



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:29 PM UTC

PDB ID : 4TGL / pdb_00004tgl
Title : CATALYSIS AT THE INTERFACE: THE ANATOMY OF A CONFORMATIONAL CHANGE IN A TRIGLYCERIDE LIPASE
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Deposited on : 1991-07-29
Resolution : 2.60 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)	:	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

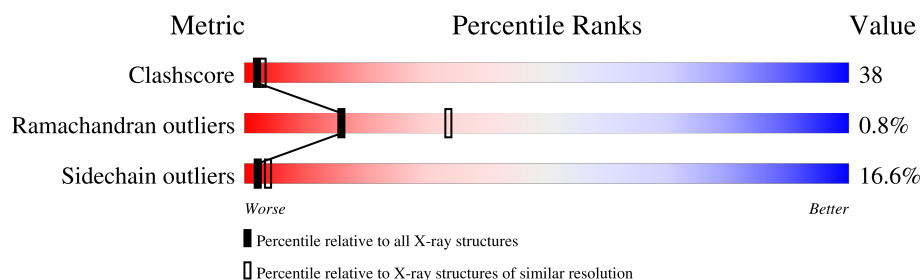
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	

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
2	DEP	A	270	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2324 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.

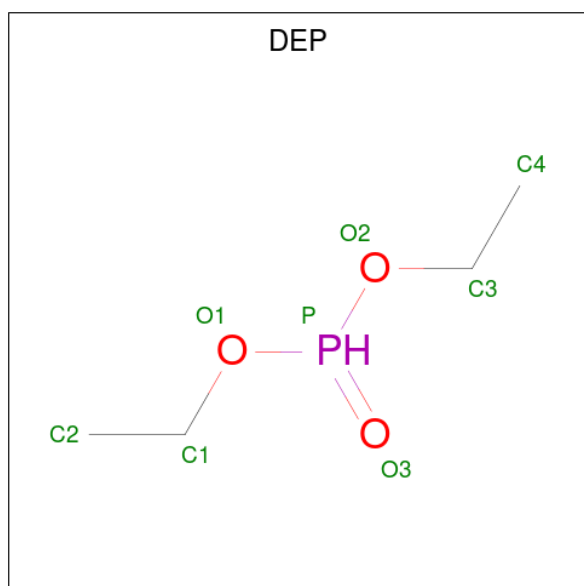
- Molecule 1 is a protein called TRIACYL-GLYCEROL ACYLHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	2078	1316	350	404	8	0	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ASN	ASP	conflict	UNP P19515
A	181	ASN	ASP	conflict	UNP P19515
A	220	SER	GLU	conflict	UNP P19515

- Molecule 2 is DIETHYL PHOSPHONATE (CCD ID: DEP) (formula: $C_4H_{11}O_3P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	8	4	3	1	0	0

- Molecule 3 is water.

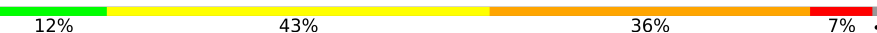
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	238	Total 238	O 238	0	0

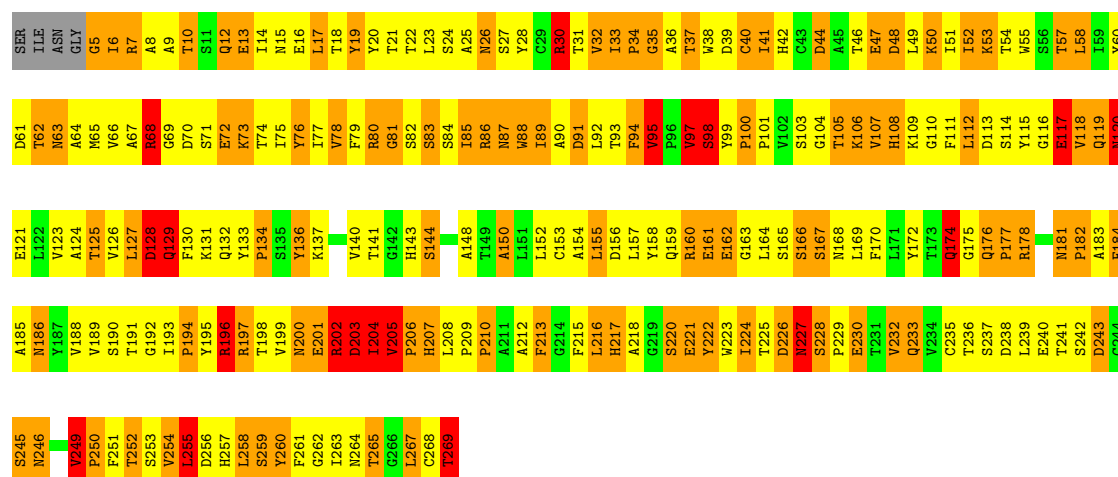
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: 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	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	48.30Å 93.90Å 122.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	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	2324	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.55	13/2149 (0.6%)	3.48	369/2934 (12.6%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86[A]	ARG	CB-CG	-11.41	1.18	1.52
1	A	86[B]	ARG	CB-CG	-11.41	1.18	1.52
1	A	30[A]	ARG	CB-CG	-11.00	1.19	1.52
1	A	30[B]	ARG	CB-CG	-11.00	1.19	1.52
1	A	30[C]	ARG	CB-CG	-11.00	1.19	1.52
1	A	80[A]	ARG	CB-CG	-7.12	1.31	1.52
1	A	80[B]	ARG	CB-CG	-7.12	1.31	1.52
1	A	100	PRO	C-O	6.50	1.31	1.24
1	A	160	ARG	NE-CZ	-5.34	1.27	1.33
1	A	81	GLY	N-CA	5.22	1.51	1.45
1	A	88	TRP	N-CA	5.18	1.52	1.46
1	A	178	ARG	C-O	5.12	1.30	1.23
1	A	75	ILE	CA-C	5.01	1.58	1.52

