



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:44 AM EDT

PDB ID : 2TRS / pdb_00002trs
Title : CRYSTAL STRUCTURES OF MUTANT (BETAK87T) TRYPTOPHAN SYNTHASE ALPHA2 BETA2 COMPLEX WITH LIGANDS BOUND TO THE ACTIVE SITES OF THE ALPHA AND BETA SUBUNITS REVEAL LIGAND-INDUCED CONFORMATIONAL CHANGES
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Deposited on : 1997-01-07
Resolution : 2.04 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](#) ①) 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

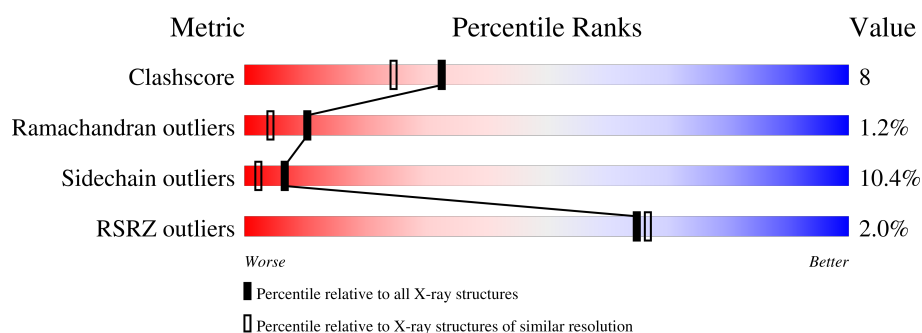
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	4% 63% 28% 7% .
2	B	397	% 63% 28% 5% . .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5153 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1976	1253	343	372	8			

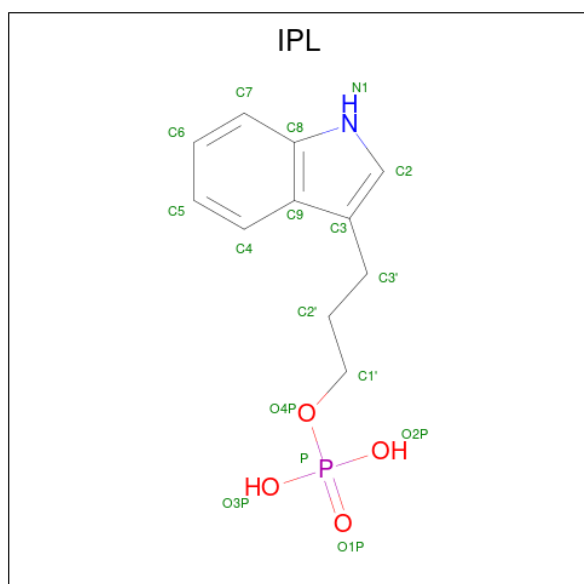
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	389	Total	C	N	O	S	0	0	0
			2948	1853	517	559	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	87	THR	LYS	engineered mutation	UNP P0A2K1
B	396	LEU	GLU	conflict	UNP P0A2K1

- Molecule 3 is INDOLE-3-PROPANOL PHOSPHATE (CCD ID: IPL) (formula: $C_{11}H_{14}NO_4P$).

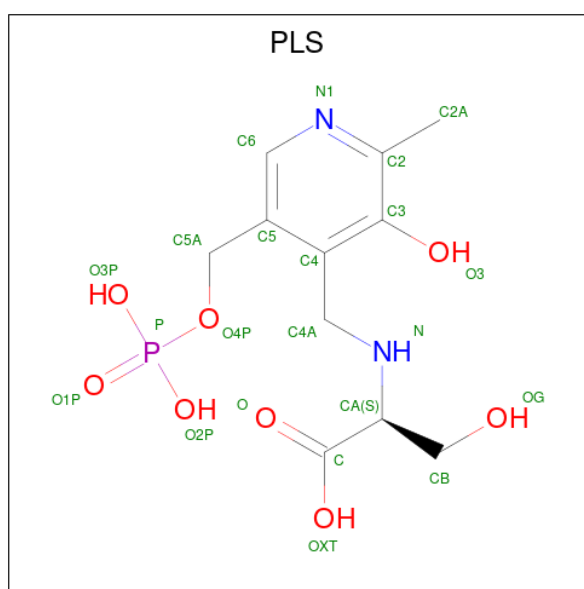


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			17	11	1	4	1		

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

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

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



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

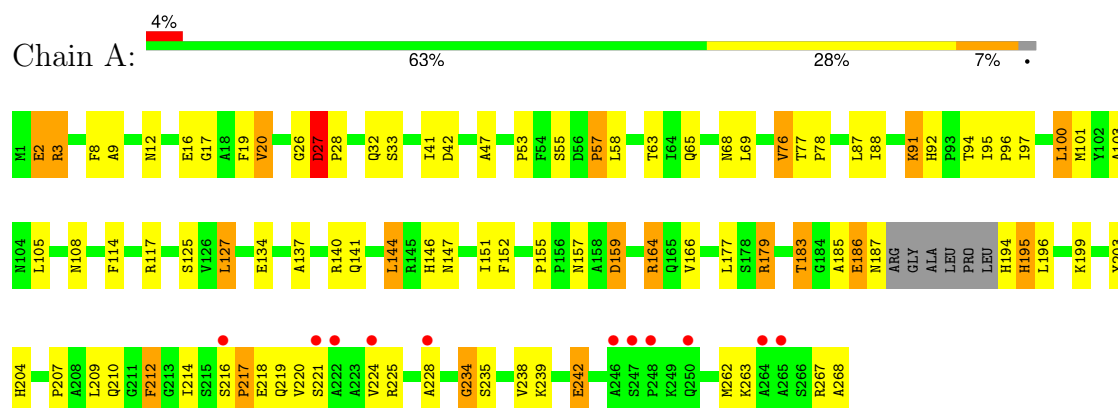
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	49	Total	O	0	0
			49	49		
6	B	140	Total	O	0	0
			140	140		

