



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 05:50 pm BST

PDB ID : 1KFJ
Title : CRYSTAL STRUCTURE OF WILD-TYPE TRYPTOPHAN SYNTHASE
COMPLEXED WITH L-SERINE
Authors : Kulik, V.; Weyand, M.; Seidel, R.; Niks, D.; Arac, D.; Dunn, M.F.; Schlichting,
I.
Deposited on : 2001-11-21
Resolution : 1.80 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 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)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

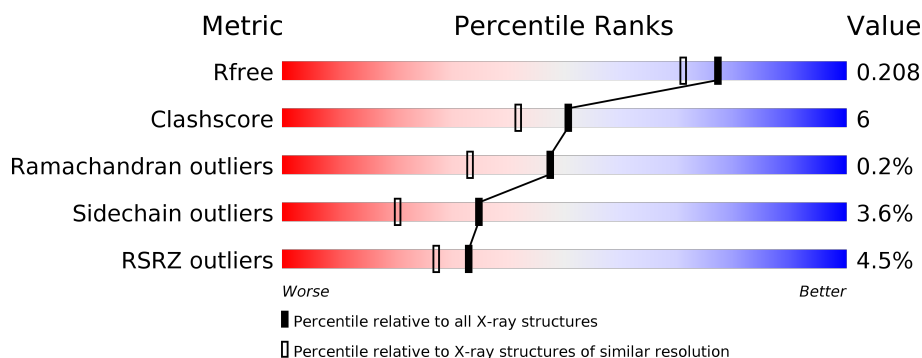
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>21%</div> <div>•</div> <div>6%</div> </div> </div>
2	B	397	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>...</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5259 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
			1912	1218	330	356	8			

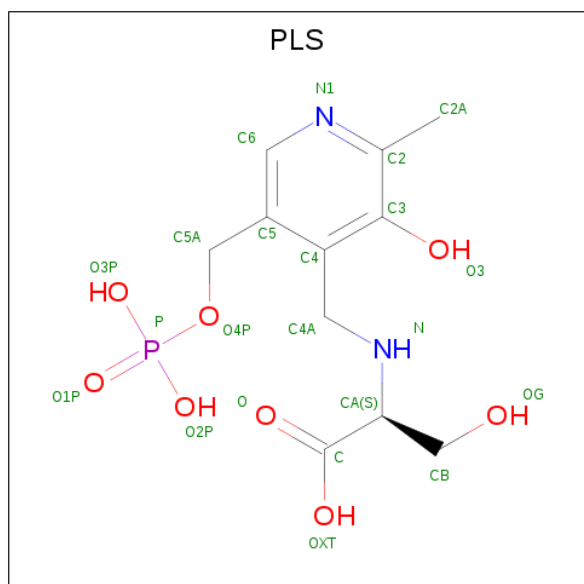
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	0	0
			2981	1873	524	565	19			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is [3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (three-letter code: PLS) (formula: C₁₁H₁₇N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

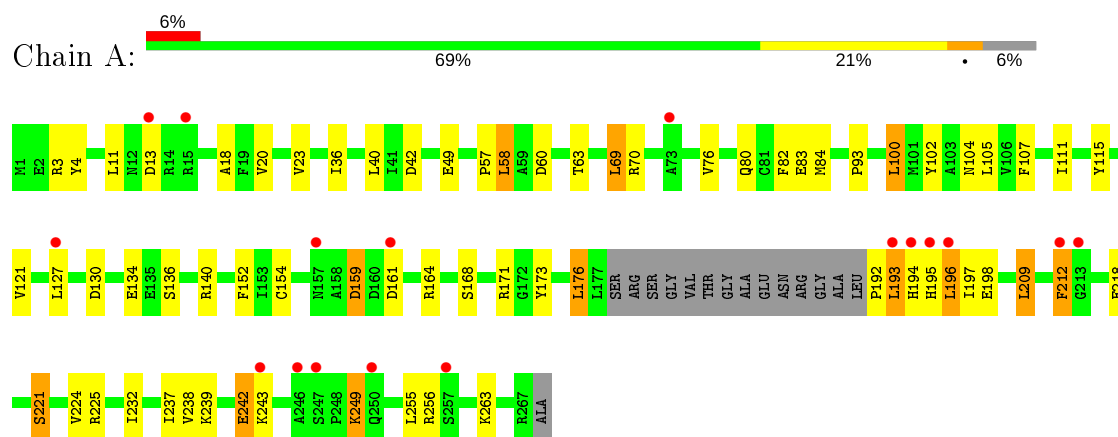
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	235	Total	O	0	0
			235	235		