All (369) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ARG	CD-NE-CZ	23.32	157.04	124.40
1	A	42	HIS	CA-CB-CG	17.30	131.10	113.80
1	A	186	ASN	OD1-CG-ND2	15.02	137.62	122.60
1	A	160	ARG	NE-CZ-NH1	14.97	136.47	121.50
1	A	186	ASN	CA-CB-CG	-14.51	98.09	112.60
1	A	68	ARG	CA-C-O	-14.45	104.75	120.36
1	A	74	THR	O-C-N	13.21	138.60	123.27
1	A	120	ASN	CA-CB-CG	-12.89	99.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	GLN	CA-C-N	12.85	136.85	122.59
1	A	132	GLN	C-N-CA	12.85	136.85	122.59
1	A	165	SER	N-CA-C	-12.75	91.75	108.19
1	A	83	SER	O-C-N	12.74	135.44	121.93
1	A	160	ARG	CD-NE-CZ	12.44	141.82	124.40
1	A	148	ALA	O-C-N	11.82	134.86	122.09
1	A	119	GLN	OE1-CD-NE2	-11.67	110.93	122.60
1	A	225	THR	CA-CB-OG1	-11.39	92.51	109.60
1	A	63	ASN	CB-CG-ND2	-11.39	99.32	116.40
1	A	61	ASP	CA-CB-CG	-11.16	101.44	112.60
1	A	13	GLU	O-C-N	11.13	134.11	122.09
1	A	220	SER	CA-CB-OG	11.13	133.37	111.10
1	A	103	SER	CA-C-O	11.10	133.40	121.19
1	A	15	ASN	CA-CB-CG	-11.09	101.51	112.60
1	A	131	LYS	N-CA-C	-11.01	99.36	111.36
1	A	240	GLU	CA-C-O	-10.95	110.00	120.95
1	A	82	SER	CA-C-O	10.89	133.34	120.92
1	A	124	ALA	O-C-N	-10.88	107.45	122.46
1	A	68	ARG	O-C-N	10.85	136.21	123.30
1	A	204	ILE	N-CA-C	10.81	121.30	110.82
1	A	104	GLY	CA-C-O	-10.77	105.99	119.13
1	A	116	GLY	O-C-N	-10.70	111.17	122.19
1	A	58	LEU	N-CA-C	10.53	122.34	111.07
1	A	196	ARG	CA-C-N	10.11	136.90	122.85
1	A	196	ARG	C-N-CA	10.11	136.90	122.85
1	A	53	LYS	CA-C-O	-10.08	109.70	120.99
1	A	58	LEU	CA-C-N	-10.07	108.43	120.72
1	A	58	LEU	C-N-CA	-10.07	108.43	120.72
1	A	68	ARG	NE-CZ-NH1	9.96	131.46	121.50
1	A	63	ASN	CB-CG-OD1	9.88	140.57	120.80
1	A	51	ILE	CA-C-O	-9.76	109.73	120.85
1	A	246	ASN	OD1-CG-ND2	-9.63	112.97	122.60
1	A	228	SER	O-C-N	9.53	132.28	121.32
1	A	40	CYS	CA-C-O	9.52	131.58	121.10
1	A	196	ARG	CD-NE-CZ	-9.33	111.34	124.40
1	A	260	TYR	CA-C-O	-9.33	110.29	120.36
1	A	6	ILE	CA-C-O	-9.31	110.24	120.67
1	A	18	THR	CA-C-O	9.31	130.86	119.31
1	A	233	GLN	OE1-CD-NE2	9.27	131.87	122.60
1	A	26	ASN	OD1-CG-ND2	9.25	131.85	122.60
1	A	174	GLN	CB-CG-CD	9.21	128.26	112.60
1	A	259	SER	CA-C-N	-9.20	110.02	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	SER	C-N-CA	-9.20	110.02	122.99
1	A	86[A]	ARG	CA-CB-CG	9.18	132.46	114.10
1	A	86[B]	ARG	CA-CB-CG	9.18	132.46	114.10
1	A	95	VAL	N-CA-CB	-9.00	98.60	111.21
1	A	44	ASP	CA-CB-CG	-8.98	103.62	112.60
1	A	195	TYR	CA-C-N	8.92	135.52	122.41
1	A	195	TYR	C-N-CA	8.92	135.52	122.41
1	A	268	CYS	O-C-N	8.92	133.28	122.58
1	A	129	GLN	CG-CD-NE2	8.91	129.76	116.40
1	A	78	VAL	O-C-N	8.84	132.62	123.07
1	A	104	GLY	O-C-N	8.83	133.44	122.41
1	A	91	ASP	O-C-N	8.80	131.45	122.12
1	A	112	LEU	CA-C-O	8.79	129.75	120.70
1	A	72	GLU	CB-CG-CD	8.70	127.39	112.60
1	A	60	TYR	CA-C-N	-8.69	109.40	123.05
1	A	60	TYR	C-N-CA	-8.69	109.40	123.05
1	A	53	LYS	O-C-N	8.69	133.15	123.33
1	A	232	VAL	CA-C-N	-8.67	110.36	122.93
1	A	232	VAL	C-N-CA	-8.67	110.36	122.93
1	A	261	PHE	CA-CB-CG	-8.66	105.14	113.80
1	A	113	ASP	N-CA-CB	-8.58	97.51	110.12
1	A	7	ARG	CD-NE-CZ	-8.52	112.47	124.40
1	A	89	ILE	CA-C-O	-8.44	111.53	120.57
1	A	205	VAL	CA-C-N	8.44	128.09	119.82
1	A	205	VAL	C-N-CA	8.44	128.09	119.82
1	A	120	ASN	CB-CG-ND2	8.40	129.01	116.40
1	A	194	PRO	CB-CA-C	8.36	120.67	111.56
1	A	26	ASN	O-C-N	8.35	133.62	122.43
1	A	261	PHE	CA-C-O	-8.35	110.52	120.12
1	A	37	THR	CA-C-O	-8.35	111.34	121.11
1	A	125	THR	CA-CB-CG2	8.30	124.61	110.50
1	A	126	VAL	O-C-N	8.29	130.48	121.94
1	A	160	ARG	NH1-CZ-NH2	-8.28	108.53	119.30
1	A	177	PRO	CA-C-O	-8.27	110.40	122.31
1	A	243	ASP	CA-C-O	-8.26	110.33	119.34
1	A	268	CYS	N-CA-CB	8.21	124.39	111.91
1	A	16	GLU	N-CA-CB	-8.20	98.00	110.13
1	A	143	HIS	CB-CA-C	-8.15	96.99	110.19
1	A	192	GLY	N-CA-C	-8.12	104.83	115.47
1	A	121	GLU	CB-CA-C	-8.11	93.37	110.31
1	A	6	ILE	O-C-N	8.09	131.76	123.10
1	A	165	SER	O-C-N	8.06	132.75	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	GLY	CA-C-N	8.05	133.17	122.30
1	A	163	GLY	C-N-CA	8.05	133.17	122.30
1	A	31	THR	CA-C-O	-8.05	108.80	119.11
1	A	66	VAL	O-C-N	8.05	131.95	123.26
1	A	21	THR	CA-C-O	-7.97	112.45	120.82
1	A	54	THR	CA-C-O	-7.95	111.81	121.11
1	A	178	ARG	CA-C-O	-7.95	112.33	121.47
1	A	61	ASP	CB-CG-OD2	7.93	136.65	118.40
1	A	254	VAL	N-CA-C	-7.92	105.05	112.96
1	A	120	ASN	CB-CG-OD1	-7.88	105.04	120.80
1	A	141	THR	CA-CB-OG1	-7.83	97.85	109.60
1	A	188	VAL	O-C-N	7.83	129.90	121.83
1	A	17	LEU	CA-C-O	-7.81	110.04	119.49
1	A	170	PHE	CA-CB-CG	-7.81	105.99	113.80
1	A	120	ASN	N-CA-C	7.80	119.56	111.14
1	A	33	ILE	CA-C-O	7.76	127.07	119.62
1	A	240	GLU	O-C-N	7.68	131.71	123.11
1	A	93	THR	CA-C-O	-7.68	113.12	122.41
1	A	88	TRP	CB-CA-C	7.65	122.99	110.90
1	A	246	ASN	CA-CB-CG	-7.63	104.97	112.60
1	A	238	ASP	CA-CB-CG	-7.60	105.00	112.60
1	A	63	ASN	CA-C-O	-7.54	112.02	120.32
1	A	237	SER	CA-C-O	-7.54	113.39	121.99
1	A	189	VAL	CA-C-O	-7.54	113.18	121.17
1	A	128	ASP	CA-CB-CG	-7.51	105.09	112.60
1	A	97	VAL	N-CA-CB	-7.51	98.84	111.23
1	A	5	GLY	CA-C-N	-7.48	112.54	122.94
1	A	5	GLY	C-N-CA	-7.48	112.54	122.94
1	A	118	VAL	CA-C-N	7.42	135.72	121.54
1	A	118	VAL	C-N-CA	7.42	135.72	121.54
1	A	128	ASP	CB-CA-C	7.42	122.53	110.88
