



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:05 PM UTC

PDB ID : 1FUY / pdb_00001fuy
Title : CRYSTAL STRUCTURE OF BETAA169L/BETAC170W DOUBLE MUTANT OF TRYPTOPHAN SYNTHASE COMPLEXED WITH 5-FLUORO-INDOLE-PROPANOL PHOSPHATE
Authors : Weyand, M.; Schlichting, I.
Deposited on : 2000-09-18
Resolution : 2.25 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

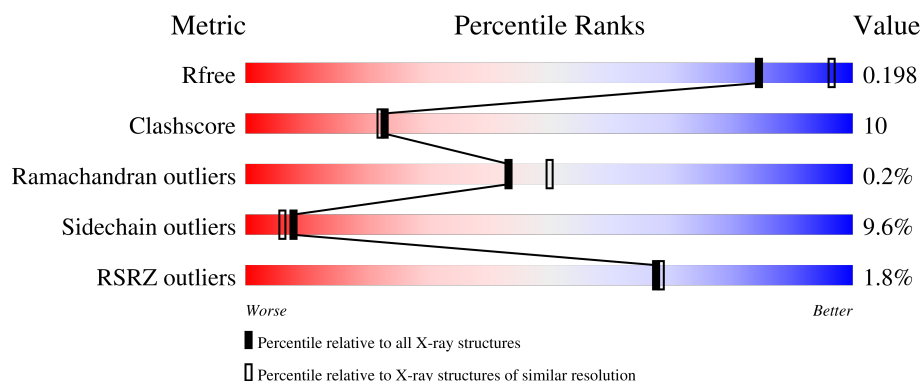
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

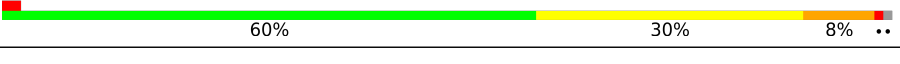
The reported resolution of this entry is 2.25 Å.

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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5187 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	262	Total	C	N	O	S	0	0	0
			1975	1255	342	370	8			

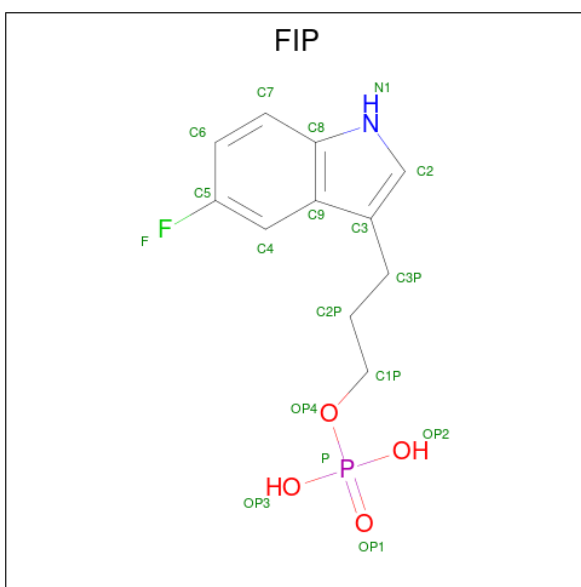
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	393	Total	C	N	O	S	0	0	0
			2988	1882	524	564	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	SER	ARG	cloning artifact	UNP P0A2K1
B	169	LEU	ALA	engineered mutation	UNP P0A2K1
B	170	TRP	CYS	engineered mutation	UNP P0A2K1

- Molecule 3 is 5-FLUOROINDOLE PROPANOL PHOSPHATE (CCD ID: FIP) (formula: C₁₁H₁₃FNO₄P).

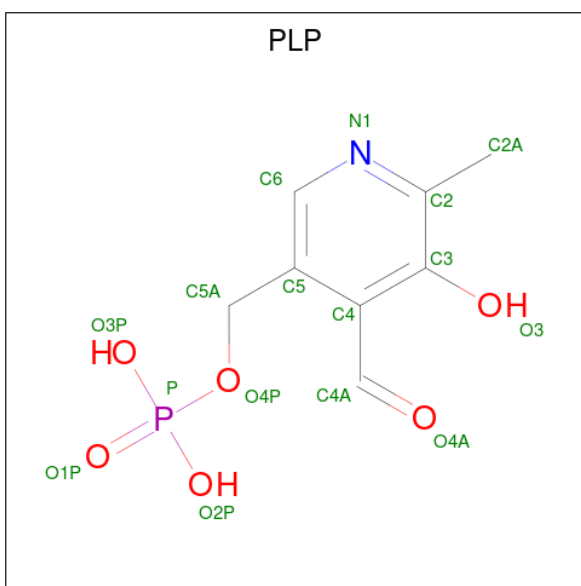


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	P	
			18	11	1	1	4	1	

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

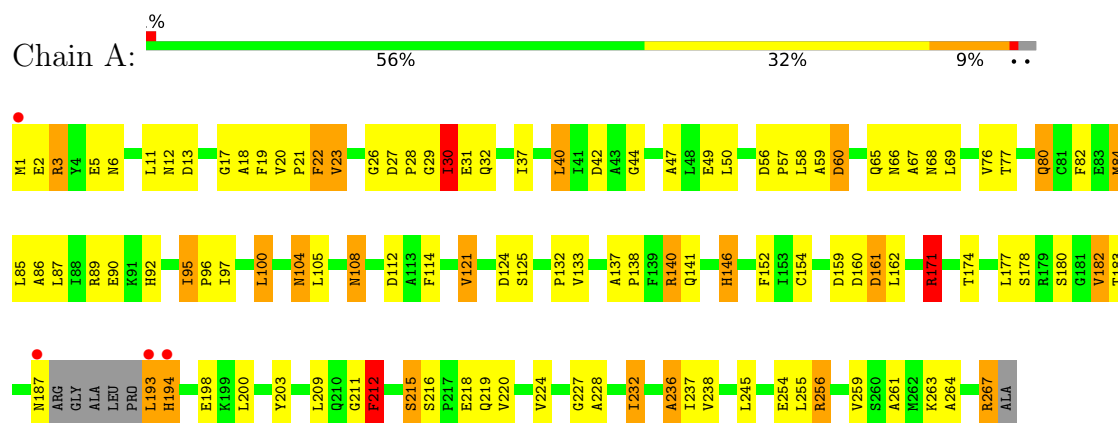
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	65	Total	O	0	0
			65	65		
6	B	125	Total	O	0	0
			125	125		

