A	180	GLY	O-C-N	5.33	131.24	122.70
1	A	187	TYR	O-C-N	-5.31	114.20	122.70
1	A	109	LYS	CA-C-O	5.31	131.25	120.10
1	A	226	ASP	O-C-N	5.30	131.19	122.70
1	A	6	ILE	O-C-N	-5.30	114.22	122.70
1	A	160	ARG	C-N-CA	5.29	134.93	121.70
1	A	213	PHE	C-N-CA	-5.29	111.20	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	VAL	CB-CA-C	5.28	121.44	111.40
1	A	202	ARG	CD-NE-CZ	5.27	130.98	123.60
1	A	65	MET	CG-SD-CE	-5.27	91.77	100.20
1	A	191	THR	C-N-CA	-5.25	111.27	122.30
1	A	100	PRO	N-CA-C	5.23	125.70	112.10
1	A	225	THR	CA-CB-OG1	-5.23	98.02	109.00
1	A	65	MET	CA-CB-CG	5.21	122.16	113.30
1	A	82	SER	O-C-N	5.21	131.04	122.70
1	A	126	VAL	CA-C-O	-5.20	109.19	120.10
1	A	14	ILE	CA-CB-CG1	-5.19	101.14	111.00
1	A	94	PHE	CZ-CE2-CD2	-5.17	113.89	120.10
1	A	158	TYR	CG-CD1-CE1	-5.17	117.16	121.30
1	A	156	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	101	PRO	N-CD-CG	-5.17	95.45	103.20
1	A	210	PRO	CA-C-N	-5.11	105.96	117.20
1	A	166	SER	CB-CA-C	5.10	119.79	110.10
1	A	115	TYR	CG-CD1-CE1	5.08	125.36	121.30
1	A	223	TRP	N-CA-CB	-5.08	101.46	110.60
1	A	226	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	6	ILE	CA-C-N	5.06	128.34	117.20
1	A	166	SER	C-N-CA	-5.06	109.05	121.70
1	A	79	PHE	N-CA-CB	5.05	119.69	110.60
1	A	213	PHE	CD1-CG-CD2	5.05	124.87	118.30
1	A	88	TRP	CD2-CE3-CZ3	-5.03	112.26	118.80
1	A	257	HIS	CE1-NE2-CD2	5.02	119.14	106.60
1	A	84	SER	O-C-N	-5.01	114.68	122.70
1	A	63	ASN	CB-CG-OD1	-5.01	111.58	121.60
1	A	230	GLU	CA-CB-CG	-5.00	102.39	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	230	0	0	12	1
All	All	2289	0	1981	61	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 15.

All (61) 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
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:140:VAL:HG12	1:A:150:VAL:CG2	2.07	0.84
1:A:141:THR:C	1:A:150:VAL:HG21	1.99	0.83
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:95:VAL:HG22	1:A:109:LYS:HB3	1.77	0.66
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:147:GLY:C	1:A:150:VAL:HG12	2.18	0.62
1:A:150:VAL:HG11	1:A:173:THR:HG22	1.84	0.59
1:A:47:GLU:CD	2:A:373:HOH:O	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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%)	15 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	97	VAL
1	A	120	ASN
1	A	131	LYS
1	A	137	LYS
1	A	195	TYR
1	A	228	SER

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Mol	Chain	Res	Type
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	87	ASN
1	A	159	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.