



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 04:08 AM EDT

PDB ID : 1K7F  
Title : CRYSTAL STRUCTURE OF WILD-TYPE TRYPTOPHAN SYNTHASE  
COMPLEXED WITH N-[1H-INDOL-3-YL-ACETYL]VALINE ACID  
Authors : Weyand, M.; Schlichting, I.; Marabotti, A.; Mozzarelli, A.  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

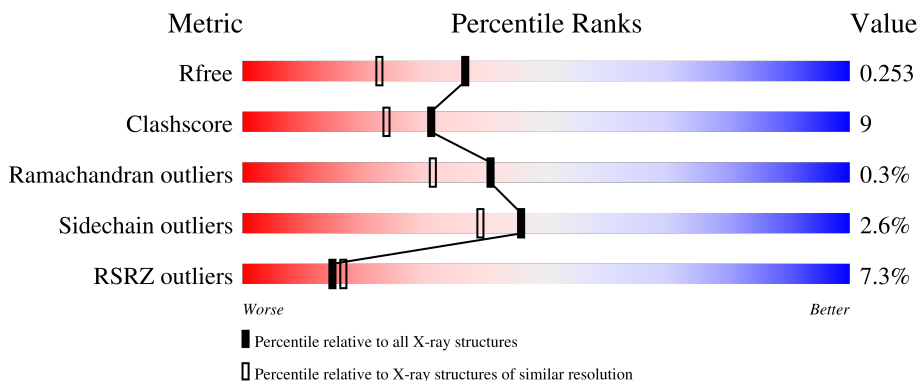
# 1 Overall quality at a glance

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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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  $\geq 3$ , 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	

## 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
			Total	C	N	O	S			
1	A	253	1911	1216	330	357	8	0	0	0

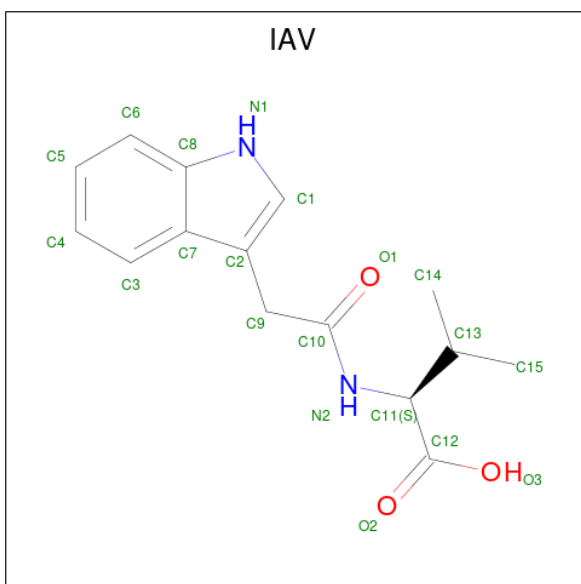
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

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

There is a discrepancy between the modelled and reference sequences:

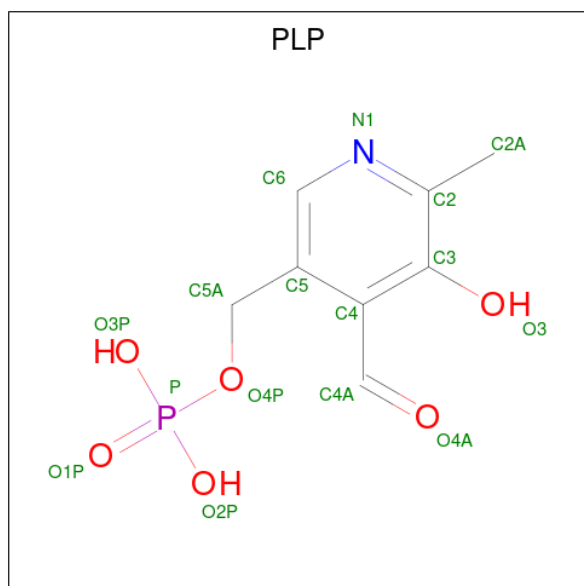
Chain	Residue	Modelled	Actual	Comment	Reference
B	34	SER	ARG	cloning artifact	UNP P0A2K1

- Molecule 3 is N-[1H-INDOL-3-YL-ACETYL]VALINE ACID (three-letter code: IAV) (formula: C<sub>15</sub>H<sub>18</sub>N<sub>2</sub>O<sub>3</sub>).