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



• Molecule 2: TRYPTOPHAN SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.20Å 61.30Å 67.90Å 90.00° 94.50° 90.00°	Depositor
Resolution (Å)	8.00 – 2.04 8.00 – 2.04	Depositor EDS
% Data completeness (in resolution range)	76.1 (8.00-2.04) 75.6 (8.00-2.04)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.05Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.214 , (Not available) 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 107.9	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	0.95	EDS
Total number of atoms	5153	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: PLS, NA, IPL

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	0.97	5/2014 (0.2%)	1.84	40/2733 (1.5%)
2	B	1.19	16/3006 (0.5%)	1.98	84/4063 (2.1%)
All	All	1.11	21/5020 (0.4%)	1.92	124/6796 (1.8%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	342	HIS	CD2-NE2	-8.19	1.28	1.37
2	B	366	PRO	CA-CB	-7.19	1.43	1.53
2	B	313	HIS	CD2-NE2	-6.98	1.30	1.37
2	B	267	HIS	CD2-NE2	-6.84	1.30	1.37
2	B	357	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	194	HIS	CD2-NE2	-6.40	1.30	1.37
2	B	273	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	195	HIS	CD2-NE2	-6.33	1.30	1.37
2	B	260	HIS	CD2-NE2	-6.17	1.31	1.37
2	B	160	HIS	CD2-NE2	-6.15	1.31	1.37
2	B	56	PRO	CA-CB	-6.04	1.42	1.53
2	B	388	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	204	HIS	CD2-NE2	-5.88	1.31	1.37
2	B	319	ILE	CA-CB	5.72	1.61	1.54
2	B	185	HIS	CD2-NE2	-5.61	1.31	1.37
2	B	74	TYR	CA-CB	-5.53	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	82	HIS	CD2-NE2	-5.49	1.31	1.37
1	A	92	HIS	CD2-NE2	-5.45	1.31	1.37
2	B	353	HIS	CD2-NE2	-5.40	1.31	1.37
2	B	86	HIS	CD2-NE2	-5.35	1.31	1.37
1	A	146	HIS	CD2-NE2	-5.09	1.32	1.37

