Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 05:44 PM EDT

PDB ID	:	4TGL
Title	:	CATALYSIS AT THE INTERFACE: THE ANATOMY OF A CONFORMATIONAL CHANGE IN A TRIGLYCERIDE LIPASE
Authors	:	Derewenda, U.; Brzozowski, A.M.; Lawson, D.; Derewenda, Z.S.
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 (i) 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 (i)) were used in the production of this report:

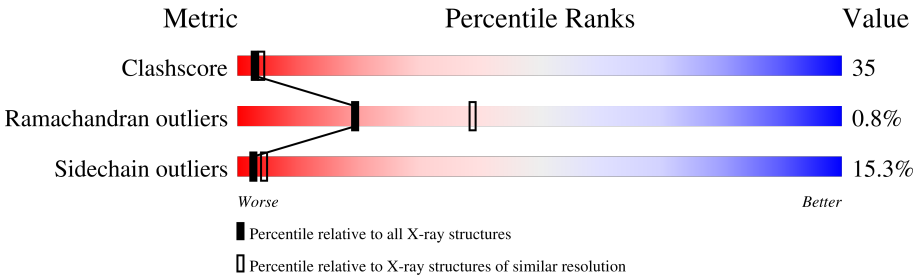
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	269	24% 45% 25% 5% •

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.

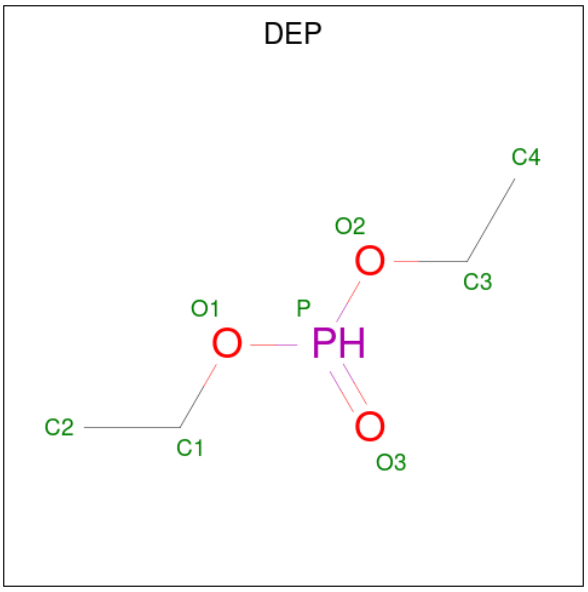
- Molecule 1 is a protein called TRIACYL-GLYCEROL ACYLHYDROLASE.

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 (three-letter code: 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
			Total	O		
3	A	238	238	238	0	0

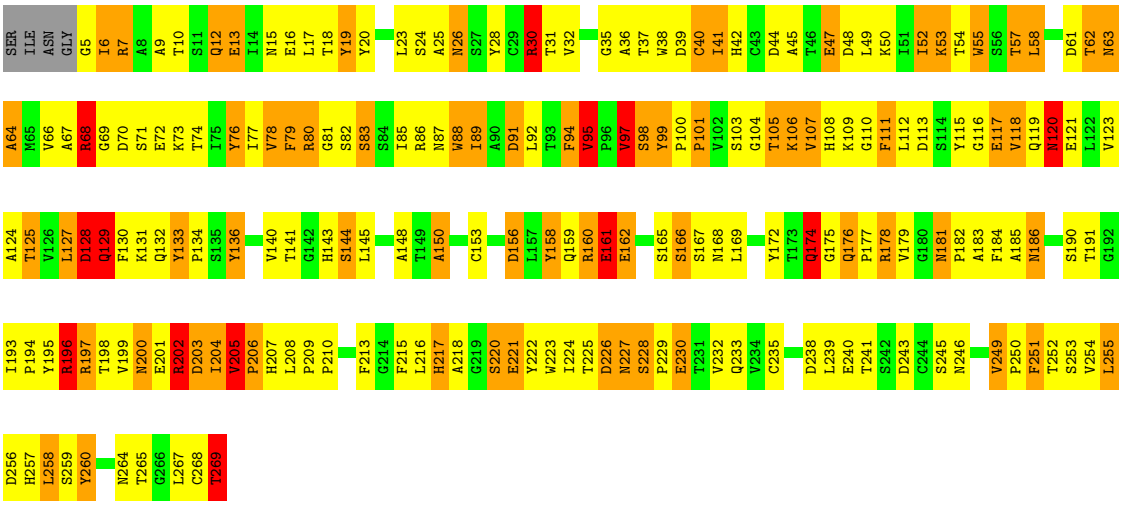
3 Residue-property plots (i)

