



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:59 PM UTC

PDB ID : 2Z71 / pdb_00002z71
Title : Structure of truncated mutant CYS1GLY of penicillin V acylase from bacillus
sphaericus co-crystallized with penicillin V
Authors : Pathak, M.C.; Brannigan, J.; Dodson, G.G.; Suresh, C.G.
Deposited on : 2007-08-10
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

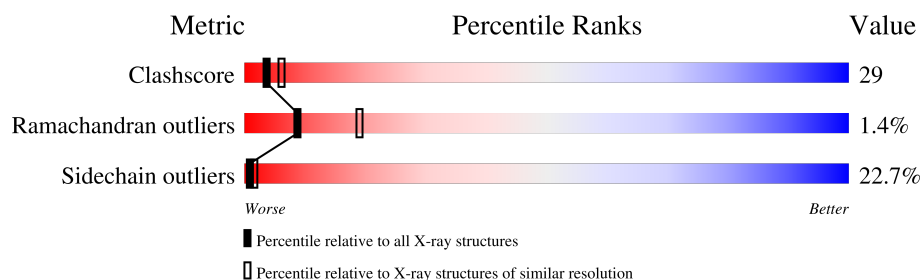
1 Overall quality at a glance

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	335	
1	C	335	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5260 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.

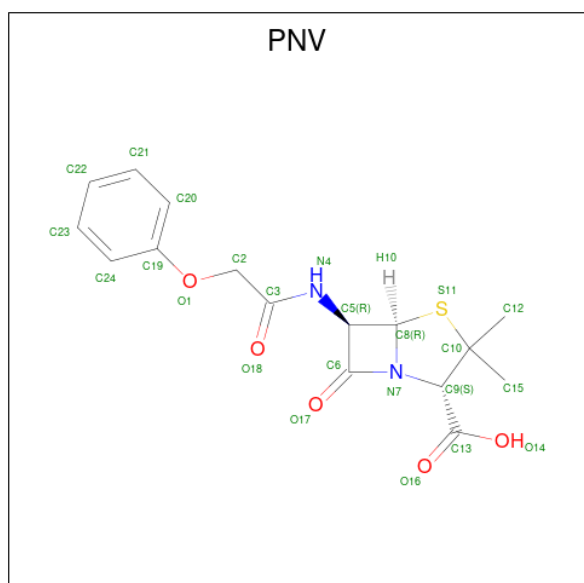
- Molecule 1 is a protein called Penicillin acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2577	1640	423	502	12			
1	C	331	Total	C	N	O	S	0	0	0
			2584	1645	424	503	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	CYS	engineered mutation	UNP P12256
A	98	ARG	THR	conflict	UNP P12256
C	1	GLY	CYS	engineered mutation	UNP P12256
C	98	ARG	THR	conflict	UNP P12256

- Molecule 2 is (2S,5R,6R)-3,3-DIMETHYL-7-OXO-6-(2-PHENOXYACETAMIDO)-4-THIA-1-AZABICYCLO(3.2.0)HEPTANE-2-CARBOXYLIC ACID (CCD ID: PNV) (formula: C₁₆H₁₈N₂O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	16	2	5	1		
2	C	1	Total	C	N	O	S	0	0
			24	16	2	5	1		

- Molecule 3 is water.

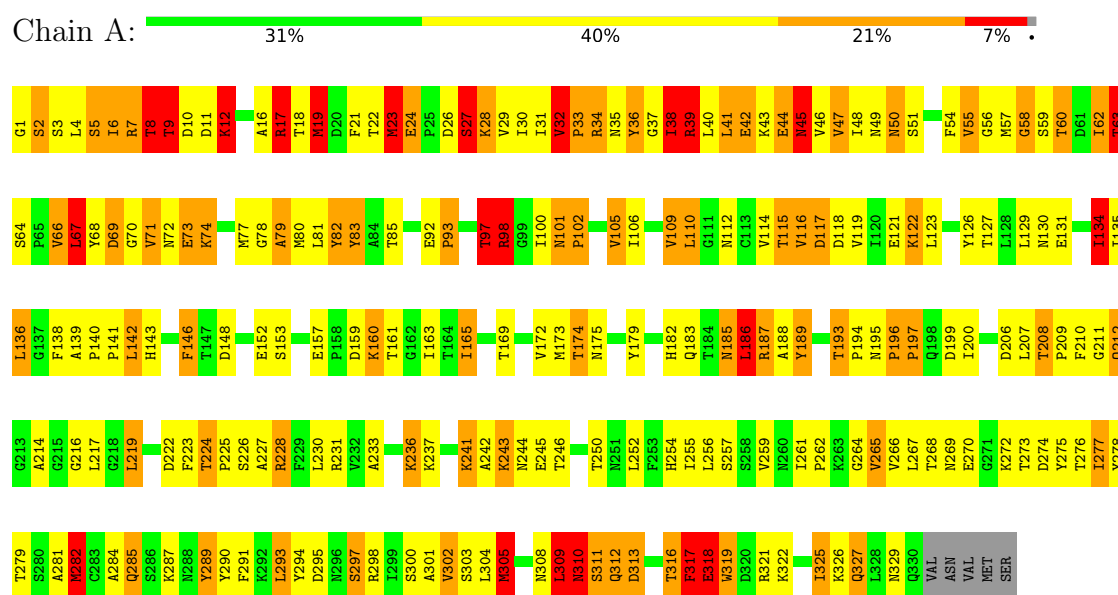
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	C	33	Total	O	0	0
			33	33		

3 Residue-property plots

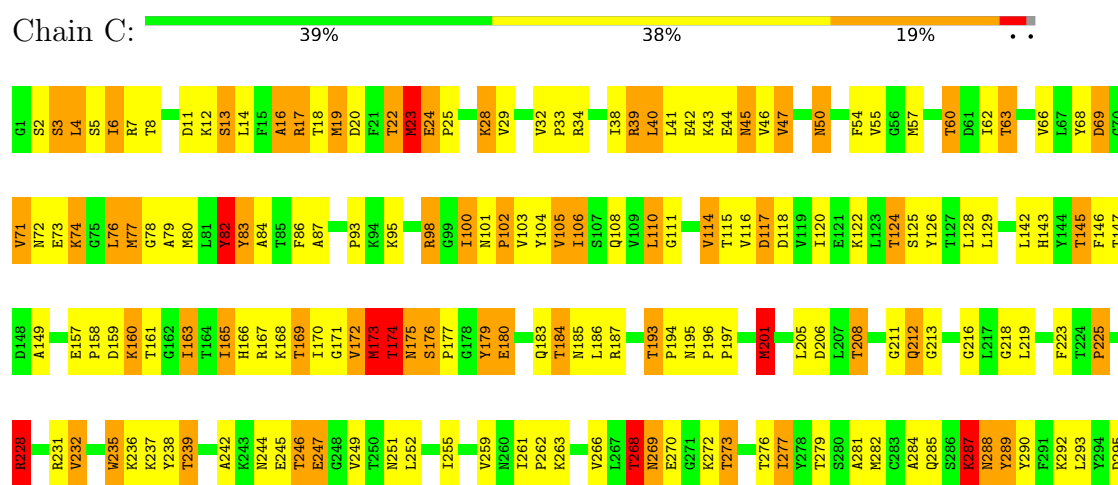
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Penicillin acylase



• Molecule 1: Penicillin acylase



K306	S297	S300	A301	V302	S303	L304	K305	A306	E307	N308	L309	N310	S311	Q312	D313	L314	T315	T316	F317	E318	W319	D320	R321	K322	K326	Q327	L328	V331	ASN	VAL	MET	SER
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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	129.73Å 158.89Å 90.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	89.7 (20.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.239 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5260	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	2.54	148/2632 (5.6%)	1.09	12/3577 (0.3%)
1	C	2.49	137/2639 (5.2%)	0.87	2/3587 (0.1%)
All	All	2.52	285/5271 (5.4%)	0.98	14/7164 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8

