



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:59 PM UTC

PDB ID : 1KFJ / pdb_00001kfj
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 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

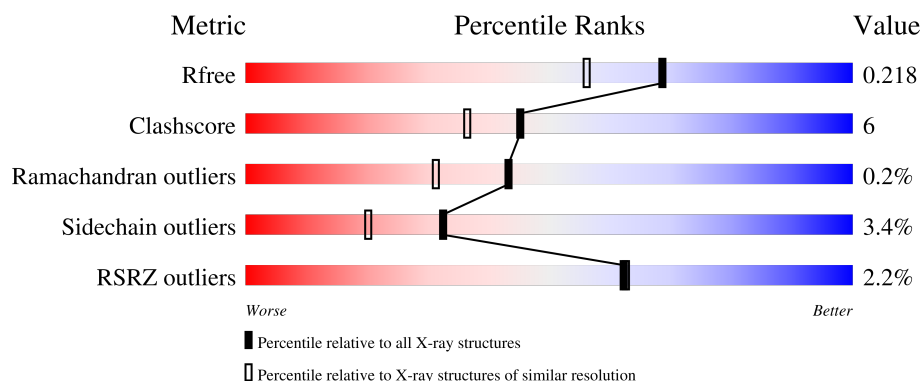
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

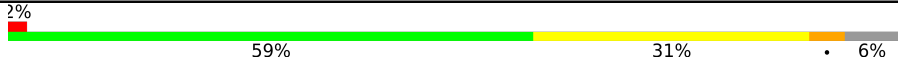
The reported resolution of this entry is 1.80 Å.

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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	

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			

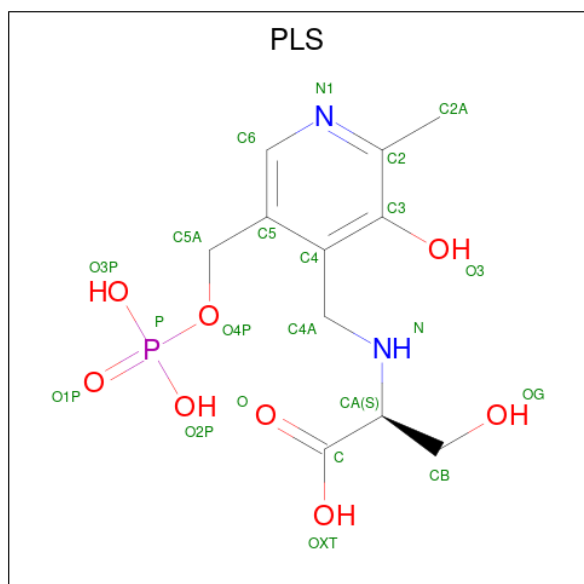
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

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 (CCD ID: 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 (CCD ID: 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		