1	A	33	ILE	N-CA-CB	7.41	120.72	111.39
1	A	89	ILE	CA-CB-CG2	7.41	123.09	110.50
1	A	184	PHE	N-CA-C	-7.39	101.71	111.24
1	A	77	ILE	CB-CG1-CD1	-7.38	98.30	113.80
1	A	186	ASN	N-CA-C	7.36	118.94	111.07
1	A	94	PHE	CA-C-N	-7.31	108.61	122.13
1	A	94	PHE	C-N-CA	-7.31	108.61	122.13
1	A	125	THR	CA-CB-OG1	-7.30	98.65	109.60
1	A	42	HIS	N-CA-CB	-7.25	101.02	111.54
1	A	254	VAL	CB-CA-C	-7.24	104.69	111.06
1	A	240	GLU	CB-CA-C	-7.22	99.68	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	THR	CA-CB-OG1	-7.19	98.81	109.60
1	A	121	GLU	CG-CD-OE2	-7.17	101.90	118.40
1	A	41	ILE	CA-CB-CG2	7.17	122.69	110.50
1	A	206	PRO	O-C-N	7.14	132.59	122.37
1	A	39	ASP	CB-CA-C	7.09	122.55	111.77
1	A	207	HIS	CA-CB-CG	-7.07	106.73	113.80
1	A	27	SER	CA-C-O	-7.06	112.12	120.10
1	A	197	ARG	CB-CA-C	-7.04	99.48	111.31
1	A	218	ALA	N-CA-C	-7.04	98.73	109.85
1	A	269	THR	CA-C-O	-7.01	99.96	121.00
1	A	32	VAL	CA-C-N	-7.00	112.26	123.46
1	A	32	VAL	C-N-CA	-7.00	112.26	123.46
1	A	120	ASN	N-CA-CB	-6.99	99.93	110.07
1	A	62	THR	CA-CB-OG1	-6.99	99.12	109.60
1	A	148	ALA	CA-C-O	-6.96	113.53	120.70
1	A	87	ASN	CA-C-O	6.92	127.96	119.79
1	A	221	GLU	CG-CD-OE2	-6.91	102.51	118.40
1	A	61	ASP	CB-CG-OD1	-6.91	102.52	118.40
1	A	195	TYR	N-CA-CB	-6.88	100.17	110.90
1	A	67	ALA	CA-C-O	-6.87	113.63	121.40
1	A	150	ALA	N-CA-C	-6.87	102.87	111.11
1	A	107	VAL	CA-C-O	-6.86	113.22	120.76
1	A	57	THR	OG1-CB-CG2	6.81	122.92	109.30
1	A	157	LEU	CA-C-O	-6.77	113.37	120.55
1	A	166	SER	N-CA-C	6.76	120.62	112.38
1	A	62	THR	O-C-N	-6.72	114.62	122.95
1	A	74	THR	CA-CB-CG2	6.72	121.92	110.50
1	A	66	VAL	CA-C-O	-6.68	113.38	120.39
1	A	178	ARG	NE-CZ-NH2	6.68	125.21	119.20
1	A	74	THR	CA-C-N	6.66	132.42	123.10
1	A	74	THR	C-N-CA	6.66	132.42	123.10
1	A	241	THR	CA-C-O	6.65	128.89	121.11
1	A	41	ILE	CA-CB-CG1	-6.62	99.14	110.40
1	A	267	LEU	CA-C-O	-6.62	111.60	119.15
1	A	21	THR	O-C-N	6.57	128.83	122.07
1	A	58	LEU	N-CA-CB	-6.50	100.58	110.01
1	A	205	VAL	CA-CB-CG1	-6.50	99.35	110.40
1	A	18	THR	CA-C-N	6.48	129.49	120.29
1	A	18	THR	C-N-CA	6.48	129.49	120.29
1	A	233	GLN	CA-C-O	-6.46	113.86	120.71
1	A	52	ILE	CA-CB-CG2	-6.45	99.53	110.50
1	A	70	ASP	CA-C-O	-6.45	112.17	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	THR	N-CA-C	-6.45	103.49	112.45
1	A	203	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	230	GLU	CB-CA-C	-6.43	99.05	109.72
1	A	18	THR	N-CA-C	6.43	120.86	112.89
1	A	245	SER	CA-CB-OG	-6.42	98.26	111.10
1	A	227	ASN	CA-CB-CG	6.39	118.99	112.60
1	A	115	TYR	N-CA-CB	6.38	119.71	110.20
1	A	212	ALA	CA-C-O	-6.38	113.74	120.63
1	A	207	HIS	CA-C-O	-6.37	111.90	119.35
1	A	155	LEU	O-C-N	6.36	129.87	122.17
1	A	207	HIS	O-C-N	6.36	130.29	122.34
1	A	129	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	A	236	THR	CA-CB-OG1	-6.36	100.06	109.60
1	A	41	ILE	CA-C-O	6.33	127.54	120.64
1	A	239	LEU	N-CA-CB	6.33	120.59	110.85
1	A	197	ARG	N-CA-CB	6.32	120.82	110.39
1	A	265	THR	CA-CB-OG1	-6.32	100.12	109.60
1	A	200	ASN	CA-C-O	6.32	127.12	120.36
1	A	268	CYS	N-CA-C	-6.31	102.68	111.52
1	A	168	ASN	O-C-N	6.30	130.72	122.15
1	A	94	PHE	CB-CA-C	-6.26	99.23	110.37
1	A	255	LEU	O-C-N	6.21	128.47	122.07
1	A	200	ASN	CB-CG-ND2	6.20	125.70	116.40
1	A	131	LYS	CB-CG-CD	6.19	125.53	111.30
1	A	255	LEU	CA-C-N	6.16	130.55	120.63
1	A	255	LEU	C-N-CA	6.16	130.55	120.63
1	A	108	HIS	CA-CB-CG	6.15	119.95	113.80
1	A	128	ASP	CB-CG-OD1	-6.15	104.26	118.40
1	A	68	ARG	CB-CA-C	-6.15	98.46	109.71
1	A	84	SER	CA-CB-OG	-6.14	98.81	111.10
1	A	74	THR	OG1-CB-CG2	-6.14	97.03	109.30
1	A	217	HIS	CB-CA-C	-6.14	99.09	109.83
1	A	226	ASP	CA-C-N	-6.13	112.99	122.49
1	A	226	ASP	C-N-CA	-6.13	112.99	122.49
1	A	14	ILE	N-CA-CB	6.13	118.13	110.47
1	A	260	TYR	O-C-N	6.12	130.58	123.30
1	A	98	SER	O-C-N	6.11	129.78	122.94
1	A	262	GLY	N-CA-C	-6.11	107.42	114.69
1	A	195	TYR	CA-C-O	6.10	127.94	120.25
1	A	26	ASN	CA-C-O	-6.09	111.89	119.38
1	A	23	LEU	CA-C-N	6.07	128.41	120.28
1	A	23	LEU	C-N-CA	6.07	128.41	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	SER	N-CA-C	-6.06	100.93	109.96
1	A	239	LEU	N-CA-C	-6.03	100.79	110.14
1	A	7	ARG	NH1-CZ-NH2	6.03	127.14	119.30
1	A	100	PRO	N-CA-C	5.98	117.99	110.70
1	A	204	ILE	CA-CB-CG2	5.98	120.66	110.50
1	A	41	ILE	CB-CG1-CD1	-5.97	101.27	113.80
1	A	235	CYS	N-CA-C	-5.94	95.92	107.62
1	A	239	LEU	CB-CG-CD2	-5.93	92.91	110.70
1	A	70	ASP	CA-CB-CG	5.92	118.53	112.60
1	A	68	ARG	NH1-CZ-NH2	-5.92	111.60	119.30
1	A	19	TYR	CA-CB-CG	-5.92	103.25	113.90
1	A	76	TYR	CA-C-O	5.90	127.70	120.92
1	A	118	VAL	CA-CB-CG2	5.88	120.40	110.40
1	A	47	GLU	CA-C-N	5.88	131.43	121.14
1	A	47	GLU	C-N-CA	5.88	131.43	121.14
1	A	168	ASN	CA-C-O	-5.87	113.41	119.51
1	A	222	TYR	N-CA-C	-5.87	98.17	108.20
1	A	201	GLU	CB-CG-CD	5.85	122.55	112.60
1	A	8	ALA	CA-C-N	5.84	129.06	120.82
1	A	8	ALA	C-N-CA	5.84	129.06	120.82
1	A	167	SER	CA-C-O	5.83	126.17	119.35
1	A	183	ALA	CB-CA-C	-5.83	100.94	110.85
1	A	13	GLU	N-CA-C	-5.83	104.85	111.14
1	A	224	ILE	CB-CG1-CD1	-5.82	101.58	113.80
1	A	196	ARG	N-CA-CB	-5.81	101.69	110.35
1	A	162	GLU	CG-CD-OE2	-5.81	105.04	118.40
1	A	50	LYS	CA-CB-CG	-5.80	102.49	114.10
1	A	10	THR	CA-C-N	5.80	128.85	120.38
1	A	10	THR	C-N-CA	5.80	128.85	120.38