All (285) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	THR	CA-C	-25.75	1.40	1.52
1	A	284	ALA	CA-CB	-14.69	1.29	1.53
1	C	6	ILE	C-O	12.88	1.37	1.23
1	C	186	LEU	C-O	-12.33	1.09	1.24
1	C	69	ASP	CA-C	-11.55	1.38	1.52
1	C	173	MET	CA-C	-10.99	1.39	1.52
1	C	103	VAL	CA-CB	10.89	1.67	1.54
1	A	298	ARG	CA-C	-10.79	1.39	1.52
1	C	289	TYR	CA-C	-10.47	1.40	1.52
1	A	326	LYS	CA-C	-10.16	1.39	1.52
1	C	79	ALA	CA-CB	-10.11	1.35	1.53
1	A	325	ILE	CA-CB	-9.95	1.42	1.54
1	C	255	ILE	C-O	-9.74	1.12	1.24
1	C	305	MET	SD-CE	9.74	2.03	1.79
1	A	208	THR	CA-CB	9.64	1.66	1.54
1	C	195	ASN	CA-C	9.58	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	TYR	CA-C	-9.56	1.41	1.52
1	C	276	THR	CA-C	-9.39	1.40	1.52
1	A	55	VAL	CA-CB	-9.18	1.44	1.55
1	A	172	VAL	CA-C	-9.16	1.41	1.52
1	A	55	VAL	C-O	9.14	1.34	1.23
1	C	196	PRO	C-O	-9.11	1.14	1.24
1	C	289	TYR	C-N	9.08	1.46	1.33
1	A	58	GLY	C-O	8.94	1.32	1.23
1	C	76	LEU	C-O	8.89	1.34	1.24
1	C	20	ASP	C-O	-8.60	1.13	1.24
1	A	119	VAL	CA-CB	-8.48	1.42	1.54
1	A	216	GLY	C-O	-8.47	1.13	1.24
1	A	32	VAL	CA-C	8.46	1.59	1.53
1	A	302	VAL	CA-CB	8.45	1.65	1.54
1	C	165	ILE	C-O	-8.43	1.15	1.24
1	C	179	TYR	CA-C	8.41	1.64	1.52
1	C	193	THR	CA-C	-8.30	1.42	1.52
1	C	219	LEU	C-O	-8.29	1.12	1.24
1	C	228	ARG	CD-NE	8.28	1.57	1.46
1	A	33	PRO	CA-C	-8.18	1.43	1.53
1	C	147	THR	CA-CB	-8.15	1.39	1.53
1	A	293	LEU	C-O	8.13	1.34	1.23
1	A	261	ILE	CA-CB	-8.08	1.45	1.53
1	A	105	VAL	CA-CB	-8.07	1.45	1.54
1	C	320	ASP	CA-C	8.02	1.62	1.53
1	C	282	MET	CG-SD	8.00	2.00	1.80
1	A	117	ASP	CA-C	-7.96	1.42	1.52
1	A	233	ALA	CA-CB	-7.95	1.40	1.53
1	A	261	ILE	N-CA	7.94	1.52	1.46
1	A	67	LEU	CA-C	-7.93	1.43	1.52
1	A	139	ALA	CA-CB	7.92	1.66	1.52
1	A	66	VAL	CA-C	-7.86	1.43	1.52
1	A	17	ARG	CA-CB	-7.84	1.40	1.53
1	A	12	LYS	CA-C	7.78	1.61	1.52
1	A	19	MET	N-CA	7.77	1.55	1.46
1	A	185	ASN	N-CA	7.67	1.55	1.46
1	A	8	THR	CA-CB	-7.57	1.41	1.53
1	C	287	LYS	CA-C	-7.57	1.43	1.53
1	C	142	LEU	CA-C	-7.54	1.43	1.52
1	A	189	TYR	N-CA	-7.53	1.38	1.46
1	A	6	ILE	C-O	7.52	1.32	1.23
1	A	268	THR	N-CA	7.50	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	THR	N-CA	-7.46	1.41	1.46
1	A	172	VAL	CA-CB	-7.43	1.46	1.55
1	C	321	ARG	CA-C	-7.43	1.40	1.52
1	C	8	THR	CA-CB	-7.41	1.42	1.53
1	A	62	ILE	C-O	7.41	1.32	1.24
1	A	39	ARG	NE-CZ	7.38	1.41	1.33
1	C	23	MET	CA-C	-7.36	1.43	1.52
1	A	276	THR	CA-C	-7.35	1.43	1.52
1	A	19	MET	CA-C	-7.25	1.44	1.52
1	C	266	VAL	C-O	-7.24	1.16	1.24
1	C	165	ILE	CA-C	-7.22	1.43	1.52
1	A	146	PHE	N-CA	7.21	1.54	1.45
1	C	175	ASN	C-O	-7.20	1.15	1.24
1	A	193	THR	N-CA	7.16	1.56	1.46
1	A	322	LYS	CA-C	7.15	1.61	1.52
1	A	282	MET	C-O	7.13	1.32	1.23
1	A	186	LEU	CA-C	7.12	1.62	1.52
1	C	216	GLY	C-O	-7.09	1.15	1.23
1	C	38	ILE	CA-CB	7.09	1.63	1.54
1	A	196	PRO	CA-C	-7.08	1.45	1.52
1	A	5	SER	C-O	7.06	1.32	1.23
1	C	237	LYS	CA-C	-7.00	1.44	1.52
1	C	160	LYS	CG-CD	7.00	1.73	1.52
1	A	79	ALA	C-O	6.98	1.32	1.23
1	C	145	THR	CA-CB	-6.92	1.37	1.53
1	C	87	ALA	CA-CB	-6.91	1.42	1.53
1	C	247	GLU	CD-OE1	6.86	1.38	1.25
1	C	166	HIS	CA-C	-6.81	1.44	1.52
1	C	46	VAL	CA-CB	-6.78	1.43	1.53
1	C	292	LYS	CB-CG	-6.75	1.32	1.52
1	A	217	LEU	CA-C	-6.73	1.43	1.52
1	C	316	THR	CA-C	-6.68	1.44	1.52
1	C	60	THR	N-CA	-6.66	1.39	1.46
1	A	188	ALA	CA-CB	-6.62	1.41	1.53
1	A	130	ASN	CA-C	-6.62	1.46	1.53
1	A	16	ALA	N-CA	6.61	1.54	1.45
1	A	206	ASP	CA-C	-6.58	1.44	1.52
1	C	201	MET	SD-CE	6.55	1.96	1.79
1	A	259	VAL	N-CA	6.53	1.52	1.46
1	C	318	GLU	CD-OE2	6.53	1.37	1.25
1	C	310	ASN	N-CA	6.53	1.53	1.46
1	C	17	ARG	CA-CB	-6.52	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	LYS	CA-C	6.47	1.61	1.52
1	C	218	GLY	C-O	-6.46	1.15	1.24
1	C	23	MET	SD-CE	6.44	1.95	1.79
1	A	38	ILE	C-O	6.43	1.31	1.24
1	C	71	VAL	C-O	-6.43	1.16	1.24
1	A	228	ARG	N-CA	-6.43	1.38	1.46
1	C	317	PHE	C-O	-6.41	1.16	1.24
1	A	301	ALA	CA-C	6.39	1.60	1.52
1	A	67	LEU	N-CA	6.38	1.53	1.46
1	C	288	ASN	N-CA	6.36	1.53	1.46
1	C	268	THR	C-O	-6.34	1.15	1.23
1	A	41	LEU	CA-C	-6.34	1.44	1.53
1	C	185	ASN	CG-OD1	-6.34	1.11	1.23
1	C	208	THR	CA-CB	6.34	1.63	1.54
1	A	119	VAL	N-CA	-6.30	1.38	1.46
1	C	13	SER	CA-CB	-6.29	1.44	1.53
1	A	193	THR	CA-C	-6.28	1.45	1.52
1	C	262	PRO	CA-C	6.28	1.60	1.52
1	C	63	THR	CA-C	6.28	1.61	1.52
1	C	18	THR	C-O	6.27	1.31	1.23
1	C	300	SER	CA-C	-6.20	1.45	1.52
1	C	82	TYR	CA-C	-6.20	1.44	1.53
1	C	225	PRO	C-N	-6.18	1.25	1.34
1	A	321	ARG	CA-C	-6.17	1.46	1.53
1	A	4	LEU	N-CA	6.16	1.53	1.46
1	A	297	SER	CA-C	-6.16	1.44	1.52
1	C	117	ASP	CA-C	-6.14	1.44	1.52
1	A	39	ARG	CD-NE	6.12	1.54	1.46
1	C	100	ILE	CA-CB	6.12	1.64	1.55
1	A	241	LYS	CA-C	-6.10	1.45	1.52
1	A	197	PRO	CA-C	-6.10	1.44	1.52
1	A	12	LYS	C-O	6.08	1.30	1.24
1	C	143	HIS	CA-C	-6.08	1.45	1.52
1	A	5	SER	N-CA	-6.07	1.38	1.45
1	C	232	VAL	CA-CB	-6.04	1.46	1.54
1	C	146	PHE	N-CA	6.03	1.53	1.45
1	C	193	THR	C-N	6.03	1.39	1.33
1	A	313	ASP	CA-C	6.01	1.60	1.52
1	C	111	GLY	CA-C	6.00	1.62	1.51
1	A	197	PRO	C-O	-5.97	1.17	1.23
1	A	285	GLN	N-CA	-5.95	1.38	1.46
1	A	243	LYS	CD-CE	5.95	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	VAL	CA-CB	5.95	1.61	1.54
1	A	49	ASN	CG-OD1	5.93	1.34	1.23
1	A	12	LYS	CE-NZ	5.91	1.67	1.49
1	C	19	MET	N-CA	5.91	1.53	1.46
1	C	142	LEU	N-CA	5.90	1.53	1.45
1	A	92	GLU	CA-C	5.89	1.58	1.52
1	C	225	PRO	C-O	-5.88	1.16	1.24
1	A	48	ILE	CA-CB	-5.87	1.48	1.54
1	A	210	PHE	N-CA	5.86	1.53	1.46
1	A	102	PRO	CA-CB	-5.86	1.45	1.53
1	C	163	ILE	CA-CB	-5.85	1.47	1.54