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	325	VAL	N-CA-CB	-12.47	97.98	112.32
2	B	176	ASP	CA-CB-CG	10.59	123.19	112.60
1	A	2	GLU	N-CA-C	9.98	123.41	111.33
1	A	212	PHE	CA-CB-CG	9.82	123.62	113.80
2	B	293	GLN	OE1-CD-NE2	-9.05	113.55	122.60
1	A	187	ASN	CA-CB-CG	8.87	121.47	112.60
2	B	291	ASP	CA-CB-CG	8.59	121.19	112.60
2	B	236	ASN	CA-CB-CG	8.27	120.87	112.60
1	A	194	HIS	CB-CG-CD2	-7.89	120.94	131.20
2	B	293	GLN	CG-CD-NE2	7.85	128.18	116.40
1	A	27	ASP	CA-CB-CG	7.55	120.15	112.60
2	B	360	LYS	CB-CG-CD	-7.49	94.08	111.30
2	B	205	GLN	OE1-CD-NE2	-7.47	115.13	122.60
2	B	161	SER	N-CA-C	-7.37	92.88	107.69
2	B	55	ARG	CA-CB-CG	7.37	128.83	114.10
1	A	195	HIS	CA-CB-CG	7.35	121.15	113.80
1	A	42	ASP	CA-CB-CG	7.27	119.87	112.60
2	B	248	THR	N-CA-C	7.21	120.00	111.71
2	B	328	THR	N-CA-CB	-7.19	99.98	110.26
2	B	3	THR	CA-CB-OG1	-7.16	98.86	109.60
2	B	189	GLY	N-CA-C	7.13	123.51	114.66
1	A	141	GLN	O-C-N	-7.04	114.77	122.09
2	B	142	GLN	OE1-CD-NE2	-7.02	115.58	122.60
2	B	147	PHE	CA-CB-CG	-6.98	106.82	113.80
2	B	235	SER	N-CA-C	6.97	118.67	111.14
2	B	325	VAL	CB-CA-C	6.97	121.09	110.91
2	B	86	HIS	CB-CG-CD2	-6.96	122.15	131.20
2	B	115	HIS	N-CA-C	-6.92	103.83	112.90
2	B	180	SER	N-CA-C	6.86	121.24	113.01
1	A	214	ILE	N-CA-C	-6.84	98.27	108.12
2	B	361	MET	N-CA-C	6.82	119.58	111.33
2	B	269	ALA	CA-C-N	6.82	126.06	118.97
2	B	269	ALA	C-N-CA	6.82	126.06	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	379	ARG	NE-CZ-NH2	6.79	125.31	119.20
2	B	313	HIS	CB-CG-CD2	-6.65	122.55	131.20
2	B	82	HIS	CB-CG-CD2	-6.64	122.57	131.20
1	A	183	THR	N-CA-C	6.64	120.00	110.24
2	B	211	GLU	N-CA-C	-6.64	103.97	111.14
1	A	195	HIS	CB-CG-CD2	-6.63	122.58	131.20
2	B	6	ASN	CA-C-N	6.60	127.78	120.45
2	B	6	ASN	C-N-CA	6.60	127.78	120.45
2	B	77	ARG	N-CA-C	6.57	120.88	110.70
1	A	94	THR	N-CA-CB	-6.56	101.10	110.81
2	B	27	GLN	OE1-CD-NE2	-6.51	116.09	122.60
2	B	27	GLN	CG-CD-NE2	6.49	126.13	116.40
1	A	164	ARG	N-CA-C	-6.45	104.17	111.14
2	B	55	ARG	CB-CA-C	6.45	118.47	108.61
2	B	317	ASN	OD1-CG-ND2	-6.43	116.17	122.60
2	B	252	LEU	N-CA-C	-6.38	97.87	108.34
2	B	160	HIS	CB-CG-CD2	-6.37	122.92	131.20
2	B	357	HIS	CA-CB-CG	-6.34	107.46	113.80
1	A	3	ARG	NE-CZ-NH2	6.32	124.89	119.20
1	A	97	ILE	CB-CA-C	-6.31	102.33	110.98
1	A	194	HIS	CB-CG-ND1	6.31	132.17	122.70
1	A	210	GLN	O-C-N	6.29	130.11	123.06
2	B	184	ALA	N-CA-C	6.28	120.12	110.20
2	B	51	ASN	OD1-CG-ND2	-6.24	116.36	122.60
2	B	55	ARG	N-CA-CB	-6.19	99.82	110.10
1	A	103	ALA	N-CA-C	6.09	118.72	111.71
1	A	210	GLN	CA-CB-CG	-6.07	101.97	114.10
2	B	329	ASP	CA-CB-CG	6.05	118.65	112.60
2	B	336	PHE	CA-CB-CG	6.01	119.81	113.80
1	A	186	GLU	N-CA-C	-6.01	99.60	108.79
2	B	273	HIS	CB-CG-CD2	-5.90	123.53	131.20
2	B	227	VAL	N-CA-C	-5.88	100.01	108.48
1	A	58	LEU	N-CA-C	5.78	119.15	111.75
1	A	144	LEU	N-CA-C	-5.74	104.93	111.07
2	B	211	GLU	CA-C-O	-5.72	114.81	120.70
2	B	115	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	A	97	ILE	CA-CB-CG2	-5.69	100.83	110.50
2	B	3	THR	CA-CB-CG2	5.64	120.09	110.50
2	B	163	SER	N-CA-C	5.63	122.80	110.80
2	B	148	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	A	33	SER	N-CA-C	-5.62	105.24	111.36
2	B	305	ASP	CA-CB-CG	5.61	118.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	267	HIS	CA-CB-CG	5.59	119.39	113.80
2	B	130	CYS	N-CA-CB	-5.57	101.70	110.77
2	B	159	VAL	CA-C-O	5.57	127.59	121.13
1	A	137	ALA	CA-C-O	-5.54	112.56	120.16
1	A	91	LYS	O-C-N	-5.54	115.84	122.27
2	B	90	GLN	OE1-CD-NE2	-5.54	117.06	122.60
2	B	130	CYS	N-CA-C	5.52	117.43	108.26
1	A	140	ARG	NE-CZ-NH2	5.50	124.15	119.20
2	B	26	ASN	CA-CB-CG	5.49	118.09	112.60
2	B	19	GLN	N-CA-C	5.49	118.77	111.75
2	B	242	ALA	CA-C-O	-5.44	115.08	121.07
1	A	92	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	A	20	VAL	O-C-N	-5.40	117.97	121.37
2	B	19	GLN	OE1-CD-NE2	-5.36	117.24	122.60
2	B	313	HIS	CB-CG-ND1	5.32	130.68	122.70
2	B	195	HIS	CB-CG-CD2	-5.30	124.31	131.20
2	B	3	THR	N-CA-CB	-5.29	102.50	111.50
2	B	160	HIS	N-CA-C	-5.29	99.54	110.80
2	B	19	GLN	CG-CD-NE2	5.28	124.32	116.40
1	A	108	ASN	CB-CG-ND2	5.27	124.31	116.40
2	B	194	PRO	N-CA-C	5.27	119.76	111.38
2	B	388	HIS	CB-CG-CD2	-5.27	124.35	131.20
2	B	386	THR	N-CA-CB	-5.25	102.40	110.01
1	A	76	VAL	N-CA-CB	-5.23	105.86	111.46
1	A	77	THR	CA-C-N	5.23	126.37	119.84
1	A	77	THR	C-N-CA	5.23	126.37	119.84
1	A	179	ARG	CB-CG-CD	-5.22	99.28	111.30
2	B	207	MET	CG-SD-CE	-5.21	89.44	100.90
2	B	306	PHE	CA-C-N	5.21	126.14	120.83
2	B	306	PHE	C-N-CA	5.21	126.14	120.83
1	A	242	GLU	CA-CB-CG	5.19	124.49	114.10
2	B	83	GLY	N-CA-C	-5.19	107.51	114.25
2	B	181	TYR	N-CA-C	5.19	121.85	110.80
1	A	147	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	159	ASP	CA-CB-CG	5.16	117.76	112.60
2	B	38	ASP	CA-C-N	5.15	124.77	119.05
2	B	38	ASP	C-N-CA	5.15	124.77	119.05
2	B	126	LEU	N-CA-C	5.13	119.52	113.16
2	B	247	ASP	N-CA-C	-5.13	97.05	107.41
1	A	212	PHE	N-CA-C	-5.10	103.67	110.55
2	B	88	THR	N-CA-C	5.09	118.26	111.75
2	B	55	ARG	N-CA-C	-5.08	103.78	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	365	GLN	CA-C-N	5.06	126.16	119.84
2	B	365	GLN	C-N-CA	5.06	126.16	119.84
1	A	164	ARG	CB-CG-CD	5.06	122.93	111.30
1	A	88	ILE	N-CA-C	-5.03	105.80	110.53
2	B	86	HIS	CB-CG-ND1	5.03	130.24	122.70
2	B	175	ARG	NE-CZ-NH2	5.03	123.72	119.20
2	B	376	LEU	N-CA-C	-5.03	99.15	107.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	324	TYR	Sidechain