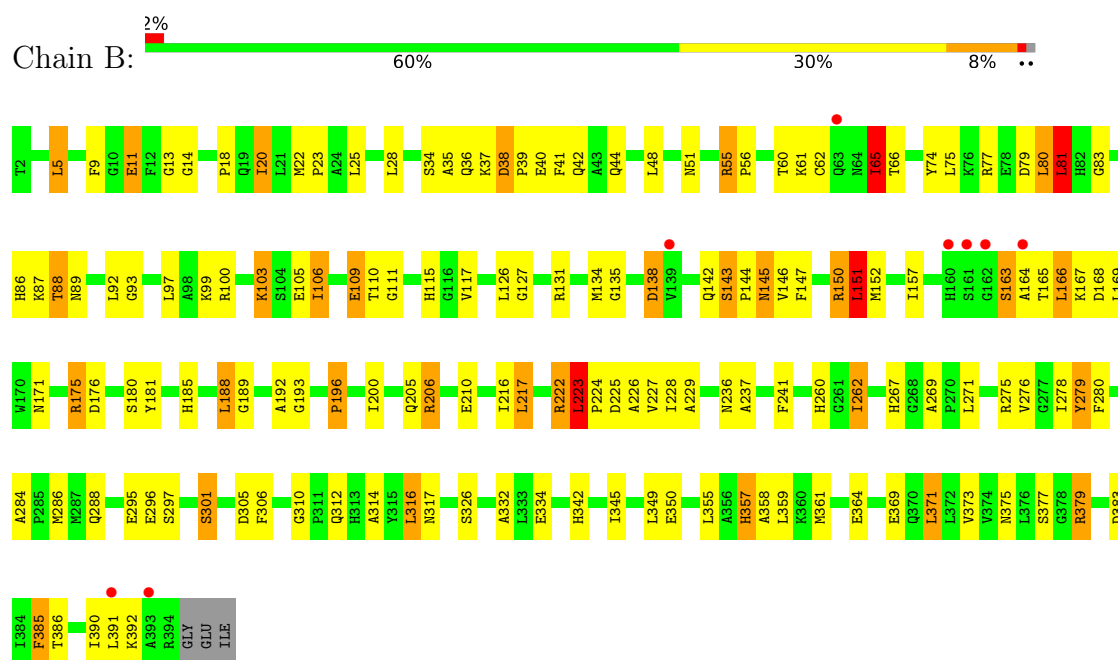
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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	184.00Å 60.70Å 67.40Å 90.00° 95.75° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 20.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	91.3 (20.00-2.25) 91.2 (20.00-2.25)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.17Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.224 0.156 , 0.198	Depositor DCC
R_{free} test set	1755 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5187	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% 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, PLP, FIP

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	0.94	0/2013	2.13	61/2733 (2.2%)
2	B	1.18	3/3048 (0.1%)	2.32	135/4119 (3.3%)
All	All	1.09	3/5061 (0.1%)	2.25	196/6852 (2.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	77	ARG	CA-CB	6.23	1.60	1.52
2	B	345	ILE	C-N	-5.65	1.28	1.33
2	B	355	LEU	C-O	-5.43	1.17	1.24

