



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:03 PM UTC

PDB ID : 2TSY / pdb_00002tsy
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
Authors : Rhee, S.; Parris, K.D.; Hyde, C.C.; Ahmed, S.A.; Miles, E.W.; Davies, D.R.
Deposited on : 1997-01-03
Resolution : 2.50 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

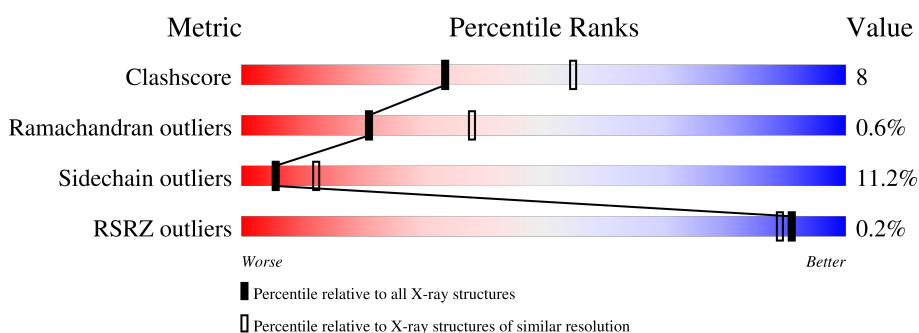
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	397	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	G3P	A	271	X	X	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5082 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			

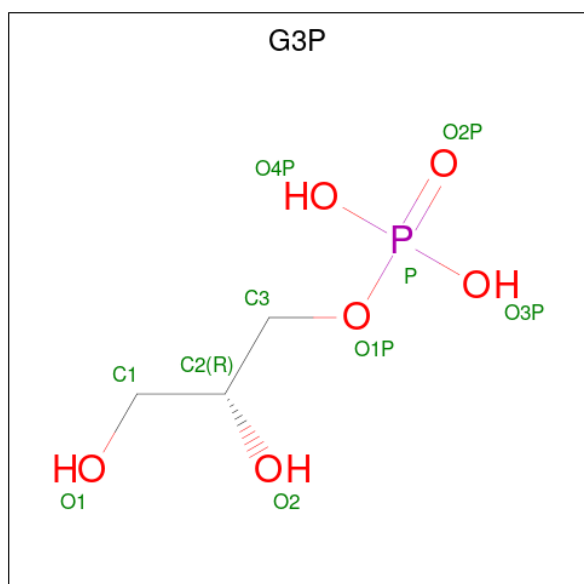
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE.

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 SN-GLYCEROL-3-PHOSPHATE (CCD ID: G3P) (formula: C₃H₉O₆P).

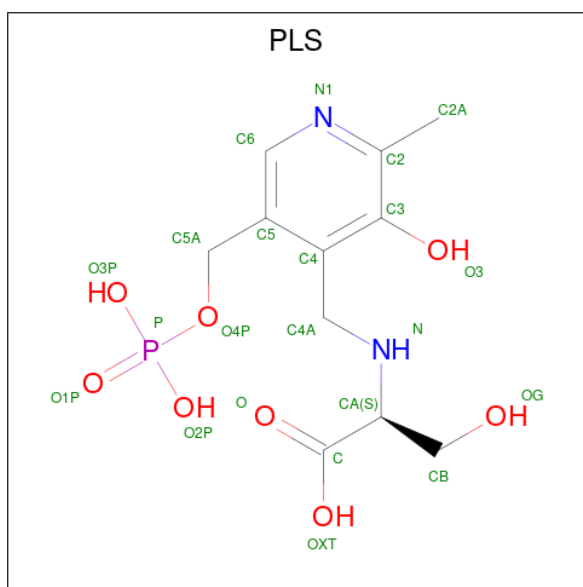


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			10	3	6	1		

- 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		

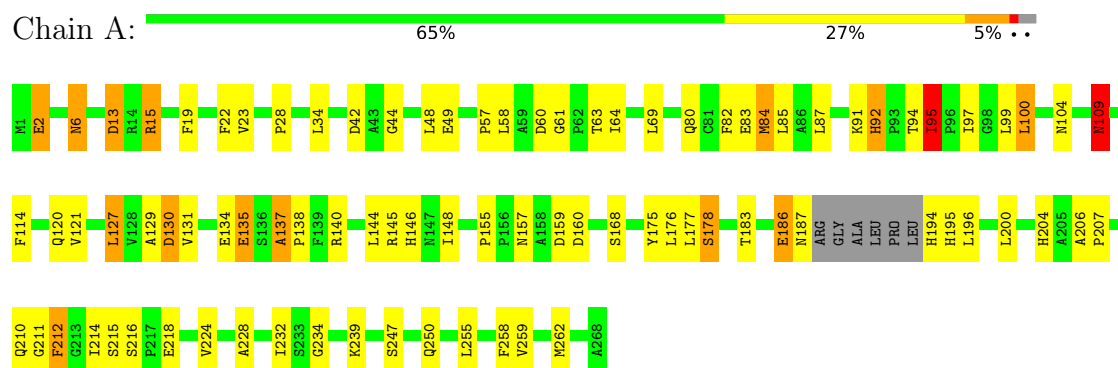
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	38	Total	O	0	0
			38	38		
6	B	87	Total	O	0	0
			87	87		