1	A	152	LEU	CA-C-O	5.79	126.69	120.20
1	A	143	HIS	N-CA-C	5.79	118.17	108.73
1	A	250	PRO	CA-C-N	-5.78	113.01	122.26
1	A	250	PRO	C-N-CA	-5.78	113.01	122.26
1	A	18	THR	CA-CB-OG1	-5.76	100.96	109.60
1	A	132	GLN	CA-CB-CG	-5.76	102.58	114.10
1	A	51	ILE	CA-C-N	-5.75	115.57	122.35
1	A	51	ILE	C-N-CA	-5.75	115.57	122.35
1	A	228	SER	N-CA-CB	5.75	120.60	110.37
1	A	195	TYR	CA-CB-CG	5.74	124.24	113.90
1	A	105	THR	N-CA-CB	5.74	120.04	110.85
1	A	28	TYR	CB-CG-CD1	5.74	129.41	120.80
1	A	47	GLU	CA-CB-CG	5.71	125.52	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	GLU	CA-C-O	-5.70	113.06	119.95
1	A	85	ILE	O-C-N	5.69	129.69	122.57
1	A	188	VAL	CA-C-N	-5.68	113.40	120.56
1	A	188	VAL	C-N-CA	-5.68	113.40	120.56
1	A	33	ILE	O-C-N	-5.68	115.84	121.12
1	A	35	GLY	N-CA-C	-5.68	105.91	112.83
1	A	46	THR	CA-CB-OG1	-5.67	101.09	109.60
1	A	249	VAL	CB-CA-C	5.67	121.68	111.36
1	A	113	ASP	CB-CA-C	5.66	120.19	110.79
1	A	131	LYS	CA-CB-CG	-5.64	102.83	114.10
1	A	242	SER	CA-C-O	-5.62	112.48	120.51
1	A	134	PRO	CA-C-N	-5.60	111.80	121.66
1	A	134	PRO	C-N-CA	-5.60	111.80	121.66
1	A	7	ARG	N-CA-C	-5.60	101.01	108.74
1	A	90	ALA	N-CA-C	-5.60	105.25	111.36
1	A	136	TYR	CA-C-N	-5.59	113.04	123.05
1	A	136	TYR	C-N-CA	-5.59	113.04	123.05
1	A	199	VAL	CA-C-N	-5.58	115.35	122.77
1	A	199	VAL	C-N-CA	-5.58	115.35	122.77
1	A	269	THR	CA-CB-CG2	5.56	119.96	110.50
1	A	6	ILE	N-CA-C	-5.56	100.17	108.46
1	A	127	LEU	CB-CA-C	-5.55	101.24	110.68
1	A	114	SER	O-C-N	5.55	128.00	122.12
1	A	128	ASP	CA-C-N	5.55	127.98	120.38
1	A	128	ASP	C-N-CA	5.55	127.98	120.38
1	A	48	ASP	CA-C-O	5.54	126.19	119.31
1	A	97	VAL	CA-C-N	-5.54	110.94	122.07
1	A	97	VAL	C-N-CA	-5.54	110.94	122.07
1	A	130	PHE	CB-CA-C	-5.53	98.42	109.99
1	A	23	LEU	CA-C-O	-5.53	115.01	120.82
1	A	196	ARG	CA-CB-CG	5.52	125.15	114.10
1	A	128	ASP	CB-CG-OD2	5.52	131.10	118.40
1	A	39	ASP	CA-C-O	5.50	131.31	120.69
1	A	258	LEU	CA-C-N	-5.50	113.17	121.86
1	A	258	LEU	C-N-CA	-5.50	113.17	121.86
1	A	144	SER	O-C-N	-5.50	115.28	122.59
1	A	20	TYR	N-CA-C	-5.50	105.37	111.36
1	A	97	VAL	CA-C-O	-5.49	113.92	120.78
1	A	13	GLU	CA-C-O	-5.48	115.06	120.70
1	A	215	PHE	N-CA-CB	5.47	120.27	110.80
1	A	42	HIS	CB-CG-ND1	5.46	130.89	122.70
1	A	92	LEU	N-CA-CB	5.46	118.51	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	THR	CA-CB-OG1	-5.45	101.42	109.60
1	A	164	LEU	CA-C-O	-5.43	114.34	120.43
1	A	54	THR	CA-CB-CG2	5.43	119.73	110.50
1	A	224	ILE	CA-C-O	-5.43	113.85	120.69
1	A	260	TYR	N-CA-CB	-5.43	101.56	110.68
1	A	182	PRO	CA-C-N	5.43	128.00	120.29
1	A	182	PRO	C-N-CA	5.43	128.00	120.29
1	A	232	VAL	O-C-N	5.42	129.03	123.18
1	A	143	HIS	O-C-N	5.41	129.38	123.22
1	A	201	GLU	O-C-N	5.41	129.78	122.59
1	A	268	CYS	CB-CA-C	-5.40	104.62	111.86
1	A	121	GLU	N-CA-CB	5.40	119.35	110.39
1	A	7	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	A	100	PRO	O-C-N	-5.39	115.10	121.46
1	A	238	ASP	OD1-CG-OD2	5.38	135.82	122.90
1	A	226	ASP	N-CA-CB	5.38	120.64	111.66
1	A	267	LEU	CD1-CG-CD2	-5.38	98.97	110.80
1	A	213	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	200	ASN	CA-CB-CG	-5.37	107.23	112.60
1	A	172	TYR	CA-C-N	-5.36	114.17	122.59
1	A	172	TYR	C-N-CA	-5.36	114.17	122.59
1	A	204	ILE	CB-CG1-CD1	-5.34	102.58	113.80
1	A	21	THR	N-CA-CB	5.31	117.70	110.01
1	A	267	LEU	N-CA-CB	-5.30	102.63	110.53
1	A	41	ILE	N-CA-C	5.29	118.47	111.17
1	A	51	ILE	CB-CG1-CD1	-5.28	102.71	113.80
1	A	22	THR	CB-CA-C	-5.28	102.03	110.79
1	A	200	ASN	CB-CG-OD1	-5.27	110.26	120.80
1	A	19	TYR	CB-CG-CD1	5.27	128.70	120.80
1	A	26	ASN	CB-CG-ND2	-5.27	108.50	116.40
1	A	73	LYS	CG-CD-CE	5.27	123.42	111.30
1	A	246	ASN	CA-C-O	-5.27	112.90	119.38
1	A	189	VAL	CA-C-N	5.26	128.72	120.82
1	A	189	VAL	C-N-CA	5.26	128.72	120.82
1	A	51	ILE	O-C-N	5.25	128.64	122.81
1	A	210	PRO	CA-C-O	-5.25	115.36	121.34
1	A	216	LEU	CA-C-O	-5.24	114.31	120.60
1	A	128	ASP	N-CA-C	-5.24	105.47	111.07
1	A	89	ILE	CB-CA-C	5.22	120.26	112.16
1	A	30[A]	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	30[B]	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	30[C]	ARG	NE-CZ-NH2	5.22	123.90	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	TYR	CA-C-N	5.21	127.22	120.44
1	A	20	TYR	C-N-CA	5.21	127.22	120.44
1	A	10	THR	N-CA-C	-5.21	101.97	110.20
1	A	166	SER	CB-CA-C	-5.21	99.33	110.32
1	A	163	GLY	CA-C-O	5.20	124.92	119.04
1	A	195	TYR	N-CA-C	5.20	116.79	107.80
1	A	227	ASN	CB-CG-ND2	5.18	124.17	116.40
1	A	174	GLN	OE1-CD-NE2	5.17	127.77	122.60
1	A	204	ILE	N-CA-CB	-5.15	103.11	110.52
1	A	263	ILE	N-CA-C	5.13	116.18	109.21
1	A	137	LYS	CB-CA-C	5.12	119.46	110.36
1	A	57	THR	CA-CB-OG1	-5.11	101.93	109.60
1	A	260	TYR	CB-CA-C	5.11	119.06	109.71
1	A	241	THR	N-CA-CB	5.10	120.65	111.37
1	A	32	VAL	N-CA-CB	-5.10	102.82	111.23
1	A	80[A]	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	80[B]	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	117	GLU	CB-CG-CD	5.09	121.25	112.60
1	A	205	VAL	O-C-N	5.08	126.89	121.10
1	A	261	PHE	O-C-N	5.05	130.15	122.03
1	A	32	VAL	N-CA-C	-5.04	98.87	109.34
1	A	87	ASN	CA-C-N	-5.03	113.61	120.44
1	A	87	ASN	C-N-CA	-5.03	113.61	120.44
1	A	90	ALA	CA-C-O	5.03	125.75	120.42
1	A	115	TYR	N-CA-C	-5.02	105.51	111.69