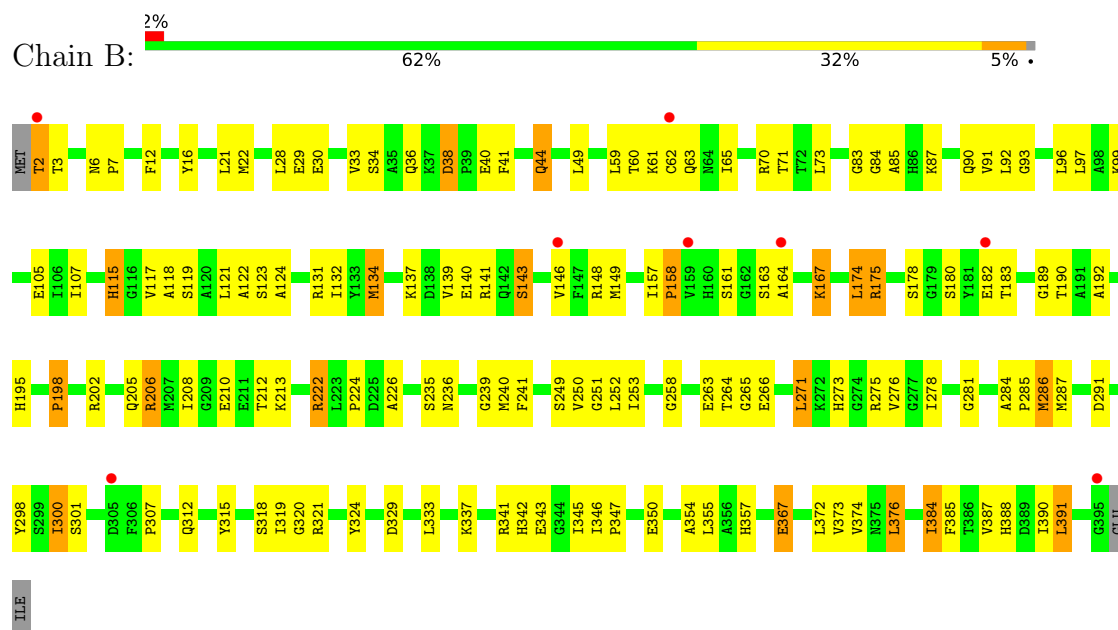
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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	183.23Å 59.68Å 67.46Å 90.00° 94.65° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-1.80) 96.8 (20.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.80Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.174 , 0.211 0.177 , 0.218	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)	0.38 , 44.3	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: 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	1.60	21/1950 (1.1%)	2.19	85/2649 (3.2%)
2	B	1.87	48/3039 (1.6%)	2.26	138/4105 (3.4%)
All	All	1.77	69/4989 (1.4%)	2.23	223/6754 (3.3%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	372	LEU	CA-C	11.65	1.66	1.52
1	A	111	ILE	CA-CB	10.90	1.68	1.54
1	A	84	MET	SD-CE	-9.31	1.56	1.79
2	B	239	GLY	C-O	9.24	1.34	1.23
2	B	96	LEU	C-O	8.93	1.35	1.24
2	B	291	ASP	CB-CG	-8.68	1.30	1.52
2	B	208	ILE	CA-CB	8.17	1.64	1.54
2	B	61	LYS	N-CA	7.83	1.56	1.46
1	A	221	SER	CA-CB	7.78	1.65	1.53
2	B	315	TYR	CD2-CE2	7.32	1.60	1.38
1	A	126	VAL	C-O	7.07	1.31	1.24
1	A	103	ALA	C-O	-7.06	1.15	1.24
2	B	192	ALA	CA-CB	7.03	1.63	1.53
2	B	149	MET	CG-SD	6.99	1.98	1.80
1	A	52	VAL	CA-C	6.87	1.58	1.53
2	B	141	ARG	C-O	6.83	1.33	1.24
2	B	213	LYS	N-CA	6.76	1.54	1.46
1	A	97	ILE	CA-C	6.58	1.61	1.52
2	B	250	VAL	C-O	-6.52	1.17	1.24
2	B	252	LEU	N-CA	6.51	1.53	1.46
2	B	320	GLY	C-O	-6.48	1.14	1.23
2	B	286	MET	CG-SD	-6.42	1.64	1.80
2	B	354	ALA	CA-CB	6.36	1.63	1.53
2	B	208	ILE	N-CA	-6.17	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	264	THR	CA-C	-6.10	1.44	1.52
2	B	44	GLN	CA-C	6.08	1.60	1.52
2	B	373	VAL	N-CA	6.08	1.53	1.46
1	A	119	GLU	C-O	6.02	1.31	1.24
1	A	144	LEU	C-O	6.02	1.31	1.24
2	B	319	ILE	CA-CB	6.02	1.62	1.54
1	A	18	ALA	N-CA	-5.98	1.38	1.46
2	B	97	LEU	CG-CD2	5.97	1.72	1.52
1	A	151	ILE	CA-CB	-5.97	1.47	1.54
1	A	55	SER	N-CA	5.79	1.53	1.46
2	B	205	GLN	CA-C	5.77	1.60	1.52
2	B	307	PRO	CA-C	5.73	1.60	1.52
2	B	33	VAL	C-O	5.68	1.30	1.24
1	A	126	VAL	CA-CB	5.61	1.61	1.54
1	A	54	PHE	N-CA	5.49	1.52	1.45
2	B	96	LEU	CA-C	-5.48	1.45	1.52
2	B	276	VAL	CA-CB	-5.48	1.48	1.54
2	B	300	ILE	CA-CB	-5.48	1.46	1.54
2	B	284	ALA	CA-CB	5.46	1.62	1.53
1	A	128	VAL	CA-CB	5.46	1.59	1.53
1	A	153	ILE	CA-CB	-5.45	1.47	1.54
2	B	134	MET	CA-C	5.40	1.58	1.52
2	B	71	THR	CA-C	5.39	1.59	1.52
2	B	374	VAL	CB-CG2	5.39	1.70	1.52
2	B	253	ILE	C-O	5.30	1.29	1.24
1	A	137	ALA	CA-CB	5.30	1.60	1.53
2	B	273	HIS	N-CA	5.29	1.52	1.46
2	B	41	PHE	CD1-CE1	5.24	1.54	1.38
2	B	59	LEU	C-O	5.24	1.30	1.24
2	B	291	ASP	CG-OD1	5.23	1.35	1.25
2	B	387	VAL	N-CA	-5.22	1.40	1.46
1	A	93	PRO	C-O	-5.21	1.17	1.24
2	B	271	LEU	CA-C	-5.17	1.46	1.52
2	B	226	ALA	CA-C	5.16	1.59	1.52
1	A	163	LEU	CA-C	-5.13	1.46	1.52
2	B	343	GLU	N-CA	5.12	1.53	1.45
2	B	85	ALA	N-CA	5.12	1.52	1.46
2	B	97	LEU	C-N	-5.12	1.27	1.33
2	B	240	MET	C-O	5.11	1.30	1.24
2	B	287	MET	SD-CE	5.10	1.92	1.79
2	B	212	THR	CA-C	5.06	1.59	1.52
1	A	210	GLN	CA-C	-5.05	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	PHE	CD1-CE1	5.05	1.53	1.38
2	B	34	SER	C-O	5.04	1.29	1.24
2	B	148	ARG	CA-C	-5.04	1.46	1.52