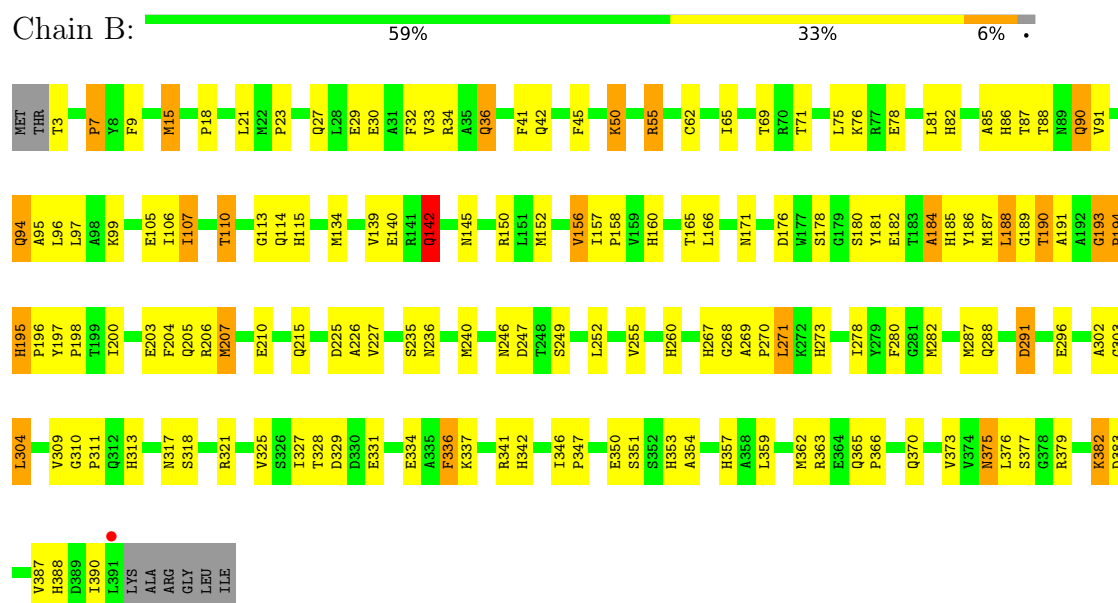
3 Residue-property plots

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	185.70Å 62.60Å 67.90Å 90.00° 94.40° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	89.5 (8.00-2.50) 87.6 (8.00-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.187 , (Not available) 0.172 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.710	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 80.1	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	5082	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G3P, PLS, NA

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	6/2014 (0.3%)	1.80	42/2733 (1.5%)
2	B	1.17	15/3006 (0.5%)	2.01	94/4063 (2.3%)
All	All	1.08	21/5020 (0.4%)	1.93	136/6796 (2.0%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	313	HIS	CD2-NE2	-7.14	1.29	1.37
2	B	267	HIS	CD2-NE2	-7.08	1.30	1.37
2	B	160	HIS	CD2-NE2	-6.86	1.30	1.37
2	B	357	HIS	CD2-NE2	-6.54	1.30	1.37
2	B	273	HIS	CD2-NE2	-6.51	1.30	1.37
2	B	366	PRO	CA-CB	-6.45	1.44	1.53
2	B	115	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	92	HIS	CD2-NE2	-6.19	1.31	1.37
2	B	388	HIS	CD2-NE2	-6.14	1.31	1.37
2	B	156	VAL	CA-CB	6.12	1.62	1.54
1	A	195	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	194	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	204	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	146	HIS	CD2-NE2	-5.78	1.31	1.37
2	B	260	HIS	CD2-NE2	-5.77	1.31	1.37
2	B	185	HIS	CD2-NE2	-5.69	1.31	1.37
2	B	82	HIS	CD2-NE2	-5.34	1.31	1.37
2	B	195	HIS	CG-ND1	-5.29	1.32	1.38
1	A	92	HIS	CG-ND1	-5.28	1.32	1.38
2	B	86	HIS	CD2-NE2	-5.22	1.32	1.37
2	B	342	HIS	CD2-NE2	-5.13	1.32	1.37