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	1976	0	1977	38	0
2	B	2948	0	2920	42	0
3	A	17	0	12	2	0
4	B	1	0	0	0	0
5	B	22	0	14	2	0
6	A	49	0	0	3	0
6	B	140	0	0	4	0
All	All	5153	0	4923	78	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 8.

All (78) 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:3:THR:HG23	2:B:5:LEU:O	1.89	0.71
1:A:185:ALA:HB2	1:A:235:SER:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LYS:HB2	6:A:550:HOH:O	1.91	0.69
2:B:160:HIS:HA	2:B:164:ALA:HB2	1.76	0.67
2:B:318:SER:HB2	6:B:575:HOH:O	1.95	0.66
2:B:91:VAL:HG13	2:B:187:MET:HE1	1.78	0.66
1:A:20:VAL:HG22	1:A:47:ALA:HB3	1.78	0.65
1:A:225:ARG:HH21	1:A:268:ALA:HB1	1.65	0.60
1:A:101:MET:HE2	1:A:114:PHE:CE1	2.38	0.58
1:A:234:GLY:O	1:A:238:VAL:HG23	2.03	0.58
2:B:34:ARG:HE	2:B:100:ARG:HE	1.52	0.58
2:B:7:PRO:HA	2:B:195:HIS:CD2	2.39	0.58
1:A:217:PRO:HA	1:A:262:MET:SD	2.45	0.57
2:B:143:SER:HA	2:B:146:VAL:HG23	1.87	0.56
2:B:116:GLY:HA3	2:B:149:MET:SD	2.46	0.55
1:A:152:PHE:HB2	1:A:166:VAL:HG23	1.88	0.55
2:B:327:ILE:HG23	2:B:331:GLU:HB2	1.89	0.55
1:A:220:VAL:O	1:A:224:VAL:HG23	2.06	0.55
1:A:157:ASN:ND2	2:B:23:PRO:HG2	2.22	0.55
2:B:193:GLY:HA2	2:B:280:PHE:O	2.07	0.53
1:A:55:SER:O	1:A:57:PRO:HD3	2.09	0.52
2:B:90:GLN:HA	2:B:204:PHE:HB3	1.92	0.52
1:A:183:THR:HG22	1:A:212:PHE:CE1	2.45	0.51
1:A:212:PHE:CD1	3:A:273:IPL:H1'2	2.46	0.51
2:B:143:SER:HA	2:B:146:VAL:CG2	2.40	0.51
2:B:91:VAL:HG11	2:B:118:ALA:O	2.12	0.49
1:A:212:PHE:HD1	3:A:273:IPL:H1'2	1.78	0.49
1:A:53:PRO:HA	1:A:68:ASN:OD1	2.13	0.49
1:A:3:ARG:HB3	1:A:96:PRO:HG3	1.94	0.49
2:B:313:HIS:HD2	2:B:324:TYR:OH	1.96	0.48
1:A:224:VAL:HA	1:A:228:ALA:O	2.14	0.48
2:B:34:ARG:HE	2:B:100:ARG:NE	2.10	0.48
1:A:157:ASN:HB2	6:A:572:HOH:O	2.14	0.47
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.96	0.47
1:A:155:PRO:HA	1:A:177:LEU:HB2	1.95	0.47
2:B:303:GLY:O	5:B:398:PLS:H5A1	2.13	0.47
1:A:157:ASN:HD22	2:B:23:PRO:HG2	1.80	0.46
2:B:78:GLU:HB2	2:B:377:SER:HA	1.96	0.46
2:B:6:ASN:HA	2:B:7:PRO:HD3	1.73	0.46
1:A:216:SER:HB3	1:A:219:GLN:HB2	1.96	0.46
1:A:164:ARG:HD2	1:A:203:TYR:CD1	2.51	0.46
2:B:147:PHE:HB2	6:B:497:HOH:O	2.15	0.45
2:B:32:PHE:CD1	2:B:200:ILE:HG12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASP:HA	1:A:28:PRO:HA	1.90	0.45
1:A:144:LEU:HD13	6:A:577:HOH:O	2.17	0.45
1:A:41:ILE:HG12	1:A:95:ILE:HD13	1.99	0.45
2:B:38:ASP:HA	2:B:39:PRO:HD2	1.82	0.45
2:B:333:LEU:O	2:B:337:LYS:HG3	2.17	0.45
2:B:34:ARG:HG3	2:B:100:ARG:HH11	1.82	0.45
2:B:89:ASN:HB3	2:B:207:MET:HE1	1.98	0.45
2:B:271:LEU:O	2:B:271:LEU:HD23	2.16	0.44
1:A:9:ALA:O	1:A:12:ASN:HB3	2.18	0.44
2:B:69:THR:HG21	2:B:362:MET:HG2	1.99	0.44
2:B:200:ILE:HD13	2:B:200:ILE:HG21	1.78	0.44
2:B:111:GLY:O	2:B:138:ASP:HB3	2.17	0.44
2:B:157:ILE:HA	2:B:158:PRO:HD3	1.77	0.44
1:A:8:PHE:CZ	1:A:209:LEU:HD21	2.53	0.43
2:B:42:GLN:HG2	6:B:505:HOH:O	2.18	0.43
2:B:254:GLY:O	2:B:324:TYR:HA	2.19	0.43
1:A:19:PHE:CE1	1:A:262:MET:HG2	2.54	0.43
1:A:101:MET:HE2	1:A:114:PHE:CZ	2.53	0.43
1:A:239:LYS:O	1:A:242:GLU:HB3	2.18	0.43
1:A:55:SER:H	2:B:293:GLN:NE2	2.17	0.42
2:B:272:LYS:HE2	2:B:324:TYR:O	2.20	0.42
1:A:26:GLY:CA	1:A:76:VAL:HG21	2.50	0.42
2:B:21:LEU:HD21	2:B:178:SER:HA	2.01	0.41
2:B:180:SER:O	2:B:182:GLU:N	2.54	0.41
2:B:206:ARG:O	2:B:210:GLU:HG3	2.21	0.41
2:B:275:ARG:HH21	2:B:275:ARG:HD3	1.76	0.41
1:A:125:SER:HB2	1:A:151:ILE:HD11	2.03	0.41
1:A:17:GLY:O	1:A:263:LYS:NZ	2.53	0.41
1:A:65:GLN:O	1:A:69:LEU:HD23	2.21	0.41
1:A:100:LEU:HD23	1:A:127:LEU:HD13	2.03	0.41
5:B:398:PLS:H5A1	5:B:398:PLS:H4A1	1.89	0.41
1:A:216:SER:O	1:A:219:GLN:HB2	2.21	0.40
2:B:376:LEU:HD12	2:B:376:LEU:HA	1.90	0.40
2:B:50:LYS:NZ	2:B:51:ASN:HD21	2.18	0.40
2:B:323:ASP:HB3	6:B:515:HOH:O	2.21	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	258/268 (96%)	239 (93%)	14 (5%)	5 (2%)	6	2
2	B	387/397 (98%)	363 (94%)	21 (5%)	3 (1%)	16	9
All	All	645/665 (97%)	602 (93%)	35 (5%)	8 (1%)	10	4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	ARG
2	B	163	SER
2	B	181	TYR
1	A	207	PRO
1	A	57	PRO
2	B	164	ALA
1	A	234	GLY
1	A	78	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	204/208 (98%)	184 (90%)	20 (10%)	7	3
2	B	305/311 (98%)	272 (89%)	33 (11%)	6	2
All	All	509/519 (98%)	456 (90%)	53 (10%)	7	2