1	A	214	ALA	CA-CB	-5.84	1.43	1.53
1	A	195	ASN	CA-C	5.82	1.60	1.52
1	C	50	ASN	N-CA	5.82	1.53	1.46
1	A	276	THR	CA-CB	-5.81	1.45	1.53
1	A	7	ARG	CZ-NH1	5.81	1.40	1.32
1	C	261	ILE	N-CA	5.81	1.51	1.46
1	A	101	ASN	C-O	5.79	1.32	1.24
1	C	239	THR	N-CA	-5.77	1.38	1.46
1	A	105	VAL	C-O	5.77	1.30	1.24
1	C	32	VAL	CA-C	5.77	1.57	1.53
1	A	85	THR	CA-C	5.76	1.60	1.52
1	A	31	ILE	CA-C	-5.76	1.46	1.53
1	A	199	ASP	CA-C	5.76	1.60	1.52
1	C	186	LEU	N-CA	5.75	1.53	1.46
1	C	185	ASN	CB-CG	-5.74	1.37	1.52
1	A	211	GLY	C-N	-5.73	1.25	1.33
1	C	149	ALA	CA-C	5.73	1.60	1.52
1	C	16	ALA	CA-C	5.72	1.59	1.52
1	A	134	ILE	CG1-CD1	5.72	1.74	1.51
1	C	300	SER	N-CA	-5.72	1.39	1.46
1	A	146	PHE	C-O	5.69	1.30	1.23
1	A	118	ASP	C-O	5.69	1.31	1.24
1	A	35	ASN	CG-OD1	5.68	1.34	1.23
1	C	159	ASP	C-O	-5.68	1.16	1.23
1	C	187	ARG	N-CA	-5.68	1.39	1.46
1	C	19	MET	CA-C	-5.66	1.45	1.52
1	A	245	GLU	CD-OE2	5.64	1.36	1.25
1	C	295	ASP	CA-C	5.63	1.60	1.52
1	C	281	ALA	N-CA	5.63	1.53	1.45
1	A	295	ASP	N-CA	5.62	1.53	1.46
1	A	139	ALA	CA-C	-5.61	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	SER	CA-C	-5.61	1.45	1.52
1	A	193	THR	CA-CB	5.61	1.62	1.53
1	A	219	LEU	CG-CD1	-5.61	1.34	1.52
1	C	5	SER	CA-CB	-5.61	1.44	1.53
1	C	83	TYR	CA-CB	5.59	1.57	1.53
1	A	319	TRP	C-O	5.58	1.30	1.24
1	A	19	MET	SD-CE	5.57	1.93	1.79
1	A	211	GLY	N-CA	5.56	1.52	1.45
1	A	255	ILE	C-O	-5.56	1.17	1.24
1	A	270	GLU	CA-C	-5.56	1.45	1.52
1	A	246	THR	C-O	5.55	1.30	1.24
1	C	71	VAL	CA-CB	-5.55	1.47	1.54
1	C	102	PRO	C-O	5.55	1.31	1.24
1	C	8	THR	CA-C	5.54	1.60	1.53
1	C	77	MET	SD-CE	-5.54	1.65	1.79
1	A	82	TYR	CA-C	-5.54	1.45	1.52
1	C	180	GLU	CA-C	-5.52	1.45	1.52
1	C	11	ASP	CG-OD1	5.52	1.35	1.25
1	C	117	ASP	C-O	-5.50	1.17	1.24
1	C	235	TRP	C-O	-5.49	1.16	1.24
1	A	212	GLN	CA-C	5.47	1.60	1.52
1	C	3	SER	C-O	-5.46	1.16	1.23
1	C	223	PHE	CA-C	5.46	1.59	1.52
1	C	282	MET	C-O	5.45	1.30	1.23
1	A	294	TYR	CA-C	-5.44	1.46	1.52
1	C	98	ARG	C-O	5.44	1.30	1.24
1	C	232	VAL	N-CA	-5.43	1.39	1.46
1	C	158	PRO	CA-CB	-5.43	1.46	1.53
1	C	124	THR	CA-CB	5.43	1.61	1.54
1	C	39	ARG	CZ-NH1	5.42	1.40	1.32
1	C	106	ILE	CA-CB	-5.41	1.48	1.54
1	C	47	VAL	CA-C	5.41	1.59	1.52
1	A	275	TYR	C-O	-5.40	1.16	1.23
1	A	329	ASN	C-O	5.36	1.30	1.23
1	C	320	ASP	C-O	5.36	1.30	1.23
1	A	160	LYS	CA-C	5.35	1.59	1.52
1	C	29	VAL	CA-CB	-5.34	1.47	1.54
1	C	125	SER	C-O	5.33	1.31	1.24
1	A	308	ASN	N-CA	5.32	1.53	1.46
1	C	244	ASN	C-N	-5.32	1.27	1.33
1	C	102	PRO	CA-CB	-5.32	1.46	1.53
1	A	291	PHE	CA-C	-5.32	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	ASN	CA-C	-5.31	1.46	1.52
1	C	290	TYR	C-O	-5.31	1.17	1.23
1	A	38	ILE	CA-C	-5.31	1.46	1.52
1	A	16	ALA	CA-C	5.29	1.58	1.52
1	C	93	PRO	C-O	-5.28	1.17	1.23
1	C	82	TYR	C-O	-5.27	1.16	1.23
1	A	274	ASP	N-CA	5.26	1.53	1.46
1	C	169	THR	CA-C	5.24	1.59	1.52
1	A	254	HIS	C-O	-5.23	1.17	1.24
1	C	284	ALA	CA-CB	-5.23	1.44	1.53
1	A	257	SER	C-O	-5.23	1.18	1.24
1	C	309	LEU	CA-C	-5.22	1.45	1.52
1	C	225	PRO	CA-C	5.20	1.60	1.52
1	C	28	LYS	CA-C	-5.20	1.46	1.52
1	C	273	THR	C-O	-5.20	1.17	1.24
1	C	282	MET	N-CA	-5.20	1.39	1.45
1	A	74	LYS	CA-C	5.18	1.60	1.52
1	A	310	ASN	CA-C	5.18	1.59	1.52
1	A	321	ARG	CZ-NH2	5.18	1.40	1.33
1	C	307	GLU	CA-C	5.18	1.58	1.52
1	C	73	GLU	CA-CB	-5.17	1.44	1.53
1	C	246	THR	N-CA	-5.17	1.40	1.46
1	A	243	LYS	N-CA	5.17	1.53	1.46
1	A	112	ASN	CG-ND2	5.17	1.44	1.33
1	A	159	ASP	C-O	-5.16	1.17	1.23
1	C	208	THR	C-O	-5.16	1.18	1.24
1	C	231	ARG	C-O	-5.15	1.18	1.24
1	A	295	ASP	CB-CG	5.13	1.64	1.52
1	A	32	VAL	C-O	5.12	1.30	1.24
1	A	187	ARG	C-O	5.12	1.30	1.24
1	C	84	ALA	CA-CB	-5.12	1.44	1.53
1	A	327	GLN	CA-C	-5.12	1.46	1.52
1	A	37	GLY	C-O	5.12	1.30	1.23
1	A	210	PHE	CB-CG	-5.11	1.38	1.50
1	A	252	LEU	C-O	-5.11	1.17	1.24
1	A	310	ASN	N-CA	5.11	1.51	1.46
1	C	44	GLU	CA-C	-5.11	1.46	1.52
1	A	11	ASP	CA-C	5.10	1.59	1.53
1	A	282	MET	SD-CE	-5.10	1.66	1.79
1	A	36	TYR	CA-C	-5.09	1.46	1.52
1	A	165	ILE	C-O	-5.09	1.18	1.24
1	C	205	LEU	C-O	-5.08	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	TYR	C-O	-5.08	1.17	1.23
1	A	257	SER	CA-CB	-5.07	1.45	1.53
1	A	6	ILE	CA-CB	-5.07	1.47	1.54
1	A	9	THR	CA-C	5.07	1.59	1.52
1	C	197	PRO	C-O	-5.06	1.17	1.23
1	A	45	ASN	CA-CB	-5.05	1.45	1.53
1	C	213	GLY	CA-C	-5.04	1.45	1.51
1	A	51	SER	CB-OG	5.04	1.52	1.42
1	A	262	PRO	N-CA	5.04	1.53	1.47
1	A	321	ARG	CZ-NH1	5.02	1.39	1.32
1	C	6	ILE	N-CA	5.02	1.51	1.46
1	C	279	THR	CA-C	-5.02	1.46	1.52
1	A	246	THR	CA-CB	-5.01	1.45	1.53
1	C	195	ASN	CB-CG	5.01	1.64	1.52
1	C	76	LEU	CA-C	-5.01	1.46	1.52
1	A	317	PHE	N-CA	5.00	1.52	1.46
1	A	293	LEU	CA-C	-5.00	1.46	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	MET	CB-CA-C	16.12	137.55	110.79
1	A	97	THR	CA-C-N	-15.31	97.41	122.21
1	A	97	THR	C-N-CA	-15.31	97.41	122.21
1	A	309	LEU	CA-C-N	-8.16	108.52	122.14
1	A	309	LEU	C-N-CA	-8.16	108.52	122.14
1	C	124	THR	N-CA-C	-7.39	105.17	114.56
1	A	98	ARG	CD-NE-CZ	-7.23	114.27	124.40
1	A	310	ASN	O-C-N	-6.78	112.98	122.26
1	A	42	GLU	CA-C-N	-5.51	112.41	122.38
1	A	42	GLU	C-N-CA	-5.51	112.41	122.38
1	A	45	ASN	N-CA-C	5.49	120.25	113.50
1	C	187	ARG	N-CA-C	5.48	117.96	111.33
1	A	261	ILE	N-CA-C	5.43	112.92	107.55
1	A	305	MET	CB-CG-SD	5.25	128.46	112.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	ASN	Mainchain,Peptide
1	A	311	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	A	317	PHE	Peptide
1	A	44	GLU	Peptide
1	A	98	ARG	Sidechain,Mainchain,Peptide