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	2078	0	2015	155	93
2	A	8	0	10	0	4
3	A	238	0	0	19	14
All	All	2324	0	2025	155	98

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 38.

All (155) 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:99:TYR:HB3	1:A:105:THR:OG1	1.56	1.04
1:A:181:ASN:HD22	1:A:181:ASN:H	1.14	0.91
1:A:181:ASN:HB2	1:A:182:PRO:HD2	1.53	0.91
1:A:220:SER:OG	3:A:409:HOH:O	1.80	0.89
1:A:181:ASN:HB2	1:A:182:PRO:CD	2.04	0.88
1:A:193:ILE:HB	3:A:422:HOH:O	1.76	0.86
1:A:169:LEU:O	1:A:194:PRO:HD2	1.77	0.84
1:A:106:LYS:H	1:A:181:ASN:HD21	1.27	0.83
1:A:181:ASN:HD22	1:A:181:ASN:N	1.76	0.80
1:A:107:VAL:HG21	1:A:112:LEU:HD13	1.64	0.78
1:A:25:ALA:HB2	1:A:265:THR:HG22	1.67	0.75
1:A:185:ALA:HB3	1:A:216:LEU:HD23	1.70	0.74
1:A:48:ASP:OD2	1:A:72:GLU:OE2	2.04	0.73
1:A:202:ARG:NE	3:A:374:HOH:O	2.23	0.72
1:A:226:ASP:OD1	1:A:227:ASN:N	2.23	0.72
1:A:202:ARG:NH1	1:A:251:PHE:HB2	2.05	0.70
1:A:202:ARG:NH1	1:A:251:PHE:CB	2.55	0.70
1:A:17:LEU:HD11	1:A:222:TYR:CD2	2.27	0.69
1:A:202:ARG:HD3	3:A:374:HOH:O	1.91	0.69
1:A:47:GLU:OE2	3:A:492:HOH:O	2.09	0.69
1:A:205:VAL:HG21	1:A:257:HIS:CE1	2.27	0.69
1:A:57:THR:OG1	1:A:117:GLU:OE1	2.12	0.67
1:A:80[B]:ARG:CZ	1:A:83:SER:HB3	2.25	0.66
1:A:191:THR:OG1	3:A:422:HOH:O	2.13	0.66
1:A:88:TRP:O	1:A:91:ASP:HB2	1.95	0.66
1:A:264:ASN:OD1	1:A:269:THR:HB	1.94	0.66
1:A:202:ARG:HG2	1:A:251:PHE:O	1.97	0.65
1:A:207:HIS:CE1	1:A:246:ASN:HD22	2.14	0.64
1:A:63:ASN:HD22	1:A:63:ASN:N	1.91	0.64
1:A:98:SER:O	1:A:100:PRO:HD3	1.97	0.64
1:A:108:HIS:CD2	1:A:111:PHE:H	2.17	0.63
1:A:49:LEU:HD22	1:A:76:TYR:CE2	2.34	0.62
1:A:185:ALA:CB	1:A:216:LEU:HD23	2.30	0.61
1:A:200:ASN:HD22	1:A:224:ILE:HB	1.64	0.61
1:A:184:PHE:O	1:A:185:ALA:C	2.40	0.61
1:A:207:HIS:CE1	1:A:246:ASN:ND2	2.69	0.61
1:A:125:THR:O	1:A:129:GLN:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:HIS:HD2	1:A:110:GLY:N	2.01	0.59
1:A:257:HIS:O	1:A:257:HIS:CG	2.56	0.58
1:A:57:THR:CB	1:A:117:GLU:OE1	2.52	0.58
1:A:128:ASP:HB2	3:A:459:HOH:O	2.03	0.58
1:A:119:GLN:HG2	1:A:120:ASN:HD22	1.69	0.58
1:A:107:VAL:O	1:A:107:VAL:HG23	2.03	0.57
1:A:144:SER:HB2	1:A:257:HIS:CE1	2.40	0.57
1:A:62:THR:C	1:A:63:ASN:HD22	2.12	0.57
1:A:10:THR:OG1	1:A:13:GLU:HG3	2.04	0.57
1:A:44:ASP:N	1:A:44:ASP:OD1	2.36	0.56
1:A:94:PHE:HD2	3:A:474:HOH:O	1.88	0.56
1:A:94:PHE:O	1:A:95:VAL:C	2.43	0.56
1:A:202:ARG:CD	3:A:374:HOH:O	2.47	0.56
1:A:156:ASP:HA	3:A:447:HOH:O	2.04	0.55
1:A:202:ARG:NH1	1:A:251:PHE:HB3	2.21	0.55
1:A:207:HIS:HE1	1:A:246:ASN:HD22	1.55	0.55
1:A:205:VAL:HG21	1:A:257:HIS:ND1	2.22	0.55
1:A:181:ASN:N	1:A:181:ASN:ND2	2.47	0.55
1:A:223:TRP:CD1	1:A:245:SER:HB3	2.42	0.54
1:A:44:ASP:O	1:A:47:GLU:HG2	2.07	0.54
1:A:68:ARG:HD2	1:A:136:TYR:CE2	2.42	0.54
1:A:57:THR:HB	1:A:117:GLU:OE1	2.07	0.54
1:A:202:ARG:HH12	1:A:251:PHE:HB2	1.72	0.54
1:A:85:ILE:HG23	1:A:89:ILE:HD12	1.88	0.54
1:A:5:GLY:C	1:A:6:ILE:HD12	2.32	0.54
1:A:62:THR:HG21	1:A:118:VAL:HG11	1.91	0.53
1:A:181:ASN:CB	1:A:182:PRO:CD	2.73	0.52
1:A:68:ARG:HD2	1:A:136:TYR:HE2	1.75	0.52
1:A:80[B]:ARG:NH2	1:A:83:SER:HB3	2.24	0.52
1:A:106:LYS:O	1:A:181:ASN:ND2	2.43	0.52
1:A:24:SER:OG	1:A:174:GLN:NE2	2.43	0.52
1:A:5:GLY:O	1:A:6:ILE:HD12	2.10	0.52
1:A:64:ALA:HB2	1:A:79:PHE:CD2	2.46	0.51
1:A:202:ARG:HB2	1:A:256:ASP:OD2	2.10	0.51
1:A:156:ASP:O	1:A:160:ARG:HG2	2.11	0.51
1:A:159:GLN:NE2	3:A:447:HOH:O	2.44	0.51
1:A:181:ASN:H	1:A:181:ASN:ND2	1.91	0.50
1:A:140:VAL:HG12	1:A:150:ALA:HB1	1.92	0.50
