



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:41 AM UTC

PDB ID : 1K7F / pdb_00001k7f
Title : CRYSTAL STRUCTURE OF WILD-TYPE TRYPTOPHAN SYNTHASE
COMPLEXED WITH N-[1H-INDOL-3-YL-ACETYL]VALINE ACID
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Deposited on : 2001-10-19
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

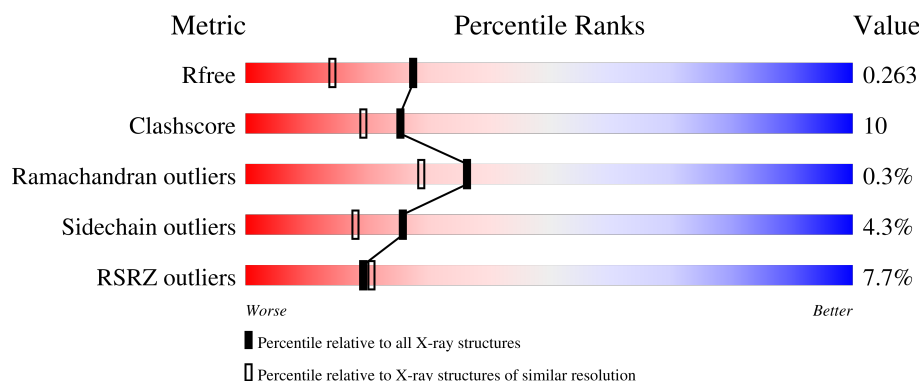
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	268	
2	B	396	

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
4	PLP	B	402	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4962 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 TRYPTOPHAN SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1911	1216	330	357	8			

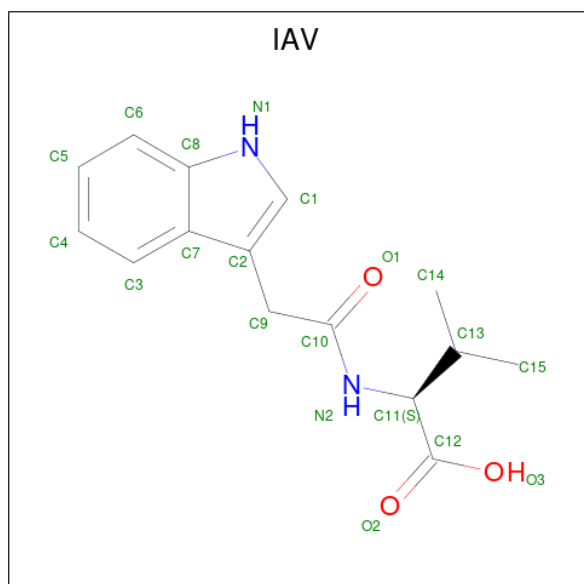
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	380	Total	C	N	O	S	0	0	0
			2866	1801	501	545	19			

There is a discrepancy between the modelled and reference sequences:

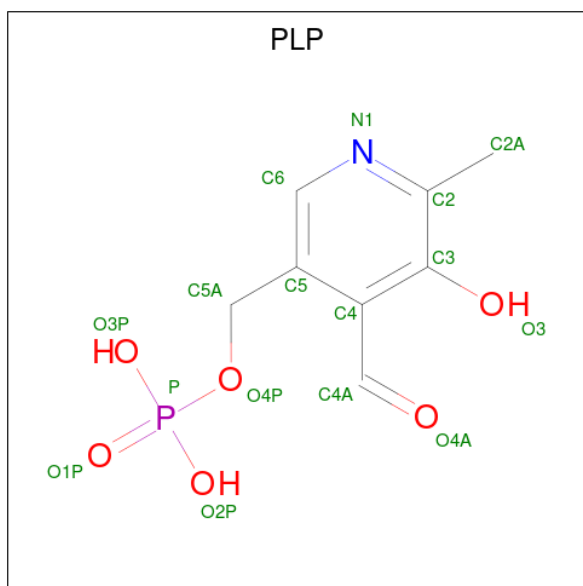
Chain	Residue	Modelled	Actual	Comment	Reference
B	34	SER	ARG	cloning artifact	UNP P0A2K1

- Molecule 3 is N-[1H-INDOL-3-YL-ACETYL]VALINE ACID (CCD ID: IAV) (formula: $C_{15}H_{18}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	15	2	3		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

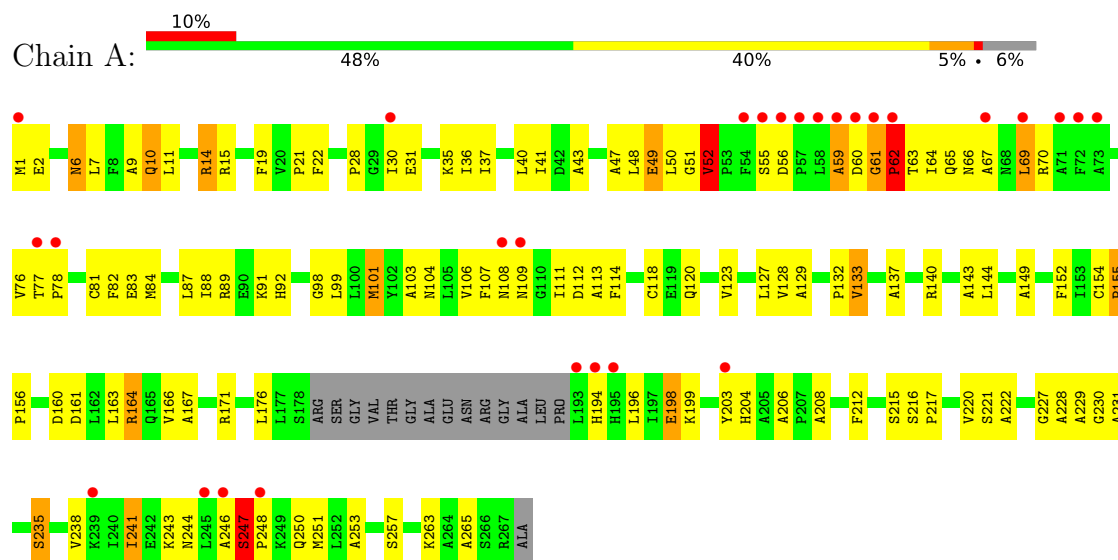
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O	0	0
			51	51		
5	B	99	Total	O	0	0
			99	99		