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	291	ASP	CB-CG-OD1	-14.86	84.22	118.40
2	B	286	MET	CA-CB-CG	-12.26	89.58	114.10
2	B	206	ARG	NE-CZ-NH1	11.88	133.38	121.50
2	B	206	ARG	CD-NE-CZ	10.62	139.26	124.40
2	B	291	ASP	OD1-CG-OD2	10.53	148.17	122.90
2	B	291	ASP	N-CA-CB	-10.46	94.44	110.44
2	B	291	ASP	CA-CB-CG	-9.55	103.05	112.60
2	B	226	ALA	O-C-N	9.08	133.65	123.48
2	B	180	SER	N-CA-C	8.88	125.47	112.94
2	B	286	MET	CA-C-O	-8.79	111.47	121.40
2	B	291	ASP	CB-CA-C	-8.74	94.28	110.01
1	A	50	LEU	CA-C-N	8.64	130.86	120.92
1	A	50	LEU	C-N-CA	8.64	130.86	120.92
1	A	14	ARG	N-CA-C	-8.50	100.96	112.94
2	B	367	GLU	CB-CG-CD	8.46	126.98	112.60
2	B	391	LEU	N-CA-C	-8.33	102.38	112.54
1	A	90	GLU	N-CA-C	-8.32	102.58	112.89
2	B	139	VAL	CB-CA-C	-8.28	101.28	111.88
1	A	140	ARG	NE-CZ-NH1	-8.27	113.23	121.50
2	B	93	GLY	N-CA-C	-8.18	102.60	112.49
1	A	216	SER	CA-C-O	8.15	127.84	120.34
2	B	319	ILE	CA-C-O	8.00	128.61	119.89
2	B	63	GLN	N-CA-C	7.92	121.01	111.82
2	B	60	THR	CA-C-N	-7.88	111.08	122.19
2	B	60	THR	C-N-CA	-7.88	111.08	122.19
1	A	124	ASP	CA-CB-CG	-7.79	104.81	112.60
1	A	232	ILE	CB-CA-C	-7.76	99.15	110.63
1	A	243	LYS	N-CA-C	7.73	121.81	112.38
2	B	206	ARG	NE-CZ-NH2	-7.69	112.28	119.20
2	B	158	PRO	CB-CA-C	-7.55	101.08	110.98
2	B	384	ILE	CA-CB-CG1	-7.37	97.88	110.40
2	B	321	ARG	CA-C-O	-7.24	111.13	119.60
2	B	249	SER	CA-C-N	-7.21	113.68	122.90
2	B	249	SER	C-N-CA	-7.21	113.68	122.90
2	B	140	GLU	CA-C-N	-7.18	111.16	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	140	GLU	C-N-CA	-7.18	111.16	122.65
2	B	38	ASP	CA-C-N	-7.16	112.26	119.56
2	B	38	ASP	C-N-CA	-7.16	112.26	119.56
1	A	234	GLY	CA-C-O	-7.14	112.44	120.30
1	A	53	PRO	CA-C-N	-7.08	110.60	122.29
1	A	53	PRO	C-N-CA	-7.08	110.60	122.29
1	A	176	LEU	CA-C-N	-7.06	108.99	121.70
1	A	176	LEU	C-N-CA	-7.06	108.99	121.70
2	B	62	CYS	CA-CB-SG	-7.05	98.17	114.40
2	B	137	LYS	N-CA-C	-6.99	103.72	111.82
2	B	287	MET	N-CA-C	-6.97	98.58	109.25
2	B	390	ILE	N-CA-C	-6.95	103.43	111.00
2	B	286	MET	O-C-N	6.94	131.56	123.17
2	B	350	GLU	N-CA-C	-6.92	103.42	110.97
1	A	111	ILE	CB-CA-C	-6.85	102.77	112.22
1	A	49	GLU	CA-CB-CG	-6.69	100.72	114.10
2	B	367	GLU	N-CA-C	-6.68	104.26	112.88
1	A	91	LYS	N-CA-C	6.66	120.62	112.23
1	A	49	GLU	CB-CG-CD	-6.61	101.37	112.60
1	A	84	MET	N-CA-CB	6.55	119.75	110.12
2	B	97	LEU	CB-CA-C	-6.55	99.71	110.85
2	B	226	ALA	CA-C-N	-6.55	114.03	123.06
2	B	226	ALA	C-N-CA	-6.55	114.03	123.06
2	B	251	GLY	CA-C-O	-6.54	115.69	121.58
2	B	36	GLN	CA-C-N	-6.50	112.24	122.65
2	B	36	GLN	C-N-CA	-6.50	112.24	122.65
2	B	263	GLU	CG-CD-OE2	-6.50	103.45	118.40
1	A	63	THR	OG1-CB-CG2	-6.49	96.31	109.30
2	B	319	ILE	CB-CA-C	-6.47	103.01	111.88
1	A	51	GLY	CA-C-N	-6.46	117.94	122.59
1	A	51	GLY	C-N-CA	-6.46	117.94	122.59
2	B	346	ILE	O-C-N	-6.45	117.31	121.37
2	B	97	LEU	CA-C-N	-6.44	112.07	120.44
2	B	97	LEU	C-N-CA	-6.44	112.07	120.44
2	B	298	TYR	CA-CB-CG	-6.42	102.35	113.90
2	B	73	LEU	CA-C-O	-6.41	113.44	120.30
2	B	198	PRO	N-CA-C	-6.41	104.62	113.53
1	A	93	PRO	CA-C-N	-6.41	112.07	122.26
1	A	93	PRO	C-N-CA	-6.41	112.07	122.26