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	206	ARG	CD-NE-CZ	31.16	168.03	124.40
2	B	222	ARG	NE-CZ-NH1	15.02	136.52	121.50
2	B	38	ASP	CA-C-O	12.31	129.70	119.36
1	A	140	ARG	NE-CZ-NH2	11.91	129.92	119.20
2	B	222	ARG	CD-NE-CZ	11.67	140.73	124.40
1	A	194	HIS	CA-CB-CG	-11.52	102.28	113.80
2	B	222	ARG	NE-CZ-NH2	-11.47	108.88	119.20
2	B	345	ILE	CA-C-N	10.80	129.95	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	345	ILE	C-N-CA	10.80	129.95	122.60
2	B	131	ARG	CD-NE-CZ	10.51	139.11	124.40
1	A	104	ASN	CA-CB-CG	-10.02	102.58	112.60
1	A	140	ARG	NE-CZ-NH1	-9.69	111.81	121.50
2	B	357	HIS	CA-CB-CG	-9.43	104.37	113.80
2	B	44	GLN	OE1-CD-NE2	9.37	131.97	122.60
2	B	62	CYS	CA-C-O	9.26	131.53	121.16
1	A	161	ASP	CA-CB-CG	-9.22	103.38	112.60
1	A	5	GLU	CA-CB-CG	9.20	132.49	114.10
2	B	62	CYS	O-C-N	-9.09	111.80	122.89
2	B	41	PHE	CA-CB-CG	-8.96	104.84	113.80
2	B	93	GLY	CA-C-O	8.87	129.89	120.75
2	B	301	SER	N-CA-CB	8.78	124.73	110.42
2	B	106	ILE	CA-CB-CG2	8.71	125.31	110.50
1	A	68	ASN	CA-CB-CG	-8.38	104.22	112.60
2	B	51	ASN	CA-CB-CG	-8.26	104.34	112.60
1	A	66	ASN	CA-CB-CG	-8.23	104.37	112.60
2	B	36	GLN	CG-CD-NE2	-8.06	104.31	116.40
2	B	138	ASP	CA-CB-CG	8.04	120.64	112.60
2	B	379	ARG	NE-CZ-NH2	7.96	126.37	119.20
2	B	369	GLU	CA-C-O	-7.89	111.68	120.60
2	B	275	ARG	NE-CZ-NH2	7.81	126.23	119.20
2	B	355	LEU	CA-C-O	-7.56	112.54	120.55
2	B	180	SER	CB-CA-C	-7.54	98.81	111.02
2	B	279	TYR	CA-C-O	-7.51	113.24	121.28
2	B	5	LEU	N-CA-CB	-7.30	99.38	111.20
2	B	106	ILE	CB-CG1-CD1	-7.29	98.49	113.80
1	A	236	ALA	CA-C-O	-7.25	111.91	120.10
2	B	93	GLY	O-C-N	-7.11	115.37	122.19
2	B	36	GLN	CB-CG-CD	7.10	124.67	112.60
2	B	147	PHE	CA-CB-CG	-7.07	106.73	113.80
2	B	369	GLU	CA-CB-CG	-6.98	100.14	114.10
2	B	34	SER	CA-C-O	-6.98	113.15	120.55
2	B	295	GLU	N-CA-C	6.96	119.97	109.95
2	B	306	PHE	O-C-N	-6.95	114.72	121.18
2	B	81	LEU	CA-C-O	-6.94	114.24	121.87
2	B	279	TYR	CA-CB-CG	-6.92	101.44	113.90
2	B	55	ARG	O-C-N	6.86	130.26	121.34
1	A	104	ASN	O-C-N	-6.86	114.85	122.12
2	B	284	ALA	N-CA-CB	-6.86	104.22	111.29
1	A	108	ASN	O-C-N	-6.83	113.51	122.59
1	A	97	ILE	CA-C-N	-6.78	117.50	122.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ILE	C-N-CA	-6.78	117.50	122.18
1	A	23	VAL	N-CA-CB	6.75	124.86	112.36
2	B	345	ILE	O-C-N	-6.65	115.32	123.10
2	B	55	ARG	CA-C-O	-6.63	113.73	120.96
2	B	334	GLU	CB-CG-CD	6.59	123.80	112.60
2	B	42	GLN	OE1-CD-NE2	-6.58	116.02	122.60
2	B	296	GLU	CB-CG-CD	6.57	123.77	112.60
2	B	105	GLU	CA-C-N	-6.54	113.85	122.94
2	B	105	GLU	C-N-CA	-6.54	113.85	122.94
1	A	159	ASP	CA-CB-CG	6.51	119.11	112.60
2	B	86	HIS	CA-CB-CG	-6.50	107.30	113.80
1	A	146	HIS	CA-CB-CG	-6.48	107.32	113.80
2	B	65	ILE	CA-C-O	-6.48	111.82	119.85
2	B	145	ASN	CA-CB-CG	-6.40	106.20	112.60
2	B	275	ARG	CA-CB-CG	6.34	126.78	114.10
2	B	222	ARG	CG-CD-NE	6.33	125.93	112.00
1	A	87	LEU	N-CA-CB	6.33	119.52	110.16
2	B	262	ILE	CA-C-N	6.33	129.39	120.28
2	B	262	ILE	C-N-CA	6.33	129.39	120.28
2	B	310	GLY	CA-C-N	6.30	125.87	119.19
2	B	310	GLY	C-N-CA	6.30	125.87	119.19
2	B	225	ASP	CA-CB-CG	-6.29	106.31	112.60
2	B	226	ALA	O-C-N	6.23	130.37	123.33
2	B	138	ASP	N-CA-CB	6.22	119.39	110.06
1	A	84	MET	CA-C-O	6.19	127.32	120.82
2	B	373	VAL	N-CA-CB	6.18	119.67	111.64
1	A	32	GLN	OE1-CD-NE2	-6.17	116.43	122.60
2	B	305	ASP	N-CA-C	6.17	119.83	112.93
1	A	212	PHE	N-CA-CB	6.13	120.86	110.49
1	A	254	GLU	O-C-N	-6.13	115.62	122.12
2	B	276	VAL	CA-C-O	6.13	128.72	120.99
2	B	286	MET	CA-C-O	-6.13	114.71	121.33
1	A	125	SER	CA-C-O	6.13	127.95	121.33
2	B	206	ARG	NE-CZ-NH1	6.12	127.62	121.50
2	B	237	ALA	CA-C-N	-6.09	110.53	120.64
2	B	237	ALA	C-N-CA	-6.09	110.53	120.64
2	B	48	LEU	CA-C-N	-6.04	112.18	120.28
2	B	48	LEU	C-N-CA	-6.04	112.18	120.28
2	B	364	GLU	CA-C-N	-6.04	115.72	123.16
2	B	364	GLU	C-N-CA	-6.04	115.72	123.16
2	B	157	ILE	N-CA-C	6.02	114.04	107.60
2	B	131	ARG	NE-CZ-NH2	5.99	124.59	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	HIS	CA-C-N	5.99	125.53	119.19
1	A	92	HIS	C-N-CA	5.99	125.53	119.19
2	B	176	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	90	GLU	CA-CB-CG	5.95	126.01	114.10
2	B	83	GLY	N-CA-C	-5.95	107.19	114.92
2	B	375	ASN	CA-C-O	-5.94	114.56	120.98
2	B	288	GLN	OE1-CD-NE2	5.92	128.52	122.60
1	A	89	ARG	O-C-N	-5.91	115.41	122.15
2	B	237	ALA	CA-C-O	-5.91	114.62	120.70
1	A	5	GLU	CA-C-N	5.87	128.07	120.44
1	A	5	GLU	C-N-CA	5.87	128.07	120.44
2	B	151	LEU	CA-C-O	-5.86	114.30	120.63