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	2577	0	2553	191	0
1	C	2584	0	2562	115	0
2	A	24	0	17	4	0
2	C	24	0	16	8	0
3	A	18	0	0	1	0
3	C	33	0	0	1	0
All	All	5260	0	5148	302	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (302) 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:C:305:MET:SD	1:C:305:MET:CE	2.03	1.46
1:A:24:GLU:HG3	1:A:277:ILE:CD1	1.49	1.41
1:A:24:GLU:CG	1:A:277:ILE:HD12	1.63	1.26
1:C:174:THR:CG2	1:C:175:ASN:H	1.50	1.20
1:A:26:ASP:O	1:A:27:SER:HB2	1.36	1.16
1:A:22:THR:O	1:A:23:MET:HB3	1.34	1.12
1:C:174:THR:HG22	1:C:175:ASN:N	1.48	1.12
1:A:317:PHE:HA	1:A:318:GLU:HB2	1.19	1.10
1:A:24:GLU:HB2	1:A:277:ILE:HG21	1.37	1.05
1:A:23:MET:HE3	1:A:272:LYS:NZ	1.75	1.01
1:A:122:LYS:HD3	1:A:126:TYR:HE2	1.23	1.01
1:A:28:LYS:CD	1:A:30:ILE:HG12	1.93	0.99
1:A:9:THR:HG23	1:A:243:LYS:HA	1.41	0.98
1:C:4:LEU:N	1:C:4:LEU:HD12	1.79	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:HD2	1:A:30:ILE:CG1	1.95	0.97
1:A:24:GLU:CB	1:A:277:ILE:HG21	1.93	0.96
1:A:28:LYS:HD2	1:A:30:ILE:HG12	1.44	0.96
1:A:23:MET:HE3	1:A:272:LYS:HZ1	1.29	0.96
1:A:97:THR:HG21	1:A:127:THR:OG1	1.65	0.95
1:A:28:LYS:HZ2	1:A:30:ILE:HG12	1.30	0.94
1:A:9:THR:CG2	1:A:243:LYS:HA	1.98	0.94
1:A:310:ASN:H	1:A:311:SER:HB2	1.31	0.93
1:A:28:LYS:CD	1:A:30:ILE:CG1	2.46	0.93
1:A:24:GLU:CG	1:A:277:ILE:CD1	2.32	0.92
1:A:28:LYS:NZ	1:A:30:ILE:HG12	1.84	0.92
1:A:24:GLU:OE2	1:A:277:ILE:HB	1.69	0.92
1:A:228:ARG:HH12	2:A:903:PNV:H21	1.36	0.91
1:C:169:THR:HG22	1:C:171:GLY:H	1.35	0.91
1:A:8:THR:HG21	1:A:10:ASP:OD1	1.69	0.91
1:A:8:THR:HG22	1:A:10:ASP:H	1.35	0.90
1:A:24:GLU:HB2	1:A:277:ILE:HD13	1.52	0.89
1:C:106:ILE:HB	3:C:934:HOH:O	1.72	0.88
1:C:40:LEU:HD12	1:C:100:ILE:HD12	1.55	0.88
1:C:4:LEU:N	1:C:4:LEU:CD1	2.35	0.88
1:A:317:PHE:CA	1:A:318:GLU:HB2	2.04	0.86
1:C:180:GLU:O	1:C:184:THR:HG23	1.74	0.86
1:A:22:THR:O	1:A:23:MET:CB	2.20	0.86
1:A:115:THR:HG22	1:A:117:ASP:H	1.40	0.86
1:A:310:ASN:N	1:A:311:SER:HB2	1.90	0.85
1:A:26:ASP:O	1:A:27:SER:CB	2.24	0.84
1:C:22:THR:HG21	1:C:272:LYS:HD2	1.60	0.82
1:A:60:THR:CG2	1:A:60:THR:O	2.28	0.82
1:C:327:GLN:HG3	1:C:331:VAL:HB	1.62	0.82
1:A:223:PHE:O	1:A:228:ARG:HD3	1.80	0.82
1:A:38:ILE:HD11	1:A:50:ASN:HB3	1.60	0.81
1:C:327:GLN:CG	1:C:331:VAL:HB	2.10	0.80
1:A:312:GLN:HG2	1:A:313:ASP:N	1.98	0.79
1:A:46:VAL:HG11	1:A:98:ARG:CZ	2.14	0.77
1:A:105:VAL:O	1:A:109:VAL:HG12	1.83	0.77
1:A:24:GLU:CB	1:A:277:ILE:HD13	2.15	0.76
1:A:28:LYS:HD3	1:A:30:ILE:HG13	1.67	0.76
1:C:22:THR:HG21	1:C:272:LYS:CD	2.15	0.75
1:C:41:LEU:HD21	1:C:129:LEU:HD12	1.67	0.75
1:C:269:ASN:H	1:C:269:ASN:ND2	1.85	0.75
1:A:17:ARG:O	1:A:17:ARG:HG3	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLU:OE1	1:A:319:TRP:HH2	1.71	0.74
1:A:122:LYS:HD3	1:A:126:TYR:CE2	2.16	0.73
1:A:28:LYS:HE3	1:A:316:THR:OG1	1.88	0.73
1:A:46:VAL:HG11	1:A:98:ARG:NH1	2.03	0.73
1:A:222:ASP:OD1	1:A:224:THR:HB	1.89	0.72
1:C:174:THR:HG22	1:C:175:ASN:H	0.63	0.72
1:A:28:LYS:CD	1:A:30:ILE:HG13	2.19	0.71
1:C:82:TYR:CZ	2:C:904:PNV:H5	2.25	0.71
1:C:114:VAL:HG22	1:C:115:THR:HG23	1.73	0.71
1:C:288:ASN:ND2	1:C:303:SER:HA	2.05	0.71
1:C:4:LEU:HD23	1:C:236:LYS:HG3	1.72	0.70
1:A:60:THR:O	1:A:60:THR:HG22	1.90	0.70
1:C:45:ASN:N	1:C:45:ASN:HD22	1.88	0.70
1:A:225:PRO:HG3	2:A:903:PNV:H22	1.73	0.70
1:A:8:THR:CG2	1:A:10:ASP:OD1	2.40	0.70
1:C:228:ARG:HG2	1:C:228:ARG:HH11	1.57	0.70
1:A:28:LYS:CE	1:A:30:ILE:HG12	2.22	0.69
1:A:24:GLU:HG3	1:A:277:ILE:HD12	0.73	0.69
1:A:24:GLU:OE1	1:A:319:TRP:CH2	2.46	0.68
1:A:28:LYS:HE2	1:A:316:THR:HA	1.75	0.68
1:A:193:THR:HB	1:A:194:PRO:CD	2.24	0.68
1:A:39:ARG:HG2	1:A:41:LEU:O	1.94	0.68
1:A:8:THR:HG22	1:A:10:ASP:N	2.09	0.67
1:C:169:THR:HG22	1:C:171:GLY:N	2.09	0.67
1:C:288:ASN:HD22	1:C:303:SER:HA	1.59	0.67
1:A:93:PRO:HB3	1:A:97:THR:HG22	1.77	0.66
1:A:24:GLU:CG	1:A:277:ILE:HD13	2.26	0.66
1:A:266:VAL:C	1:A:267:LEU:HD23	2.20	0.66
1:A:138:PHE:CD1	1:A:138:PHE:C	2.73	0.66
1:A:62:ILE:C	1:A:63:THR:HG22	2.21	0.65
1:C:57:MET:HB2	1:C:289:TYR:OH	1.97	0.65
1:A:300:SER:HB3	1:C:328:LEU:HD11	1.76	0.65
1:A:28:LYS:CE	1:A:316:THR:HA	2.27	0.65
1:C:45:ASN:N	1:C:45:ASN:ND2	2.45	0.64
1:C:180:GLU:O	1:C:184:THR:CG2	2.44	0.64
1:A:310:ASN:N	1:A:311:SER:CB	2.59	0.64
1:A:71:VAL:HG22	1:A:282:MET:HB3	1.79	0.63
1:C:22:THR:O	1:C:22:THR:CG2	2.46	0.63
1:C:272:LYS:HD2	2:C:904:PNV:H153	1.80	0.63
1:A:224:THR:HG22	1:A:227:ALA:H	1.64	0.63