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

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

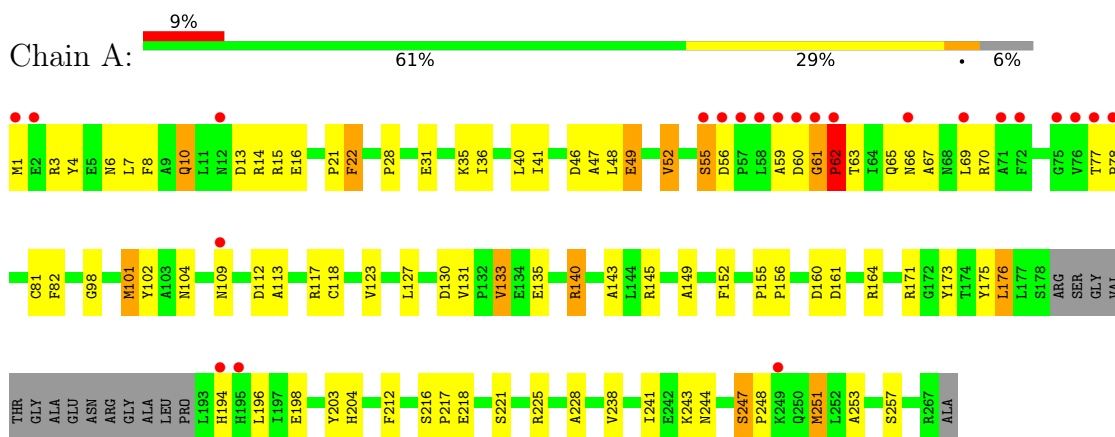
- Molecule 5 is water.

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

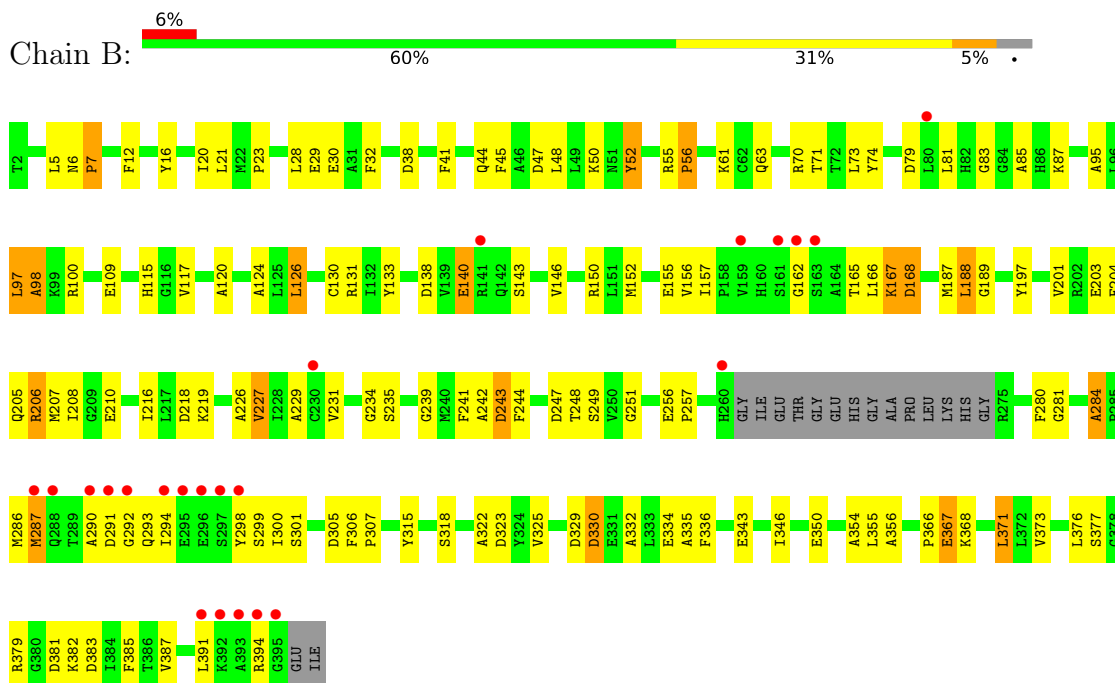
### 3 Residue-property plots i

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 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, $\alpha$ , $\beta$ , $\gamma$	183.66Å 59.07Å 67.47Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 43.67 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.8 (20.00-1.90) 93.8 (43.67-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.89Å)	Xtrriage
Refinement program	CNS, REFMAC	Depositor
R, $R_{free}$	0.197 , 0.251 0.198 , 0.253	Depositor DCC
$R_{free}$ test set	2684 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtrriage
Anisotropy	0.723	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 54.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.84	39/1948 (2.0%)	1.52	30/2646 (1.1%)
2	B	2.12	89/2919 (3.0%)	1.69	50/3944 (1.3%)
All	All	2.01	128/4867 (2.6%)	1.62	80/6590 (1.2%)