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: 24% 45% 25% 5%



4 Data and refinement statistics (i)

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	1.34	7/2149 (0.3%)	2.98	222/2934 (7.6%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86[A]	ARG	CB-CG	-13.53	1.16	1.52
1	A	86[B]	ARG	CB-CG	-13.53	1.16	1.52
1	A	30[A]	ARG	CB-CG	-13.49	1.16	1.52
1	A	30[B]	ARG	CB-CG	-13.49	1.16	1.52
1	A	30[C]	ARG	CB-CG	-13.49	1.16	1.52
1	A	80[A]	ARG	CB-CG	-7.96	1.31	1.52
1	A	80[B]	ARG	CB-CG	-7.96	1.31	1.52

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	160	ARG	NE-CZ-NH1	32.34	136.47	120.30
1	A	202	ARG	CD-NE-CZ	23.89	157.04	123.60
1	A	68	ARG	NE-CZ-NH1	22.31	131.46	120.30
1	A	61	ASP	CB-CG-OD2	20.38	136.65	118.30
1	A	61	ASP	CB-CG-OD1	-17.54	102.52	118.30
1	A	128	ASP	CB-CG-OD1	-15.60	104.26	118.30
1	A	128	ASP	CB-CG-OD2	14.22	131.10	118.30
1	A	28	TYR	CB-CG-CD1	14.01	129.41	121.00
1	A	160	ARG	CD-NE-CZ	13.02	141.82	123.60
1	A	19	TYR	CB-CG-CD1	12.84	128.70	121.00
1	A	7	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	A	28	TYR	CB-CG-CD2	-10.97	114.42	121.00
1	A	115	TYR	CB-CG-CD2	10.77	127.46	121.00
1	A	160	ARG	NE-CZ-NH2	-10.67	114.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	239	LEU	CB-CG-CD2	-10.64	92.91	111.00
1	A	30[A]	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	A	30[B]	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	A	30[C]	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	A	99	TYR	CB-CG-CD2	10.37	127.22	121.00
1	A	42	HIS	CA-CB-CG	10.29	131.10	113.60
1	A	115	TYR	CB-CG-CD1	-10.21	114.87	121.00
1	A	74	THR	O-C-N	9.94	138.60	122.70
1	A	160	ARG	NH1-CZ-NH2	-9.88	108.53	119.40
1	A	178	ARG	NE-CZ-NH2	9.82	125.21	120.30
1	A	269	THR	CA-C-O	-9.59	99.96	120.10
1	A	124	ALA	O-C-N	-9.53	107.45	122.70
1	A	19	TYR	CB-CG-CD2	-9.52	115.29	121.00
1	A	238	ASP	CB-CG-OD1	-9.52	109.73	118.30
1	A	172	TYR	CB-CG-CD1	-9.50	115.30	121.00
1	A	63	ASN	CB-CG-OD1	9.48	140.57	121.60
1	A	80[A]	ARG	CA-CB-CG	8.88	132.93	113.40
1	A	80[B]	ARG	CA-CB-CG	8.88	132.93	113.40
1	A	196	ARG	CD-NE-CZ	-8.76	111.34	123.60
1	A	125	THR	CA-CB-CG2	8.72	124.61	112.40
1	A	86[A]	ARG	CA-CB-CG	8.66	132.46	113.40
1	A	86[B]	ARG	CA-CB-CG	8.66	132.46	113.40
1	A	121	GLU	CB-CA-C	-8.52	93.37	110.40
1	A	113	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	A	120	ASN	CB-CG-OD1	-8.28	105.04	121.60
1	A	220	SER	CA-CB-OG	8.21	133.37	111.20
1	A	121	GLU	CG-CD-OE2	-8.20	101.90	118.30
1	A	258	LEU	CB-CG-CD1	-8.14	97.16	111.00
1	A	30[A]	ARG	NH1-CZ-NH2	-8.13	110.45	119.40
1	A	30[B]	ARG	NH1-CZ-NH2	-8.13	110.45	119.40