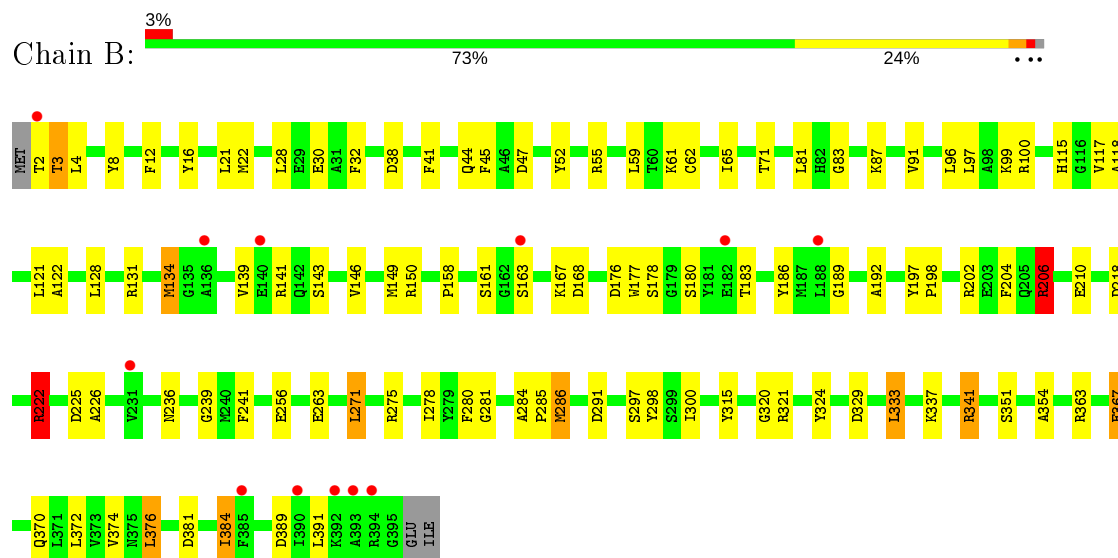
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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	183.23 Å 59.68 Å 67.46 Å 90.00° 94.65° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 29.25 – 1.81	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-1.80) 97.0 (29.25-1.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.80 Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.174 , 0.211 0.170 , 0.208	Depositor DCC
R_{free} test set	3267 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5259	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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

5.1 Standard geometry

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

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	1.27	9/1950 (0.5%)	1.84	48/2649 (1.8%)
2	B	1.55	24/3039 (0.8%)	2.05	83/4105 (2.0%)
All	All	1.45	33/4989 (0.7%)	1.97	131/6754 (1.9%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	TYR	CD2-CE2	14.17	1.60	1.39
2	B	291	ASP	CB-CG	-10.20	1.30	1.51
2	B	374	VAL	CB-CG2	8.33	1.70	1.52
1	A	221	SER	CA-CB	8.32	1.65	1.52
2	B	256	GLU	CD-OE1	7.74	1.34	1.25
2	B	41	PHE	CD1-CE1	7.57	1.54	1.39
1	A	82	PHE	CD1-CE1	7.28	1.53	1.39
2	B	239	GLY	C-O	7.01	1.34	1.23
2	B	204	PHE	CE2-CZ	6.83	1.50	1.37
2	B	149	MET	CG-SD	6.57	1.98	1.81
2	B	286	MET	CG-SD	-6.32	1.64	1.81
2	B	96	LEU	C-O	6.31	1.35	1.23
2	B	139	VAL	CB-CG2	5.96	1.65	1.52
1	A	111	ILE	CA-CB	5.92	1.68	1.54
2	B	320	GLY	C-O	-5.78	1.14	1.23
2	B	177	TRP	CE3-CZ3	-5.71	1.28	1.38
2	B	8	TYR	CD2-CE2	5.69	1.47	1.39
1	A	136	SER	CB-OG	5.60	1.49	1.42
2	B	97	LEU	CG-CD2	5.51	1.72	1.51
2	B	45	PHE	CE1-CZ	5.49	1.47	1.37
2	B	370	GLN	CG-CD	5.37	1.63	1.51
1	A	82	PHE	CE2-CZ	5.29	1.47	1.37
2	B	372	LEU	CA-C	5.28	1.66	1.52
1	A	20	VAL	CB-CG1	5.28	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	VAL	CB-CG2	5.26	1.63	1.52
2	B	354	ALA	CA-CB	5.21	1.63	1.52
2	B	192	ALA	CA-CB	5.16	1.63	1.52
2	B	141	ARG	C-O	5.14	1.33	1.23
2	B	177	TRP	CZ3-CH2	5.13	1.48	1.40
2	B	351	SER	CA-CB	5.12	1.60	1.52
1	A	3	ARG	CG-CD	5.10	1.64	1.51
1	A	115	TYR	CD2-CE2	-5.01	1.31	1.39
2	B	61	LYS	CB-CG	5.00	1.66	1.52