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	16	GLU
1	A	27	ASP
1	A	32	GLN
1	A	63	THR
1	A	87	LEU
1	A	100	LEU
1	A	105	LEU
1	A	117	ARG
1	A	127	LEU
1	A	134	GLU
1	A	159	ASP
1	A	186	GLU
1	A	195	HIS
1	A	196	LEU
1	A	199	LYS
1	A	217	PRO
1	A	218	GLU
1	A	221	SER
1	A	267	ARG
2	B	3	THR
2	B	5	LEU
2	B	18	PRO
2	B	37	LYS
2	B	42	GLN
2	B	44	GLN
2	B	55	ARG
2	B	63	GLN
2	B	75	LEU
2	B	90	GLN
2	B	99	LYS
2	B	106	ILE
2	B	126	LEU
2	B	129	LYS
2	B	137	LYS
2	B	140	GLU
2	B	147	PHE
2	B	155	GLU
2	B	161	SER
2	B	163	SER
2	B	165	THR
2	B	166	LEU
2	B	180	SER

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Mol	Chain	Res	Type
2	B	182	GLU
2	B	198	PRO
2	B	207	MET
2	B	216	ILE
2	B	223	LEU
2	B	249	SER
2	B	325	VAL
2	B	337	LYS
2	B	347	PRO
2	B	351	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	204	HIS
1	A	244	ASN
2	B	36	GLN
2	B	44	GLN
2	B	51	ASN
2	B	64	ASN
2	B	195	HIS
2	B	215	GLN
2	B	260	HIS
2	B	288	GLN
2	B	293	GLN
2	B	313	HIS
2	B	342	HIS
2	B	365	GLN

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 [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
5	PLS	B	398	-	22,22,22	3.55	11 (50%)	28,31,31	3.55	12 (42%)
3	IPL	A	273	-	18,18,18	2.09	6 (33%)	25,25,25	3.24	4 (16%)