1	A	30[C]	ARG	NH1-CZ-NH2	-8.13	110.45	119.40
1	A	104	GLY	CA-C-O	-8.12	105.99	120.60
1	A	158	TYR	CB-CG-CD2	7.97	125.78	121.00
1	A	83	SER	O-C-N	7.96	135.44	122.70
1	A	7	ARG	CD-NE-CZ	-7.95	112.47	123.60
1	A	221	GLU	CG-CD-OE2	-7.89	102.51	118.30
1	A	225	THR	CA-CB-OG1	-7.85	92.51	109.00
1	A	136	TYR	CB-CG-CD2	7.75	125.65	121.00
1	A	20	TYR	CB-CG-CD2	7.74	125.64	121.00
1	A	205	VAL	CA-CB-CG1	-7.70	99.35	110.90
1	A	251	PHE	CB-CG-CD1	-7.66	115.44	120.80
1	A	268	CYS	N-CA-CB	7.66	124.39	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ARG	O-C-N	7.65	136.21	123.20
1	A	148	ALA	O-C-N	7.60	134.86	122.70
1	A	158	TYR	CB-CG-CD1	-7.55	116.47	121.00
1	A	172	TYR	CG-CD2-CE2	-7.48	115.32	121.30
1	A	86[A]	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	A	86[B]	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	A	80[A]	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	80[B]	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	30[A]	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	A	30[B]	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	A	30[C]	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	A	68	ARG	CA-C-O	-7.31	104.75	120.10
1	A	113	ASP	N-CA-CB	-7.27	97.51	110.60
1	A	63	ASN	CB-CG-ND2	-7.24	99.32	116.70
1	A	55	TRP	CD1-NE1-CE2	7.24	115.52	109.00
1	A	116	GLY	O-C-N	-7.21	111.17	122.70
1	A	13	GLU	O-C-N	7.13	134.11	122.70
1	A	165	SER	N-CA-C	-7.13	91.75	111.00
1	A	68	ARG	NH1-CZ-NH2	-7.09	111.60	119.40
1	A	7	ARG	NH1-CZ-NH2	7.04	127.14	119.40
1	A	16	GLU	N-CA-CB	-7.00	98.00	110.60
1	A	16	GLU	OE1-CD-OE2	7.00	131.69	123.30
1	A	127	LEU	CB-CG-CD2	-6.98	99.13	111.00
1	A	186	ASN	CA-CB-CG	-6.96	98.09	113.40
1	A	99	TYR	CG-CD2-CE2	6.95	126.86	121.30
1	A	68	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	186	ASN	OD1-CG-ND2	6.84	137.62	121.90
1	A	26	ASN	O-C-N	6.83	133.62	122.70
1	A	74	THR	CA-CB-CG2	6.80	121.92	112.40
1	A	30[A]	ARG	CB-CG-CD	-6.75	94.06	111.60
1	A	30[B]	ARG	CB-CG-CD	-6.75	94.06	111.60
1	A	30[C]	ARG	CB-CG-CD	-6.75	94.06	111.60
1	A	172	TYR	CD1-CE1-CZ	-6.75	113.73	119.80
1	A	228	SER	N-CA-CB	6.73	120.60	110.50
1	A	156	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	104	GLY	O-C-N	6.71	133.44	122.70
1	A	143	HIS	CB-CA-C	-6.71	96.99	110.40
1	A	162	GLU	CG-CD-OE2	-6.63	105.04	118.30
1	A	268	CYS	O-C-N	6.62	133.28	122.70
1	A	238	ASP	OD1-CG-OD2	6.59	135.82	123.30
1	A	113	ASP	CB-CG-OD1	6.57	124.21	118.30
1	A	80[A]	ARG	CB-CG-CD	6.56	128.66	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80[B]	ARG	CB-CG-CD	6.56	128.66	111.60
1	A	53	LYS	O-C-N	6.53	133.15	122.70