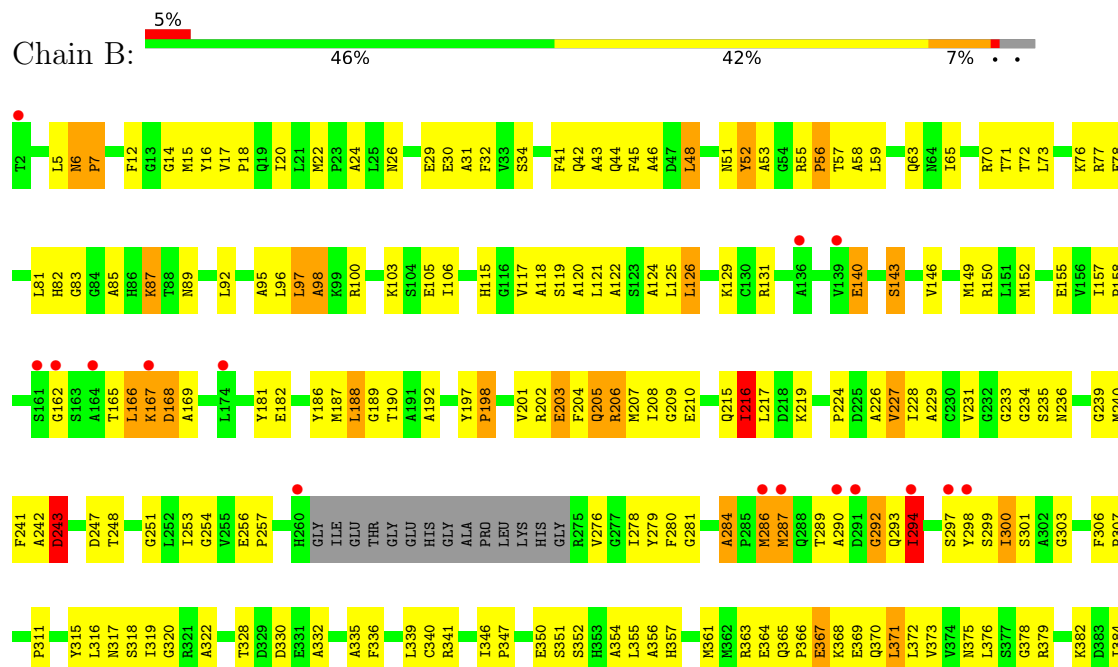
3 Residue-property plots [i](#)

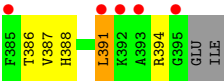
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: TRYPTOPHAN SYNTHASE ALPHA CHAIN



• Molecule 2: TRYPTOPHAN SYNTHASE BETA CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.66Å 59.07Å 67.47Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.8 (20.00-1.90) 93.7 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.89Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.197 , 0.251 0.210 , 0.263	Depositor DCC
R_{free} test set	2684 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4962	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: IAV, PLP

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	2.26	70/1948 (3.6%)	1.87	46/2646 (1.7%)
2	B	2.56	157/2919 (5.4%)	2.03	108/3944 (2.7%)
All	All	2.44	227/4867 (4.7%)	1.97	154/6590 (2.3%)