1:A:108:HIS:CD2	1:A:110:GLY:N	2.79	0.50
1:A:217:HIS:HA	3:A:273:HOH:O	2.10	0.50
1:A:17:LEU:HD21	1:A:196:ARG:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LYS:O	1:A:110:GLY:C	2.53	0.50
1:A:62:THR:HG21	1:A:118:VAL:CG1	2.42	0.49
1:A:200:ASN:HB2	1:A:260:TYR:CE1	2.48	0.49
1:A:106:LYS:H	1:A:181:ASN:ND2	2.04	0.49
1:A:160:ARG:O	1:A:161:GLU:C	2.56	0.49
1:A:202:ARG:HH12	1:A:251:PHE:CB	2.22	0.49
1:A:205:VAL:N	1:A:206:PRO:CD	2.76	0.49
1:A:80[B]:ARG:CZ	1:A:83:SER:CB	2.90	0.48
1:A:230:GLU:N	3:A:353:HOH:O	2.47	0.48
1:A:85:ILE:HG23	1:A:89:ILE:CD1	2.44	0.48
1:A:64:ALA:HA	1:A:78:VAL:O	2.14	0.48
1:A:246:ASN:HD22	1:A:246:ASN:HA	1.53	0.48
1:A:129:GLN:O	1:A:133:TYR:HD2	1.97	0.48
1:A:257:HIS:O	1:A:257:HIS:CD2	2.67	0.48
1:A:264:ASN:OD1	1:A:267:LEU:HB2	2.13	0.48
1:A:176:GLN:HG2	1:A:177:PRO:O	2.15	0.47
1:A:160:ARG:O	1:A:162:GLU:HG2	2.14	0.47
1:A:32:VAL:O	1:A:36:ALA:N	2.43	0.47
1:A:153:CYS:O	1:A:156:ASP:N	2.48	0.47
1:A:26:ASN:ND2	3:A:394:HOH:O	2.47	0.47
1:A:41:ILE:O	1:A:41:ILE:HG13	2.15	0.47
1:A:107:VAL:CG2	1:A:112:LEU:HD22	2.44	0.47
1:A:203:ASP:OD1	1:A:257:HIS:HB2	2.14	0.47
1:A:200:ASN:ND2	1:A:224:ILE:HD12	2.30	0.46
1:A:19:TYR:C	1:A:19:TYR:CD1	2.94	0.46
1:A:62:THR:HA	3:A:472:HOH:O	2.16	0.46
1:A:144:SER:HB2	1:A:257:HIS:HE1	1.81	0.46
1:A:174:GLN:O	1:A:175:GLY:C	2.59	0.45
1:A:197:ARG:O	1:A:221:GLU:HA	2.16	0.45
1:A:107:VAL:O	1:A:107:VAL:CG2	2.63	0.45
1:A:182:PRO:HA	1:A:216:LEU:CD2	2.47	0.45
1:A:245:SER:HB2	3:A:279:HOH:O	2.17	0.45
1:A:80[A]:ARG:HG2	1:A:81:GLY:O	2.17	0.45
1:A:35:GLY:O	1:A:36:ALA:HB3	2.17	0.45
1:A:53:LYS:HB3	1:A:55:TRP:CH2	2.52	0.45
1:A:119:GLN:HG2	1:A:120:ASN:ND2	2.32	0.45
1:A:127:LEU:HD23	1:A:127:LEU:N	2.17	0.45
1:A:123:VAL:HG21	1:A:156:ASP:OD2	2.18	0.44
1:A:205:VAL:CG2	1:A:257:HIS:ND1	2.81	0.44
1:A:108:HIS:CD2	1:A:108:HIS:C	2.95	0.44
1:A:158:TYR:C	1:A:158:TYR:CD1	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80[B]:ARG:HG2	1:A:81:GLY:N	2.33	0.43
1:A:198:THR:HA	1:A:222:TYR:O	2.18	0.43
1:A:80[B]:ARG:NE	1:A:83:SER:HB2	2.32	0.43
1:A:120:ASN:HB2	3:A:466:HOH:O	2.18	0.43
1:A:26:ASN:HD22	1:A:26:ASN:HA	1.47	0.43
1:A:38:TRP:CD1	1:A:47:GLU:HA	2.53	0.43
1:A:203:ASP:CG	1:A:257:HIS:HB2	2.43	0.43
1:A:97:VAL:O	1:A:106:LYS:HG3	2.18	0.43
1:A:205:VAL:C	1:A:207:HIS:H	2.26	0.43
1:A:153:CYS:O	1:A:154:ALA:C	2.61	0.42
1:A:99:TYR:CZ	1:A:101:PRO:HG2	2.54	0.42
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.40	0.42
1:A:30[C]:ARG:NH2	3:A:312:HOH:O	2.52	0.42
1:A:223:TRP:NE1	1:A:245:SER:HB3	2.35	0.42
1:A:52:ILE:O	1:A:52:ILE:HG22	2.16	0.42
1:A:69:GLY:HA3	1:A:72:GLU:OE1	2.18	0.42
1:A:12:GLN:HE21	1:A:12:GLN:HB2	1.67	0.42
1:A:85:ILE:O	1:A:89:ILE:HD12	2.20	0.42
1:A:80[B]:ARG:NH2	1:A:87:ASN:OD1	2.51	0.42
1:A:7:ARG:HH11	1:A:7:ARG:HD2	1.46	0.42
1:A:197:ARG:HH11	1:A:197:ARG:HD2	1.71	0.41
1:A:33:ILE:HD11	1:A:65:MET:HE2	2.01	0.41
1:A:153:CYS:C	1:A:155:LEU:N	2.77	0.41
1:A:133:TYR:N	1:A:134:PRO:HD3	2.34	0.41
1:A:158:TYR:CD1	1:A:158:TYR:O	2.74	0.41
1:A:202:ARG:HH11	1:A:251:PHE:CB	2.29	0.41
1:A:224:ILE:HG21	1:A:224:ILE:HD13	1.58	0.41
1:A:9:ALA:CB	1:A:232:VAL:HB	2.51	0.41
1:A:34:PRO:O	1:A:35:GLY:C	2.62	0.41
1:A:178:ARG:HB2	1:A:209:PRO:HD2	2.02	0.41
1:A:182:PRO:HA	1:A:216:LEU:HD23	2.03	0.41
1:A:226:ASP:CG	3:A:418:HOH:O	2.63	0.41
1:A:208:LEU:HA	1:A:209:PRO:C	2.46	0.40
1:A:38:TRP:CG	1:A:47:GLU:HA	2.56	0.40
1:A:205:VAL:C	1:A:207:HIS:N	2.80	0.40
1:A:228:SER:HA	1:A:229:PRO:HA	1.82	0.40