1	A	202	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	A	145	LEU	CA-CB-CG	6.44	130.11	115.30
1	A	174	GLN	CB-CG-CD	6.41	128.26	111.60
1	A	101	PRO	CA-C-N	6.38	131.23	117.20
1	A	179	VAL	CG1-CB-CG2	-6.34	100.75	110.90
1	A	103	SER	CA-C-O	6.33	133.40	120.10
1	A	118	VAL	CA-CB-CG2	6.33	120.40	110.90
1	A	82	SER	CA-C-O	6.30	133.34	120.10
1	A	88	TRP	CB-CA-C	6.29	122.99	110.40
1	A	165	SER	O-C-N	6.28	132.75	122.70
1	A	133	TYR	CG-CD1-CE1	-6.27	116.28	121.30
1	A	41	ILE	CA-CB-CG1	-6.24	99.14	111.00
1	A	120	ASN	CA-CB-CG	-6.22	99.71	113.40
1	A	78	VAL	O-C-N	6.20	132.62	122.70
1	A	47	GLU	OE1-CD-OE2	-6.18	115.88	123.30
1	A	206	PRO	O-C-N	6.18	132.59	122.70
1	A	70	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	183	ALA	CB-CA-C	-6.11	100.94	110.10
1	A	89	ILE	CA-CB-CG2	6.09	123.09	110.90
1	A	55	TRP	CG-CD1-NE1	-6.08	104.02	110.10
1	A	196	ARG	C-N-CA	6.08	136.90	121.70
1	A	39	ASP	CB-CA-C	6.07	122.55	110.40
1	A	128	ASP	CB-CA-C	6.07	122.53	110.40
1	A	132	GLN	C-N-CA	6.06	136.85	121.70
1	A	196	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	130	PHE	CB-CA-C	-5.99	98.42	110.40
1	A	68	ARG	CB-CA-C	-5.97	98.46	110.40
1	A	120	ASN	N-CA-CB	-5.92	99.93	110.60
1	A	41	ILE	CA-CB-CG2	5.89	122.69	110.90
1	A	228	SER	O-C-N	5.88	132.28	121.10
1	A	20	TYR	CB-CG-CD1	-5.86	117.48	121.00
1	A	95	VAL	N-CA-CB	-5.86	98.60	111.50
1	A	45	ALA	CB-CA-C	-5.83	101.36	110.10
1	A	195	TYR	N-CA-CB	-5.79	100.17	110.60
1	A	66	VAL	O-C-N	5.78	131.95	122.70
1	A	235	CYS	CA-CB-SG	5.76	124.37	114.00
1	A	97	VAL	N-CA-CB	-5.75	98.84	111.50
1	A	23	LEU	CB-CG-CD1	-5.75	101.22	111.00
1	A	80[A]	ARG	NH1-CZ-NH2	-5.74	113.08	119.40
1	A	80[B]	ARG	NH1-CZ-NH2	-5.74	113.08	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	VAL	CA-CB-CG2	-5.71	102.33	110.90
1	A	195	TYR	CA-CB-CG	5.70	124.24	113.40
1	A	52	ILE	CA-CB-CG2	-5.68	99.53	110.90
1	A	197	ARG	N-CA-CB	5.68	120.82	110.60
1	A	230	GLU	CB-CA-C	-5.67	99.05	110.40
1	A	200	ASN	CB-CG-OD1	-5.67	110.26	121.60
1	A	166	SER	CB-CA-C	-5.67	99.33	110.10
1	A	6	ILE	O-C-N	5.66	131.76	122.70
1	A	218	ALA	CB-CA-C	5.66	118.59	110.10
1	A	217	HIS	CB-CA-C	-5.66	99.09	110.40
1	A	74	THR	OG1-CB-CG2	-5.64	97.03	110.00
1	A	240	GLU	O-C-N	5.63	131.71	122.70
1	A	58	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	A	57	THR	OG1-CB-CG2	5.62	122.92	110.00
1	A	150	ALA	CB-CA-C	5.62	118.52	110.10
1	A	118	VAL	C-N-CA	5.61	135.72	121.70
1	A	94	PHE	CB-CA-C	-5.58	99.23	110.40
1	A	235	CYS	N-CA-C	-5.58	95.92	111.00
1	A	226	ASP	N-CA-CB	5.58	120.64	110.60
1	A	77	ILE	CB-CG1-CD1	-5.57	98.30	113.90
1	A	161	GLU	CG-CD-OE1	-5.54	107.23	118.30
1	A	195	TYR	C-N-CA	5.53	135.52	121.70