1:A:22:THR:O	1:A:22:THR:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:VAL:CG2	1:A:282:MET:HB3	2.29	0.62
1:A:42:GLU:HB2	1:A:131:GLU:OE2	1.97	0.62
1:A:8:THR:CG2	1:A:10:ASP:H	2.09	0.62
1:A:264:GLY:H	1:A:273:THR:CG2	2.13	0.62
1:A:305:MET:SD	1:A:309:LEU:HD21	2.41	0.61
1:A:169:THR:HB	1:A:179:TYR:CZ	2.35	0.61
1:A:19:MET:HE3	1:A:24:GLU:OE2	2.01	0.61
1:C:174:THR:CG2	1:C:175:ASN:N	2.23	0.61
1:A:69:ASP:HA	1:A:78:GLY:O	2.01	0.61
1:C:45:ASN:ND2	1:C:45:ASN:H	1.98	0.60
1:C:228:ARG:HH11	1:C:228:ARG:CG	2.14	0.60
1:C:268:THR:HG22	1:C:270:GLU:H	1.65	0.60
1:A:68:TYR:O	1:A:79:ALA:HA	2.02	0.60
1:C:62:ILE:HD11	1:C:66:VAL:CG2	2.31	0.60
1:A:72:ASN:OD1	1:A:72:ASN:C	2.44	0.59
1:A:62:ILE:O	1:A:63:THR:HG22	2.01	0.59
1:A:264:GLY:H	1:A:273:THR:HG23	1.68	0.59
1:C:272:LYS:CD	2:C:904:PNV:H153	2.32	0.59
1:C:71:VAL:HG13	1:C:71:VAL:O	2.03	0.58
1:C:106:ILE:O	1:C:110:LEU:HB2	2.04	0.58
1:A:2:SER:HB3	1:A:174:THR:HG22	1.85	0.58
1:A:21:PHE:HB3	1:A:277:ILE:HD11	1.86	0.58
1:A:8:THR:CG2	1:A:9:THR:N	2.67	0.58
1:C:4:LEU:O	1:C:4:LEU:HD13	2.03	0.57
1:A:312:GLN:CG	1:A:313:ASP:N	2.68	0.57
1:C:268:THR:CG2	1:C:269:ASN:N	2.67	0.57
1:A:317:PHE:HA	1:A:318:GLU:CB	2.12	0.57
1:C:86:PHE:CZ	1:C:177:PRO:HB3	2.40	0.57
1:A:169:THR:HB	1:A:179:TYR:OH	2.05	0.56
1:A:189:TYR:CE1	1:A:230:LEU:HD11	2.40	0.56
1:C:102:PRO:O	1:C:105:VAL:HG13	2.05	0.56
1:C:327:GLN:HG2	1:C:331:VAL:HB	1.86	0.56
1:A:115:THR:HG22	1:A:117:ASP:N	2.14	0.56
1:A:45:ASN:O	1:A:47:VAL:HG12	2.05	0.55
1:A:71:VAL:HG13	1:A:77:MET:HG3	1.88	0.55
1:C:145:THR:HB	1:C:173:MET:HE2	1.88	0.55
1:A:24:GLU:CB	1:A:277:ILE:CD1	2.79	0.55
1:A:34:ARG:HH21	1:A:309:LEU:HD23	1.72	0.55
1:A:10:ASP:OD1	1:A:12:LYS:HD3	2.07	0.55
1:C:308:ASN:O	1:C:311:SER:HB2	2.07	0.55
1:A:9:THR:HG22	1:A:242:ALA:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:THR:HG21	1:C:225:PRO:O	2.06	0.54
1:A:28:LYS:CE	1:A:316:THR:OG1	2.56	0.54
1:A:57:MET:HB2	1:A:289:TYR:OH	2.07	0.54
1:C:120:ILE:HG12	1:C:165:ILE:HG21	1.89	0.54
1:C:169:THR:HG23	1:C:179:TYR:CE1	2.43	0.54
1:A:193:THR:HB	1:A:194:PRO:HD2	1.91	0.53
1:C:268:THR:HG22	1:C:270:GLU:N	2.23	0.53
1:C:4:LEU:HD12	1:C:4:LEU:H	1.64	0.53
1:C:6:ILE:HG12	1:C:252:LEU:HD21	1.90	0.53
1:A:325:ILE:HG21	1:C:301:ALA:HB2	1.90	0.52
1:C:268:THR:HG23	1:C:269:ASN:N	2.24	0.52
1:C:72:ASN:HB3	1:C:110:LEU:O	2.10	0.52
1:A:23:MET:O	1:A:23:MET:SD	2.67	0.52
1:A:224:THR:CG2	1:A:226:SER:OG	2.58	0.52
1:A:38:ILE:CD1	1:A:50:ASN:HB3	2.36	0.52
1:C:232:VAL:O	1:C:236:LYS:HB2	2.09	0.52
1:A:228:ARG:HH12	2:A:903:PNV:C21	2.15	0.51
1:C:4:LEU:CD1	1:C:4:LEU:H	2.17	0.51
1:A:62:ILE:HG13	1:A:63:THR:H	1.75	0.51
1:A:200:ILE:HG13	1:A:207:LEU:HB2	1.93	0.51
1:A:62:ILE:C	1:A:63:THR:CG2	2.84	0.51
1:C:272:LYS:CE	2:C:904:PNV:H153	2.41	0.51
1:A:185:ASN:O	1:A:186:LEU:C	2.53	0.51
1:A:58:GLY:HA3	1:A:66:VAL:O	2.11	0.50
1:A:109:VAL:HG11	1:A:146:PHE:CZ	2.46	0.50
1:A:140:PRO:O	1:A:142:LEU:HD22	2.11	0.50
1:A:70:GLY:O	1:A:282:MET:HE3	2.11	0.50
1:A:302:VAL:HG11	1:A:317:PHE:CE1	2.47	0.50
1:C:22:THR:O	1:C:22:THR:HG23	2.11	0.50
1:A:68:TYR:HD1	1:A:80:MET:HE2	1.76	0.50
1:C:17:ARG:O	1:C:17:ARG:HD3	2.12	0.50
1:C:54:PHE:HB3	1:C:72:ASN:HA	1.92	0.50
1:C:201:MET:HG3	1:C:206:ASP:OD1	2.12	0.50
1:A:59:SER:OG	1:A:60:THR:N	2.45	0.49
1:A:60:THR:O	1:A:60:THR:HG23	2.09	0.49
1:C:270:GLU:OE1	2:C:904:PNV:H151	2.13	0.49
1:A:28:LYS:HE2	1:A:29:VAL:O	2.12	0.49
1:A:312:GLN:HE21	1:A:313:ASP:HB2	1.78	0.49
1:A:17:ARG:NH2	1:A:80:MET:O	2.45	0.49
1:A:208:THR:OG1	1:A:209:PRO:HD2	2.12	0.48
1:C:74:LYS:HD2	1:C:74:LYS:HA	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ARG:O	1:A:17:ARG:CG	2.58	0.48
1:C:42:GLU:OE1	1:C:63:THR:OG1	2.31	0.48
1:A:36:TYR:O	1:A:50:ASN:OD1	2.30	0.48
1:A:54:PHE:HA	1:A:72:ASN:HA	1.96	0.48
1:A:24:GLU:HB2	1:A:277:ILE:CG2	2.26	0.48
1:A:17:ARG:HH21	1:A:68:TYR:HB3	1.79	0.48
1:A:27:SER:HA	1:A:58:GLY:O	2.13	0.48
1:A:70:GLY:C	1:A:110:LEU:HD11	2.38	0.48
1:C:4:LEU:HD13	1:C:4:LEU:C	2.37	0.48
1:C:287:LYS:HD3	1:C:305:MET:HG2	1.96	0.48
1:C:268:THR:HG21	2:C:904:PNV:H151	1.96	0.48
1:A:312:GLN:NE2	1:A:313:ASP:H	2.12	0.47
1:C:3:SER:C	1:C:4:LEU:HD12	2.36	0.47
1:C:175:ASN:OD1	2:C:904:PNV:H21	2.14	0.47
1:C:24:GLU:HA	1:C:25:PRO:HD2	1.76	0.47
1:C:82:TYR:CE2	2:C:904:PNV:H5	2.49	0.47
1:C:268:THR:HG23	1:C:269:ASN:H	1.79	0.47
1:C:42:GLU:OE1	1:C:104:TYR:OH	2.27	0.47
1:C:16:ALA:HB2	1:C:252:LEU:HD13	1.97	0.47
1:A:266:VAL:O	1:A:267:LEU:HD23	2.15	0.47
1:A:24:GLU:CG	1:A:277:ILE:HG21	2.44	0.46