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	TYR	CE2-CZ	14.70	1.57	1.38
2	B	227	VAL	CB-CG1	13.41	1.81	1.52
2	B	41	PHE	CD1-CE1	11.43	1.62	1.39
1	A	133	VAL	CB-CG1	-10.79	1.30	1.52
2	B	284	ALA	CA-CB	10.79	1.75	1.52
2	B	167	LYS	CA-CB	10.75	1.77	1.53
2	B	204	PHE	CE2-CZ	10.62	1.57	1.37
2	B	30	GLU	CD-OE2	10.55	1.37	1.25
1	A	10	GLN	CB-CG	10.21	1.80	1.52
2	B	45	PHE	CG-CD1	9.94	1.53	1.38
2	B	197	TYR	CE1-CZ	9.69	1.51	1.38
2	B	231	VAL	CB-CG2	9.40	1.72	1.52
2	B	379	ARG	CZ-NH1	9.36	1.45	1.33
2	B	315	TYR	CD1-CE1	9.31	1.53	1.39
2	B	45	PHE	CE2-CZ	8.84	1.54	1.37
2	B	204	PHE	CD1-CE1	8.69	1.56	1.39
2	B	235	SER	CB-OG	8.63	1.53	1.42
2	B	30	GLU	CD-OE1	8.37	1.34	1.25
2	B	117	VAL	CB-CG2	7.94	1.69	1.52
2	B	74	TYR	CD2-CE2	7.93	1.51	1.39
2	B	242	ALA	CA-CB	7.83	1.68	1.52
1	A	135	GLU	CD-OE2	-7.77	1.17	1.25
2	B	63	GLN	CG-CD	7.74	1.68	1.51
2	B	241	PHE	CE2-CZ	7.71	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	ARG	CG-CD	7.64	1.71	1.51
2	B	98	ALA	CA-CB	7.55	1.68	1.52
1	A	149	ALA	CA-CB	7.55	1.68	1.52
1	A	173	TYR	CD1-CE1	7.49	1.50	1.39
2	B	325	VAL	CB-CG2	7.47	1.68	1.52
2	B	81	LEU	C-O	7.42	1.37	1.23
1	A	55	SER	CB-OG	7.38	1.51	1.42
2	B	30	GLU	CG-CD	7.32	1.62	1.51
2	B	336	PHE	CD2-CE2	7.28	1.53	1.39
2	B	56	PRO	N-CD	7.13	1.57	1.47
2	B	229	ALA	CA-CB	7.10	1.67	1.52
1	A	164	ARG	CZ-NH1	7.08	1.42	1.33
2	B	382	LYS	CB-CG	6.89	1.71	1.52
2	B	247	ASP	C-O	6.82	1.36	1.23
1	A	173	TYR	CD2-CE2	6.80	1.49	1.39
2	B	32	PHE	CG-CD1	-6.77	1.28	1.38
2	B	150	ARG	CZ-NH2	6.70	1.41	1.33
1	A	218	GLU	CD-OE2	6.68	1.33	1.25
2	B	204	PHE	CD2-CE2	6.65	1.52	1.39
1	A	82	PHE	CB-CG	6.61	1.62	1.51
2	B	367	GLU	C-O	6.60	1.35	1.23
2	B	332	ALA	CA-CB	6.60	1.66	1.52
2	B	371	LEU	CG-CD2	6.58	1.76	1.51
2	B	290	ALA	CA-CB	6.58	1.66	1.52
1	A	10	GLN	C-O	6.57	1.35	1.23
2	B	226	ALA	CA-CB	-6.53	1.38	1.52
2	B	120	ALA	CA-CB	6.21	1.65	1.52
1	A	225	ARG	CG-CD	6.19	1.67	1.51
2	B	124	ALA	CA-CB	6.17	1.65	1.52
2	B	373	VAL	CB-CG1	6.14	1.65	1.52
2	B	187	MET	CB-CG	6.10	1.70	1.51
2	B	30	GLU	CA-CB	6.10	1.67	1.53
2	B	241	PHE	CG-CD1	6.07	1.47	1.38
1	A	98	GLY	C-O	6.01	1.33	1.23
1	A	3	ARG	CG-CD	5.99	1.67	1.51
2	B	208	ILE	CA-CB	5.96	1.68	1.54
2	B	248	THR	CA-CB	5.93	1.68	1.53
1	A	161	ASP	CG-OD2	5.90	1.39	1.25
1	A	102	TYR	CE2-CZ	-5.88	1.30	1.38