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
5	PLS	B	398	-	-	5/17/17/17	0/1/1/1
3	IPL	A	273	-	-	2/8/8/8	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	398	PLS	P-O1P	-10.00	1.19	1.50
5	B	398	PLS	P-O4P	-6.59	1.39	1.60
5	B	398	PLS	C3-C2	4.91	1.46	1.41
5	B	398	PLS	OXT-C	-4.58	1.16	1.30
3	A	273	IPL	C8-N1	-4.58	1.30	1.37
5	B	398	PLS	C3-C4	4.34	1.46	1.40
5	B	398	PLS	C6-C5	4.03	1.45	1.37
3	A	273	IPL	O4P-C1'	-4.00	1.28	1.44
5	B	398	PLS	P-O3P	-3.59	1.41	1.54
3	A	273	IPL	C5-C4	3.46	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	273	IPL	C2-N1	3.09	1.42	1.37
5	B	398	PLS	C2A-C2	3.02	1.55	1.50
5	B	398	PLS	CA-C	2.73	1.59	1.52
5	B	398	PLS	CB-CA	-2.58	1.45	1.53
3	A	273	IPL	C2-C3	-2.34	1.33	1.36
5	B	398	PLS	C4A-N	-2.15	1.40	1.46
3	A	273	IPL	C4-C9	2.14	1.43	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	273	IPL	C3'-C2'-C1'	13.02	138.45	112.33
5	B	398	PLS	O3P-P-O4P	12.57	139.46	106.67
5	B	398	PLS	C4A-N-CA	9.04	130.80	113.84
3	A	273	IPL	P-O4P-C1'	7.19	137.76	118.21
5	B	398	PLS	OXT-C-O	-4.15	114.66	124.08
5	B	398	PLS	OG-CB-CA	3.98	121.98	111.18
5	B	398	PLS	O4P-C5A-C5	3.28	115.51	109.36
5	B	398	PLS	O3-C3-C2	3.25	124.31	117.58
5	B	398	PLS	O3P-P-O1P	-3.20	98.37	110.83
5	B	398	PLS	C6-N1-C2	3.07	124.76	119.20
3	A	273	IPL	O4P-C1'-C2'	2.95	119.75	109.28
5	B	398	PLS	O2P-P-O4P	-2.65	99.75	106.67
3	A	273	IPL	C3-C2-N1	-2.43	107.64	110.31
5	B	398	PLS	CB-CA-N	2.37	115.96	109.05
5	B	398	PLS	C5-C6-N1	-2.29	120.10	123.83
5	B	398	PLS	C3-C2-N1	-2.17	118.22	120.96

There are no chirality outliers.

All (7) torsion outliers are listed below:

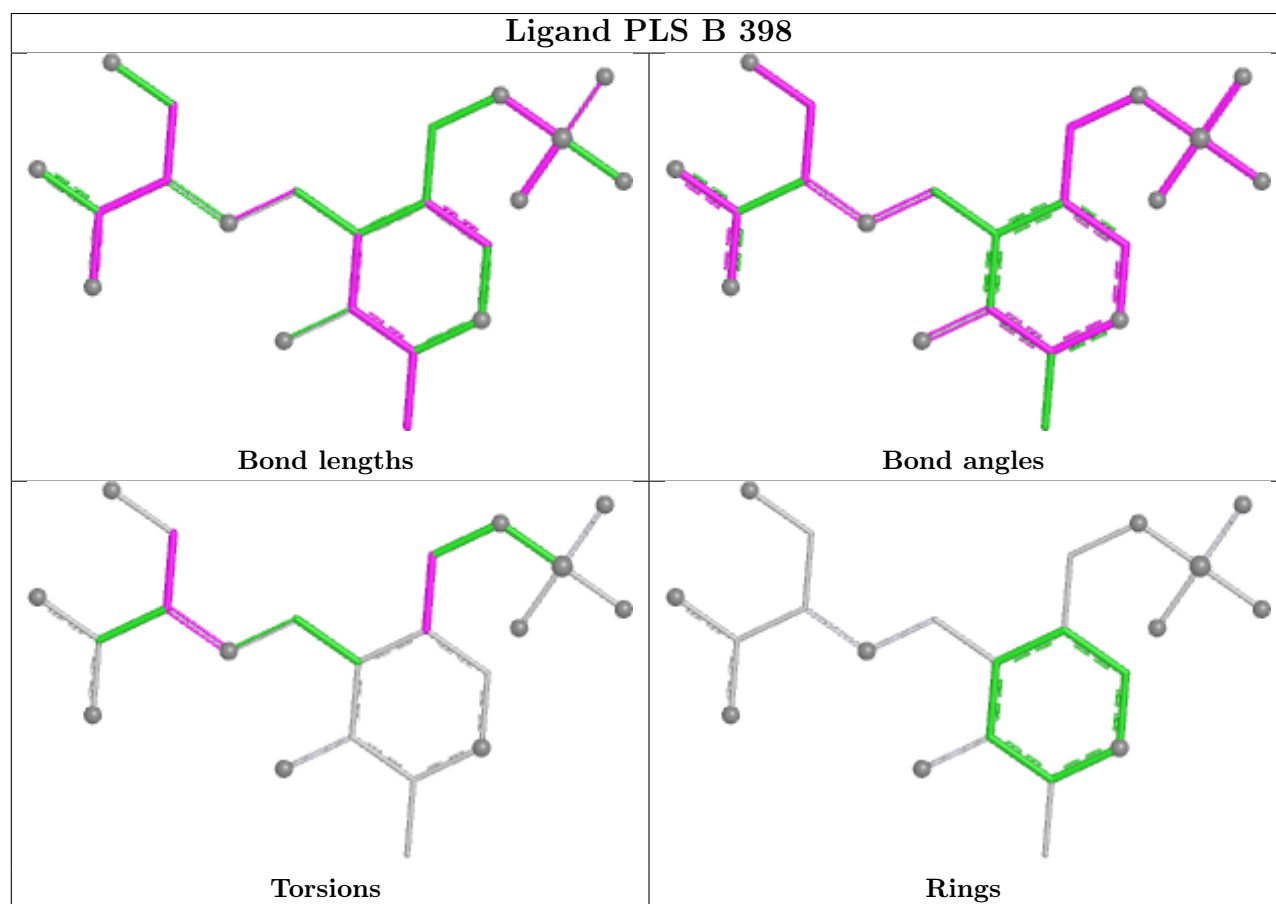
Mol	Chain	Res	Type	Atoms
3	A	273	IPL	C1'-C2'-C3'-C3
5	B	398	PLS	CB-CA-N-C4A
5	B	398	PLS	C4-C5-C5A-O4P
3	A	273	IPL	O4P-C1'-C2'-C3'
5	B	398	PLS	C6-C5-C5A-O4P
5	B	398	PLS	N-CA-CB-OG
5	B	398	PLS	C-CA-N-C4A