1	A	92	LEU	CB-CG-CD1	5.51	120.37	111.00
1	A	47	GLU	CA-CB-CG	5.51	125.52	113.40
1	A	64	ALA	CB-CA-C	5.49	118.34	110.10
1	A	91	ASP	O-C-N	5.47	131.45	122.70
1	A	218	ALA	N-CA-CB	5.47	117.76	110.10
1	A	40	CYS	CA-C-O	5.46	131.58	120.10
1	A	144	SER	CA-C-N	5.46	129.22	117.20
1	A	197	ARG	CB-CA-C	-5.46	99.48	110.40
1	A	241	THR	N-CA-CB	5.45	120.65	110.30
1	A	129	GLN	CG-CD-NE2	5.44	129.76	116.70
1	A	61	ASP	CA-CB-CG	-5.44	101.44	113.40
1	A	239	LEU	CA-CB-CG	5.42	127.78	115.30
1	A	178	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	A	249	VAL	CB-CA-C	5.41	121.68	111.40
1	A	15	ASN	CA-CB-CG	-5.40	101.51	113.40
1	A	269	THR	CA-CB-CG2	5.40	119.96	112.40
1	A	31	THR	CA-C-O	-5.38	108.80	120.10
1	A	221	GLU	OE1-CD-OE2	5.37	129.75	123.30
1	A	215	PHE	N-CA-CB	5.37	120.27	110.60
1	A	240	GLU	CB-CA-C	-5.36	99.68	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	131	LYS	CB-CG-CD	5.36	125.53	111.60
1	A	116	GLY	CA-C-N	5.35	128.97	117.20
1	A	19	TYR	CA-CB-CG	-5.34	103.25	113.40
1	A	162	GLU	OE1-CD-OE2	5.34	129.71	123.30
1	A	196	ARG	CA-CB-CG	5.34	125.15	113.40
1	A	39	ASP	CA-C-O	5.34	131.31	120.10
1	A	30[A]	ARG	CG-CD-NE	5.33	123.00	111.80
1	A	30[B]	ARG	CG-CD-NE	5.33	123.00	111.80
1	A	30[C]	ARG	CG-CD-NE	5.33	123.00	111.80
1	A	42	HIS	N-CA-CB	-5.32	101.02	110.60
1	A	141	THR	CA-CB-OG1	-5.31	97.85	109.00
1	A	58	LEU	C-N-CA	-5.31	108.43	121.70
1	A	121	GLU	CG-CD-OE1	5.28	128.86	118.30
1	A	80[A]	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	80[B]	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	54	THR	CA-CB-CG2	5.24	119.73	112.40
1	A	94	PHE	C-N-CA	-5.24	108.61	121.70
1	A	178	ARG	CA-C-N	5.23	128.71	117.20
1	A	79	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	A	199	VAL	CG1-CB-CG2	5.16	119.15	110.90
1	A	111	PHE	CB-CG-CD1	5.13	124.39	120.80
1	A	120	ASN	CB-CG-ND2	5.13	129.01	116.70
1	A	105	THR	N-CA-CB	5.12	120.04	110.30
1	A	18	THR	CA-C-O	5.12	130.86	120.10
1	A	239	LEU	N-CA-CB	5.10	120.59	110.40
1	A	79	PHE	CD1-CE1-CZ	-5.09	113.99	120.10
1	A	186	ASN	CB-CG-OD1	-5.09	111.42	121.60
1	A	179	VAL	CA-CB-CG2	5.08	118.52	110.90
1	A	76	TYR	CZ-CE2-CD2	-5.08	115.23	119.80
1	A	115	TYR	N-CA-CB	5.06	119.71	110.60
1	A	166	SER	N-CA-CB	-5.06	102.92	110.50
1	A	74	THR	CA-C-N	-5.05	106.08	117.20
1	A	62	THR	O-C-N	-5.05	114.62	122.70
1	A	268	CYS	CA-CB-SG	-5.04	104.93	114.00
1	A	95	VAL	CG1-CB-CG2	5.04	118.96	110.90
1	A	260	TYR	N-CA-CB	-5.02	101.56	110.60
1	A	107	VAL	CG1-CB-CG2	5.01	118.92	110.90
1	A	55	TRP	CD1-CG-CD2	5.01	110.31	106.30
1	A	168	ASN	O-C-N	5.01	130.72	122.70
1	A	67	ALA	CB-CA-C	-5.01	102.58	110.10