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	176	ASP	CA-CB-CG	11.38	123.98	112.60
2	B	236	ASN	CA-CB-CG	11.02	123.62	112.60
1	A	2	GLU	N-CA-C	9.71	123.08	111.33
1	A	13	ASP	CA-CB-CG	8.46	121.06	112.60
2	B	184	ALA	N-CA-C	8.32	123.00	109.76
2	B	226	ALA	CA-C-O	-8.17	111.84	120.99
1	A	186	GLU	O-C-N	8.08	133.38	123.44
2	B	55	ARG	CA-CB-CG	7.99	130.08	114.10
2	B	45	PHE	N-CA-C	-7.91	102.59	111.14
2	B	291	ASP	CA-CB-CG	7.86	120.46	112.60
2	B	375	ASN	OD1-CG-ND2	-7.85	114.75	122.60
1	A	130	ASP	CA-CB-CG	7.55	120.15	112.60
1	A	137	ALA	CA-C-O	-7.48	109.91	120.16
1	A	109	ASN	CA-CB-CG	7.46	120.06	112.60
2	B	375	ASN	CA-CB-CG	7.30	119.90	112.60
2	B	15	MET	CG-SD-CE	-7.22	85.02	100.90
2	B	171	ASN	CA-CB-CG	7.16	119.75	112.60
2	B	115	HIS	CB-CG-CD2	-7.13	121.92	131.20
2	B	273	HIS	CB-CG-CD2	-7.10	121.97	131.20
1	A	6	ASN	CA-CB-CG	7.09	119.69	112.60
1	A	95	ILE	CB-CA-C	-6.96	102.68	110.68
2	B	310	GLY	CA-C-N	6.93	126.74	119.05
2	B	310	GLY	C-N-CA	6.93	126.74	119.05
1	A	195	HIS	CA-CB-CG	6.89	120.69	113.80
2	B	205	GLN	OE1-CD-NE2	-6.89	115.71	122.60
2	B	142	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	A	42	ASP	CA-CB-CG	6.81	119.41	112.60
1	A	19	PHE	CA-CB-CG	-6.79	107.01	113.80
2	B	152	MET	CG-SD-CE	-6.76	86.04	100.90
1	A	168	SER	N-CA-C	6.74	118.71	111.36
2	B	145	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	A	186	GLU	N-CA-C	6.63	120.42	108.48
2	B	207	MET	CG-SD-CE	-6.59	86.39	100.90
1	A	159	ASP	CA-CB-CG	6.54	119.14	112.60
2	B	7	PRO	N-CA-C	6.51	121.45	114.68
2	B	90	GLN	OE1-CD-NE2	-6.46	116.14	122.60
1	A	160	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	84	MET	CA-CB-CG	6.44	126.97	114.10
2	B	194	PRO	N-CA-C	6.43	121.28	111.19
2	B	160	HIS	CB-CG-CD2	-6.41	122.86	131.20
2	B	325	VAL	CA-C-O	-6.39	115.37	121.64
2	B	55	ARG	CB-CA-C	6.36	118.75	109.20
2	B	288	GLN	CG-CD-NE2	6.32	125.88	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	260	HIS	CB-CG-CD2	-6.30	123.01	131.20
2	B	205	GLN	O-C-N	-6.28	115.25	122.09
2	B	36	GLN	OE1-CD-NE2	-6.25	116.35	122.60
2	B	342	HIS	CA-CB-CG	-6.22	107.58	113.80
1	A	95	ILE	N-CA-CB	6.17	117.02	110.17
2	B	115	HIS	N-CA-C	-6.16	103.88	112.45
2	B	329	ASP	CA-CB-CG	6.16	118.76	112.60
2	B	86	HIS	CB-CG-CD2	-6.13	123.23	131.20
1	A	109	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	A	177	LEU	O-C-N	6.07	130.20	123.16
2	B	328	THR	CA-CB-OG1	-6.05	100.53	109.60
2	B	185	HIS	CB-CG-CD2	-6.02	123.37	131.20
2	B	282	MET	O-C-N	6.01	130.11	123.25
2	B	95	ALA	N-CA-C	-5.98	104.84	111.36
2	B	88	THR	O-C-N	-5.95	115.42	122.20
2	B	82	HIS	CB-CG-CD2	-5.94	123.47	131.20
2	B	350	GLU	CA-C-O	-5.94	114.78	120.90
2	B	370	GLN	N-CA-C	5.93	118.11	108.26
2	B	142	GLN	N-CA-CB	-5.93	101.65	111.49
2	B	193	GLY	CA-C-N	5.93	125.69	119.76
2	B	193	GLY	C-N-CA	5.93	125.69	119.76
2	B	383	ASP	N-CA-C	5.92	120.58	113.23
2	B	313	HIS	CB-CG-CD2	-5.90	123.53	131.20
2	B	107	ILE	N-CA-C	-5.88	99.95	108.89