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	291	ASP	CB-CG-OD1	-37.87	84.22	118.30
2	B	206	ARG	NE-CZ-NH1	26.15	133.38	120.30
2	B	206	ARG	NE-CZ-NH2	-16.05	112.28	120.30
1	A	140	ARG	NE-CZ-NH1	-14.14	113.23	120.30
2	B	286	MET	CA-CB-CG	-13.95	89.58	113.30
2	B	291	ASP	OD1-CG-OD2	13.09	148.17	123.30
1	A	159	ASP	CB-CG-OD2	11.82	128.94	118.30
1	A	164	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	A	164	ARG	NE-CZ-NH2	-11.57	114.52	120.30
2	B	206	ARG	CD-NE-CZ	11.19	139.26	123.60
2	B	176	ASP	CB-CG-OD2	10.90	128.11	118.30
2	B	329	ASP	CB-CG-OD1	10.71	127.94	118.30
2	B	291	ASP	CB-CG-OD2	10.34	127.61	118.30
2	B	225	ASP	CB-CG-OD2	9.67	127.00	118.30
2	B	315	TYR	CG-CD2-CE2	-9.56	113.65	121.30
1	A	42	ASP	CB-CG-OD2	9.42	126.78	118.30
2	B	376	LEU	CB-CG-CD1	-9.21	95.34	111.00
2	B	291	ASP	N-CA-CB	-8.97	94.44	110.60
2	B	141	ARG	NE-CZ-NH2	-8.80	115.90	120.30
2	B	62	CYS	CA-CB-SG	-8.79	98.17	114.00
1	A	176	LEU	CB-CG-CD2	-8.75	96.12	111.00
1	A	159	ASP	CB-CG-OD1	-8.74	110.43	118.30
1	A	171	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	A	130	ASP	CB-CG-OD2	8.54	125.99	118.30
2	B	341	ARG	NE-CZ-NH2	-8.54	116.03	120.30
2	B	168	ASP	CB-CG-OD2	8.41	125.86	118.30
1	A	42	ASP	CB-CG-OD1	-8.20	110.92	118.30
2	B	363	ARG	NE-CZ-NH1	8.18	124.39	120.30
2	B	291	ASP	CB-CA-C	-8.06	94.28	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	GLU	OE1-CD-OE2	7.97	132.86	123.30
1	A	176	LEU	CB-CG-CD1	-7.61	98.07	111.00
2	B	286	MET	CG-SD-CE	-7.57	88.09	100.20
1	A	134	GLU	OE1-CD-OE2	-7.56	114.22	123.30
2	B	45	PHE	CB-CG-CD2	-7.55	115.51	120.80
2	B	241	PHE	CB-CG-CD2	-7.49	115.55	120.80
2	B	372	LEU	CB-CG-CD1	-7.48	98.28	111.00
2	B	263	GLU	CG-CD-OE2	-7.43	103.45	118.30
1	A	11	LEU	CB-CG-CD1	-7.42	98.38	111.00
2	B	168	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	A	107	PHE	CB-CG-CD2	-7.25	115.73	120.80
2	B	315	TYR	CB-CG-CD1	-7.23	116.66	121.00
2	B	47	ASP	CB-CG-OD2	7.21	124.79	118.30
1	A	171	ARG	NE-CZ-NH1	7.03	123.81	120.30
2	B	100	ARG	NE-CZ-NH1	-6.95	116.83	120.30
1	A	69	LEU	CB-CG-CD1	6.94	122.80	111.00
2	B	367	GLU	CG-CD-OE1	-6.94	104.42	118.30
2	B	384	ILE	CA-CB-CG1	-6.91	97.88	111.00
2	B	4	LEU	CB-CG-CD1	-6.87	99.32	111.00
2	B	367	GLU	CG-CD-OE2	6.87	132.04	118.30
2	B	186	TYR	CG-CD1-CE1	6.85	126.78	121.30
1	A	13	ASP	CB-CG-OD2	6.84	124.46	118.30
2	B	226	ALA	O-C-N	6.84	133.65	122.70
2	B	186	TYR	CG-CD2-CE2	-6.83	115.83	121.30
2	B	315	TYR	CD1-CG-CD2	6.80	125.38	117.90
1	A	82	PHE	CB-CG-CD2	-6.79	116.05	120.80
1	A	3	ARG	NE-CZ-NH2	-6.75	116.93	120.30
2	B	241	PHE	CB-CA-C	-6.66	97.08	110.40
1	A	256	ARG	NE-CZ-NH1	-6.55	117.02	120.30
2	B	38	ASP	CB-CG-OD2	6.50	124.15	118.30
2	B	71	THR	CA-CB-CG2	-6.43	103.39	112.40
2	B	117	VAL	CA-CB-CG2	-6.39	101.32	110.90
2	B	30	GLU	OE1-CD-OE2	-6.38	115.65	123.30
2	B	146	VAL	CA-CB-CG2	-6.35	101.37	110.90
2	B	222	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	A	58	LEU	CB-CG-CD1	-6.30	100.29	111.00