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	2078	0	2015	145	93
2	A	8	0	10	0	4
3	A	238	0	0	19	14
All	All	2324	0	2025	145	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 35.

All (145) 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:30[A]:ARG:NH1	3:A:346:HOH:O	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:VAL:HG21	1:A:257:HIS:CE1	2.27	0.69
1:A:181:ASN:H	1:A:181:ASN:ND2	1.91	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:181:ASN:N	1:A:181:ASN:ND2	2.47	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: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
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:184:PHE:O	1:A:185:ALA:C	2.40	0.57
1:A:144:SER:HB2	1:A:257:HIS:CE1	2.40	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: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: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:62:THR:HG21	1:A:118:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:THR:C	1:A:63:ASN:HD22	2.12	0.52
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:94:PHE:O	1:A:95:VAL:C	2.43	0.51
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: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
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:5:GLY:C	1:A:6:ILE:HD12	2.32	0.49
1:A:106:LYS:H	1:A:181:ASN:ND2	2.04	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:LYS:O	1:A:110:GLY:C	2.53	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:160:ARG:O	1:A:161:GLU:C	2.56	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: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:97:VAL:O	1:A:106:LYS:HG3	2.18	0.43
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:19:TYR:CD1	1:A:19:TYR:C	2.94	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: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:174:GLN:O	1:A:175:GLY:C	2.59	0.41
1:A:38:TRP:CG	1:A:47:GLU:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	22 43

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%)	196 (84%)	37 (16%)	2 4

All (37) 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	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	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

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Mol	Chain	Res	Type
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
1	A	233	GLN
1	A	243	ASP
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
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

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)

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	5.70	1 (25%)	2,7,7	5.21	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	-11.35	1.17	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	270	DEP	O2-C3-C4	7.32	166.03	110.88

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.