2	B	185	HIS	CB-CG-ND1	5.85	131.47	122.70
2	B	189	GLY	N-CA-C	5.83	119.94	112.83
1	A	204	HIS	CB-CG-CD2	-5.83	123.63	131.20
2	B	106	ILE	N-CA-C	-5.82	99.68	108.17
1	A	212	PHE	N-CA-C	5.80	118.66	109.96
2	B	341	ARG	O-C-N	-5.80	114.72	122.43
1	A	61	GLY	CA-C-N	5.73	125.09	118.85
1	A	61	GLY	C-N-CA	5.73	125.09	118.85
1	A	23	VAL	CG1-CB-CG2	-5.71	98.24	110.80
1	A	250	GLN	OE1-CD-NE2	-5.71	116.89	122.60
2	B	142	GLN	CG-CD-NE2	5.67	124.91	116.40
2	B	246	ASN	CA-CB-CG	5.67	118.27	112.60
1	A	58	LEU	N-CA-C	5.64	118.97	111.75
2	B	105	GLU	N-CA-C	-5.64	101.86	110.14
2	B	185	HIS	CA-CB-CG	5.61	119.41	113.80
2	B	318	SER	N-CA-C	5.59	118.09	111.33
2	B	373	VAL	O-C-N	-5.55	117.31	123.03
1	A	211	GLY	N-CA-C	5.55	126.33	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	GLU	CA-C-N	5.54	131.68	121.70
1	A	186	GLU	C-N-CA	5.54	131.68	121.70
1	A	92	HIS	CB-CG-CD2	-5.50	124.05	131.20
2	B	288	GLN	OE1-CD-NE2	-5.49	117.11	122.60
2	B	27	GLN	OE1-CD-NE2	-5.48	117.12	122.60
2	B	88	THR	CA-C-O	-5.48	114.06	120.20
2	B	9	PHE	N-CA-C	-5.48	96.83	107.62
2	B	273	HIS	CB-CG-ND1	5.47	130.91	122.70
2	B	302	ALA	O-C-N	-5.47	115.32	122.59
1	A	195	HIS	CB-CG-CD2	-5.46	124.10	131.20
2	B	336	PHE	CA-CB-CG	5.46	119.26	113.80
1	A	218	GLU	CB-CG-CD	5.45	121.87	112.60
2	B	390	ILE	N-CA-C	-5.41	98.09	109.34
1	A	206	ALA	CA-C-N	5.39	126.58	119.84
1	A	206	ALA	C-N-CA	5.39	126.58	119.84
2	B	334	GLU	CB-CG-CD	5.39	121.77	112.60
2	B	236	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	A	247	SER	CA-C-N	5.36	125.43	119.32
1	A	247	SER	C-N-CA	5.36	125.43	119.32
2	B	388	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	A	121	VAL	CG1-CB-CG2	-5.33	99.07	110.80
1	A	129	ALA	N-CA-C	5.33	118.57	111.75
2	B	311	PRO	N-CA-C	5.31	120.92	113.53
1	A	82	PHE	CA-CB-CG	-5.31	108.49	113.80
2	B	337	LYS	CB-CG-CD	5.30	123.48	111.30
2	B	382	LYS	CA-C-O	5.30	125.90	119.49
2	B	156	VAL	N-CA-C	-5.29	100.86	108.48
2	B	346	ILE	CA-C-O	-5.28	116.03	119.15
2	B	365	GLN	CA-C-N	5.25	124.92	119.56
2	B	365	GLN	C-N-CA	5.25	124.92	119.56
2	B	287	MET	N-CA-C	-5.20	100.05	108.52
2	B	197	TYR	CA-C-O	-5.19	113.86	118.63
2	B	317	ASN	OD1-CG-ND2	-5.18	117.42	122.60
2	B	375	ASN	CB-CG-ND2	5.18	124.18	116.40
2	B	50	LYS	N-CA-C	5.18	116.78	111.03
2	B	235	SER	N-CA-C	5.16	116.72	111.14
2	B	113	GLY	N-CA-C	-5.16	108.87	115.42
1	A	144	LEU	CA-C-O	-5.14	115.61	121.00
2	B	207	MET	N-CA-C	-5.13	105.76	112.23
2	B	357	HIS	CB-CG-CD2	-5.12	124.55	131.20
2	B	205	GLN	N-CA-C	-5.11	106.16	114.09
2	B	269	ALA	CA-C-N	5.11	126.23	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	ALA	C-N-CA	5.11	126.23	119.84
2	B	225	ASP	N-CA-C	-5.09	106.23	112.90
2	B	55	ARG	O-C-N	-5.09	116.59	121.94
2	B	379	ARG	N-CA-C	-5.09	102.93	110.46
1	A	64	ILE	N-CA-C	-5.06	105.77	110.53
1	A	145	ARG	CB-CG-CD	-5.04	99.70	111.30
2	B	304	LEU	N-CA-C	-5.04	107.08	114.39
2	B	353	HIS	CB-CG-ND1	5.02	130.24	122.70
2	B	247	ASP	N-CA-C	-5.02	97.73	107.62