1:A:148:ASP:OD1	1:A:148:ASP:C	2.57	0.46
1:C:45:ASN:O	1:C:47:VAL:HG23	2.14	0.46
1:C:169:THR:HG23	1:C:179:TYR:CZ	2.50	0.46
1:C:69:ASP:HA	1:C:78:GLY:O	2.15	0.46
1:C:269:ASN:H	1:C:269:ASN:HD22	1.60	0.46
1:A:297:SER:O	1:C:297:SER:OG	2.34	0.46
1:C:312:GLN:NE2	1:C:313:ASP:OD2	2.49	0.46
1:A:47:VAL:O	1:A:47:VAL:CG2	2.63	0.46
1:A:267:LEU:HD23	1:A:267:LEU:N	2.29	0.46
1:C:62:ILE:HD11	1:C:66:VAL:HG23	1.97	0.46
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.69	0.46
1:A:32:VAL:CG1	1:A:54:PHE:CE1	2.99	0.46
1:C:22:THR:HG21	1:C:272:LYS:HD3	1.95	0.46
1:C:122:LYS:HE3	1:C:126:TYR:CE2	2.51	0.46
1:C:176:SER:CB	1:C:177:PRO:HA	2.44	0.46
1:A:1:GLY:N	1:A:175:ASN:OD1	2.44	0.45
1:A:115:THR:CG2	1:A:116:VAL:N	2.78	0.45
1:C:12:LYS:HG2	1:C:285:GLN:HB2	1.97	0.45
1:C:83:TYR:CZ	1:C:157:GLU:HG2	2.51	0.45
1:A:241:LYS:HB3	1:A:241:LYS:HE3	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:TYR:OH	1:A:183:GLN:NE2	2.50	0.45
1:C:238:TYR:O	1:C:239:THR:C	2.57	0.45
1:C:268:THR:HG23	1:C:269:ASN:HD22	1.81	0.45
1:A:8:THR:HG22	1:A:9:THR:N	2.31	0.45
1:A:140:PRO:HA	1:A:141:PRO:HD2	1.62	0.44
1:A:12:LYS:HA	1:A:285:GLN:OE1	2.18	0.44
1:A:231:ARG:HD2	3:A:914:HOH:O	2.17	0.44
1:A:19:MET:HG3	1:A:278:TYR:CE2	2.52	0.44
1:A:29:VAL:HA	1:A:56:GLY:O	2.16	0.44
1:A:40:LEU:HD12	1:A:100:ILE:HD12	1.99	0.44
1:A:45:ASN:O	1:A:47:VAL:CG1	2.64	0.44
1:A:28:LYS:HD2	1:A:30:ILE:CD1	2.46	0.44
1:A:115:THR:HG22	1:A:116:VAL:N	2.31	0.44
1:A:175:ASN:OD1	1:A:228:ARG:NH2	2.51	0.44
1:C:242:ALA:HB2	1:C:251:ASN:ND2	2.33	0.44
1:C:268:THR:CG2	1:C:270:GLU:H	2.29	0.44
1:A:39:ARG:HA	1:A:47:VAL:HB	1.99	0.44
1:C:145:THR:O	1:C:145:THR:HG23	2.16	0.44
1:C:268:THR:HG21	1:C:270:GLU:OE1	2.18	0.44
1:A:17:ARG:NH1	1:A:19:MET:HG2	2.33	0.44
1:A:21:PHE:CB	1:A:277:ILE:HD11	2.48	0.43
1:A:42:GLU:OE2	1:A:63:THR:HG23	2.17	0.43
1:C:245:GLU:O	1:C:249:VAL:HG23	2.18	0.43
1:A:54:PHE:HE1	1:A:67:LEU:HD13	1.83	0.43
1:A:71:VAL:HG13	1:A:77:MET:CG	2.48	0.43
1:A:138:PHE:C	1:A:138:PHE:HD1	2.24	0.43
1:A:143:HIS:HB2	1:A:157:GLU:HG2	2.01	0.43
1:C:71:VAL:HA	1:C:76:LEU:O	2.18	0.43
1:C:320:ASP:C	1:C:322:LYS:H	2.26	0.43
1:A:23:MET:CE	1:A:272:LYS:NZ	2.66	0.43
1:C:232:VAL:HG23	1:C:259:VAL:HG11	2.00	0.43
1:A:5:SER:O	1:A:236:LYS:NZ	2.35	0.43
1:C:68:TYR:HD1	1:C:80:MET:HE2	1.84	0.43
1:C:304:LEU:C	1:C:306:ALA:H	2.26	0.43
1:A:55:VAL:O	1:A:70:GLY:HA2	2.19	0.43
1:A:24:GLU:CD	1:A:277:ILE:HD12	2.34	0.43
1:A:101:ASN:O	1:A:102:PRO:C	2.62	0.43
1:C:50:ASN:OD1	1:C:50:ASN:N	2.52	0.43
1:C:115:THR:O	1:C:118:ASP:HB2	2.19	0.42
1:A:282:MET:HG2	1:A:289:TYR:HD2	1.84	0.42
1:A:135:ILE:H	1:A:135:ILE:HG12	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:O	1:A:187:ARG:N	2.52	0.42
1:C:24:GLU:O	1:C:24:GLU:HG2	2.19	0.42
1:A:79:ALA:C	1:A:106:ILE:HD11	2.45	0.42
1:A:281:ALA:C	1:A:282:MET:HG3	2.44	0.42
1:A:72:ASN:HB3	1:A:110:LEU:O	2.19	0.42
2:A:903:PNV:C6	1:C:212:GLN:HE22	2.32	0.42
1:A:32:VAL:HA	1:A:33:PRO:HD3	1.97	0.42
1:C:17:ARG:HD3	1:C:17:ARG:C	2.44	0.42
1:A:175:ASN:HB2	1:A:225:PRO:HB3	2.01	0.41
1:A:73:GLU:H	1:A:73:GLU:HG3	1.53	0.41
1:C:77:MET:HE3	1:C:77:MET:HB2	1.95	0.41
1:A:24:GLU:OE2	1:A:277:ILE:CB	2.56	0.41
1:A:81:LEU:HB2	1:A:173:MET:HE3	2.01	0.41
1:A:136:LEU:HD13	1:A:136:LEU:HA	1.86	0.41
1:A:196:PRO:HA	1:A:197:PRO:HD2	1.91	0.41
1:A:303:SER:HB2	1:C:331:VAL:HG22	2.03	0.41
1:C:55:VAL:O	1:C:55:VAL:HG13	2.21	0.41
1:A:17:ARG:NH2	1:A:68:TYR:HB3	2.35	0.41
1:A:47:VAL:O	1:A:47:VAL:HG22	2.21	0.41
1:A:224:THR:HG23	1:A:226:SER:H	1.85	0.41
1:A:8:THR:HB	1:A:12:LYS:O	2.21	0.41
1:C:22:THR:C	1:C:23:MET:HG3	2.46	0.41
1:C:170:ILE:HG13	1:C:172:VAL:HG13	2.03	0.41
1:A:54:PHE:CD2	1:A:54:PHE:N	2.88	0.41
1:C:62:ILE:HD12	1:C:104:TYR:OH	2.21	0.41
1:C:269:ASN:ND2	1:C:269:ASN:N	2.60	0.41
1:A:305:MET:SD	1:A:309:LEU:CD2	3.07	0.41
1:C:33:PRO:O	1:C:50:ASN:ND2	2.54	0.41
1:A:83:TYR:O	1:A:141:PRO:HB2	2.22	0.41
1:C:40:LEU:HD13	1:C:108:GLN:NE2	2.36	0.41
1:A:127:THR:O	1:A:129:LEU:HD13	2.21	0.40
1:A:175:ASN:O	1:A:182:HIS:HE1	2.05	0.40
1:A:134:ILE:H	1:A:134:ILE:HG13	1.57	0.40
1:A:24:GLU:CD	1:A:277:ILE:HB	2.42	0.40
1:A:28:LYS:H	1:A:28:LYS:HG3	1.66	0.40
1:A:219:LEU:HD12	1:A:219:LEU:HA	1.87	0.40
1:C:277:ILE:H	1:C:277:ILE:HG12	1.65	0.40
1:A:50:ASN:OD1	1:A:50:ASN:N	2.48	0.40
1:A:98:ARG:HH11	1:A:98:ARG:HD3	1.58	0.40
1:A:219:LEU:HD21	1:A:231:ARG:HG2	2.03	0.40
1:C:101:ASN:OD1	1:C:102:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:THR:HB	1:C:194:PRO:CD	2.51	0.40