2	B	355	LEU	N-CA-C	-5.86	104.89	111.28
2	B	200	ILE	CB-CA-C	-5.86	104.14	112.22
1	A	3	ARG	NE-CZ-NH2	5.84	124.46	119.20
2	B	152	MET	CA-CB-CG	-5.84	102.43	114.10
1	A	95	ILE	CA-C-O	5.82	124.24	119.47
1	A	19	PHE	N-CA-CB	5.81	119.71	110.65
2	B	196	PRO	CA-C-N	5.81	127.35	120.09
2	B	196	PRO	C-N-CA	5.81	127.35	120.09
2	B	111	GLY	CA-C-N	5.81	127.99	120.44
2	B	111	GLY	C-N-CA	5.81	127.99	120.44
2	B	326	SER	CA-C-O	5.79	128.21	121.44
2	B	60	THR	CA-C-O	5.75	126.70	120.43
2	B	192	ALA	CA-C-O	-5.72	115.05	121.40
2	B	28	LEU	N-CA-C	-5.71	105.13	111.36
1	A	182	VAL	N-CA-C	5.71	117.14	108.80
1	A	30	ILE	CB-CA-C	5.66	119.43	112.02
2	B	185	HIS	CA-C-O	-5.65	114.26	120.36
2	B	227	VAL	O-C-N	-5.65	117.38	123.14
2	B	206	ARG	NH1-CZ-NH2	-5.61	112.00	119.30
2	B	241	PHE	N-CA-C	5.61	118.33	111.82
2	B	316	LEU	N-CA-CB	-5.61	101.59	110.22
2	B	312	GLN	OE1-CD-NE2	5.60	128.20	122.60
1	A	261	ALA	CA-C-N	-5.59	112.35	120.29
1	A	261	ALA	C-N-CA	-5.59	112.35	120.29
2	B	127	GLY	CA-C-N	-5.58	113.88	122.87
2	B	127	GLY	C-N-CA	-5.58	113.88	122.87
2	B	51	ASN	CA-C-O	5.53	126.17	119.31
2	B	14	GLY	CA-C-N	5.53	130.44	123.03
2	B	14	GLY	C-N-CA	5.53	130.44	123.03
2	B	332	ALA	CA-C-O	-5.53	114.56	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	PHE	CB-CG-CD1	5.50	130.05	120.70
2	B	151	LEU	N-CA-CB	5.50	118.31	110.06
2	B	260	HIS	CA-CB-CG	-5.50	108.30	113.80
2	B	357	HIS	O-C-N	-5.50	116.15	122.09
1	A	65	GLN	N-CA-CB	5.49	118.19	110.12
2	B	66	THR	N-CA-CB	-5.48	102.56	110.56
2	B	237	ALA	O-C-N	5.48	128.00	122.09
1	A	141	GLN	CA-CB-CG	-5.47	103.16	114.10
1	A	44	GLY	CA-C-O	-5.47	112.90	118.97
2	B	175	ARG	O-C-N	-5.47	116.40	122.09
2	B	109	GLU	CA-C-O	-5.46	114.72	121.06
2	B	35	ALA	CA-C-N	5.46	127.59	120.28
2	B	35	ALA	C-N-CA	5.46	127.59	120.28
1	A	114	PHE	N-CA-C	-5.45	105.42	111.36
1	A	152	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	125	SER	O-C-N	-5.42	117.07	123.25
2	B	383	ASP	CA-CB-CG	-5.42	107.18	112.60
1	A	256	ARG	CD-NE-CZ	5.42	131.98	124.40
1	A	218	GLU	N-CA-C	-5.41	105.47	111.36
2	B	229	ALA	CA-C-O	-5.41	114.93	120.99
2	B	236	ASN	CB-CG-ND2	5.40	124.50	116.40
2	B	151	LEU	N-CA-C	-5.37	104.83	111.33
2	B	88	THR	CA-CB-OG1	-5.37	101.55	109.60
1	A	82	PHE	CB-CG-CD2	-5.36	111.58	120.70
2	B	13	GLY	N-CA-C	-5.34	105.65	111.21
1	A	154	CYS	CB-CA-C	5.32	115.75	110.33
1	A	80	GLN	CA-C-O	-5.31	114.92	120.55
1	A	60	ASP	N-CA-C	5.29	117.53	108.90
1	A	171	ARG	CD-NE-CZ	-5.29	116.99	124.40
1	A	187	ASN	CA-C-O	5.27	129.75	120.80
2	B	350	GLU	CG-CD-OE1	5.26	130.51	118.40
1	A	92	HIS	CA-C-O	5.25	127.35	120.74
1	A	215	SER	N-CA-CB	-5.23	104.07	110.98
1	A	193	LEU	CD1-CG-CD2	-5.23	99.30	110.80
1	A	232	ILE	CA-C-O	-5.22	114.77	121.40
2	B	11	GLU	CB-CG-CD	5.22	121.47	112.60
2	B	223	LEU	N-CA-CB	-5.21	102.55	110.05
1	A	17	GLY	N-CA-C	-5.20	105.64	112.82
2	B	350	GLU	N-CA-CB	5.20	117.50	109.91
2	B	103	LYS	CA-C-O	-5.19	115.50	121.47
2	B	383	ASP	CB-CA-C	-5.15	101.50	110.09
2	B	80	LEU	N-CA-CB	-5.14	102.58	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	GLY	CA-C-O	-5.14	115.67	121.68
1	A	100	LEU	CA-C-O	-5.13	114.97	120.46
2	B	106	ILE	CB-CA-C	5.12	118.39	110.50
2	B	37	LYS	CA-C-N	5.12	130.67	121.76
2	B	37	LYS	C-N-CA	5.12	130.67	121.76
1	A	82	PHE	CA-CB-CG	-5.12	108.68	113.80
1	A	174	THR	N-CA-CB	5.10	118.74	110.43
2	B	100	ARG	NH1-CZ-NH2	-5.09	112.68	119.30
2	B	18	PRO	CA-C-N	5.08	127.34	120.38
2	B	18	PRO	C-N-CA	5.08	127.34	120.38
1	A	132	PRO	O-C-N	-5.08	116.57	122.86
2	B	350	GLU	CB-CA-C	-5.07	103.15	110.96
2	B	143	SER	O-C-N	5.07	124.99	120.48
2	B	150	ARG	NH1-CZ-NH2	5.06	125.88	119.30
1	A	22	PHE	CA-CB-CG	-5.05	108.75	113.80
2	B	9	PHE	N-CA-C	-5.05	97.54	107.69
2	B	334	GLU	CA-C-O	-5.04	115.21	120.55
2	B	377	SER	CA-C-O	-5.01	114.43	120.10
2	B	99	LYS	CA-CB-CG	-5.01	104.07	114.10
2	B	36	GLN	CA-CB-CG	5.01	124.12	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	317	ASN	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1975	0	1979	55	0
2	B	2988	0	2965	53	0
3	A	18	0	11	1	0
4	B	1	0	0	0	0
5	B	15	0	7	1	0
6	A	65	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	125	0	0	2	0
All	All	5187	0	4962	104	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 (104) 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:358:ALA:HA	2:B:361:MET:HE3	1.34	1.06
2:B:267:HIS:HD2	2:B:269:ALA:H	1.15	0.94
2:B:89:ASN:HD22	2:B:205:GLN:HE22	1.21	0.89
2:B:358:ALA:HA	2:B:361:MET:CE	2.13	0.77
1:A:56:ASP:HB3	2:B:279:TYR:OH	1.85	0.76
2:B:81:LEU:HD13	2:B:88:THR:HB	1.67	0.76