2	B	174	LEU	CA-C-N	-6.40	111.62	120.38
2	B	174	LEU	C-N-CA	-6.40	111.62	120.38
1	A	231	ALA	CA-C-O	6.37	128.25	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	83	GLY	CA-C-O	-6.35	112.67	119.27
2	B	30	GLU	CA-C-O	-6.34	113.83	120.55
1	A	229	ALA	CA-C-N	-6.31	112.77	121.23
1	A	229	ALA	C-N-CA	-6.31	112.77	121.23
1	A	95	ILE	CA-C-O	6.29	124.63	119.47
1	A	112	ASP	CB-CA-C	-6.24	100.43	110.79
2	B	119	SER	N-CA-C	-6.24	104.58	111.82
1	A	212	PHE	CA-C-N	-6.22	111.57	122.09
1	A	212	PHE	C-N-CA	-6.22	111.57	122.09
1	A	93	PRO	CA-C-O	-6.21	110.30	119.00
1	A	69	LEU	CA-C-N	-6.20	111.97	120.28
1	A	69	LEU	C-N-CA	-6.20	111.97	120.28
1	A	232	ILE	N-CA-C	6.20	116.79	108.11
2	B	241	PHE	CB-CA-C	-6.18	97.08	109.99
1	A	9	ALA	N-CA-C	-6.17	104.63	111.36
1	A	93	PRO	N-CD-CG	-6.15	93.98	103.20
1	A	143	ALA	CA-C-O	6.13	127.44	121.00
2	B	123	SER	CA-CB-OG	-6.13	98.84	111.10
1	A	164	ARG	CA-C-O	-6.12	114.06	120.55
1	A	108	ASN	N-CA-C	6.10	118.46	111.02
1	A	221	SER	N-CA-CB	6.09	119.08	110.12
2	B	367	GLU	CG-CD-OE1	-6.08	104.42	118.40
1	A	204	HIS	CB-CA-C	-6.05	102.97	111.80
2	B	28	LEU	N-CA-C	-6.05	104.76	111.36
1	A	156	PRO	N-CA-C	-6.03	105.32	113.40
2	B	301	SER	CA-C-O	6.03	127.36	120.54
1	A	133	VAL	O-C-N	6.03	127.95	121.87
1	A	29	GLY	CA-C-O	-5.99	115.32	121.61
1	A	55	SER	N-CA-C	5.99	119.41	111.75
2	B	70	ARG	N-CA-C	-5.97	105.31	112.59
2	B	84	GLY	CA-C-O	-5.96	111.86	119.13
2	B	321	ARG	N-CA-CB	-5.96	101.39	110.33
1	A	47	ALA	N-CA-C	-5.95	100.10	108.96
1	A	168	SER	N-CA-C	5.94	118.72	111.82
2	B	367	GLU	CG-CD-OE2	5.93	132.04	118.40
1	A	207	PRO	CB-CA-C	-5.91	104.05	111.56
1	A	176	LEU	CA-C-O	5.89	126.85	120.43
2	B	324	TYR	CA-CB-CG	-5.88	103.31	113.90
2	B	357	HIS	CA-CB-CG	-5.87	107.93	113.80
1	A	54	PHE	N-CA-C	-5.87	100.14	109.23
2	B	7	PRO	CB-CA-C	-5.84	102.74	110.27
2	B	41	PHE	N-CA-C	-5.83	104.84	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	286	MET	CG-SD-CE	-5.82	88.09	100.90
2	B	202	ARG	CA-C-N	-5.81	111.91	120.28
2	B	202	ARG	C-N-CA	-5.81	111.91	120.28
1	A	243	LYS	CA-CB-CG	-5.80	102.50	114.10
1	A	140	ARG	CD-NE-CZ	-5.78	116.31	124.40
2	B	107	ILE	CB-CA-C	-5.77	102.09	110.63
1	A	209	LEU	N-CA-CB	5.76	119.62	110.57
2	B	157	ILE	N-CA-C	5.75	113.75	107.60
2	B	250	VAL	CB-CA-C	-5.72	103.14	110.98
1	A	148	ILE	CB-CA-C	-5.71	102.11	110.62
1	A	140	ARG	CB-CA-C	5.69	120.52	110.85
2	B	239	GLY	CA-C-O	-5.68	114.63	120.66
2	B	167	LYS	N-CA-C	-5.68	105.23	111.82
2	B	183	THR	OG1-CB-CG2	-5.68	97.94	109.30
2	B	266	GLU	CA-CB-CG	-5.67	102.75	114.10
2	B	12	PHE	CA-CB-CG	-5.67	108.13	113.80
2	B	143	SER	N-CA-C	5.65	121.31	113.45
2	B	235	SER	N-CA-C	5.64	117.23	111.14
2	B	251	GLY	CA-C-N	-5.59	115.11	122.99
2	B	251	GLY	C-N-CA	-5.59	115.11	122.99
2	B	132	ILE	N-CA-C	5.59	115.93	108.11
1	A	5	GLU	N-CA-C	-5.58	105.10	111.07
2	B	22	MET	CA-C-O	5.58	123.76	118.63
1	A	196	LEU	N-CA-C	-5.56	105.12	111.07
1	A	161	ASP	N-CA-C	-5.56	105.22	111.28
2	B	347	PRO	CA-C-O	-5.55	115.20	122.19
2	B	175	ARG	CA-C-O	5.53	126.61	120.63
2	B	342	HIS	CA-CB-CG	-5.49	108.31	113.80
2	B	123	SER	N-CA-C	-5.49	105.31	112.23
1	A	146	HIS	N-CA-CB	-5.48	102.15	110.92