1	A	60	ASP	C-O	5.88	1.34	1.23
1	A	228	ALA	CA-CB	5.88	1.64	1.52
2	B	368	LYS	N-CA	5.83	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	231	VAL	CB-CG1	5.82	1.65	1.52
2	B	29	GLU	CB-CG	5.80	1.63	1.52
2	B	12	PHE	CD2-CE2	5.76	1.50	1.39
2	B	334	GLU	CG-CD	5.75	1.60	1.51
2	B	52	TYR	CE2-CZ	-5.71	1.31	1.38
1	A	164	ARG	NE-CZ	5.69	1.40	1.33
1	A	67	ALA	CA-CB	5.68	1.64	1.52
2	B	330	ASP	CB-CG	5.66	1.63	1.51
2	B	44	GLN	CG-CD	5.66	1.64	1.51
1	A	117	ARG	CG-CD	5.63	1.66	1.51
2	B	197	TYR	CG-CD1	5.62	1.46	1.39
2	B	83	GLY	C-O	5.59	1.32	1.23
2	B	249	SER	CB-OG	5.58	1.49	1.42
2	B	56	PRO	CB-CG	5.58	1.77	1.50
2	B	377	SER	CA-CB	5.56	1.61	1.52
2	B	146	VAL	CA-CB	5.55	1.66	1.54
2	B	346	ILE	CB-CG2	5.51	1.70	1.52
1	A	113	ALA	CA-CB	-5.50	1.40	1.52
2	B	61	LYS	CE-NZ	5.49	1.62	1.49
2	B	133	TYR	CE1-CZ	-5.45	1.31	1.38
1	A	47	ALA	CA-CB	5.45	1.63	1.52
2	B	204	PHE	CE1-CZ	-5.45	1.26	1.37
1	A	143	ALA	CA-CB	5.43	1.63	1.52
2	B	234	GLY	C-O	5.43	1.32	1.23
1	A	16	GLU	CD-OE2	5.42	1.31	1.25
2	B	387	VAL	CB-CG2	5.42	1.64	1.52
1	A	175	TYR	CD1-CE1	5.41	1.47	1.39
2	B	85	ALA	CA-CB	5.40	1.63	1.52
2	B	32	PHE	CD1-CE1	5.40	1.50	1.39
2	B	50	LYS	CE-NZ	5.37	1.62	1.49
2	B	130	CYS	CB-SG	-5.36	1.73	1.81
1	A	221	SER	C-O	5.36	1.33	1.23
1	A	22	PHE	CG-CD1	5.33	1.46	1.38
1	A	218	GLU	CG-CD	5.29	1.59	1.51
2	B	354	ALA	CA-CB	5.28	1.63	1.52
1	A	253	ALA	CA-CB	5.28	1.63	1.52
2	B	152	MET	SD-CE	-5.27	1.48	1.77
2	B	251	GLY	CA-C	5.25	1.60	1.51
2	B	201	VAL	CB-CG1	5.24	1.63	1.52
2	B	5	LEU	C-O	5.24	1.33	1.23
1	A	49	GLU	C-O	5.23	1.33	1.23
1	A	8	PHE	CD1-CE1	5.20	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	385	PHE	CB-CG	-5.17	1.42	1.51
2	B	239	GLY	CA-C	5.16	1.60	1.51
1	A	112	ASP	CB-CG	-5.15	1.41	1.51
1	A	22	PHE	CE2-CZ	5.14	1.47	1.37
2	B	335	ALA	CA-CB	5.14	1.63	1.52
1	A	131	VAL	CB-CG1	5.10	1.63	1.52
2	B	251	GLY	C-O	5.09	1.31	1.23
2	B	133	TYR	CE2-CZ	5.08	1.45	1.38
2	B	301	SER	CB-OG	-5.08	1.35	1.42
1	A	15	ARG	C-O	5.07	1.32	1.23
2	B	287	MET	SD-CE	5.06	2.06	1.77
2	B	244	PHE	CE1-CZ	5.05	1.47	1.37
1	A	164	ARG	CB-CG	5.05	1.66	1.52
1	A	21	PRO	CG-CD	5.05	1.67	1.50
2	B	23	PRO	CG-CD	5.04	1.67	1.50
2	B	318	SER	CA-CB	5.03	1.60	1.52
2	B	356	ALA	CA-CB	5.03	1.63	1.52
2	B	376	LEU	C-O	5.03	1.32	1.23
2	B	156	VAL	CB-CG2	5.03	1.63	1.52
2	B	322	ALA	C-O	5.02	1.32	1.23