1	A	140	ARG	NE-CZ-NH2	6.27	123.43	120.30
2	B	204	PHE	CB-CG-CD1	-6.23	116.44	120.80
1	A	232	ILE	CB-CA-C	-6.22	99.15	111.60
2	B	128	LEU	CB-CG-CD2	-6.17	100.50	111.00
2	B	100	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	A	93	PRO	N-CD-CG	-6.15	93.98	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	GLU	OE1-CD-OE2	-6.08	116.00	123.30
2	B	381	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	63	THR	OG1-CB-CG2	-5.95	96.31	110.00
2	B	134	MET	CG-SD-CE	5.92	109.68	100.20
1	A	209	LEU	CB-CG-CD2	5.88	121.00	111.00
1	A	20	VAL	CA-CB-CG1	-5.86	102.11	110.90
2	B	22	MET	CA-CB-CG	-5.84	103.37	113.30
2	B	333	LEU	CA-CB-CG	-5.82	101.91	115.30
2	B	298	TYR	CA-CB-CG	-5.82	102.35	113.40
1	A	49	GLU	CA-CB-CG	-5.76	100.72	113.40
2	B	12	PHE	CG-CD1-CE1	-5.74	114.49	120.80
2	B	271	LEU	CB-CG-CD1	-5.74	101.24	111.00
2	B	81	LEU	CB-CG-CD1	-5.73	101.26	111.00
2	B	321	ARG	NE-CZ-NH1	-5.73	117.44	120.30
2	B	218	ASP	CB-CG-OD2	5.73	123.46	118.30
2	B	32	PHE	CB-CG-CD1	-5.72	116.80	120.80
1	A	221	SER	N-CA-CB	5.72	119.08	110.50
2	B	117	VAL	CA-CB-CG1	5.71	119.46	110.90
1	A	105	LEU	CB-CG-CD2	5.69	120.68	111.00
2	B	59	LEU	CB-CG-CD2	-5.69	101.33	111.00
1	A	224	VAL	CG1-CB-CG2	-5.68	101.81	110.90
2	B	263	GLU	OE1-CD-OE2	5.65	130.09	123.30
2	B	28	LEU	CB-CG-CD1	5.64	120.60	111.00
1	A	60	ASP	CB-CG-OD2	5.61	123.35	118.30
2	B	275	ARG	CG-CD-NE	5.61	123.58	111.80
1	A	196	LEU	CB-CG-CD2	-5.60	101.48	111.00
1	A	115	TYR	CD1-CE1-CZ	-5.55	114.81	119.80
2	B	286	MET	O-C-N	5.54	131.56	122.70
1	A	152	PHE	CB-CG-CD1	-5.53	116.93	120.80
2	B	97	LEU	CB-CA-C	-5.52	99.71	110.20
1	A	18	ALA	N-CA-CB	-5.45	102.47	110.10
2	B	3	THR	CA-CB-CG2	-5.44	104.79	112.40
1	A	82	PHE	CB-CG-CD1	5.42	124.60	120.80
2	B	202	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	168	SER	N-CA-CB	-5.40	102.40	110.50
2	B	180	SER	N-CA-C	5.36	125.47	111.00
1	A	4	TYR	CD1-CE1-CZ	-5.33	115.00	119.80
2	B	139	VAL	CB-CA-C	-5.33	101.28	111.40
2	B	376	LEU	CA-CB-CG	-5.33	103.04	115.30
2	B	324	TYR	CA-CB-CG	-5.31	103.31	113.40
2	B	52	TYR	CB-CG-CD2	-5.28	117.83	121.00
2	B	38	ASP	C-N-CD	5.25	139.41	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	183	THR	OG1-CB-CG2	-5.24	97.94	110.00
1	A	140	ARG	CD-NE-CZ	-5.21	116.31	123.60
2	B	315	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	A	263	LYS	CD-CE-NZ	5.17	123.60	111.70
2	B	4	LEU	CB-CG-CD2	-5.17	102.22	111.00
2	B	284	ALA	CB-CA-C	-5.13	102.41	110.10
2	B	55	ARG	NE-CZ-NH2	5.12	122.86	120.30
2	B	389	ASP	CB-CG-OD2	5.12	122.90	118.30
2	B	321	ARG	N-CA-CB	-5.11	101.39	110.60
1	A	212	PHE	C-N-CA	-5.11	111.57	122.30
2	B	197	TYR	CD1-CE1-CZ	-5.11	115.20	119.80
2	B	197	TYR	CG-CD2-CE2	-5.09	117.23	121.30
1	A	84	MET	N-CA-CB	5.08	119.75	110.60
1	A	176	LEU	C-N-CA	-5.08	108.99	121.70
2	B	83	GLY	CA-C-N	5.08	126.36	116.20
2	B	150	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	A	140	ARG	CB-CA-C	5.06	120.52	110.40
1	A	82	PHE	CZ-CE2-CD2	5.03	126.13	120.10