2	B	265	GLY	CA-C-N	-5.46	114.68	122.77
2	B	265	GLY	C-N-CA	-5.46	114.68	122.77
2	B	240	MET	CA-C-N	-5.44	111.62	121.14
2	B	240	MET	C-N-CA	-5.44	111.62	121.14
2	B	224	PRO	CB-CA-C	-5.44	103.83	110.95
1	A	216	SER	CB-CA-C	-5.42	101.57	109.97
1	A	53	PRO	CA-C-O	-5.41	115.42	121.32
1	A	69	LEU	N-CA-C	-5.41	105.30	111.14
2	B	38	ASP	CB-CA-C	5.41	115.53	110.17
2	B	115	HIS	N-CA-C	-5.41	105.54	111.82
2	B	92	LEU	N-CA-C	-5.39	105.48	111.36
2	B	132	ILE	CA-C-N	-5.39	114.62	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	132	ILE	C-N-CA	-5.39	114.62	122.65
1	A	151	ILE	CB-CA-C	-5.37	102.65	110.81
2	B	22	MET	CA-CB-CG	-5.37	103.37	114.10
2	B	117	VAL	CA-CB-CG2	-5.34	101.32	110.40
1	A	109	ASN	CB-CA-C	-5.33	102.14	110.94
2	B	117	VAL	CA-CB-CG1	5.33	119.46	110.40
1	A	154	CYS	CA-C-N	5.33	125.87	120.38
1	A	154	CYS	C-N-CA	5.33	125.87	120.38
2	B	195	HIS	CA-CB-CG	-5.32	108.48	113.80
2	B	62	CYS	CB-CA-C	-5.32	103.97	112.05
1	A	139	PHE	N-CA-C	-5.31	105.40	111.14
1	A	221	SER	CB-CA-C	-5.31	101.97	110.79
2	B	146	VAL	CA-CB-CG2	-5.31	101.37	110.40
1	A	92	HIS	CA-C-N	5.29	124.90	119.56
1	A	92	HIS	C-N-CA	5.29	124.90	119.56
2	B	388	HIS	O-C-N	-5.28	116.63	122.07
1	A	141	GLN	CA-C-O	-5.28	115.28	120.82
2	B	312	GLN	N-CA-C	-5.27	105.71	111.82
2	B	275	ARG	CG-CD-NE	5.26	123.58	112.00
1	A	95	ILE	N-CA-C	-5.25	104.11	108.63
2	B	182	GLU	CA-C-N	-5.25	113.80	121.99
2	B	182	GLU	C-N-CA	-5.25	113.80	121.99
1	A	210	GLN	CA-C-N	-5.24	116.91	122.67
1	A	210	GLN	C-N-CA	-5.24	116.91	122.67
2	B	90	GLN	CA-C-O	-5.24	113.61	119.79
2	B	258	GLY	N-CA-C	-5.24	106.50	115.61
1	A	164	ARG	NE-CZ-NH2	-5.20	114.52	119.20
2	B	49	LEU	O-C-N	5.20	127.63	122.12
2	B	345	ILE	CA-C-N	-5.20	116.92	122.85
2	B	345	ILE	C-N-CA	-5.20	116.92	122.85
2	B	105	GLU	CA-CB-CG	-5.19	103.72	114.10
1	A	227	GLY	CA-C-O	5.16	124.70	118.97
2	B	124	ALA	N-CA-C	-5.15	105.56	111.07
2	B	164	ALA	CA-C-N	-5.14	115.37	122.16
2	B	164	ALA	C-N-CA	-5.14	115.37	122.16
1	A	51	GLY	O-C-N	-5.14	118.57	122.99
1	A	49	GLU	N-CA-C	-5.13	100.54	108.90
2	B	263	GLU	N-CA-C	5.13	118.31	111.75
2	B	376	LEU	CB-CG-CD1	-5.12	95.34	110.70
2	B	29	GLU	O-C-N	5.12	127.98	122.15
2	B	6	ASN	CA-C-O	-5.10	114.70	119.80
2	B	132	ILE	CB-CG1-CD1	-5.09	103.10	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	190	THR	CA-C-N	-5.09	114.67	122.21
2	B	190	THR	C-N-CA	-5.09	114.67	122.21
1	A	168	SER	N-CA-CB	-5.08	102.40	110.28
1	A	120	GLN	N-CA-CB	-5.07	102.67	110.12
2	B	2	THR	CB-CA-C	5.07	120.25	109.10
2	B	226	ALA	CA-C-O	-5.06	115.32	120.89
2	B	373	VAL	N-CA-C	-5.06	100.83	108.12
2	B	252	LEU	CA-C-N	-5.06	115.80	122.98
2	B	252	LEU	C-N-CA	-5.06	115.80	122.98
2	B	385	PHE	CA-C-O	5.05	125.77	119.97
2	B	318	SER	CA-C-N	-5.04	115.12	122.28
2	B	318	SER	C-N-CA	-5.04	115.12	122.28
1	A	149	ALA	CA-C-O	5.04	123.34	119.46
2	B	61	LYS	O-C-N	-5.03	117.48	123.22
1	A	52	VAL	CB-CA-C	-5.03	105.33	110.71
2	B	315	TYR	CG-CD2-CE2	-5.03	113.65	121.20
1	A	18	ALA	N-CA-CB	-5.03	102.47	110.06
1	A	103	ALA	N-CA-C	5.01	116.75	111.28
2	B	355	LEU	O-C-N	5.01	127.43	122.12
2	B	252	LEU	N-CA-C	-5.00	100.75	108.90