There are no symmetry-related clashes.

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	328/335 (98%)	297 (90%)	24 (7%)	7 (2%)	5	11
1	C	329/335 (98%)	302 (92%)	25 (8%)	2 (1%)	21	42
All	All	657/670 (98%)	599 (91%)	49 (8%)	9 (1%)	9	19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	MET
1	A	27	SER
1	A	83	TYR
1	C	23	MET
1	C	211	GLY
1	A	186	LEU
1	A	318	GLU
1	A	63	THR
1	A	93	PRO

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	286/291 (98%)	216 (76%)	70 (24%)	1	1
1	C	287/291 (99%)	227 (79%)	60 (21%)	1	2
All	All	573/582 (98%)	443 (77%)	130 (23%)	1	1

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	6	ILE
1	A	7	ARG
1	A	8	THR
1	A	9	THR
1	A	12	LYS
1	A	17	ARG
1	A	18	THR
1	A	19	MET
1	A	23	MET
1	A	24	GLU
1	A	27	SER
1	A	28	LYS
1	A	32	VAL
1	A	34	ARG
1	A	38	ILE
1	A	39	ARG
1	A	43	LYS
1	A	44	GLU
1	A	45	ASN
1	A	47	VAL
1	A	60	THR
1	A	63	THR
1	A	64	SER
1	A	67	LEU
1	A	69	ASP
1	A	71	VAL
1	A	73	GLU
1	A	74	LYS
1	A	82	TYR
1	A	97	THR
1	A	98	ARG
1	A	109	VAL
1	A	110	LEU

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Mol	Chain	Res	Type
1	A	114	VAL
1	A	115	THR
1	A	116	VAL
1	A	121	GLU
1	A	122	LYS
1	A	123	LEU
1	A	134	ILE
1	A	136	LEU
1	A	142	LEU
1	A	152	GLU
1	A	153	SER
1	A	160	LYS
1	A	161	THR
1	A	163	ILE
1	A	165	ILE
1	A	212	GLN
1	A	224	THR
1	A	237	LYS
1	A	244	ASN
1	A	250	THR
1	A	265	VAL
1	A	269	ASN
1	A	277	ILE
1	A	279	THR
1	A	282	MET
1	A	287	LYS
1	A	293	LEU
1	A	304	LEU
1	A	305	MET
1	A	309	LEU
1	A	310	ASN
1	A	312	GLN
1	A	316	THR
1	A	317	PHE
1	A	318	GLU
1	A	327	GLN
1	C	2	SER
1	C	4	LEU
1	C	7	ARG
1	C	13	SER
1	C	14	LEU
1	C	19	MET

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Mol	Chain	Res	Type
1	C	22	THR
1	C	23	MET
1	C	24	GLU
1	C	28	LYS
1	C	34	ARG
1	C	39	ARG
1	C	40	LEU
1	C	43	LYS
1	C	45	ASN
1	C	60	THR
1	C	74	LYS
1	C	82	TYR
1	C	95	LYS
1	C	98	ARG
1	C	105	VAL
1	C	110	LEU
1	C	114	VAL
1	C	116	VAL
1	C	117	ASP
1	C	124	THR
1	C	128	LEU
1	C	160	LYS
1	C	161	THR
1	C	163	ILE
1	C	167	ARG
1	C	168	LYS
1	C	172	VAL
1	C	173	MET
1	C	174	THR
1	C	176	SER
1	C	183	GLN
1	C	184	THR
1	C	201	MET
1	C	208	THR
1	C	212	GLN
1	C	228	ARG
1	C	235	TRP
1	C	246	THR
1	C	247	GLU
1	C	263	LYS
1	C	268	THR
1	C	269	ASN

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Mol	Chain	Res	Type
1	C	273	THR
1	C	277	ILE
1	C	287	LYS
1	C	293	LEU
1	C	303	SER
1	C	304	LEU
1	C	305	MET
1	C	311	SER
1	C	314	LEU
1	C	322	LYS
1	C	326	LYS
1	C	331	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	49	ASN
1	A	130	ASN
1	A	182	HIS
1	A	183	GLN
1	A	185	ASN
1	A	195	ASN
1	A	198	GLN
1	A	251	ASN
1	A	312	GLN
1	C	35	ASN
1	C	45	ASN
1	C	108	GLN
1	C	183	GLN
1	C	185	ASN
1	C	212	GLN
1	C	260	ASN
1	C	269	ASN
1	C	288	ASN
1	C	310	ASN
1	C	312	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	PNV	A	903	-	26,26,26	1.22	3 (11%)	39,39,39	3.10	14 (35%)
2	PNV	C	904	-	26,26,26	1.45	4 (15%)	39,39,39	3.39	19 (48%)