All (227) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	167	LYS	CA-CB	14.28	1.77	1.53
2	B	284	ALA	CA-CB	14.23	1.75	1.54
2	B	208	ILE	CA-CB	13.45	1.68	1.54
2	B	152	MET	SD-CE	-12.48	1.48	1.79
2	B	81	LEU	C-O	10.97	1.37	1.23
2	B	287	MET	SD-CE	10.66	2.06	1.79
2	B	146	VAL	CA-CB	10.26	1.66	1.54
1	A	10	GLN	C-O	10.20	1.35	1.24
2	B	242	ALA	CA-CB	10.03	1.68	1.53
1	A	84	MET	SD-CE	-9.90	1.54	1.79
2	B	98	ALA	CA-CB	9.62	1.68	1.53
2	B	247	ASP	C-O	9.26	1.36	1.23
2	B	368	LYS	N-CA	9.24	1.58	1.46
1	A	10	GLN	CB-CG	9.22	1.80	1.52
2	B	226	ALA	CA-CB	-9.18	1.38	1.53
1	A	163	LEU	CA-C	-9.02	1.41	1.52
1	A	88	ILE	CA-CB	8.98	1.65	1.54
2	B	379	ARG	CZ-NH1	8.90	1.45	1.32
2	B	30	GLU	CA-CB	8.88	1.67	1.53
2	B	386	THR	CA-C	-8.77	1.41	1.52
2	B	286	MET	SD-CE	8.71	2.01	1.79
2	B	248	THR	CA-CB	8.64	1.68	1.53
2	B	227	VAL	CB-CG1	8.63	1.81	1.52
2	B	367	GLU	C-O	8.61	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	289	THR	CA-CB	-8.60	1.40	1.53
1	A	149	ALA	CA-CB	8.48	1.68	1.52
2	B	332	ALA	CA-CB	8.34	1.66	1.53
2	B	17	VAL	N-CA	-8.25	1.39	1.46
1	A	60	ASP	C-O	8.24	1.34	1.24
2	B	290	ALA	CA-CB	8.15	1.66	1.53
2	B	106	ILE	CA-C	8.14	1.62	1.52
1	A	15	ARG	C-O	8.11	1.32	1.23
2	B	315	TYR	CE2-CZ	8.09	1.57	1.38
1	A	221	SER	C-O	8.05	1.33	1.24
2	B	71	THR	N-CA	8.03	1.56	1.45
2	B	58	ALA	CA-C	8.00	1.63	1.52
2	B	235	SER	CA-C	7.94	1.62	1.52
2	B	251	GLY	C-O	7.91	1.31	1.23
2	B	229	ALA	CA-CB	7.89	1.67	1.53
2	B	120	ALA	CA-CB	7.82	1.65	1.53
2	B	41	PHE	CD1-CE1	7.82	1.62	1.38
1	A	49	GLU	C-O	7.73	1.33	1.24
2	B	124	ALA	CA-CB	7.62	1.65	1.53
2	B	5	LEU	C-O	7.52	1.33	1.23
1	A	113	ALA	CA-CB	-7.47	1.40	1.53
2	B	6	ASN	C-N	-7.45	1.26	1.33
2	B	42	GLN	C-O	7.45	1.32	1.24
2	B	347	PRO	CA-CB	-7.45	1.45	1.54
2	B	322	ALA	C-O	7.42	1.32	1.23
2	B	369	GLU	C-O	7.40	1.32	1.24
2	B	192	ALA	CA-C	7.31	1.61	1.52
2	B	119	SER	C-O	-7.26	1.15	1.24
2	B	371	LEU	CG-CD2	7.17	1.76	1.52
1	A	161	ASP	CG-OD2	7.15	1.39	1.25
2	B	56	PRO	N-CD	7.13	1.57	1.47
2	B	363	ARG	CA-C	7.13	1.62	1.52
2	B	76	LYS	C-O	7.11	1.32	1.24
2	B	368	LYS	CA-C	7.08	1.61	1.52
1	A	167	ALA	CA-C	-7.08	1.43	1.52
2	B	45	PHE	CG-CD1	7.05	1.53	1.38
1	A	1	MET	SD-CE	7.04	1.97	1.79
1	A	137	ALA	CA-CB	6.99	1.62	1.53
1	A	67	ALA	CA-CB	6.93	1.64	1.53
1	A	98	GLY	C-O	6.92	1.33	1.23
2	B	56	PRO	CB-CG	6.87	1.77	1.51
2	B	251	GLY	CA-C	6.86	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	ARG	CZ-NH1	6.79	1.42	1.32
1	A	133	VAL	CB-CG1	-6.78	1.30	1.52
1	A	143	ALA	CA-CB	6.77	1.63	1.53
2	B	235	SER	C-O	6.77	1.31	1.24
2	B	376	LEU	C-O	6.77	1.32	1.23
1	A	154	CYS	C-O	-6.76	1.15	1.24
2	B	168	ASP	N-CA	-6.73	1.38	1.46
1	A	164	ARG	NE-CZ	6.73	1.40	1.33
2	B	118	ALA	N-CA	6.72	1.54	1.46
2	B	63	GLN	CG-CD	6.72	1.68	1.52
1	A	228	ALA	CA-CB	6.72	1.64	1.53
2	B	318	SER	CA-C	-6.71	1.44	1.52
2	B	22	MET	N-CA	6.69	1.52	1.46
1	A	220	VAL	C-O	6.64	1.31	1.24
2	B	229	ALA	C-O	6.62	1.31	1.23
1	A	215	SER	N-CA	-6.58	1.39	1.46
2	B	354	ALA	CA-CB	6.57	1.63	1.53
1	A	253	ALA	CA-CB	6.56	1.63	1.53
2	B	239	GLY	CA-C	6.55	1.60	1.51
1	A	37	ILE	CA-CB	6.55	1.62	1.54
2	B	371	LEU	C-O	6.49	1.31	1.24
2	B	41	PHE	C-O	6.45	1.31	1.24
2	B	120	ALA	C-O	-6.44	1.16	1.24
1	A	132	PRO	C-O	6.42	1.32	1.23
1	A	222	ALA	C-O	-6.41	1.16	1.24
2	B	373	VAL	C-O	6.41	1.30	1.24
2	B	150	ARG	CZ-NH2	6.39	1.41	1.33
1	A	230	GLY	CA-C	6.35	1.58	1.52
2	B	52	TYR	N-CA	6.35	1.54	1.46
2	B	352	SER	C-O	-6.35	1.16	1.24
2	B	65	ILE	CA-CB	6.31	1.63	1.54
1	A	208	ALA	CA-C	6.31	1.61	1.52
2	B	276	VAL	CA-CB	-6.31	1.46	1.54
2	B	204	PHE	CE2-CZ	6.29	1.57	1.38
2	B	30	GLU	CD-OE2	6.27	1.37	1.25
2	B	335	ALA	CA-CB	6.26	1.63	1.53
1	A	83	GLU	N-CA	6.25	1.53	1.46
2	B	70	ARG	N-CA	-6.25	1.38	1.46
2	B	317	ASN	CA-C	6.25	1.60	1.52
2	B	382	LYS	CB-CG	6.24	1.71	1.52
2	B	379	ARG	N-CA	6.22	1.53	1.45
2	B	82	HIS	CA-C	-6.21	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	122	ALA	N-CA	6.21	1.53	1.46
1	A	164	ARG	CG-CD	6.20	1.71	1.52
2	B	167	LYS	CA-C	-6.18	1.44	1.52
1	A	98	GLY	C-N	-6.18	1.24	1.33