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	30	0
2	B	2981	0	2959	29	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	58	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 (58) 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
1:A:58:LEU:C	1:A:58:LEU:HD12	2.28	0.58
2:B:206:ARG:HD3	2:B:210:GLU:OE2	2.05	0.57
2:B:271:LEU:HD23	2:B:271:LEU:C	2.31	0.56
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
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
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
1:A:127:LEU:C	1:A:127:LEU:HD23	2.37	0.49
2:B:206:ARG:CD	2:B:210:GLU:OE2	2.60	0.49
2:B:285:PRO:C	2:B:286:MET:HG3	2.37	0.49
1:A:36:ILE:HG23	1:A:255:LEU:HD13	1.93	0.49
1:A:100:LEU:C	1:A:100:LEU:CD1	2.86	0.49
1:A:100:LEU:C	1:A:100:LEU:HD13	2.38	0.48
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:1:MET:HE3	1:A:1:MET:HB2	1.81	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
2:B:121:LEU:HD12	2:B:121:LEU:C	2.41	0.46
1:A:239:LYS:O	1:A:243:LYS:HG3	2.16	0.46
1:A:70:ARG:NH1	1:A:242:GLU:HG2	2.31	0.45
2:B:131:ARG:O	2:B:131:ARG:HG3	2.16	0.45
1:A:221:SER:HB2	1:A:225:ARG:HH12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:ILE:HB	2:B:329:ASP:CG	2.43	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
1:A:193:LEU:N	1:A:193:LEU:CD2	2.82	0.43
2:B:16:TYR:O	2:B:281:GLY:HA2	2.19	0.43
2:B:271:LEU:HD23	2:B:271:LEU:O	2.19	0.43
1:A:249:LYS:H	1:A:249:LYS:HG3	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
2:B:38:ASP:OD1	2:B:38:ASP:C	2.61	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:115:HIS:CE1	2:B:189:GLY:HA2	2.55	0.41
2:B:134:MET:O	2:B:158:PRO:HA	2.21	0.40
2:B:174:LEU:O	2:B:175:ARG:C	2.60	0.40
1:A:176:LEU:HD12	1:A:176:LEU:HA	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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	249/268 (93%)	245 (98%)	3 (1%)	1 (0%)	30	19
2	B	392/397 (99%)	382 (97%)	10 (3%)	0	100	100
All	All	641/665 (96%)	627 (98%)	13 (2%)	1 (0%)	43	31