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	PNV	A	903	-	-	7/13/44/44	0/3/3/3
2	PNV	C	904	-	-	6/13/44/44	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	904	PNV	C10-S11	-3.92	1.77	1.85
2	A	903	PNV	C10-S11	-3.36	1.78	1.85
2	C	904	PNV	C8-S11	-3.21	1.76	1.81
2	C	904	PNV	C6-N7	-2.70	1.31	1.37
2	A	903	PNV	C8-S11	-2.70	1.77	1.81
2	C	904	PNV	C5-C6	-2.35	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	903	PNV	C6-N7	-2.28	1.32	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	903	PNV	S11-C8-N7	-9.29	92.37	104.93
2	A	903	PNV	C5-N4-C3	7.94	137.48	121.80
2	C	904	PNV	S11-C8-N7	-7.63	94.62	104.93
2	C	904	PNV	C2-O1-C19	6.68	129.60	117.63
2	C	904	PNV	C5-N4-C3	6.53	134.70	121.80
2	C	904	PNV	C5-C8-S11	6.18	128.91	119.22
2	C	904	PNV	C5-C8-N7	-6.05	80.80	88.01
2	C	904	PNV	C8-N7-C9	6.00	124.34	117.30
2	C	904	PNV	C8-N7-C6	5.40	100.53	93.92
2	A	903	PNV	C2-O1-C19	5.33	127.18	117.63
2	C	904	PNV	C10-C9-C13	5.26	120.84	112.87
2	C	904	PNV	O17-C6-N7	5.14	138.84	131.75
2	A	903	PNV	C8-N7-C9	4.89	123.04	117.30
2	A	903	PNV	C10-C9-C13	4.74	120.04	112.87
2	A	903	PNV	C5-C8-S11	4.03	125.54	119.22
2	A	903	PNV	C8-N7-C6	4.00	98.82	93.92
2	A	903	PNV	C9-N7-C6	3.92	137.25	126.38
2	C	904	PNV	C2-C3-N4	-3.91	109.66	116.41
2	C	904	PNV	C8-C5-N4	3.87	126.51	118.49
2	A	903	PNV	C5-C8-N7	-3.73	83.56	88.01
2	A	903	PNV	C6-C5-N4	3.72	125.80	115.29
2	C	904	PNV	C13-C9-N7	3.52	117.94	112.10
2	A	903	PNV	O17-C6-N7	3.51	136.59	131.75
2	A	903	PNV	O14-C13-C9	3.11	121.39	112.47
2	C	904	PNV	C9-N7-C6	2.79	134.13	126.38
2	A	903	PNV	C13-C9-N7	2.67	116.54	112.10
2	C	904	PNV	C10-C9-N7	-2.60	102.67	106.43
2	C	904	PNV	C8-C5-C6	2.56	89.04	85.15
2	C	904	PNV	C5-C6-N7	-2.53	88.61	91.95
2	C	904	PNV	C15-C10-C9	-2.46	106.30	111.61
2	C	904	PNV	C12-C10-C9	2.36	116.70	111.61
2	A	903	PNV	C10-C9-N7	-2.19	103.26	106.43
2	C	904	PNV	C20-C19-C24	-2.05	117.16	120.16

There are no chirality outliers.

All (13) torsion outliers are listed below:

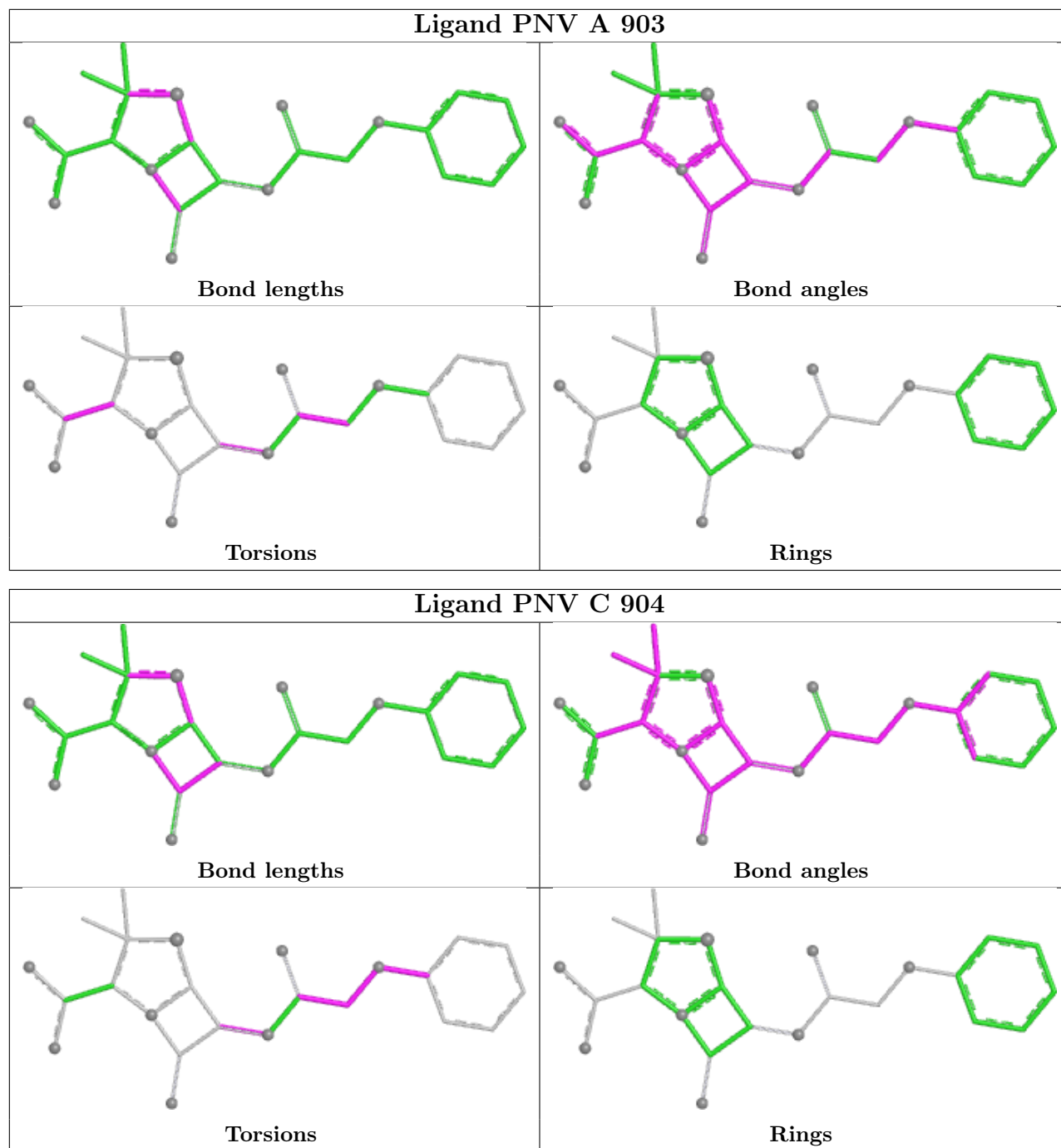
Mol	Chain	Res	Type	Atoms
2	A	903	PNV	O14-C13-C9-N7
2	A	903	PNV	O16-C13-C9-N7
2	A	903	PNV	O14-C13-C9-C10
2	A	903	PNV	O16-C13-C9-C10
2	A	903	PNV	O1-C2-C3-N4
2	C	904	PNV	C20-C19-O1-C2
2	C	904	PNV	C24-C19-O1-C2
2	A	903	PNV	O1-C2-C3-O18
2	C	904	PNV	C6-C5-N4-C3
2	C	904	PNV	C3-C2-O1-C19
2	C	904	PNV	O1-C2-C3-N4
2	C	904	PNV	O1-C2-C3-O18
2	A	903	PNV	C6-C5-N4-C3

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	903	PNV	4	0
2	C	904	PNV	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.