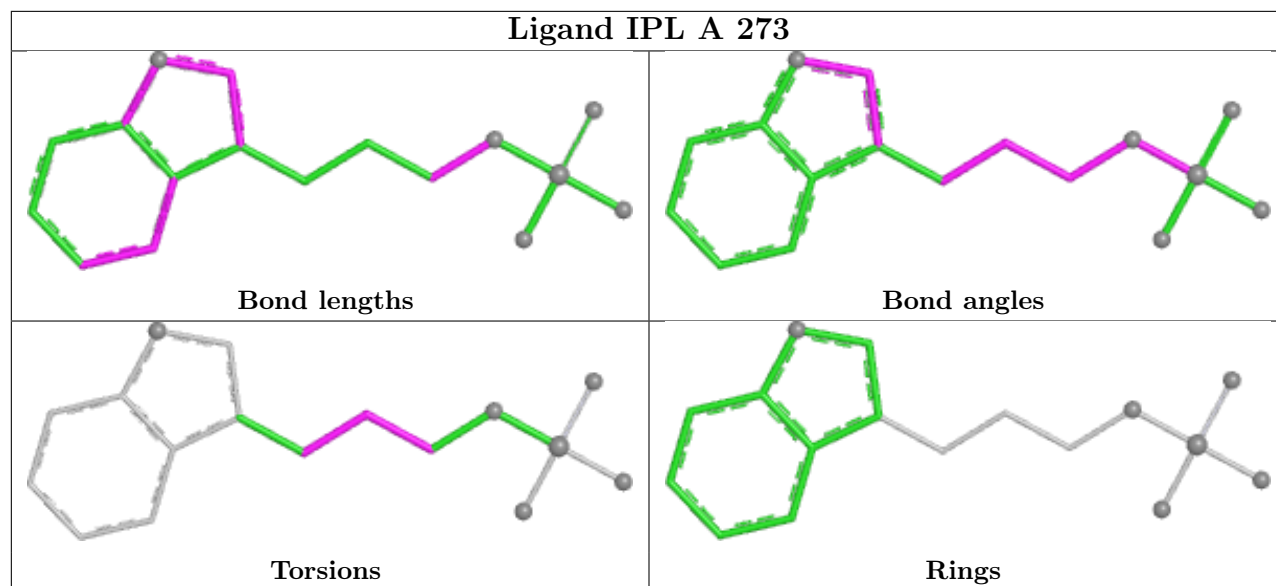
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	398	PLS	2	0
3	A	273	IPL	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, 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%)	0.08	11 (4%) 40 40	19, 54, 98, 120	1 (0%)
2	B	389/397 (97%)	-0.75	2 (0%) 87 89	11, 28, 64, 106	2 (0%)
All	All	651/665 (97%)	-0.41	13 (1%) 65 67	11, 35, 91, 120	3 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	SER	4.8
1	A	221	SER	3.9
1	A	222	ALA	3.5
1	A	264	ALA	3.0
1	A	246	ALA	2.8
2	B	163	SER	2.7
1	A	224	VAL	2.6
1	A	265	ALA	2.3
1	A	248	PRO	2.3
1	A	250	GLN	2.2
2	B	161	SER	2.1
1	A	228	ALA	2.1
1	A	247	SER	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](#)