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%)	32	19
2	B	308/311 (99%)	298 (97%)	10 (3%)	34	22
All	All	506/519 (98%)	489 (97%)	17 (3%)	32	20

All (17) 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	193	LEU
1	A	196	LEU
1	A	218	GLU
1	A	249	LYS
2	B	40	GLU
2	B	65	ILE
2	B	99	LYS
2	B	143	SER
2	B	161	SER
2	B	198	PRO
2	B	222	ARG
2	B	236	ASN
2	B	367	GLU
2	B	384	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN

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Mol	Chain	Res	Type
2	B	26	ASN
2	B	236	ASN
2	B	246	ASN
2	B	375	ASN
2	B	388	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 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	-	22,22,22	1.53	7 (31%)	28,31,31	2.53	14 (50%)

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	-	-	4/17/17/17	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	PLS	C3-C2	-3.06	1.37	1.41
4	B	400	PLS	P-O2P	-2.85	1.44	1.54
4	B	400	PLS	C5A-C5	2.55	1.57	1.50
4	B	400	PLS	C5-C4	-2.19	1.37	1.40
4	B	400	PLS	O-C	2.16	1.28	1.22
4	B	400	PLS	C2-N1	-2.09	1.30	1.33
4	B	400	PLS	P-O3P	-2.09	1.47	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	400	PLS	C2A-C2-C3	6.19	128.04	120.80
4	B	400	PLS	C4A-N-CA	4.73	122.71	113.84
4	B	400	PLS	O-C-CA	-3.88	109.74	122.26
4	B	400	PLS	O3-C3-C2	3.84	125.55	117.58
4	B	400	PLS	C2A-C2-N1	-3.63	110.80	117.64
4	B	400	PLS	OG-CB-CA	-3.32	102.17	111.18
4	B	400	PLS	O4P-C5A-C5	2.85	114.70	109.36
4	B	400	PLS	O3P-P-O1P	-2.40	101.50	110.83
4	B	400	PLS	OXT-C-O	2.37	129.46	124.08
4	B	400	PLS	C4A-C4-C3	2.37	123.13	119.98
4	B	400	PLS	O3P-P-O2P	2.19	116.00	107.80
4	B	400	PLS	OXT-C-CA	2.15	120.80	113.51
4	B	400	PLS	O2P-P-O4P	-2.09	101.21	106.67
4	B	400	PLS	O3-C3-C4	-2.03	112.29	118.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

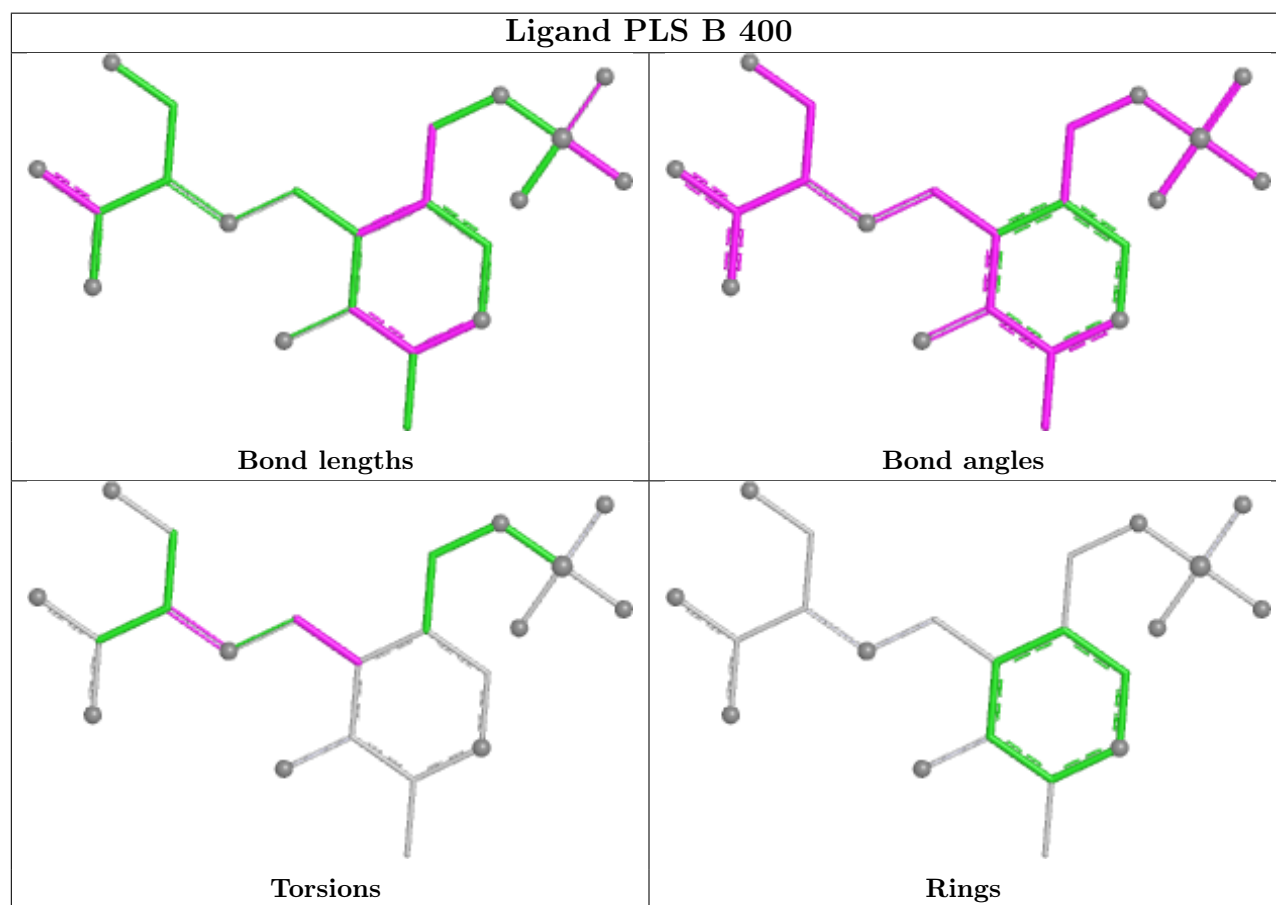
Mol	Chain	Res	Type	Atoms
4	B	400	PLS	C-CA-N-C4A
4	B	400	PLS	C3-C4-C4A-N
4	B	400	PLS	C5-C4-C4A-N
4	B	400	PLS	CB-CA-N-C4A