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	1912	0	1922	29	0
2	B	2981	0	2959	28	0
3	B	1	0	0	0	0
4	B	22	0	13	1	0
5	A	108	0	0	1	0
5	B	235	0	0	2	0
All	All	5259	0	4894	56	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 6.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:HIS:O	1:A:198:GLU:HG3	1.64	0.97
1:A:176:LEU:HD11	1:A:196:LEU:HD23	1.57	0.85
2:B:222:ARG:NH1	5:B:635:HOH:O	2.22	0.72
1:A:192:PRO:O	1:A:195:HIS:N	2.25	0.68
2:B:2:THR:HG22	2:B:3:THR:H	1.64	0.61
1:A:176:LEU:HD11	1:A:196:LEU:CD2	2.32	0.58
2:B:337:LYS:CE	2:B:391:LEU:HD21	2.32	0.58
2:B:337:LYS:NZ	2:B:391:LEU:HD21	2.19	0.58
2:B:206:ARG:HD3	2:B:210:GLU:OE2	2.05	0.57
2:B:121:LEU:HD12	2:B:122:ALA:N	2.20	0.55
2:B:300:ILE:CD1	2:B:333:LEU:HD11	2.37	0.54
1:A:58:LEU:HD12	1:A:58:LEU:C	2.28	0.53
2:B:91:VAL:HG21	2:B:118:ALA:HB1	1.90	0.53
1:A:173:TYR:CD1	1:A:209:LEU:HD12	2.43	0.52
2:B:44:GLN:HG3	5:B:502:HOH:O	2.07	0.52
2:B:163:SER:OG	2:B:167:LYS:HE3	2.10	0.52
2:B:337:LYS:HE2	2:B:391:LEU:HD21	1.92	0.52
2:B:21:LEU:HD21	2:B:178:SER:HA	1.91	0.52
2:B:271:LEU:C	2:B:271:LEU:HD23	2.31	0.51
1:A:193:LEU:O	1:A:197:ILE:HG13	2.09	0.51
1:A:193:LEU:HD23	1:A:193:LEU:H	1.77	0.50
1:A:154:CYS:HB3	1:A:176:LEU:HD12	1.92	0.49
2:B:206:ARG:CD	2:B:210:GLU:OE2	2.60	0.49
1:A:36:ILE:HG23	1:A:255:LEU:HD13	1.93	0.49
1:A:100:LEU:HD12	5:A:305:HOH:O	2.13	0.47
1:A:23:VAL:CG1	1:A:237:ILE:HG21	2.44	0.47
1:A:57:PRO:HA	1:A:102:TYR:CZ	2.50	0.47
1:A:194:HIS:O	1:A:198:GLU:CG	2.52	0.46
1:A:239:LYS:O	1:A:243:LYS:HG3	2.16	0.46
1:A:127:LEU:HD23	1:A:127:LEU:C	2.37	0.45
1:A:70:ARG:NH1	1:A:242:GLU:HG2	2.31	0.45
2:B:131:ARG:HG3	2:B:131:ARG:O	2.16	0.45
1:A:221:SER:HB2	1:A:225:ARG:HH12	1.82	0.45
2:B:285:PRO:C	2:B:286:MET:HG3	2.37	0.45
1:A:100:LEU:C	1:A:100:LEU:CD1	2.86	0.44
1:A:100:LEU:C	1:A:100:LEU:HD13	2.38	0.44
1:A:104:ASN:HB2	2:B:278:ILE:O	2.17	0.44
1:A:70:ARG:CZ	1:A:242:GLU:HG2	2.48	0.43
1:A:70:ARG:NH2	1:A:242:GLU:HG2	2.33	0.43
1:A:36:ILE:O	1:A:40:LEU:HG	2.18	0.43
2:B:341:ARG:O	2:B:341:ARG:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:CD2	1:A:193:LEU:N	2.82	0.43
2:B:16:TYR:O	2:B:281:GLY:HA2	2.19	0.43
2:B:271:LEU:O	2:B:271:LEU:HD23	2.19	0.43
1:A:249:LYS:HG3	1:A:249:LYS:H	1.31	0.42
1:A:238:VAL:O	1:A:242:GLU:HG3	2.19	0.42
2:B:87:LYS:CE	4:B:400:PLS:H4A1	2.49	0.42
1:A:76:VAL:HA	1:A:80:GLN:OE1	2.19	0.42
2:B:376:LEU:HD12	2:B:376:LEU:HA	1.78	0.42
2:B:121:LEU:C	2:B:121:LEU:HD12	2.41	0.41
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.55	0.41
2:B:280:PHE:O	2:B:280:PHE:CG	2.74	0.41
2:B:286:MET:HB2	2:B:286:MET:HE2	1.69	0.40
2:B:134:MET:O	2:B:158:PRO:HA	2.21	0.40
1:A:176:LEU:HA	1:A:176:LEU:HD12	1.90	0.40
2:B:300:ILE:HD12	2:B:333:LEU:HD11	2.04	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%)	245 (98%)	3 (1%)	1 (0%)	34	21
2	B	392/397 (99%)	382 (97%)	10 (3%)	0	100	100
All	All	641/665 (96%)	627 (98%)	13 (2%)	1 (0%)	47	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE

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%)	191 (96%)	7 (4%)	36	21
2	B	308/311 (99%)	297 (96%)	11 (4%)	35	20
All	All	506/519 (98%)	488 (96%)	18 (4%)	35	20

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	100	LEU
1	A	159	ASP
1	A	161	ASP
1	A	193	LEU
1	A	218	GLU
1	A	249	LYS
2	B	65	ILE
2	B	99	LYS
2	B	143	SER
2	B	161	SER
2	B	198	PRO
2	B	206	ARG
2	B	222	ARG
2	B	236	ASN
2	B	297	SER
2	B	367	GLU
2	B	384	ILE

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

Mol	Chain	Res	Type
2	B	26	ASN
2	B	44	GLN
2	B	236	ASN
2	B	246	ASN

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Mol	Chain	Res	Type
2	B	375	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	PLS	B	400	-	19,22,22	1.52	5 (26%)	25,31,31	2.86	11 (44%)

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	PLS	B	400	-	-	4/13/17/17	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	PLS	C3-C2	-3.10	1.37	1.40
4	B	400	PLS	P-O2P	-2.76	1.44	1.54
4	B	400	PLS	C5A-C5	2.45	1.57	1.50
4	B	400	PLS	C5-C4	-2.17	1.37	1.40
4	B	400	PLS	P-O3P	-2.03	1.47	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	400	PLS	C4-C4A-N	7.16	131.49	111.78
4	B	400	PLS	C2A-C2-C3	5.79	128.04	120.89
4	B	400	PLS	C4A-N-CA	4.63	122.71	113.83
4	B	400	PLS	OG-CB-CA	-4.21	102.17	111.51
4	B	400	PLS	O3-C3-C2	3.70	125.55	117.49