All (98) 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)
1:A:254:VAL:O	1:A:254:VAL:CG1[3_456]	0.73	1.47
1:A:209:PRO:C	1:A:250:PRO:N[3_456]	0.78	1.42
1:A:208:LEU:CA	1:A:250:PRO:C[3_456]	0.81	1.39
1:A:210:PRO:CD	1:A:249:VAL:O[3_456]	0.87	1.33
1:A:208:LEU:C	1:A:250:PRO:C[3_456]	0.91	1.29
1:A:209:PRO:CG	1:A:251:PHE:CD2[3_456]	0.92	1.28
1:A:210:PRO:N	1:A:249:VAL:O[3_456]	0.98	1.22
1:A:209:PRO:O	1:A:250:PRO:CD[3_456]	1.00	1.20
1:A:208:LEU:C	1:A:251:PHE:N[3_456]	1.01	1.19
1:A:210:PRO:N	1:A:249:VAL:C[3_456]	1.02	1.18
1:A:204:ILE:CA	1:A:204:ILE:CD1[3_456]	1.05	1.15
2:A:270:DEP:O2	3:A:376:HOH:O[3_456]	1.08	1.12
1:A:209:PRO:CG	1:A:251:PHE:CE2[3_456]	1.17	1.03
1:A:209:PRO:O	1:A:250:PRO:N[3_456]	1.20	1.00
1:A:210:PRO:CG	3:A:371:HOH:O[3_456]	1.21	0.99
1:A:209:PRO:C	1:A:250:PRO:CD[3_456]	1.22	0.98
1:A:209:PRO:C	1:A:249:VAL:C[3_456]	1.22	0.98
1:A:213:PHE:CD1	3:A:372:HOH:O[3_456]	1.27	0.93
1:A:204:ILE:CB	1:A:204:ILE:CB[3_456]	1.28	0.92
1:A:208:LEU:N	1:A:250:PRO:O[3_456]	1.38	0.82
2:A:270:DEP:C3	3:A:376:HOH:O[3_456]	1.39	0.81
1:A:204:ILE:O	1:A:252:THR:OG1[3_456]	1.43	0.77
1:A:257:HIS:CD2	3:A:401:HOH:O[3_456]	1.43	0.77
1:A:213:PHE:CE1	3:A:372:HOH:O[3_456]	1.44	0.76
1:A:254:VAL:C	1:A:254:VAL:CG1[3_456]	1.45	0.75
1:A:205:VAL:CG1	1:A:252:THR:O[3_456]	1.46	0.74
1:A:204:ILE:CG2	1:A:253:SER:O[3_456]	1.47	0.73
1:A:254:VAL:O	1:A:254:VAL:CB[3_456]	1.49	0.71
1:A:208:LEU:CA	1:A:250:PRO:CA[3_456]	1.52	0.68
1:A:208:LEU:CA	1:A:251:PHE:N[3_456]	1.54	0.66
1:A:208:LEU:N	1:A:250:PRO:C[3_456]	1.57	0.63
1:A:208:LEU:O	1:A:250:PRO:C[3_456]	1.58	0.62
1:A:208:LEU:CD1	1:A:252:THR:CA[3_456]	1.59	0.61
1:A:209:PRO:O	1:A:250:PRO:CG[3_456]	1.59	0.61
1:A:209:PRO:CD	1:A:251:PHE:CD2[3_456]	1.61	0.59
1:A:178:ARG:O	1:A:251:PHE:CE1[3_456]	1.63	0.57
1:A:208:LEU:O	1:A:250:PRO:O[3_456]	1.63	0.57
1:A:209:PRO:N	1:A:251:PHE:N[3_456]	1.63	0.57
1:A:208:LEU:CB	1:A:251:PHE:C[3_456]	1.67	0.53
1:A:88:TRP:CH2	3:A:375:HOH:O[3_456]	1.68	0.52
1:A:208:LEU:CA	1:A:250:PRO:O[3_456]	1.69	0.51
1:A:210:PRO:CD	1:A:249:VAL:C[3_456]	1.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:PRO:C	1:A:249:VAL:O[3_456]	1.71	0.49
1:A:209:PRO:CA	1:A:250:PRO:N[3_456]	1.71	0.49
1:A:209:PRO:CD	1:A:251:PHE:CE2[3_456]	1.71	0.49
1:A:254:VAL:CA	1:A:254:VAL:CA[3_456]	1.73	0.47
1:A:254:VAL:CG2	1:A:257:HIS:CB[3_456]	1.77	0.43
1:A:205:VAL:CB	1:A:252:THR:O[3_456]	1.79	0.41
1:A:209:PRO:O	1:A:250:PRO:CB[3_456]	1.79	0.41
1:A:210:PRO:N	1:A:250:PRO:N[3_456]	1.79	0.41
1:A:91:ASP:O	1:A:202:ARG:NH2[3_456]	1.80	0.40
1:A:208:LEU:C	1:A:250:PRO:CA[3_456]	1.82	0.38
1:A:208:LEU:CB	1:A:252:THR:N[3_456]	1.83	0.37
1:A:208:LEU:CB	1:A:251:PHE:N[3_456]	1.83	0.37
1:A:209:PRO:CA	1:A:250:PRO:CD[3_456]	1.85	0.35
1:A:209:PRO:O	1:A:250:PRO:CA[3_456]	1.85	0.35
1:A:205:VAL:CA	1:A:252:THR:O[3_456]	1.88	0.32
1:A:208:LEU:C	1:A:250:PRO:O[3_456]	1.90	0.30
1:A:213:PHE:CG	3:A:372:HOH:O[3_456]	1.90	0.30
2:A:270:DEP:C4	3:A:374:HOH:O[3_456]	1.90	0.30
1:A:208:LEU:O	1:A:251:PHE:N[3_456]	1.91	0.29
1:A:209:PRO:CA	1:A:249:VAL:C[3_456]	1.92	0.28
1:A:208:LEU:CG	1:A:252:THR:CG2[3_456]	1.95	0.25
1:A:204:ILE:CG2	1:A:253:SER:C[3_456]	1.96	0.24
1:A:208:LEU:N	1:A:250:PRO:CA[3_456]	1.96	0.24
1:A:208:LEU:CD1	1:A:252:THR:N[3_456]	1.99	0.21
1:A:204:ILE:N	1:A:204:ILE:CD1[3_456]	2.00	0.20
1:A:208:LEU:CB	1:A:250:PRO:C[3_456]	2.00	0.20
1:A:208:LEU:CG	1:A:252:THR:N[3_456]	2.01	0.19
1:A:209:PRO:CD	1:A:251:PHE:CG[3_456]	2.02	0.18
1:A:178:ARG:NH1	1:A:250:PRO:CB[3_456]	2.03	0.17
1:A:204:ILE:C	1:A:252:THR:OG1[3_456]	2.03	0.17
1:A:204:ILE:C	1:A:204:ILE:CD1[3_456]	2.03	0.17
3:A:417:HOH:O	3:A:474:HOH:O[3_456]	2.03	0.17
1:A:213:PHE:CE1	3:A:368:HOH:O[3_456]	2.04	0.16
1:A:205:VAL:O	1:A:250:PRO:O[3_456]	2.05	0.15
1:A:208:LEU:CB	1:A:251:PHE:CA[3_456]	2.05	0.15
1:A:254:VAL:C	1:A:254:VAL:O[3_456]	2.05	0.15
1:A:91:ASP:C	1:A:202:ARG:NH2[3_456]	2.08	0.12
1:A:210:PRO:CD	1:A:249:VAL:N[3_456]	2.08	0.12
1:A:204:ILE:CA	1:A:204:ILE:CG1[3_456]	2.09	0.11
1:A:255:LEU:CD1	1:A:258:LEU:CD2[3_456]	2.09	0.11
1:A:209:PRO:N	1:A:250:PRO:CD[3_456]	2.10	0.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:CA	1:A:254:VAL:O[3_456]	2.10	0.10
1:A:255:LEU:CG	1:A:258:LEU:CD2[3_456]	2.10	0.10
1:A:210:PRO:CA	1:A:249:VAL:CG1[3_456]	2.11	0.09
2:A:270:DEP:C4	3:A:402:HOH:O[3_456]	2.11	0.09
1:A:178:ARG:O	1:A:251:PHE:CZ[3_456]	2.12	0.08
1:A:213:PHE:CZ	3:A:372:HOH:O[3_456]	2.12	0.08
1:A:254:VAL:CB	1:A:257:HIS:CB[3_456]	2.12	0.08
1:A:254:VAL:C	1:A:254:VAL:CB[3_456]	2.12	0.08
1:A:209:PRO:N	1:A:250:PRO:N[3_456]	2.14	0.06
1:A:257:HIS:NE2	3:A:401:HOH:O[3_456]	2.14	0.06
1:A:204:ILE:CG1	1:A:252:THR:CB[3_456]	2.15	0.05
1:A:209:PRO:N	1:A:250:PRO:C[3_456]	2.16	0.04
1:A:209:PRO:CA	1:A:249:VAL:O[3_456]	2.17	0.03
1:A:208:LEU:C	1:A:251:PHE:CA[3_456]	2.18	0.02
1:A:210:PRO:CG	1:A:249:VAL:O[3_456]	2.19	0.01