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	168	ASP	CB-CG-OD2	12.15	129.23	118.30
2	B	97	LEU	CB-CG-CD2	-10.93	92.42	111.00
1	A	56	ASP	CB-CG-OD2	10.84	128.06	118.30
2	B	55	ARG	NE-CZ-NH1	10.39	125.50	120.30
2	B	70	ARG	NE-CZ-NH1	-10.35	115.12	120.30
2	B	126	LEU	CB-CG-CD1	-9.35	95.10	111.00
2	B	79	ASP	CB-CG-OD2	8.94	126.35	118.30
2	B	315	TYR	CD1-CE1-CZ	-8.93	111.76	119.80
1	A	13	ASP	CB-CG-OD2	8.77	126.19	118.30
2	B	383	ASP	CB-CG-OD2	8.35	125.82	118.30
2	B	305	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	171	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	62	PRO	N-CA-C	7.91	132.67	112.10
2	B	38	ASP	CB-CG-OD1	7.85	125.36	118.30
1	A	130	ASP	CB-CG-OD2	7.79	125.31	118.30
2	B	55	ARG	CA-CB-CG	7.72	130.39	113.40
2	B	355	LEU	CB-CG-CD1	-7.66	97.98	111.00
2	B	219	LYS	CD-CE-NZ	-7.62	94.17	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	100	ARG	NE-CZ-NH1	-7.56	116.52	120.30
2	B	227	VAL	CG1-CB-CG2	-7.30	99.22	110.90
2	B	379	ARG	NE-CZ-NH1	7.18	123.89	120.30
2	B	100	ARG	NE-CZ-NH2	7.17	123.89	120.30
2	B	241	PHE	CB-CG-CD2	-7.07	115.85	120.80
1	A	164	ARG	NE-CZ-NH2	-7.00	116.80	120.30
2	B	188	LEU	CA-CB-CG	6.97	131.33	115.30
2	B	188	LEU	CB-CG-CD2	-6.94	99.21	111.00
2	B	368	LYS	N-CA-CB	-6.93	98.13	110.60
1	A	101	MET	CG-SD-CE	-6.67	89.54	100.20
2	B	206	ARG	NE-CZ-NH1	6.65	123.63	120.30
2	B	376	LEU	CB-CG-CD2	-6.56	99.84	111.00
2	B	376	LEU	CB-CG-CD1	-6.49	99.97	111.00
1	A	56	ASP	CB-CG-OD1	-6.47	112.48	118.30
1	A	164	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	221	SER	O-C-N	6.46	133.03	122.70
2	B	32	PHE	CB-CG-CD1	-6.45	116.29	120.80
1	A	61	GLY	CA-C-O	-6.44	109.01	120.60
2	B	32	PHE	CD1-CE1-CZ	-6.40	112.42	120.10
2	B	330	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	133	VAL	CG1-CB-CG2	-6.40	100.66	110.90
2	B	28	LEU	CB-CG-CD1	-6.39	100.14	111.00
2	B	218	ASP	CB-CG-OD2	6.38	124.05	118.30
2	B	55	ARG	NE-CZ-NH2	-6.25	117.18	120.30
2	B	286	MET	CB-CG-SD	6.24	131.13	112.40
1	A	101	MET	CA-CB-CG	6.22	123.88	113.30
1	A	117	ARG	NE-CZ-NH1	6.17	123.39	120.30
2	B	329	ASP	CB-CG-OD1	6.14	123.83	118.30
2	B	291	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	140	ARG	NE-CZ-NH1	-6.13	117.23	120.30
2	B	29	GLU	OE1-CD-OE2	-6.13	115.94	123.30
1	A	251	MET	CG-SD-CE	6.13	110.01	100.20
1	A	7	LEU	CA-CB-CG	-6.07	101.34	115.30
2	B	97	LEU	CB-CG-CD1	6.04	121.27	111.00
1	A	46	ASP	CB-CG-OD2	5.97	123.67	118.30
2	B	138	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	4	TYR	CD1-CE1-CZ	-5.95	114.45	119.80
1	A	14	ARG	NE-CZ-NH1	-5.94	117.33	120.30
2	B	381	ASP	CB-CG-OD2	5.91	123.62	118.30
2	B	81	LEU	CB-CG-CD1	-5.91	100.95	111.00
1	A	176	LEU	CB-CG-CD2	-5.86	101.04	111.00
2	B	47	ASP	CB-CG-OD2	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	97	LEU	CA-CB-CG	5.71	128.43	115.30
1	A	160	ASP	CB-CG-OD2	5.70	123.43	118.30
2	B	323	ASP	CB-CG-OD1	5.67	123.40	118.30
2	B	7	PRO	N-CD-CG	-5.63	94.75	103.20
2	B	379	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	112	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	A	145	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	60	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	52	VAL	CB-CA-C	-5.38	101.18	111.40
2	B	73	LEU	CD1-CG-CD2	-5.34	94.49	110.50
2	B	168	ASP	CB-CG-OD1	-5.34	113.50	118.30
2	B	329	ASP	CB-CG-OD2	-5.31	113.52	118.30
2	B	343	GLU	CG-CD-OE1	5.21	128.73	118.30
2	B	350	GLU	CA-CB-CG	5.18	124.79	113.40
1	A	60	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	127	LEU	CB-CG-CD2	5.17	119.78	111.00
2	B	71	THR	N-CA-CB	-5.13	100.56	110.30
1	A	1	MET	CG-SD-CE	5.11	108.37	100.20
1	A	60	ASP	OD1-CG-OD2	-5.08	113.64	123.30
2	B	21	LEU	CB-CG-CD2	-5.03	102.44	111.00