2	B	125	LEU	C-O	6.15	1.31	1.24
1	A	155	PRO	C-O	6.15	1.31	1.24
2	B	187	MET	CB-CG	6.14	1.70	1.52
1	A	49	GLU	N-CA	-6.11	1.38	1.46
2	B	356	ALA	CA-CB	6.10	1.63	1.53
2	B	201	VAL	C-O	6.09	1.31	1.24
1	A	47	ALA	CA-CB	6.08	1.63	1.53
2	B	231	VAL	CB-CG2	6.07	1.72	1.52
1	A	231	ALA	C-O	6.07	1.31	1.23
1	A	199	LYS	C-O	6.06	1.31	1.24
2	B	182	GLU	CA-C	-6.05	1.44	1.52
2	B	96	LEU	CB-CG	-6.05	1.41	1.53
1	A	206	ALA	CA-CB	6.03	1.61	1.53
2	B	340	CYS	CA-CB	6.00	1.62	1.53
2	B	372	LEU	N-CA	6.00	1.53	1.46
2	B	234	GLY	C-O	6.00	1.32	1.24
2	B	204	PHE	CD1-CE1	5.99	1.56	1.38
2	B	202	ARG	C-O	5.97	1.30	1.24
2	B	24	ALA	CA-CB	5.91	1.62	1.53
2	B	44	GLN	CA-C	5.91	1.60	1.52
2	B	103	LYS	N-CA	-5.90	1.38	1.45
1	A	92	HIS	C-O	-5.90	1.17	1.24
1	A	171	ARG	C-O	-5.89	1.16	1.23
2	B	368	LYS	CA-CB	5.88	1.61	1.53
1	A	265	ALA	C-O	-5.88	1.16	1.24
2	B	48	LEU	C-O	5.85	1.30	1.24
1	A	228	ALA	N-CA	5.82	1.53	1.46
2	B	105	GLU	C-O	-5.82	1.17	1.23
1	A	222	ALA	CA-CB	-5.81	1.44	1.53
2	B	357	HIS	N-CA	-5.80	1.39	1.46
2	B	63	GLN	CD-OE1	5.75	1.34	1.23
1	A	161	ASP	CG-OD1	5.72	1.36	1.25
1	A	64	ILE	CA-C	-5.70	1.45	1.52
2	B	83	GLY	C-O	5.69	1.32	1.24
1	A	89	ARG	CA-CB	5.68	1.62	1.53
2	B	253	ILE	CG1-CD1	5.67	1.73	1.51
2	B	235	SER	CB-OG	5.66	1.53	1.42
2	B	85	ALA	CA-CB	5.66	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	15	MET	CA-C	-5.64	1.45	1.53
2	B	236	ASN	N-CA	5.62	1.53	1.46
1	A	69	LEU	CA-C	-5.57	1.45	1.52
1	A	128	VAL	N-CA	5.53	1.53	1.46
2	B	241	PHE	CA-C	5.50	1.60	1.52
2	B	202	ARG	NE-CZ	-5.49	1.27	1.33
2	B	207	MET	SD-CE	5.49	1.93	1.79
2	B	12	PHE	CA-C	-5.49	1.45	1.52
2	B	301	SER	N-CA	-5.48	1.39	1.46
2	B	215	GLN	C-O	5.47	1.30	1.24
2	B	203	GLU	N-CA	-5.46	1.39	1.46
2	B	166	LEU	C-O	5.45	1.30	1.24
1	A	107	PHE	CA-C	5.45	1.60	1.52
2	B	31	ALA	CA-C	5.45	1.60	1.52
2	B	351	SER	C-O	-5.45	1.17	1.24
1	A	263	LYS	CA-CB	5.45	1.61	1.53
1	A	166	VAL	CA-CB	-5.42	1.47	1.54
2	B	375	ASN	C-O	-5.42	1.17	1.24
2	B	315	TYR	CA-C	-5.42	1.46	1.52
1	A	14	ARG	C-O	-5.41	1.17	1.24
1	A	83	GLU	CA-CB	5.40	1.61	1.53
2	B	328	THR	CA-CB	5.40	1.61	1.53
1	A	87	LEU	N-CA	5.40	1.53	1.46
2	B	371	LEU	CA-CB	-5.38	1.46	1.53
2	B	197	TYR	CE1-CZ	5.37	1.51	1.38
2	B	224	PRO	CA-C	5.37	1.59	1.52
2	B	387	VAL	C-O	-5.37	1.18	1.24
2	B	143	SER	C-O	-5.36	1.19	1.24
1	A	106	VAL	C-O	5.35	1.30	1.24
2	B	197	TYR	CA-CB	5.35	1.61	1.53
1	A	99	LEU	N-CA	5.35	1.53	1.46
2	B	51	ASN	C-N	-5.34	1.26	1.33
1	A	127	LEU	CG-CD1	5.33	1.70	1.52
2	B	372	LEU	CG-CD2	5.33	1.70	1.52
2	B	240	MET	SD-CE	5.31	1.92	1.79
2	B	216	ILE	CA-C	5.30	1.59	1.52
2	B	228	ILE	C-O	5.30	1.29	1.24
1	A	108	ASN	N-CA	5.28	1.52	1.46
2	B	346	ILE	CB-CG2	5.26	1.70	1.52
2	B	122	ALA	CA-CB	5.24	1.61	1.53
2	B	388	HIS	CA-CB	5.24	1.61	1.53
1	A	241	ILE	CA-C	5.23	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	77	ARG	N-CA	5.23	1.53	1.46
2	B	192	ALA	CA-CB	5.22	1.62	1.53
2	B	186	TYR	N-CA	5.20	1.52	1.46
2	B	14	GLY	N-CA	5.20	1.52	1.45
1	A	82	PHE	CB-CG	5.19	1.62	1.50
2	B	129	LYS	CA-C	-5.18	1.46	1.52
2	B	339	LEU	CA-CB	5.18	1.61	1.53
1	A	227	GLY	CA-C	5.16	1.59	1.51
2	B	45	PHE	CE2-CZ	5.16	1.54	1.38
2	B	316	LEU	CA-CB	5.15	1.61	1.53
1	A	21	PRO	N-CA	-5.15	1.41	1.46
2	B	117	VAL	CB-CG2	5.14	1.69	1.52
1	A	144	LEU	C-O	5.13	1.30	1.24
2	B	169	ALA	CA-CB	5.13	1.61	1.53
1	A	120	GLN	CA-CB	5.12	1.61	1.53
2	B	197	TYR	C-O	-5.12	1.19	1.24
1	A	6	ASN	N-CA	-5.08	1.40	1.46
2	B	370	GLN	CD-NE2	-5.08	1.22	1.33
2	B	206	ARG	N-CA	5.07	1.52	1.46
2	B	346	ILE	CG1-CD1	5.07	1.71	1.51
2	B	355	LEU	C-O	-5.07	1.18	1.24
2	B	361	MET	SD-CE	-5.06	1.66	1.79
1	A	43	ALA	CA-CB	-5.06	1.44	1.53
1	A	250	GLN	N-CA	-5.06	1.40	1.46
2	B	341	ARG	CA-C	-5.06	1.45	1.52
2	B	336	PHE	CD2-CE2	5.05	1.53	1.38
2	B	143	SER	CA-CB	5.04	1.59	1.53
2	B	340	CYS	CA-C	5.04	1.59	1.52
1	A	229	ALA	C-O	-5.03	1.17	1.24
2	B	43	ALA	CA-C	5.02	1.59	1.52
2	B	278	ILE	CA-CB	5.01	1.60	1.53
2	B	55	ARG	NE-CZ	5.01	1.38	1.33
2	B	30	GLU	CD-OE1	5.00	1.34	1.25
2	B	391	LEU	N-CA	-5.00	1.40	1.46
2	B	29	GLU	CA-CB	-5.00	1.45	1.53