2:B:357:HIS:CD2	2:B:361:MET:HE2	2.23	0.74
1:A:23:VAL:HG21	1:A:37:ILE:HD11	1.69	0.73
1:A:180:SER:OG	2:B:20:ILE:HD11	1.91	0.70
2:B:228:ILE:CD1	2:B:361:MET:HE1	2.23	0.69
2:B:55:ARG:HB3	2:B:56:PRO:HA	1.77	0.67
1:A:137:ALA:HB3	1:A:138:PRO:HD3	1.78	0.65
1:A:211:GLY:O	1:A:212:PHE:HB2	1.96	0.65
2:B:386:THR:O	2:B:390:ILE:HD13	1.96	0.65
2:B:143:SER:N	2:B:144:PRO:HD2	2.13	0.63
1:A:30:ILE:HD13	1:A:31:GLU:N	2.14	0.62
2:B:11:GLU:HG2	2:B:11:GLU:O	2.01	0.61
1:A:23:VAL:CG2	1:A:37:ILE:HD11	2.32	0.60
1:A:86:ALA:HB2	1:A:121:VAL:HG22	1.83	0.60
1:A:2:GLU:HG3	1:A:6:ASN:ND2	2.18	0.58
1:A:177:LEU:HD11	1:A:212:PHE:CD2	2.38	0.58
2:B:228:ILE:HD13	2:B:361:MET:HE1	1.86	0.57
1:A:183:THR:HG22	1:A:212:PHE:CE1	2.41	0.56
2:B:267:HIS:CD2	2:B:269:ALA:H	2.08	0.56
1:A:56:ASP:OD2	2:B:167:LYS:HG2	2.05	0.56
1:A:42:ASP:OD2	1:A:256:ARG:NH1	2.41	0.54
1:A:40:LEU:HD12	1:A:259:VAL:HG21	1.89	0.54
2:B:217:LEU:HD11	2:B:223:LEU:HD13	1.91	0.53
2:B:89:ASN:HD22	2:B:205:GLN:NE2	2.01	0.52
2:B:193:GLY:HA2	2:B:280:PHE:O	2.09	0.52
2:B:61:LYS:HB2	2:B:74:TYR:CE2	2.45	0.52
1:A:264:ALA:HA	1:A:267:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ASP:OD2	1:A:146:HIS:HE1	1.93	0.51
1:A:96:PRO:HA	1:A:124:ASP:OD2	2.12	0.49
1:A:22:PHE:C	1:A:22:PHE:CD1	2.90	0.49
2:B:135:GLY:HA3	2:B:164:ALA:HB1	1.93	0.49
1:A:216:SER:O	1:A:219:GLN:HB2	2.13	0.49
2:B:165:THR:O	2:B:166:LEU:C	2.55	0.49
2:B:165:THR:HG22	2:B:168:ASP:OD2	2.14	0.48
2:B:271:LEU:HD11	2:B:314:ALA:HA	1.95	0.48
2:B:103:LYS:NZ	2:B:181:TYR:O	2.45	0.48
2:B:171:ASN:O	2:B:175:ARG:HG3	2.13	0.48
1:A:194:HIS:O	1:A:198:GLU:HG2	2.12	0.48
1:A:177:LEU:HD11	1:A:212:PHE:CE2	2.48	0.48
2:B:188:LEU:HD23	6:B:510:HOH:O	2.14	0.47
2:B:385:PHE:N	2:B:385:PHE:CD1	2.82	0.47
1:A:263:LYS:HE2	6:A:301:HOH:O	2.15	0.47
2:B:262:ILE:HG12	6:B:436:HOH:O	2.14	0.47
2:B:385:PHE:H	2:B:385:PHE:HD1	1.62	0.47
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.96	0.47
2:B:217:LEU:CD1	2:B:223:LEU:HD13	2.45	0.47
1:A:58:LEU:C	1:A:58:LEU:HD12	2.39	0.47
2:B:391:LEU:HD23	2:B:391:LEU:HA	1.81	0.47
1:A:22:PHE:HA	1:A:49:GLU:O	2.14	0.47
1:A:77:THR:HG23	1:A:80:GLN:NE2	2.30	0.47
1:A:1:MET:HE3	1:A:3:ARG:NH2	2.30	0.46
1:A:95:ILE:HA	1:A:96:PRO:HD3	1.83	0.46
2:B:79:ASP:HB2	2:B:379:ARG:HB3	1.98	0.46
2:B:22:MET:N	2:B:23:PRO:CD	2.78	0.46
2:B:117:VAL:HG21	2:B:145:ASN:HD22	1.79	0.46
2:B:206:ARG:HD3	2:B:210:GLU:OE2	2.15	0.46
2:B:216:ILE:HG21	2:B:224:PRO:HD3	1.97	0.46
1:A:108:ASN:HA	6:A:288:HOH:O	2.16	0.46
1:A:20:VAL:O	1:A:232:ILE:HA	2.17	0.45
1:A:21:PRO:HD2	1:A:47:ALA:O	2.17	0.45
2:B:134:MET:CE	2:B:142:GLN:HB2	2.47	0.45
2:B:163:SER:O	2:B:164:ALA:HB3	2.17	0.45
1:A:263:LYS:HD2	1:A:263:LYS:HA	1.77	0.44
1:A:227:GLY:O	1:A:228:ALA:C	2.57	0.44
1:A:100:LEU:C	1:A:100:LEU:HD13	2.42	0.44
1:A:193:LEU:O	1:A:194:HIS:C	2.61	0.44
1:A:215:SER:OG	1:A:236:ALA:HB2	2.17	0.44
1:A:37:ILE:N	1:A:37:ILE:HD13	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:GLN:O	2:B:146:VAL:HG23	2.17	0.44
1:A:57:PRO:HB2	1:A:60:ASP:HB2	1.99	0.43
2:B:357:HIS:HD2	2:B:361:MET:HE2	1.78	0.43
2:B:228:ILE:HD11	2:B:361:MET:HE1	2.00	0.43
1:A:2:GLU:HG3	1:A:6:ASN:HD21	1.83	0.43
1:A:104:ASN:HB2	2:B:278:ILE:O	2.19	0.43
2:B:38:ASP:HA	2:B:39:PRO:HD3	1.77	0.43
2:B:150:ARG:O	2:B:151:LEU:C	2.62	0.43
1:A:112:ASP:CG	1:A:146:HIS:HE1	2.27	0.43
1:A:26:GLY:H	1:A:84:MET:HE1	1.84	0.42
2:B:143:SER:N	2:B:144:PRO:CD	2.82	0.42
2:B:205:GLN:NE2	2:B:205:GLN:HA	2.34	0.42
1:A:171:ARG:HH11	1:A:171:ARG:HD2	1.60	0.42
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.54	0.42
1:A:58:LEU:HD12	1:A:59:ALA:N	2.35	0.42
2:B:87:LYS:NZ	5:B:401:PLP:O3	2.53	0.41
1:A:95:ILE:HG13	1:A:96:PRO:CD	2.51	0.41
1:A:178:SER:OG	1:A:212:PHE:O	2.34	0.41
2:B:65:ILE:HG23	2:B:342:HIS:HB2	2.02	0.41
1:A:220:VAL:O	1:A:224:VAL:HG23	2.20	0.41
1:A:11:LEU:CD1	1:A:18:ALA:HB2	2.50	0.41
1:A:182:VAL:HG23	1:A:183:THR:O	2.20	0.41
2:B:385:PHE:N	2:B:385:PHE:HD1	2.18	0.41
1:A:67:ALA:HB2	1:A:238:VAL:HG11	2.02	0.41
2:B:224:PRO:HA	2:B:371:LEU:HD13	2.03	0.41
1:A:182:VAL:O	1:A:183:THR:C	2.61	0.41
1:A:183:THR:HG21	3:A:269:FIP:C8	2.51	0.41
1:A:27:ASP:HA	1:A:28:PRO:HA	1.82	0.40
1:A:160:ASP:OD1	1:A:203:TYR:OH	2.22	0.40
2:B:110:THR:O	2:B:169:LEU:HD13	2.20	0.40
1:A:140:ARG:HH11	1:A:140:ARG:HD3	1.57	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	258/268 (96%)	248 (96%)	9 (4%)	1 (0%)	30	31
2	B	391/396 (99%)	382 (98%)	9 (2%)	0	100	100
All	All	649/664 (98%)	630 (97%)	18 (3%)	1 (0%)	43	50