There are no chirality outliers.

There are no planarity outliers.

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	1976	0	1977	28	0
2	B	2948	0	2920	50	0
3	A	10	0	4	4	0
4	B	1	0	0	0	0
5	B	22	0	13	2	0
6	A	38	0	0	0	0
6	B	87	0	0	1	0
All	All	5082	0	4914	76	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 (76) 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)
3:A:271:G3P:C3	3:A:271:G3P:O1P	1.68	1.37
2:B:94:GLN:HB3	2:B:187:MET:HE2	1.58	0.83
1:A:210:GLN:HE21	1:A:214:ILE:HD11	1.47	0.79
2:B:21:LEU:HD21	2:B:178:SER:HA	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:HB3	1:A:234:GLY:HA2	1.67	0.74
2:B:3:THR:HG21	2:B:15:MET:HE1	1.70	0.74
1:A:92:HIS:HB3	1:A:95:ILE:HD11	1.72	0.70
2:B:359:LEU:O	2:B:363:ARG:HG2	1.92	0.68
2:B:69:THR:HG22	2:B:71:THR:H	1.59	0.67
2:B:271:LEU:HB2	2:B:309:VAL:HG11	1.79	0.63
1:A:175:TYR:CE2	1:A:232:ILE:HD12	2.35	0.62
3:A:271:G3P:C3	3:A:271:G3P:P	2.87	0.61
2:B:91:VAL:HG13	2:B:187:MET:SD	2.41	0.61
1:A:100:LEU:HD23	1:A:127:LEU:HB3	1.84	0.60
2:B:134:MET:HG2	2:B:139:VAL:HG23	1.83	0.60
1:A:157:ASN:HD22	2:B:23:PRO:HG2	1.67	0.59
1:A:157:ASN:ND2	2:B:23:PRO:HG2	2.20	0.57
2:B:69:THR:HG21	2:B:362:MET:CG	2.34	0.57
2:B:271:LEU:HD12	2:B:271:LEU:O	2.04	0.57
1:A:183:THR:HG22	3:A:271:G3P:H32	1.88	0.56
1:A:183:THR:CG2	3:A:271:G3P:H32	2.35	0.56
2:B:78:GLU:HB2	2:B:377:SER:HA	1.87	0.56
2:B:107:ILE:HD11	2:B:184:ALA:HB1	1.88	0.56
2:B:303:GLY:O	5:B:398:PLS:H5A1	2.05	0.55
2:B:327:ILE:HG23	2:B:331:GLU:HB2	1.88	0.55
2:B:240:MET:HE2	2:B:375:ASN:OD1	2.06	0.55
1:A:57:PRO:HB2	1:A:60:ASP:HB2	1.89	0.55
2:B:30:GLU:O	2:B:34:ARG:HG3	2.07	0.54
2:B:69:THR:HG21	2:B:362:MET:HG3	1.89	0.54
2:B:29:GLU:HB2	2:B:196:PRO:HG3	1.90	0.53
2:B:186:TYR:CE2	2:B:188:LEU:HG	2.43	0.53
1:A:258:PHE:O	1:A:262:MET:HG2	2.09	0.52
1:A:104:ASN:HD22	2:B:278:ILE:H	1.57	0.51
1:A:85:LEU:HD11	1:A:99:LEU:HD21	1.93	0.51
2:B:62:CYS:SG	2:B:65:ILE:HD11	2.51	0.50
2:B:255:VAL:HG21	2:B:354:ALA:HA	1.94	0.50
2:B:193:GLY:HA2	2:B:280:PHE:O	2.12	0.50
2:B:76:LYS:HZ2	2:B:215:GLN:HE22	1.59	0.49
2:B:142:GLN:OE1	2:B:382:LYS:HD2	2.12	0.49
1:A:224:VAL:HA	1:A:228:ALA:O	2.12	0.48
2:B:90:GLN:HE21	2:B:94:GLN:NE2	2.12	0.48
2:B:194:PRO:HG3	6:B:427:HOH:O	2.11	0.48
2:B:303:GLY:HA3	5:B:398:PLS:H4A2	1.95	0.47
2:B:268:GLY:C	2:B:270:PRO:HD2	2.38	0.47
1:A:34:LEU:HD21	1:A:84:MET:HB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:THR:HG21	2:B:362:MET:HG2	1.96	0.47
1:A:104:ASN:ND2	2:B:278:ILE:H	2.13	0.47
2:B:87:THR:HG21	2:B:114:GLN:O	2.14	0.47
2:B:157:ILE:HA	2:B:158:PRO:HD3	1.74	0.46
2:B:190:THR:OG1	2:B:191:ALA:N	2.47	0.46
1:A:255:LEU:O	1:A:259:VAL:HG23	2.16	0.46
2:B:41:PHE:HD2	2:B:42:GLN:NE2	2.14	0.45
1:A:137:ALA:HB3	1:A:138:PRO:HD3	1.97	0.45
2:B:81:LEU:HD23	2:B:85:ALA:O	2.16	0.45
1:A:22:PHE:HD2	1:A:49:GLU:HB3	1.81	0.45
2:B:29:GLU:O	2:B:33:VAL:HG23	2.17	0.45
1:A:91:LYS:HG3	1:A:92:HIS:CD2	2.52	0.44
2:B:110:THR:HG23	2:B:134:MET:HE3	1.99	0.44
2:B:376:LEU:HD12	2:B:376:LEU:HA	1.85	0.44
1:A:131:VAL:HG13	1:A:135:GLU:HB3	2.00	0.44
2:B:206:ARG:O	2:B:210:GLU:HG3	2.17	0.44
1:A:109:ASN:HD21	1:A:114:PHE:HB2	1.82	0.44
2:B:180:SER:O	2:B:182:GLU:N	2.51	0.43
2:B:110:THR:HG22	2:B:134:MET:HB2	2.01	0.43
1:A:15:ARG:NE	1:A:15:ARG:HA	2.34	0.43
2:B:336:PHE:CE2	2:B:387:VAL:HG11	2.53	0.43
2:B:32:PHE:CD1	2:B:200:ILE:HG12	2.55	0.42
1:A:48:LEU:HB2	1:A:97:ILE:HG22	2.02	0.41
2:B:41:PHE:HD2	2:B:42:GLN:HE21	1.68	0.41
1:A:95:ILE:HD13	1:A:95:ILE:H	1.85	0.41
2:B:227:VAL:HG22	2:B:252:LEU:HD23	2.02	0.41
2:B:7:PRO:HB3	2:B:195:HIS:CG	2.56	0.41
2:B:90:GLN:HA	2:B:204:PHE:HB3	2.02	0.41
1:A:137:ALA:HA	1:A:140:ARG:HG2	2.03	0.41
1:A:178:SER:OG	1:A:212:PHE:N	2.54	0.40
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.99	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%)	230 (89%)	25 (10%)	3 (1%)	10	20
2	B	387/397 (98%)	364 (94%)	22 (6%)	1 (0%)	36	55
All	All	645/665 (97%)	594 (92%)	47 (7%)	4 (1%)	21	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	181	TYR
1	A	15	ARG
1	A	13	ASP
1	A	44	GLY