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	208	ILE	N-CA-C	11.53	122.22	110.23
2	B	318	SER	N-CA-C	-10.72	99.67	111.36
1	A	221	SER	O-C-N	10.30	133.03	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	PRO	N-CA-C	9.81	132.67	112.47
1	A	11	LEU	N-CA-C	-9.64	100.64	111.82
1	A	61	GLY	CA-C-N	9.51	131.72	119.84
1	A	61	GLY	C-N-CA	9.51	131.72	119.84
1	A	160	ASP	N-CA-C	8.95	120.64	111.07
1	A	61	GLY	CA-C-O	-8.75	109.01	121.52
1	A	52	VAL	CB-CA-C	-8.41	101.18	110.85
2	B	315	TYR	N-CA-C	8.35	120.00	111.07
2	B	205	GLN	N-CA-C	-8.17	100.98	113.89
2	B	55	ARG	CA-CB-CG	8.14	130.39	114.10
2	B	198	PRO	N-CA-C	-8.05	102.33	113.53
2	B	367	GLU	CA-C-N	-7.91	111.03	122.19
2	B	367	GLU	C-N-CA	-7.91	111.03	122.19
2	B	240	MET	N-CA-C	-7.84	102.05	111.69
1	A	114	PHE	N-CA-C	-7.80	102.86	111.36
2	B	303	GLY	N-CA-C	7.79	123.05	114.40
2	B	63	GLN	N-CA-C	7.46	120.29	111.71
2	B	73	LEU	CD1-CG-CD2	-7.41	94.49	110.80
2	B	320	GLY	N-CA-C	7.39	124.81	115.21
2	B	368	LYS	N-CA-CB	-7.29	98.13	110.16
2	B	364	GLU	CA-C-N	-7.28	114.85	122.85
2	B	364	GLU	C-N-CA	-7.28	114.85	122.85
2	B	70	ARG	N-CA-C	-7.21	103.58	112.88
2	B	34	SER	N-CA-C	7.20	119.75	111.11
1	A	229	ALA	N-CA-C	-7.16	104.54	113.28
1	A	67	ALA	N-CA-C	-6.72	104.09	112.90
2	B	92	LEU	CA-C-N	6.70	127.42	119.98
2	B	92	LEU	C-N-CA	6.70	127.42	119.98
2	B	235	SER	N-CA-C	6.70	118.37	111.14
1	A	92	HIS	CA-C-N	6.61	126.20	119.19
1	A	92	HIS	C-N-CA	6.61	126.20	119.19
2	B	335	ALA	N-CA-C	-6.56	104.21	111.36
2	B	226	ALA	N-CA-C	6.51	118.41	108.52
1	A	89	ARG	N-CA-C	6.46	118.32	111.28
1	A	129	ALA	N-CA-C	6.45	119.12	111.71
1	A	61	GLY	O-C-N	6.41	128.18	121.77
2	B	32	PHE	N-CA-C	-6.40	103.81	111.69
2	B	202	ARG	CA-C-N	-6.40	110.03	120.72
2	B	202	ARG	C-N-CA	-6.40	110.03	120.72
2	B	365	GLN	CB-CG-CD	6.40	123.48	112.60
2	B	55	ARG	CB-CA-C	6.38	118.68	109.11
2	B	70	ARG	NE-CZ-NH1	-6.38	115.12	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	149	MET	N-CA-C	6.35	118.73	111.11
2	B	209	GLY	N-CA-C	-6.34	104.87	113.37
2	B	289	THR	CA-C-N	6.33	129.05	120.38
2	B	289	THR	C-N-CA	6.33	129.05	120.38
2	B	217	LEU	N-CA-C	-6.27	104.37	111.14
1	A	51	GLY	CA-C-O	-6.23	114.83	120.94
2	B	30	GLU	N-CA-C	-6.23	104.41	111.14
1	A	7	LEU	N-CA-C	-6.17	104.56	111.28
2	B	286	MET	CB-CG-SD	6.14	131.13	112.70
2	B	97	LEU	CB-CG-CD2	-6.09	92.42	110.70
2	B	46	ALA	N-CA-C	6.06	118.38	111.11
2	B	319	ILE	CA-C-N	-6.05	112.58	122.20
2	B	319	ILE	C-N-CA	-6.05	112.58	122.20
2	B	71	THR	N-CA-CB	-6.04	100.56	110.41
1	A	82	PHE	N-CA-C	6.04	118.82	111.82
1	A	246	ALA	CA-C-N	-6.03	116.22	122.85
1	A	246	ALA	C-N-CA	-6.03	116.22	122.85
2	B	72	THR	N-CA-C	-6.02	99.09	108.90
2	B	294	ILE	N-CA-C	6.01	117.05	108.93
1	A	221	SER	CA-C-O	-5.96	114.24	120.55
1	A	235	SER	N-CA-C	5.95	118.53	111.33
2	B	169	ALA	N-CA-C	-5.88	104.77	111.07
2	B	236	ASN	N-CA-C	-5.85	104.91	111.28
1	A	103	ALA	N-CA-C	5.83	117.64	111.28
1	A	2	GLU	N-CA-CB	-5.78	102.69	111.19
1	A	84	MET	N-CA-CB	5.78	118.45	110.07
2	B	254	GLY	CA-C-N	-5.78	115.41	123.10
2	B	254	GLY	C-N-CA	-5.78	115.41	123.10
1	A	69	LEU	N-CA-C	-5.73	105.12	111.36
2	B	51	ASN	O-C-N	5.72	130.16	122.49
1	A	9	ALA	N-CA-C	-5.71	105.14	111.36
2	B	241	PHE	N-CA-C	5.68	118.41	111.82
1	A	60	ASP	N-CA-C	5.65	118.61	109.40
1	A	59	ALA	N-CA-C	-5.64	104.98	112.94
2	B	7	PRO	N-CD-CG	-5.63	94.75	103.20
1	A	62	PRO	CB-CA-C	-5.62	102.28	111.56
2	B	368	LYS	CB-CG-CD	5.62	124.22	111.30
2	B	379	ARG	N-CA-C	-5.62	101.72	110.42
2	B	78	GLU	N-CA-C	-5.61	106.28	113.01
2	B	89	ASN	N-CA-C	5.59	117.84	111.02
2	B	26	ASN	N-CA-C	-5.58	104.83	111.69
1	A	56	ASP	N-CA-C	5.56	118.72	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	216	ILE	O-C-N	5.56	127.48	121.87
2	B	190	THR	CA-C-O	-5.55	115.49	121.38
2	B	31	ALA	N-CA-C	5.55	118.10	111.71
2	B	7	PRO	CB-CA-C	-5.54	103.07	110.88
2	B	219	LYS	CD-CE-NZ	-5.54	94.17	111.90
1	A	247	SER	O-C-N	5.48	125.67	121.23
2	B	292	GLY	N-CA-C	5.46	123.13	115.43
1	A	137	ALA	N-CA-C	5.46	120.35	113.25
2	B	233	GLY	N-CA-C	-5.46	108.17	115.32
2	B	181	TYR	CA-C-O	-5.44	112.73	120.51
2	B	150	ARG	N-CA-C	5.43	117.28	111.36
1	A	50	LEU	CA-C-N	-5.42	117.35	122.66
1	A	50	LEU	C-N-CA	-5.42	117.35	122.66
1	A	108	ASN	N-CA-C	5.42	120.25	111.37
2	B	121	LEU	N-CA-C	-5.41	105.46	111.36
1	A	19	PHE	CA-CB-CG	-5.41	108.39	113.80
2	B	373	VAL	CB-CA-C	-5.41	102.63	110.63
2	B	29	GLU	N-CA-C	-5.40	105.39	111.28
2	B	56	PRO	CA-C-N	-5.40	112.91	122.74
2	B	56	PRO	C-N-CA	-5.40	112.91	122.74
2	B	300	ILE	CB-CG1-CD1	-5.36	102.55	113.80
2	B	207	MET	CA-C-N	-5.35	113.76	120.77
2	B	207	MET	C-N-CA	-5.35	113.76	120.77
1	A	198	GLU	CB-CA-C	-5.35	101.91	110.79
2	B	248	THR	OG1-CB-CG2	-5.35	98.60	109.30
2	B	311	PRO	CA-C-O	-5.35	111.48	119.34
2	B	350	GLU	CA-CB-CG	5.35	124.79	114.10
2	B	203	GLU	N-CA-C	5.34	119.06	112.54
2	B	352	SER	N-CA-C	-5.34	105.63	111.82
2	B	367	GLU	N-CA-C	-5.33	106.01	112.88
2	B	158	PRO	CA-C-N	-5.32	115.97	122.93
2	B	158	PRO	C-N-CA	-5.32	115.97	122.93
2	B	243	ASP	CA-CB-CG	-5.32	107.28	112.60
2	B	18	PRO	CB-CA-C	-5.31	104.43	111.23
2	B	87	LYS	CB-CG-CD	-5.30	99.10	111.30
1	A	76	VAL	CB-CA-C	-5.29	104.56	110.96
2	B	12	PHE	CA-C-O	-5.28	115.22	121.66
2	B	227	VAL	CG1-CB-CG2	-5.26	99.22	110.80
2	B	168	ASP	N-CA-CB	-5.25	102.39	110.16
2	B	378	GLY	CA-C-O	-5.25	115.95	121.56
2	B	56	PRO	CB-CG-CD	-5.24	93.36	105.40
2	B	70	ARG	CA-CB-CG	-5.23	103.63	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	GLN	CA-CB-CG	-5.21	103.67	114.10
2	B	197	TYR	N-CA-C	5.21	120.57	113.16
2	B	59	LEU	CA-C-N	-5.21	114.89	122.65
2	B	59	LEU	C-N-CA	-5.21	114.89	122.65
2	B	100	ARG	NE-CZ-NH2	5.21	123.89	119.20
2	B	297	SER	CA-C-N	-5.20	115.14	122.94
2	B	297	SER	C-N-CA	-5.20	115.14	122.94
2	B	126	LEU	CB-CG-CD1	-5.20	95.10	110.70
2	B	57	THR	CA-C-N	5.18	128.57	120.75
2	B	57	THR	C-N-CA	5.18	128.57	120.75
1	A	101	MET	CG-SD-CE	-5.17	89.54	100.90
2	B	328	THR	OG1-CB-CG2	-5.16	98.99	109.30
2	B	53	ALA	CA-C-N	5.15	128.58	121.26
2	B	53	ALA	C-N-CA	5.15	128.58	121.26
2	B	375	ASN	CA-C-N	-5.14	114.12	122.34
2	B	375	ASN	C-N-CA	-5.14	114.12	122.34
1	A	52	VAL	CA-C-N	5.12	125.41	119.93
1	A	52	VAL	C-N-CA	5.12	125.41	119.93
1	A	149	ALA	CA-C-O	5.11	123.39	119.46
2	B	81	LEU	N-CA-C	5.10	117.29	110.35
2	B	192	ALA	N-CA-C	-5.08	101.73	108.74
2	B	251	GLY	O-C-N	-5.08	117.61	122.84
2	B	379	ARG	CD-NE-CZ	-5.05	117.33	124.40
1	A	91	LYS	CA-C-N	-5.01	116.26	122.42
1	A	91	LYS	C-N-CA	-5.01	116.26	122.42