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	42	0
2	B	2866	0	2835	47	0
3	A	20	0	18	2	0
4	B	15	0	6	0	0
5	A	51	0	0	2	0
5	B	99	0	0	2	0
All	All	4962	0	4778	87	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 9.

All (87) 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	0.72
1:A:241:ILE:HG23	1:A:251:MET:CE	2.19	0.71
1:A:241:ILE:HA	1:A:251:MET:HE2	1.71	0.70
1:A:77:THR:HB	1:A:78:PRO:HD2	1.75	0.68
1:A:241:ILE:HG23	1:A:251:MET:HE1	1.78	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
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
1:A:62:PRO:HA	1:A:65:GLN:HB2	1.87	0.55
2:B:210:GLU:HG3	2:B:243:ASP:OD1	2.07	0.55
1:A:22:PHE:C	1:A:22:PHE:CD1	2.80	0.54
1:A:217:PRO:HD2	5:A:450:HOH:O	2.06	0.54
1:A:241:ILE:CA	1:A:251:MET:HE2	2.37	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: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:241:ILE:HG23	1:A:251:MET:HE2	1.90	0.53
1:A:52:VAL:HG21	1:A:101:MET:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ALA:CB	2:B:284:ALA:C	2.73	0.51
2:B:216:ILE:HG13	2:B:216:ILE:O	2.10	0.50
1:A:10:GLN:CG	1:A:10:GLN:CA	2.81	0.49
2:B:95:ALA:HB1	2:B:126:LEU:HD12	1.93	0.49
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:165:THR:O	2:B:166:LEU:C	2.51	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: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:61:GLY:C	1:A:65:GLN:HE21	2.21	0.44
1:A:140:ARG:HH11	1:A:140:ARG:HD3	1.59	0.44
2:B:298:TYR:CD2	2:B:298:TYR:C	2.86	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:97:LEU:O	2:B:98:ALA:C	2.55	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
1:A:41:ILE:HD11	1:A:48:LEU:HD11	2.00	0.42
2:B:166:LEU:O	2:B:167:LYS:C	2.58	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	249/268 (93%)	239 (96%)	8 (3%)	2 (1%)	19	9
2	B	376/396 (95%)	367 (98%)	9 (2%)	0	100	100
All	All	625/664 (94%)	606 (97%)	17 (3%)	2 (0%)	41	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE
1	A	62	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	198/208 (95%)	192 (97%)	6 (3%)	41	33
2	B	296/310 (96%)	289 (98%)	7 (2%)	49	43
All	All	494/518 (95%)	481 (97%)	13 (3%)	46	39

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PRO
1	A	69	LEU
1	A	109	ASN
1	A	243	LYS
1	A	247	SER
1	A	257	SER
2	B	20	ILE
2	B	109	GLU
2	B	140	GLU
2	B	143	SER
2	B	207	MET
2	B	243	ASP
2	B	367	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	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 monosaccharides 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
4	PLP	B	402	2	15,15,16	2.06	5 (33%)	20,22,23	3.37	9 (45%)
3	IAV	A	401	-	20,21,21	2.07	5 (25%)	23,29,29	2.89	8 (34%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	IAV	O1-C10	5.17	1.33	1.23
3	A	401	IAV	O2-C12	4.69	1.36	1.22
4	B	402	PLP	C3-C2	-4.32	1.36	1.40
4	B	402	PLP	C6-N1	3.23	1.41	1.34
4	B	402	PLP	O3-C3	-2.90	1.30	1.37
4	B	402	PLP	O4P-C5A	-2.79	1.34	1.45
3	A	401	IAV	O3-C12	2.61	1.39	1.30
4	B	402	PLP	P-O4P	-2.34	1.52	1.60
3	A	401	IAV	C5-C6	2.26	1.41	1.36
3	A	401	IAV	C3-C7	-2.21	1.37	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	IAV	C11-N2-C10	-8.44	105.67	121.83
4	B	402	PLP	C6-C5-C4	7.83	124.32	118.16
4	B	402	PLP	C5A-C5-C6	-6.81	108.17	119.37
4	B	402	PLP	O4P-C5A-C5	6.55	121.83	109.35
4	B	402	PLP	C5-C6-N1	-6.09	113.68	123.82
3	A	401	IAV	C9-C10-N2	5.49	124.72	115.88
3	A	401	IAV	C12-C11-N2	-4.77	99.86	110.28
3	A	401	IAV	C4-C3-C7	-3.64	115.84	120.89
3	A	401	IAV	C3-C7-C8	3.32	122.57	118.17
3	A	401	IAV	C13-C11-C12	-3.01	104.20	111.05
4	B	402	PLP	O2P-P-O4P	2.82	114.23	106.73
4	B	402	PLP	C3-C4-C5	-2.67	115.85	118.74
4	B	402	PLP	O3P-P-O4P	2.65	113.79	106.73
4	B	402	PLP	O3P-P-O2P	-2.55	97.89	107.64
3	A	401	IAV	O1-C10-N2	-2.54	118.67	122.95
4	B	402	PLP	C6-N1-C2	2.46	123.73	119.17
3	A	401	IAV	O1-C10-C9	-2.42	116.52	122.03

