



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:14 PM UTC

PDB ID : 5EKD / pdb_00005ekd
Title : Human mitochondrial tryptophanyl-tRNA synthetase bound by indolmycin and Mn*ATP.
Authors : Williams, T.L.; Carter Jr., C.W.
Deposited on : 2015-11-03
Resolution : 1.82 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

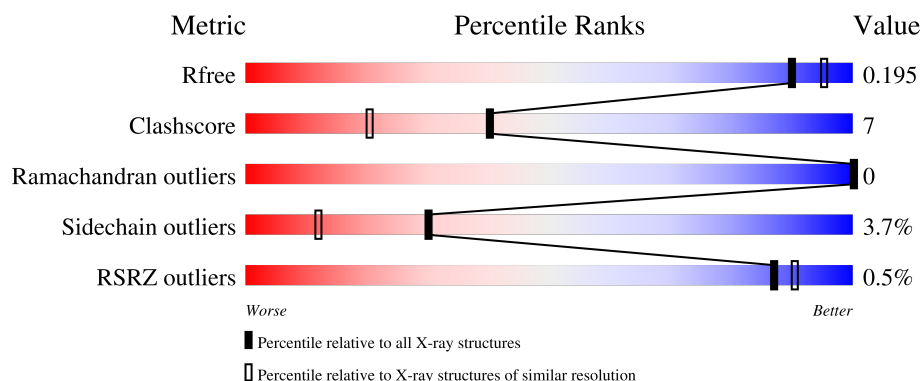
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	343	
1	B	343	

2 Entry composition [i](#)

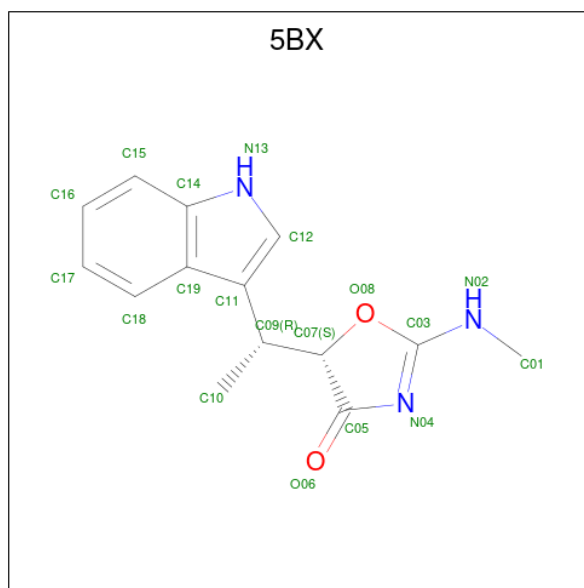
There are 6 unique types of molecules in this entry. The entry contains 11183 atoms, of which 5378 are hydrogens and 0 are deuteriums.

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-tRNA ligase, mitochondrial.

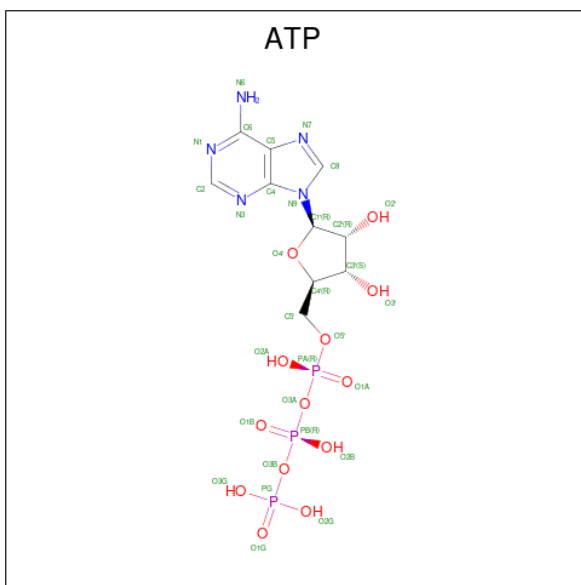
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	327	Total	C	H	N	O	S	0	0	0
			5225	1637	2660	442	477	9			
1	B	327	Total	C	H	N	O	S	0	4	0
			5261	1649	2678	443	482	9			