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	1911	0	1919	45	0
2	B	2866	0	2835	49	0
3	A	20	0	18	2	0
4	B	15	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	51	0	0	2	0
5	B	99	0	0	2	0
All	All	4962	0	4778	92	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 10.

All (92) 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)
2:B:371:LEU:CD2	2:B:371:LEU:CG	1.76	1.60
2:B:167:LYS:CA	2:B:167:LYS:CB	1.77	1.58
2:B:284:ALA:CA	2:B:284:ALA:CB	1.75	1.58
2:B:227:VAL:CB	2:B:227:VAL:CG1	1.81	1.56
1:A:10:GLN:CG	1:A:10:GLN:CB	1.80	1.54
2:B:56:PRO:CG	2:B:56:PRO:CB	1.77	1.43
2:B:287:MET:SD	2:B:287:MET:CE	2.06	1.43
1:A:63:THR:HG22	1:A:238:VAL:HG12	1.43	0.96
1:A:52:VAL:HG23	1:A:101:MET:SD	2.12	0.90
1:A:59:ALA:O	3:A:401:IAV:C1	2.20	0.88
1:A:52:VAL:CG2	1:A:101:MET:SD	2.66	0.83
1:A:59:ALA:O	3:A:401:IAV:HC1	1.79	0.80
2:B:227:VAL:CG1	2:B:227:VAL:CG2	2.58	0.80
2:B:371:LEU:CD2	2:B:371:LEU:CD1	2.59	0.78
2:B:167:LYS:CB	2:B:167:LYS:C	2.56	0.76
2:B:279:TYR:H	2:B:286:MET:HE1	1.55	0.72
1:A:241:ILE:HG23	1:A:251:MET:CE	2.19	0.71
1:A:241:ILE:HA	1:A:251:MET:HE2	1.73	0.70
1:A:77:THR:HB	1:A:78:PRO:HD2	1.75	0.68
2:B:279:TYR:N	2:B:286:MET:HE1	2.12	0.64
2:B:371:LEU:CD2	2:B:371:LEU:CB	2.72	0.64
1:A:176:LEU:HD11	1:A:196:LEU:HD23	1.81	0.62
1:A:52:VAL:HG21	1:A:101:MET:SD	2.40	0.61
1:A:52:VAL:HG21	1:A:101:MET:HE1	1.81	0.61
1:A:241:ILE:HG23	1:A:251:MET:HE2	1.82	0.60
1:A:22:PHE:C	1:A:22:PHE:CD1	2.80	0.59
1:A:241:ILE:HG23	1:A:251:MET:HE1	1.86	0.57
2:B:284:ALA:CB	2:B:284:ALA:N	2.62	0.56
1:A:31:GLU:O	1:A:35:LYS:HG3	2.05	0.56
2:B:284:ALA:CB	2:B:284:ALA:C	2.73	0.56
1:A:62:PRO:HA	1:A:65:GLN:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:GLU:HG3	2:B:243:ASP:OD1	2.07	0.55
1:A:217:PRO:HD2	5:A:450:HOH:O	2.06	0.54
1:A:22:PHE:HA	1:A:49:GLU:O	2.08	0.54
1:A:77:THR:HB	1:A:78:PRO:CD	2.38	0.54
1:A:241:ILE:CA	1:A:251:MET:HE2	2.37	0.53
1:A:63:THR:HG22	1:A:238:VAL:CG1	2.29	0.53
2:B:131:ARG:HG3	2:B:157:ILE:HD11	1.89	0.53
2:B:366:PRO:HG3	5:B:501:HOH:O	2.07	0.53
1:A:118:CYS:HB3	1:A:123:VAL:HB	1.89	0.53
1:A:203:TYR:O	1:A:204:HIS:HB2	2.07	0.53
1:A:52:VAL:HG21	1:A:101:MET:CE	2.39	0.52
2:B:216:ILE:O	2:B:216:ILE:HG13	2.10	0.50
1:A:10:GLN:CG	1:A:10:GLN:CA	2.81	0.49
1:A:61:GLY:C	1:A:65:GLN:HE21	2.21	0.49
2:B:95:ALA:HB1	2:B:126:LEU:HD12	1.93	0.49
2:B:165:THR:O	2:B:166:LEU:C	2.51	0.49
2:B:298:TYR:CD2	2:B:298:TYR:C	2.86	0.49
2:B:97:LEU:O	2:B:98:ALA:C	2.55	0.48
2:B:227:VAL:CG1	2:B:227:VAL:CA	2.83	0.48
1:A:66:ASN:O	1:A:70:ARG:HG3	2.14	0.48
2:B:298:TYR:CG	2:B:299:SER:N	2.80	0.47
2:B:294:ILE:N	2:B:294:ILE:HD13	2.30	0.47
2:B:287:MET:CE	2:B:287:MET:CG	2.91	0.47
2:B:166:LEU:O	2:B:167:LYS:C	2.58	0.47
2:B:162:GLY:HA3	2:B:168:ASP:OD1	2.15	0.47
2:B:140:GLU:O	2:B:140:GLU:HG3	2.16	0.46
2:B:131:ARG:NE	2:B:155:GLU:OE1	2.47	0.45
2:B:203:GLU:OE2	2:B:206:ARG:NH1	2.41	0.45
1:A:247:SER:N	1:A:248:PRO:CD	2.79	0.45
2:B:131:ARG:CG	2:B:157:ILE:HD11	2.47	0.45
2:B:48:LEU:O	2:B:52:TYR:HB3	2.17	0.45
1:A:241:ILE:CG2	1:A:251:MET:HE2	2.47	0.44
1:A:140:ARG:HH11	1:A:140:ARG:HD3	1.59	0.44
1:A:52:VAL:HG13	1:A:81:CYS:SG	2.56	0.44
1:A:176:LEU:CD1	1:A:196:LEU:HD23	2.48	0.43
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.53	0.43
2:B:6:ASN:HA	2:B:7:PRO:HD3	1.77	0.43
2:B:391:LEU:HD23	2:B:391:LEU:HA	1.74	0.43
2:B:95:ALA:CB	2:B:126:LEU:HD12	2.48	0.43
2:B:330:ASP:OD1	2:B:394:ARG:NH1	2.48	0.43
2:B:300:ILE:HD13	2:B:300:ILE:HG21	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ILE:HD11	1:A:48:LEU:HD11	2.00	0.42
1:A:78:PRO:O	1:A:81:CYS:HB2	2.19	0.42
2:B:306:PHE:HA	2:B:307:PRO:HD3	1.84	0.42
2:B:157:ILE:HG21	2:B:157:ILE:HD13	1.71	0.42
1:A:194:HIS:O	1:A:198:GLU:HG2	2.20	0.42
1:A:55:SER:HB3	2:B:293:GLN:HB3	2.01	0.42
1:A:244:ASN:HB3	1:A:251:MET:HB2	2.01	0.41
1:A:111:ILE:O	1:A:112:ASP:C	2.62	0.41
1:A:133:VAL:HG12	1:A:152:PHE:CD1	2.55	0.41
1:A:104:ASN:ND2	2:B:292:GLY:O	2.53	0.41
1:A:36:ILE:O	1:A:40:LEU:HG	2.20	0.41
1:A:155:PRO:HA	1:A:156:PRO:HD3	1.89	0.41
2:B:87:LYS:HE3	5:B:427:HOH:O	2.20	0.41
2:B:205:GLN:OE1	2:B:205:GLN:HA	2.21	0.41
2:B:16:TYR:O	2:B:281:GLY:HA2	2.20	0.40
1:A:6:ASN:O	1:A:10:GLN:HG3	2.21	0.40
2:B:188:LEU:HD21	2:B:280:PHE:CZ	2.56	0.40
2:B:256:GLU:HB3	2:B:257:PRO:HD2	2.04	0.40
1:A:216:SER:HB2	5:A:450:HOH:O	2.22	0.40
2:B:126:LEU:HD23	2:B:126:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	249/268 (93%)	239 (96%)	8 (3%)	2 (1%)	16	8
2	B	376/396 (95%)	367 (98%)	9 (2%)	0	100	100
All	All	625/664 (94%)	606 (97%)	17 (3%)	2 (0%)	36	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE
1	A	62	PRO