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

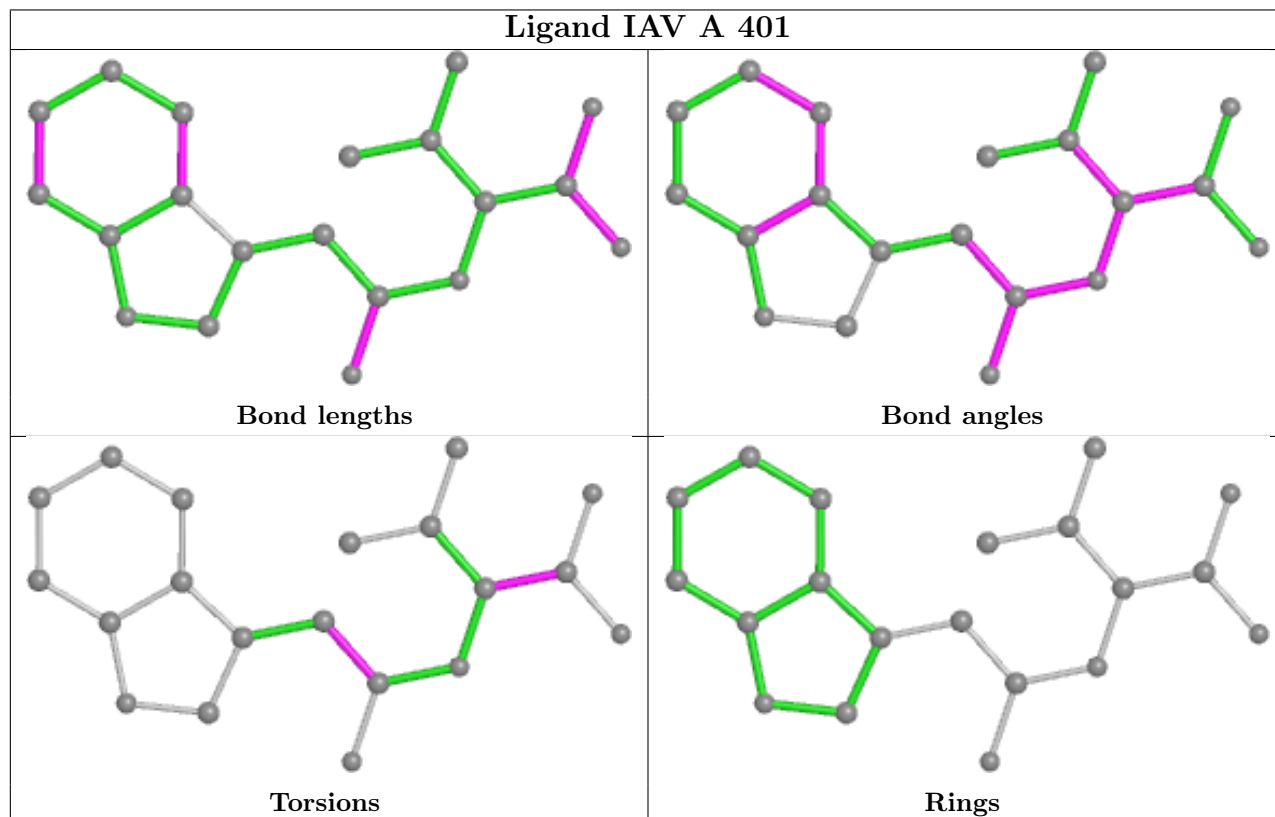
There are no ring outliers.