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%)	176 (86%)	28 (14%)	3	7
2	B	305/311 (98%)	276 (90%)	29 (10%)	8	17
All	All	509/519 (98%)	452 (89%)	57 (11%)	6	12

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	6	ASN
1	A	28	PRO
1	A	63	THR
1	A	69	LEU
1	A	80	GLN
1	A	83	GLU
1	A	87	LEU
1	A	94	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	95	ILE
1	A	100	LEU
1	A	109	ASN
1	A	120	GLN
1	A	127	LEU
1	A	130	ASP
1	A	134	GLU
1	A	135	GLU
1	A	148	ILE
1	A	155	PRO
1	A	176	LEU
1	A	178	SER
1	A	186	GLU
1	A	187	ASN
1	A	196	LEU
1	A	207	PRO
1	A	215	SER
1	A	216	SER
1	A	239	LYS
2	B	18	PRO
2	B	36	GLN
2	B	50	LYS
2	B	55	ARG
2	B	75	LEU
2	B	94	GLN
2	B	96	LEU
2	B	97	LEU
2	B	99	LYS
2	B	110	THR
2	B	140	GLU
2	B	142	GLN
2	B	150	ARG
2	B	156	VAL
2	B	165	THR
2	B	166	LEU
2	B	188	LEU
2	B	190	THR
2	B	198	PRO
2	B	203	GLU
2	B	207	MET
2	B	249	SER
2	B	271	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	291	ASP
2	B	296	GLU
2	B	304	LEU
2	B	321	ARG
2	B	347	PRO
2	B	351	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	109	ASN
1	A	195	HIS
1	A	210	GLN
1	A	250	GLN
2	B	90	GLN
2	B	171	ASN
2	B	195	HIS
2	B	215	GLN

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	$\# Z > 2$
5	PLS	B	398	-	22,22,22	2.49	12 (54%)	28,31,31	3.37	9 (32%)
3	G3P	A	271	-	9,9,9	4.30	8 (88%)	10,12,12	2.41	4 (40%)

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	-	-	4/17/17/17	0/1/1/1
3	G3P	A	271	-	1/1/2/2	1/8/8/8	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	271	G3P	C1-C2	-8.13	1.20	1.51
3	A	271	G3P	O1P-C3	6.25	1.68	1.44
5	B	398	PLS	P-O1P	-5.70	1.32	1.50
5	B	398	PLS	P-O4P	-5.65	1.42	1.60
3	A	271	G3P	P-O3P	-4.50	1.38	1.54
3	A	271	G3P	P-O2P	3.51	1.61	1.50
5	B	398	PLS	C4A-N	-3.26	1.37	1.46
3	A	271	G3P	O2-C2	3.21	1.52	1.43
5	B	398	PLS	C3-C2	3.07	1.44	1.41
5	B	398	PLS	OXT-C	-2.85	1.21	1.30
3	A	271	G3P	O1-C1	2.85	1.54	1.42
5	B	398	PLS	C5-C4	-2.60	1.36	1.40
5	B	398	PLS	CA-C	2.46	1.58	1.52
3	A	271	G3P	C3-C2	2.40	1.59	1.51
5	B	398	PLS	O-C	2.32	1.29	1.22
5	B	398	PLS	C6-C5	2.31	1.42	1.37
5	B	398	PLS	P-O3P	-2.29	1.46	1.54
5	B	398	PLS	C3-C4	2.27	1.43	1.40
5	B	398	PLS	C5A-C5	2.20	1.56	1.50
3	A	271	G3P	P-O1P	2.07	1.66	1.60