5.3.2 Protein sidechains ⓘ

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	198/208 (95%)	187 (94%)	11 (6%)	19	11
2	B	296/310 (96%)	286 (97%)	10 (3%)	32	25
All	All	494/518 (95%)	473 (96%)	21 (4%)	26	18

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	28	PRO
1	A	30	ILE
1	A	52	VAL
1	A	69	LEU
1	A	109	ASN
1	A	164	ARG
1	A	235	SER
1	A	243	LYS
1	A	247	SER
1	A	257	SER
2	B	20	ILE
2	B	140	GLU
2	B	143	SER
2	B	188	LEU
2	B	198	PRO
2	B	216	ILE
2	B	243	ASP
2	B	294	ILE
2	B	367	GLU
2	B	384	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	109	ASN
2	B	27	GLN
2	B	114	GLN
2	B	236	ASN
2	B	246	ASN
2	B	375	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	IAV	A	401	-	21,21,21	2.40	6 (28%)	29,29,29	2.96	13 (44%)
4	PLP	B	402	2	15,15,16	2.08	6 (40%)	21,22,23	3.33	10 (47%)

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
3	IAV	A	401	-	-	4/16/16/16	0/2/2/2
4	PLP	B	402	2	-	2/6/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	IAV	C7-C2	-5.93	1.34	1.44
3	A	401	IAV	O1-C10	5.30	1.33	1.23
3	A	401	IAV	O2-C12	4.85	1.36	1.22
4	B	402	PLP	C3-C2	-4.23	1.36	1.41
4	B	402	PLP	C6-N1	3.35	1.41	1.34
4	B	402	PLP	O3-C3	-2.91	1.30	1.36
4	B	402	PLP	O4P-C5A	-2.79	1.34	1.44
3	A	401	IAV	C8-N1	-2.78	1.33	1.37
3	A	401	IAV	O3-C12	2.66	1.39	1.30
4	B	402	PLP	P-O4P	-2.42	1.52	1.60
3	A	401	IAV	C5-C4	2.15	1.43	1.38
4	B	402	PLP	C4A-C4	-2.04	1.47	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	IAV	C11-N2-C10	-8.17	105.67	121.80
4	B	402	PLP	C6-C5-C4	7.59	124.32	118.10
4	B	402	PLP	C5A-C5-C6	-6.86	108.17	119.36
4	B	402	PLP	O4P-C5A-C5	6.65	121.83	109.36
4	B	402	PLP	C5-C6-N1	-6.24	113.68	123.83
3	A	401	IAV	C7-C2-C1	5.33	111.61	106.16
3	A	401	IAV	C2-C1-N1	-5.04	104.77	110.31
3	A	401	IAV	C9-C10-N2	4.92	124.72	116.31
3	A	401	IAV	C12-C11-N2	-4.70	99.86	110.17
3	A	401	IAV	C3-C7-C8	3.60	122.57	118.84
3	A	401	IAV	C9-C2-C1	-3.59	121.93	126.84
3	A	401	IAV	C13-C11-C12	-3.12	104.20	111.04
3	A	401	IAV	O1-C10-C9	-3.10	116.52	121.40
4	B	402	PLP	O2P-P-O4P	2.90	114.23	106.67
4	B	402	PLP	O3P-P-O4P	2.73	113.79	106.67
4	B	402	PLP	O3P-P-O2P	-2.64	97.89	107.80
3	A	401	IAV	O1-C10-N2	-2.53	118.67	122.95
4	B	402	PLP	C6-N1-C2	2.50	123.73	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	PLP	C5A-C5-C4	2.45	127.48	122.64
3	A	401	IAV	C5-C4-C3	2.38	123.17	120.24
4	B	402	PLP	C3-C4-C5	-2.28	115.85	118.59
3	A	401	IAV	C4-C3-C7	-2.19	115.84	119.80
3	A	401	IAV	C8-C7-C2	-2.17	104.97	107.17

There are no chirality outliers.

All (6) torsion outliers are listed below:

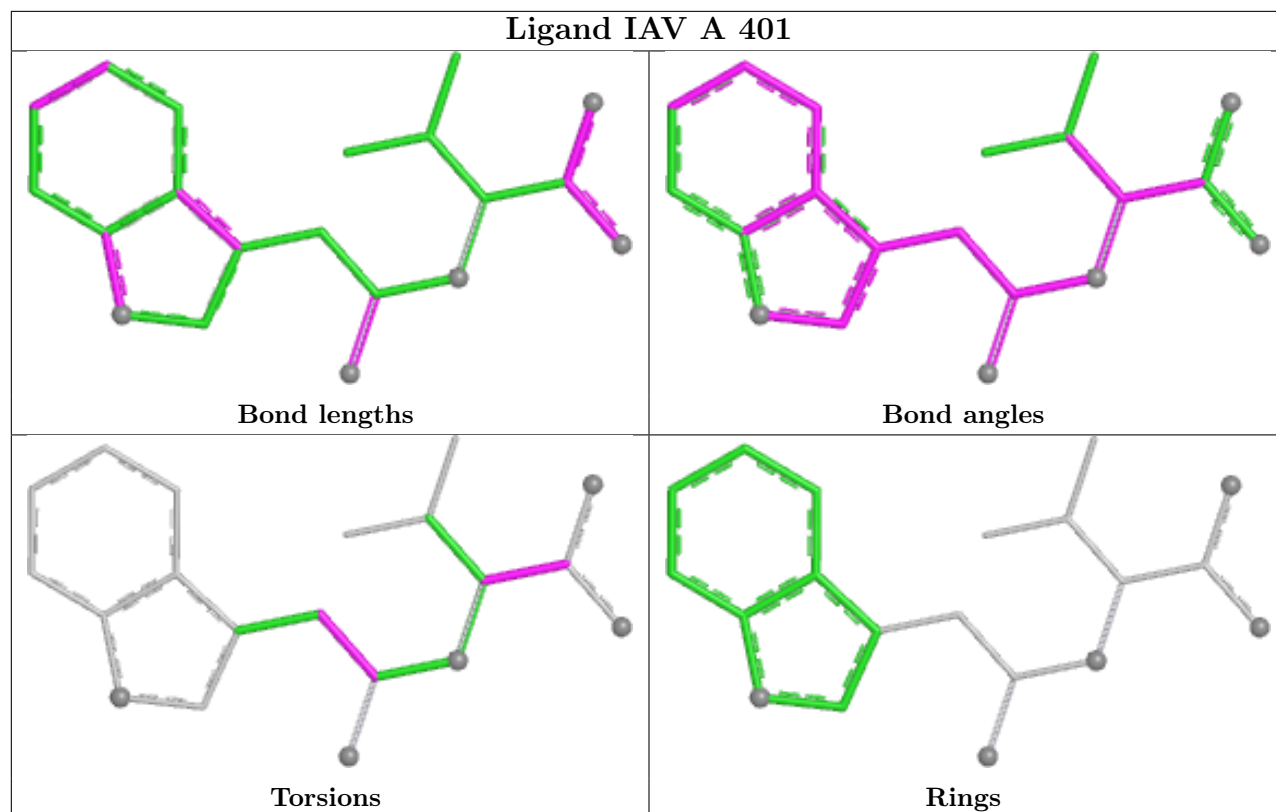
Mol	Chain	Res	Type	Atoms
3	A	401	IAV	N2-C10-C9-C2
4	B	402	PLP	C6-C5-C5A-O4P
3	A	401	IAV	C13-C11-C12-O2
3	A	401	IAV	C13-C11-C12-O3
4	B	402	PLP	C4-C5-C5A-O4P
3	A	401	IAV	O1-C10-C9-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	IAV	2	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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	253/268 (94%)	0.71	28 (11%)	10 11	28, 41, 66, 77	0
2	B	380/396 (95%)	0.20	21 (5%)	30 32	23, 33, 67, 86	0
All	All	633/664 (95%)	0.40	49 (7%)	19 21	23, 37, 67, 86	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	290	ALA	5.5
2	B	395	GLY	4.8
1	A	59	ALA	4.7
1	A	193	LEU	4.7
1	A	58	LEU	4.4
1	A	55	SER	4.4
1	A	78	PRO	4.4
1	A	109	ASN	4.3
1	A	61	GLY	3.9
2	B	162	GLY	3.8
1	A	1	MET	3.8
1	A	56	ASP	3.7
1	A	54	PHE	3.6
2	B	294	ILE	3.6
1	A	246	ALA	3.5
1	A	57	PRO	3.5
1	A	77	THR	3.4
1	A	60	ASP	3.4
1	A	194	HIS	3.3
1	A	69	LEU	3.3
2	B	297	SER	3.3
2	B	139	VAL	3.2
2	B	298	TYR	3.2
2	B	291	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	287	MET	3.0
1	A	62	PRO	2.9
2	B	164	ALA	2.8
1	A	108	ASN	2.8
1	A	248	PRO	2.7
2	B	391	LEU	2.7
1	A	73	ALA	2.6
2	B	260	HIS	2.6
2	B	385	PHE	2.5
2	B	393	ALA	2.5
2	B	286	MET	2.5
1	A	71	ALA	2.3
2	B	392	LYS	2.3
1	A	30	ILE	2.3
2	B	174	LEU	2.2
2	B	161	SER	2.2
1	A	195	HIS	2.2
1	A	245	LEU	2.2
1	A	72	PHE	2.2
1	A	203	TYR	2.2
1	A	239	LYS	2.2
2	B	2	THR	2.2
1	A	67	ALA	2.1
2	B	136	ALA	2.0
2	B	167	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

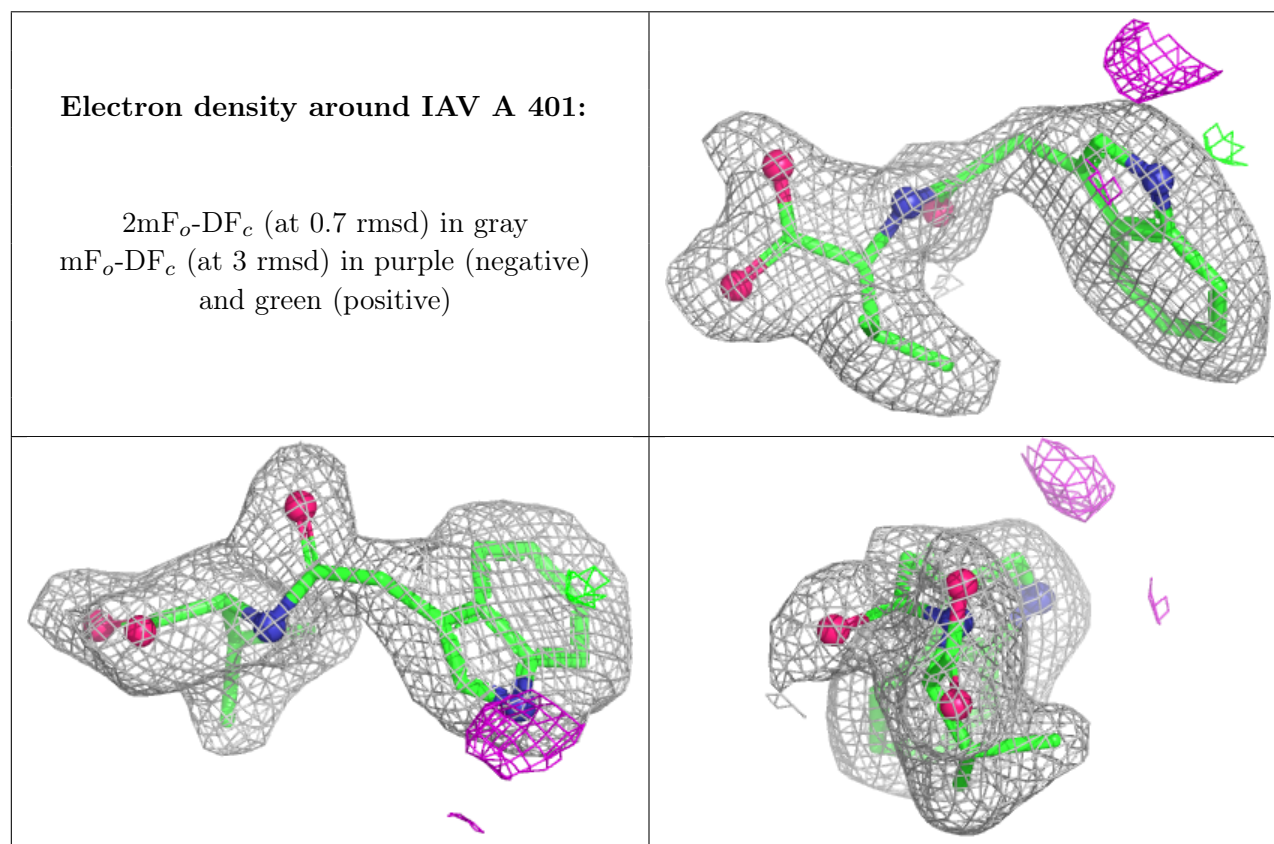
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IAV	A	401	20/20	0.91	0.09	38,46,52,54	0
4	PLP	B	402	15/16	0.98	0.05	22,28,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.