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	253/268 (94%)	0.38	23 (9%) <b>9</b> <b>10</b>	28, 41, 66, 77	0
2	B	380/396 (95%)	0.37	23 (6%) <b>21</b> <b>24</b>	23, 33, 67, 86	0
All	All	633/664 (95%)	0.38	46 (7%) <b>15</b> <b>16</b>	23, 37, 67, 86	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	294	ILE	6.3
1	A	61	GLY	5.9
1	A	55	SER	5.6
1	A	72	PHE	5.6
2	B	298	TYR	4.7
1	A	71	ALA	4.6
2	B	291	ASP	4.6
2	B	297	SER	4.3
1	A	69	LEU	4.3
2	B	296	GLU	4.2
1	A	59	ALA	4.2
1	A	78	PRO	4.2
1	A	58	LEU	4.0
2	B	295	GLU	3.9
1	A	56	ASP	3.9
2	B	163	SER	3.9
2	B	162	GLY	3.8
1	A	109	ASN	3.7
1	A	1	MET	3.5
2	B	161	SER	3.5
1	A	195	HIS	3.4
2	B	287	MET	3.4
2	B	141	ARG	3.4
1	A	194	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	292	GLY	3.2
2	B	392	LYS	3.1
1	A	66	ASN	3.0
1	A	62	PRO	3.0
2	B	290	ALA	2.9
1	A	77	THR	2.8
1	A	60	ASP	2.8
2	B	394	ARG	2.8
2	B	395	GLY	2.8
2	B	260	HIS	2.5
1	A	76	VAL	2.5
2	B	391	LEU	2.5
2	B	288	GLN	2.4
1	A	75	GLY	2.4
1	A	57	PRO	2.2
2	B	230	CYS	2.2
1	A	2	GLU	2.2
2	B	159	VAL	2.2
1	A	12	ASN	2.1
2	B	393	ALA	2.1
2	B	80	LEU	2.1
1	A	249	LYS	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

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, 95<sup>th</sup> 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.

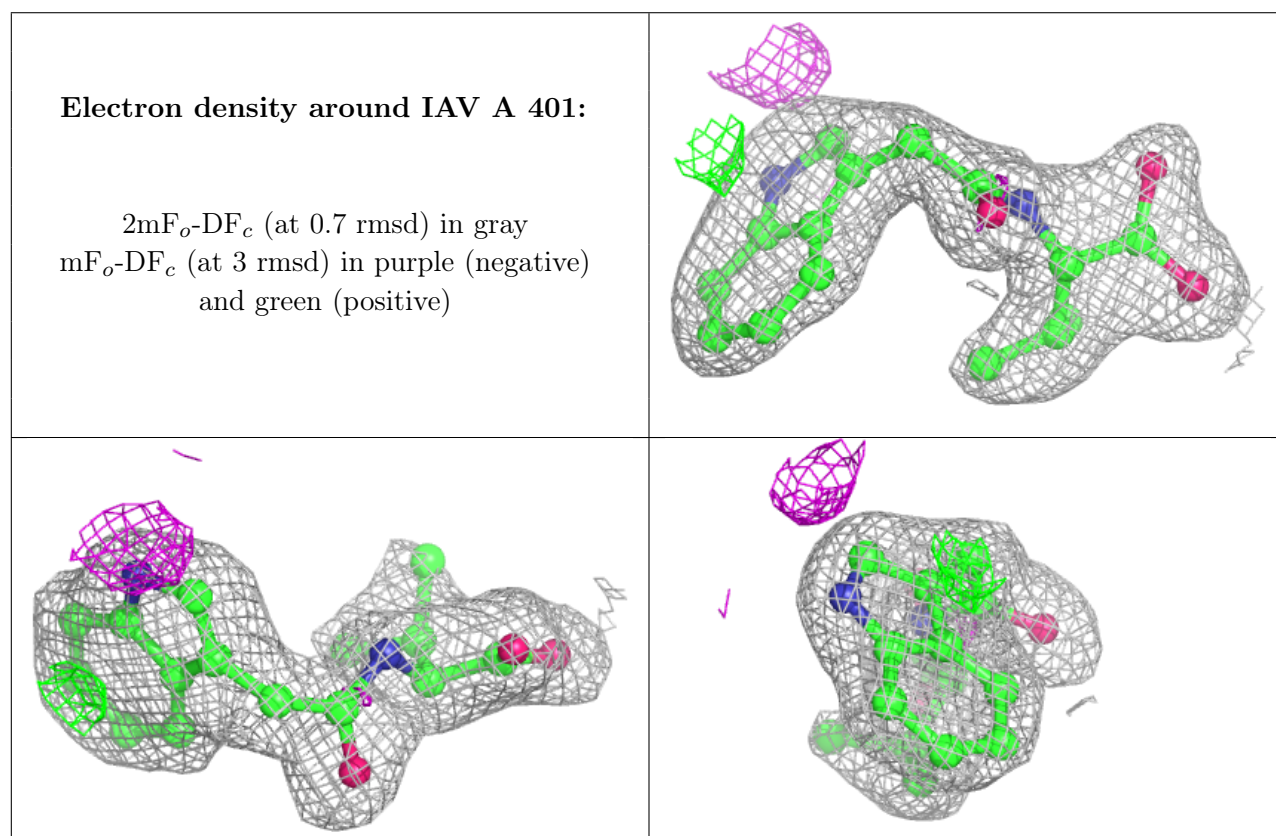
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	IAV	A	401	20/20	0.93	0.12	38,46,52,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PLP	B	402	15/16	0.99	0.13	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.