4	B	400	PLS	C2A-C2-N1	-3.52	110.80	117.67
4	B	400	PLS	C4A-C4-C3	2.88	123.13	120.04
4	B	400	PLS	O4P-C5A-C5	2.81	114.70	109.35
4	B	400	PLS	O3P-P-O1P	-2.35	101.50	110.68
4	B	400	PLS	O3P-P-O2P	2.19	116.00	107.64
4	B	400	PLS	O2P-P-O4P	-2.08	101.21	106.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	400	PLS	C3-C4-C4A-N
4	B	400	PLS	C5-C4-C4A-N
4	B	400	PLS	C-CA-N-C4A
4	B	400	PLS	CB-CA-N-C4A

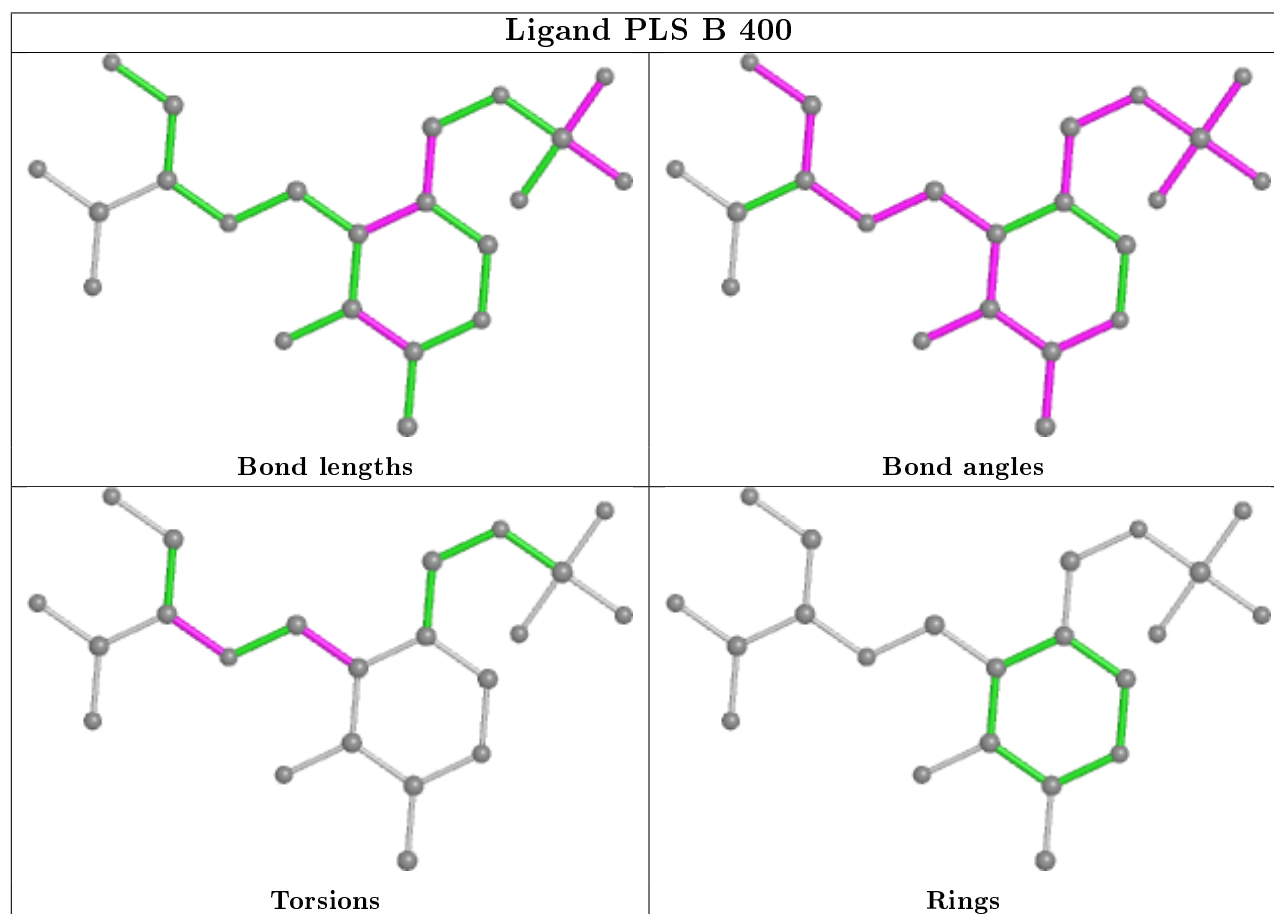
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	400	PLS	1	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%)	0.22	17 (6%)	17 14	21, 36, 55, 88	0
2	B	394/397 (99%)	0.08	12 (3%)	50 44	18, 26, 44, 75	0
All	All	647/665 (97%)	0.14	29 (4%)	33 27	18, 30, 51, 88	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	HIS	6.5
1	A	193	LEU	4.5
1	A	13	ASP	4.3
2	B	2	THR	3.5
1	A	195	HIS	3.4
2	B	182	GLU	3.4
1	A	246	ALA	3.0
1	A	212	PHE	3.0
2	B	385	PHE	2.9
2	B	392	LYS	2.8
2	B	393	ALA	2.7
2	B	394	ARG	2.6
2	B	163	SER	2.5
1	A	15	ARG	2.5
1	A	127	LEU	2.4
1	A	161	ASP	2.4
2	B	140	GLU	2.4
1	A	250	GLN	2.4
2	B	188	LEU	2.3
1	A	73	ALA	2.3
2	B	390	ILE	2.3
1	A	196	LEU	2.3
1	A	213	GLY	2.2
1	A	247	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	157	ASN	2.2
1	A	257	SER	2.1
2	B	231	VAL	2.1
2	B	136	ALA	2.1
1	A	243	LYS	2.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