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	204/208 (98%)	185 (91%)	19 (9%)	8	6
2	B	309/311 (99%)	279 (90%)	30 (10%)	8	6
All	All	513/519 (99%)	464 (90%)	49 (10%)	8	6

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	ASP
1	A	30	ILE
1	A	40	LEU
1	A	50	LEU
1	A	69	LEU
1	A	85	LEU
1	A	105	LEU
1	A	121	VAL
1	A	133	VAL
1	A	161	ASP
1	A	162	LEU

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Mol	Chain	Res	Type
1	A	171	ARG
1	A	200	LEU
1	A	209	LEU
1	A	237	ILE
1	A	245	LEU
1	A	255	LEU
1	A	267	ARG
2	B	5	LEU
2	B	20	ILE
2	B	25	LEU
2	B	40	GLU
2	B	65	ILE
2	B	75	LEU
2	B	80	LEU
2	B	81	LEU
2	B	92	LEU
2	B	97	LEU
2	B	106	ILE
2	B	109	GLU
2	B	126	LEU
2	B	138	ASP
2	B	151	LEU
2	B	163	SER
2	B	166	LEU
2	B	188	LEU
2	B	196	PRO
2	B	217	LEU
2	B	222	ARG
2	B	223	LEU
2	B	297	SER
2	B	301	SER
2	B	316	LEU
2	B	349	LEU
2	B	359	LEU
2	B	371	LEU
2	B	385	PHE
2	B	392	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN

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Mol	Chain	Res	Type
1	A	12	ASN
1	A	66	ASN
1	A	80	GLN
1	A	146	HIS
1	A	157	ASN
1	A	244	ASN
2	B	44	GLN
2	B	145	ASN
2	B	205	GLN
2	B	246	ASN
2	B	267	HIS

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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
3	FIP	A	269	-	19,19,19	0.98	1 (5%)	27,27,27	1.43	5 (18%)
5	PLP	B	401	2	15,15,16	2.15	5 (33%)	21,22,23	2.78	9 (42%)

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	FIP	A	269	-	-	1/8/8/8	0/2/2/2
5	PLP	B	401	2	-	0/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	PLP	C3-C2	-4.87	1.35	1.41
5	B	401	PLP	C5-C4	-4.36	1.35	1.40
5	B	401	PLP	C2-N1	2.76	1.38	1.33
5	B	401	PLP	P-O3P	-2.70	1.44	1.54
3	A	269	FIP	C4-C5	2.18	1.41	1.37
5	B	401	PLP	C2A-C2	2.01	1.53	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	PLP	C3-C4-C5	6.31	126.16	118.59
5	B	401	PLP	C6-C5-C4	-5.09	113.92	118.10
5	B	401	PLP	O4P-C5A-C5	4.46	117.72	109.36
5	B	401	PLP	C4A-C4-C3	-3.86	114.09	120.52
5	B	401	PLP	C2A-C2-C3	3.81	125.26	120.80
3	A	269	FIP	C2P-C3P-C3	-3.73	104.82	113.92
5	B	401	PLP	O3-C3-C2	3.39	124.61	117.58
5	B	401	PLP	C3-C2-N1	-3.01	117.17	120.96
5	B	401	PLP	O2P-P-O4P	-2.53	100.07	106.67
3	A	269	FIP	OP3-P-OP4	-2.16	101.04	106.67
5	B	401	PLP	C5A-C5-C4	2.14	126.86	122.64
3	A	269	FIP	C7-C6-C5	2.05	120.48	118.38
3	A	269	FIP	F-C5-C4	2.04	121.18	118.28
3	A	269	FIP	OP3-P-OP1	2.03	118.74	110.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

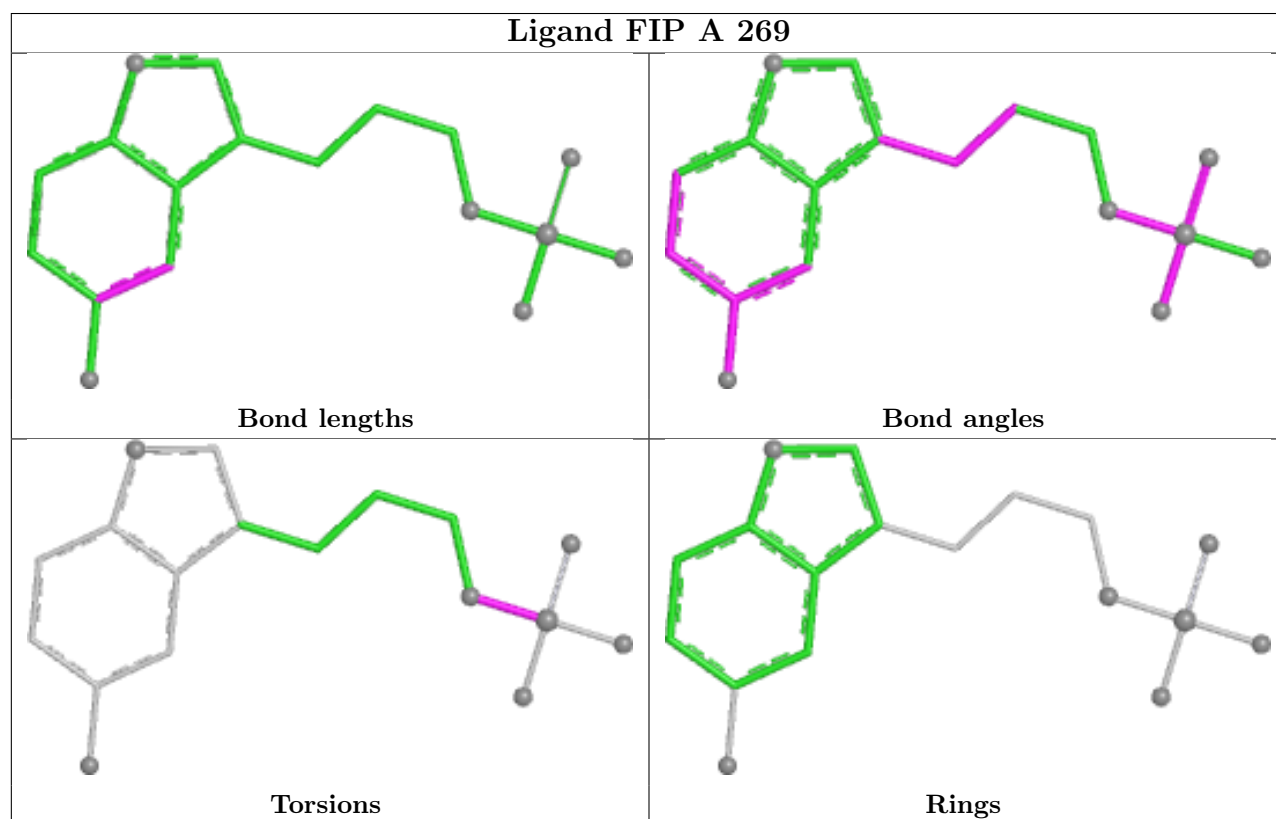
Mol	Chain	Res	Type	Atoms
3	A	269	FIP	C1P-OP4-P-OP3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	269	FIP	1	0
5	B	401	PLP	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 ⓘ