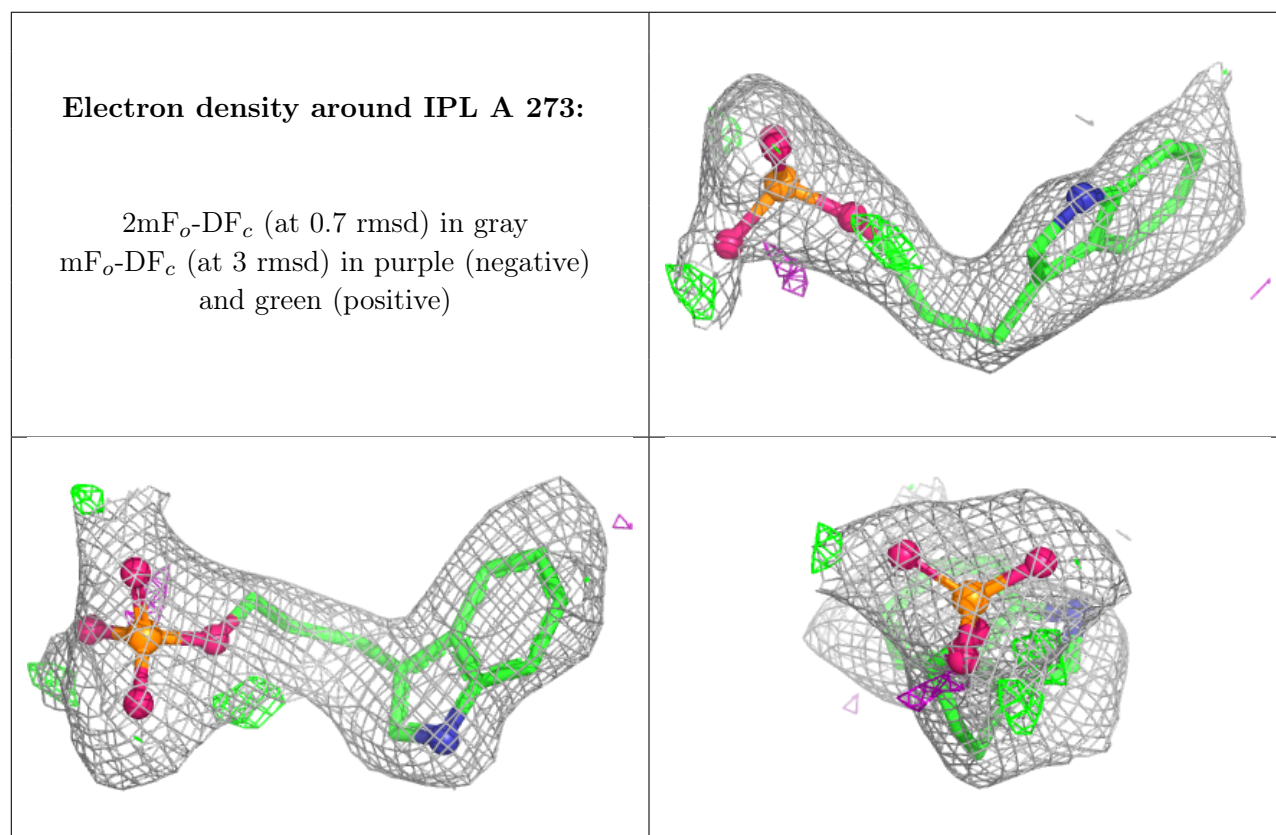
There are no oligosaccharides in this entry.

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.

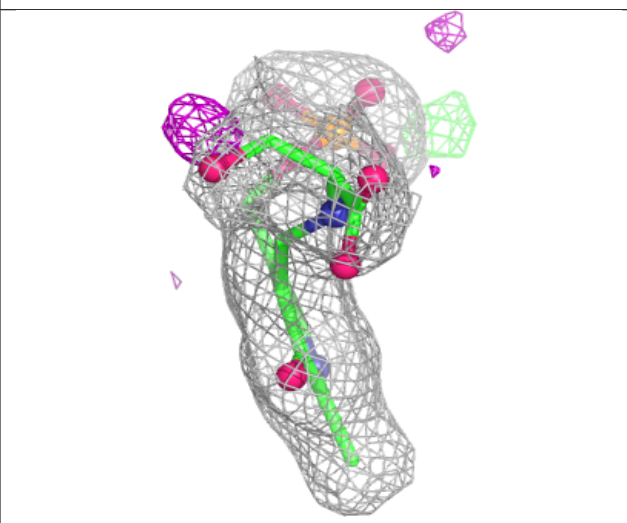
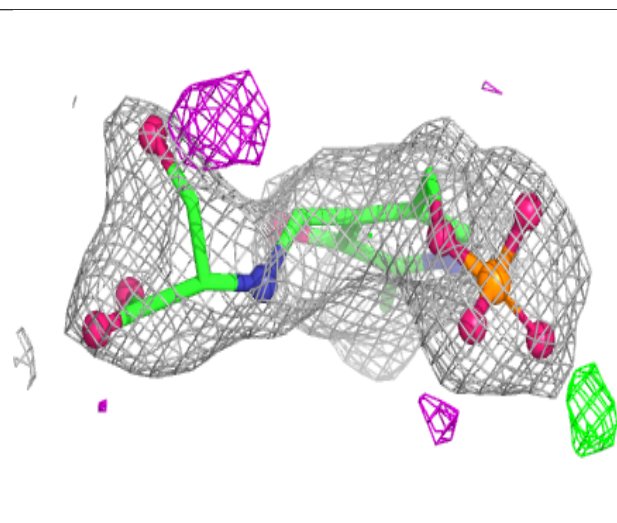
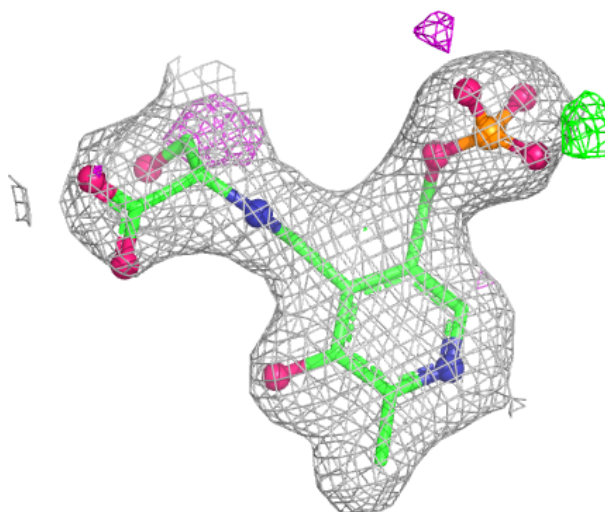
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IPL	A	273	17/17	0.89	0.07	42,52,67,68	0
4	NA	B	400	1/1	0.97	0.04	35,35,35,35	0
5	PLS	B	398	22/22	0.97	0.05	24,32,45,51	0

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 398:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.