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	267/269 (99%)	238 (89%)	27 (10%)	2 (1%)	18 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	GLU
1	A	203	ASP

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	233/232 (100%)	192 (82%)	41 (18%)	2 3

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	30[A]	ARG
1	A	30[B]	ARG
1	A	30[C]	ARG
1	A	34	PRO
1	A	37	THR
1	A	40	CYS
1	A	50	LYS
1	A	58	LEU
1	A	68	ARG
1	A	71	SER
1	A	73	LYS
1	A	86[A]	ARG
1	A	86[B]	ARG
1	A	95	VAL
1	A	97	VAL
1	A	98	SER
1	A	106	LYS
1	A	117	GLU
1	A	120	ASN
1	A	128	ASP
1	A	129	GLN
1	A	161	GLU
1	A	166	SER
1	A	167	SER
1	A	174	GLN
1	A	176	GLN
1	A	181	ASN
1	A	186	ASN
1	A	190	SER
1	A	196	ARG
1	A	202	ARG
1	A	204	ILE
1	A	205	VAL
1	A	227	ASN

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Mol	Chain	Res	Type
1	A	233	GLN
1	A	243	ASP
1	A	249	VAL
1	A	255	LEU
1	A	259	SER
1	A	269	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	15	ASN
1	A	26	ASN
1	A	63	ASN
1	A	108	HIS
1	A	120	ASN
1	A	159	GLN
1	A	174	GLN
1	A	176	GLN
1	A	181	ASN
1	A	186	ASN
1	A	200	ASN
1	A	246	ASN
1	A	257	HIS

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	$\# Z > 2$
2	DEP	A	270	1	4,7,7	4.74	1 (25%)	2,7,7	5.68	1 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DEP	A	270	1	-	0/2/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	270	DEP	O2-C3	-9.42	1.17	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	270	DEP	O2-C3-C4	7.99	166.03	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	270	DEP	0	4

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.