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 ⓘ

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	253/268 (94%)	0.28	6 (2%) 59 60	21, 36, 55, 88	0
2	B	394/397 (99%)	-0.11	8 (2%) 65 65	18, 26, 44, 75	0
All	All	647/665 (97%)	0.04	14 (2%) 62 62	18, 30, 51, 88	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	LEU	4.8
2	B	395	GLY	4.3
1	A	192	PRO	4.0
1	A	194	HIS	3.6
2	B	159	VAL	2.6
2	B	2	THR	2.5
2	B	62	CYS	2.4
1	A	13	ASP	2.4
1	A	195	HIS	2.3
2	B	146	VAL	2.3
2	B	305	ASP	2.2
2	B	182	GLU	2.2
2	B	164	ALA	2.1
1	A	213	GLY	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 ⓘ

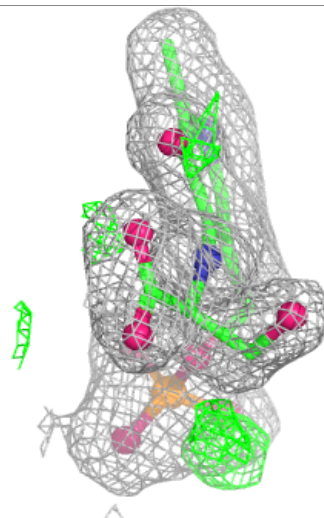
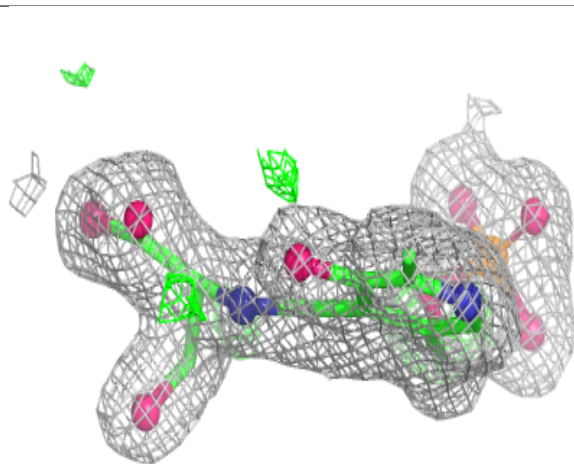
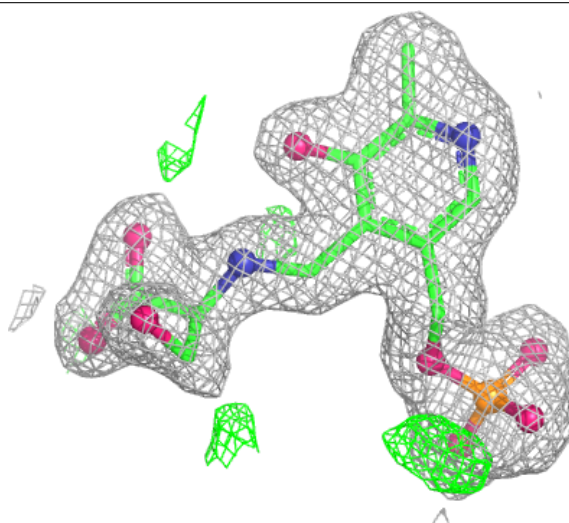
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PLS	B	400	22/22	0.97	0.06	21,28,34,37	0
3	NA	B	399	1/1	0.99	0.06	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.