- Molecule 2 is (5S)-5-[(1R)-1-(1H-indol-3-yl)ethyl]-2-(methylamino)-1,3-oxazol-4(5H)-one (CCD ID: 5BX) (formula: C₁₄H₁₅N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	14	3	2		
2	B	1	Total	C	N	O	0	0
			19	14	3	2		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

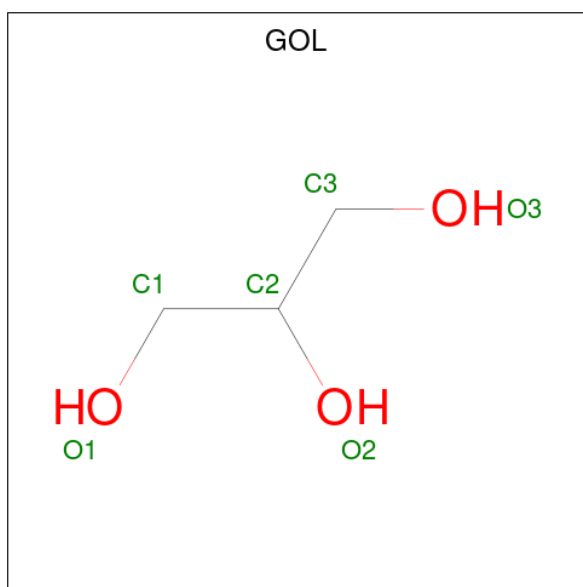


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0	0
3	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0	0

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mn 2 2	0	0
4	B	2	Total Mn 2 2	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		

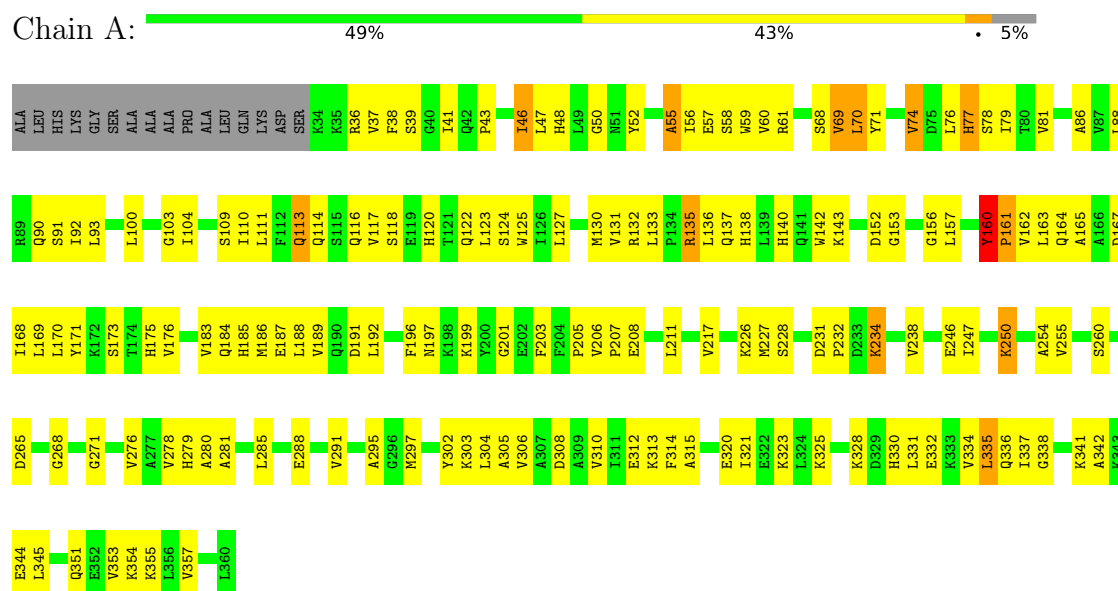
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	283	Total	O	0	0
			283	283		
6	B	258	Total	O	0	0
			258	258		