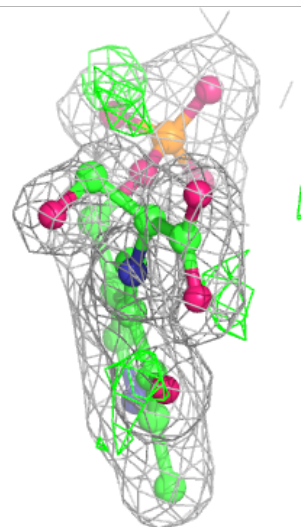
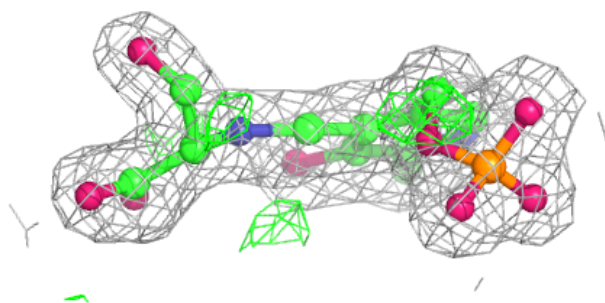
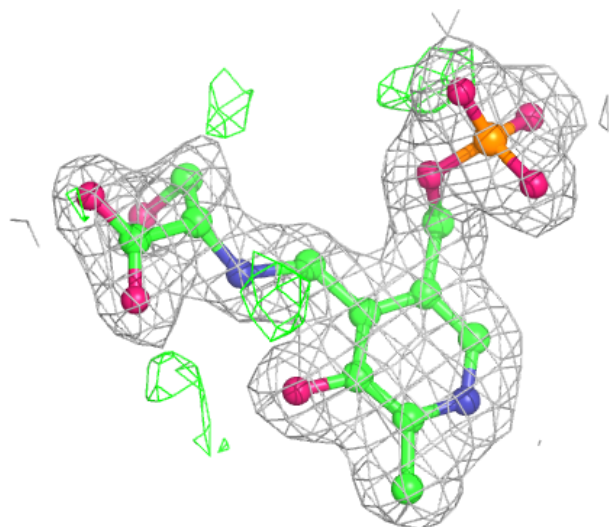
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PLS	B	400	22/22	0.97	0.12	21,28,34,37	0
3	NA	B	399	1/1	0.99	0.07	26,26,26,26	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.

Electron density around PLS B 400:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.