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	398	PLS	O3P-P-O4P	10.90	135.08	106.67
5	B	398	PLS	C4A-N-CA	10.22	133.01	113.84
3	A	271	G3P	C3-C2-C1	4.30	126.24	111.77
5	B	398	PLS	O4P-C5A-C5	3.68	116.26	109.36
5	B	398	PLS	O3-C3-C2	3.58	125.00	117.58
3	A	271	G3P	O2-C2-C1	-3.51	94.66	109.18
3	A	271	G3P	O1-C1-C2	3.28	125.13	110.38
5	B	398	PLS	OXT-C-O	-3.05	117.15	124.08
5	B	398	PLS	OG-CB-CA	2.85	118.91	111.18
3	A	271	G3P	O3P-P-O2P	-2.83	99.81	110.83
5	B	398	PLS	C6-N1-C2	2.69	124.07	119.20
5	B	398	PLS	C5-C6-N1	-2.67	119.49	123.83
5	B	398	PLS	O2P-P-O4P	-2.48	100.20	106.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	271	G3P	C2

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	271	G3P	C3-O1P-P-O3P
5	B	398	PLS	CB-CA-N-C4A
5	B	398	PLS	C3-C4-C4A-N
5	B	398	PLS	C4-C5-C5A-O4P
5	B	398	PLS	C-CA-N-C4A

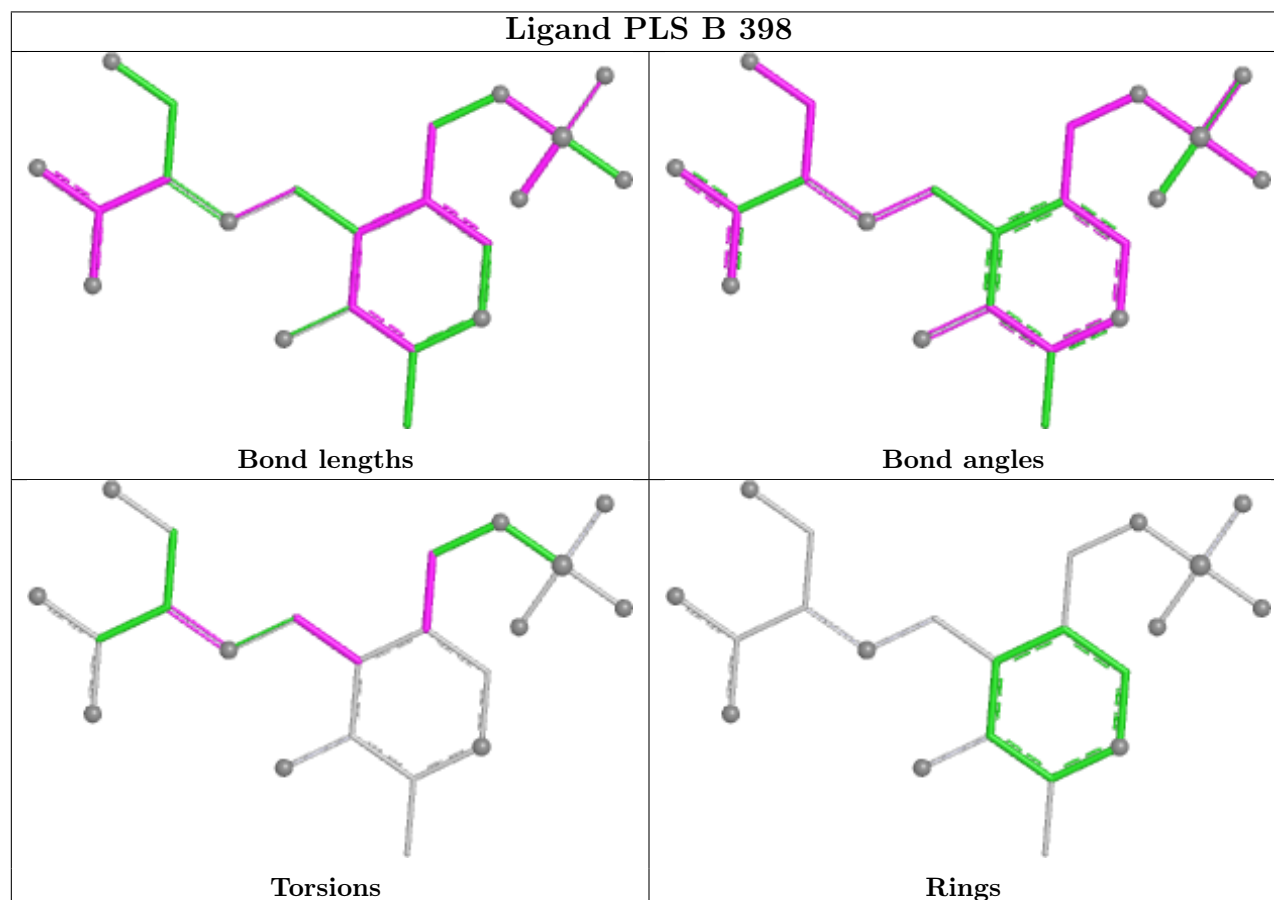
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	398	PLS	2	0
3	A	271	G3P	4	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%)	-0.65	0	100 100	21, 49, 86, 106	1 (0%)
2	B	389/397 (97%)	-1.05	1 (0%)	90 87	12, 28, 51, 84	2 (0%)
All	All	651/665 (97%)	-0.89	1 (0%)	91 89	12, 36, 74, 106	3 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	391	LEU	2.5