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, 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	262/268 (97%)	-0.13	4 (1%) 72 73	20, 40, 75, 106	0
2	B	393/396 (99%)	-0.55	8 (2%) 65 65	14, 25, 62, 109	0
All	All	655/664 (98%)	-0.38	12 (1%) 67 68	14, 31, 73, 109	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	ASN	4.2
2	B	63	GLN	4.1
2	B	139	VAL	3.7
2	B	161	SER	3.3
2	B	162	GLY	2.8
1	A	1	MET	2.7
2	B	164	ALA	2.6
2	B	393	ALA	2.5
1	A	193	LEU	2.5
2	B	160	HIS	2.3
1	A	194	HIS	2.2
2	B	391	LEU	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](#)

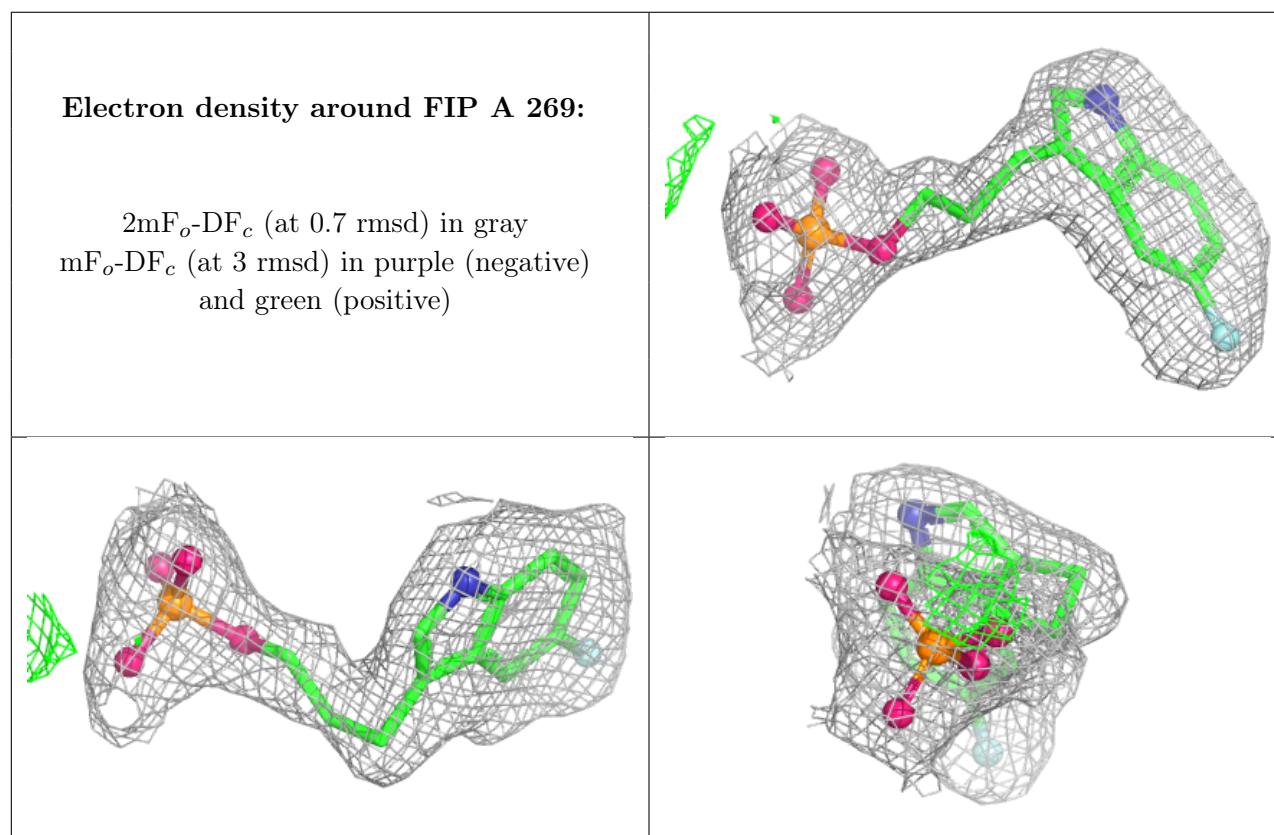
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
3	FIP	A	269	18/18	0.94	0.07	37,40,45,47	0
4	NA	B	400	1/1	0.97	0.03	21,21,21,21	0
5	PLP	B	401	15/16	0.98	0.05	14,18,22,22	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.