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](#)

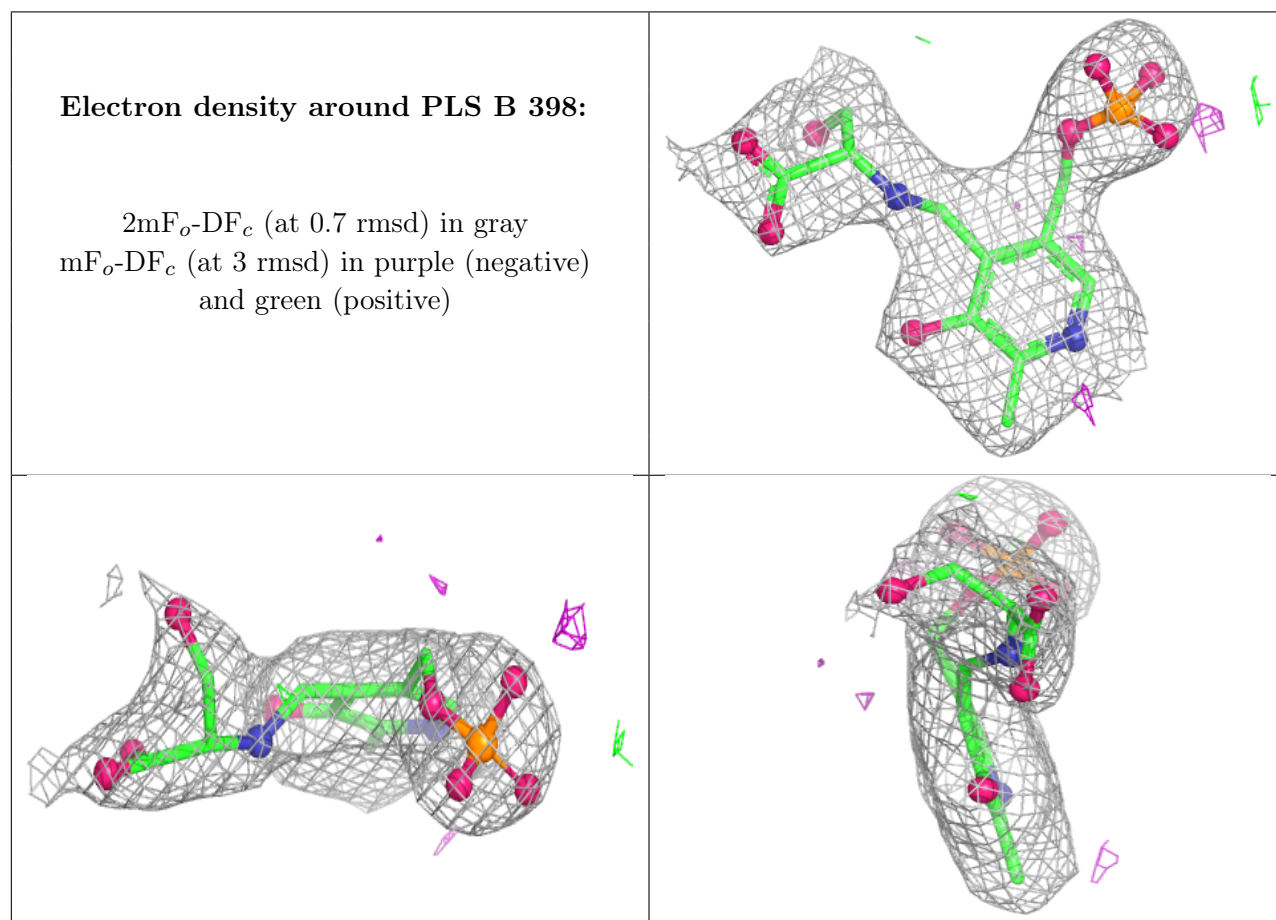
There are no oligosaccharides in this entry.

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	G3P	A	271	10/10	0.94	0.08	54,59,65,68	0
4	NA	B	400	1/1	0.98	0.05	26,26,26,26	0
5	PLS	B	398	22/22	0.98	0.05	29,35,52,53	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 ⓘ

There are no such residues in this entry.