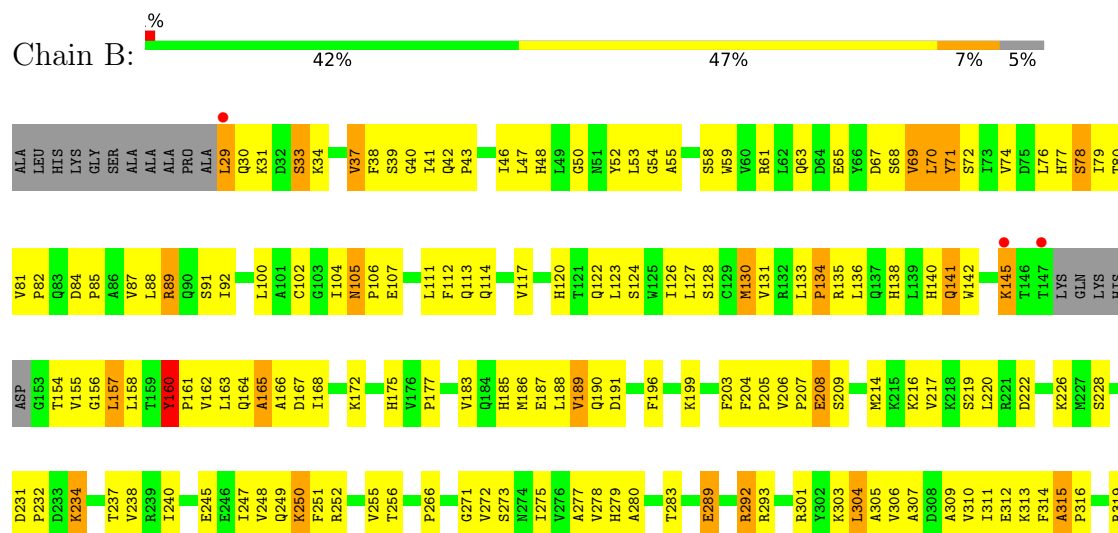
3 Residue-property plots

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-tRNA ligase, mitochondrial



- Molecule 1: Tryptophan-tRNA ligase, mitochondrial



E320	I321	E322	K323	L324
K328	D329	H330	L331	E332
K333	V334	I337	G338	A342
K343	E344	L345	A346	Y347
E352	V353	K354	K355	L356
V357	G358	F359	L360	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	58.29Å 78.09Å 154.00Å 90.00° 96.55° 90.00°	Depositor
Resolution (Å)	29.06 – 1.82 29.06 – 1.82	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.06-1.82) 98.4 (29.06-1.82)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.170 , 0.207 0.173 , 0.195	Depositor DCC
R_{free} test set	3070 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11183	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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: ATP, 5BX, GOL, MN

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	2.26	146/2612 (5.6%)	1.11	7/3534 (0.2%)
1	B	2.37	169/2640 (6.4%)	1.19	23/3570 (0.6%)
All	All	2.31	315/5252 (6.0%)	1.15	30/7104 (0.4%)

All (315) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89[A]	ARG	CA-C	14.08	1.71	1.52
1	B	89[B]	ARG	CA-C	14.08	1.71	1.52
1	A	160	TYR	C-O	-9.72	1.15	1.24
1	A	127	LEU	C-O	-8.97	1.13	1.24
1	A	315	ALA	C-O	-8.72	1.16	1.24
1	A	48	HIS	CG-ND1	-8.70	1.28	1.38
1	B	48	HIS	CG-ND1	-8.59	1.28	1.38
1	B	330	HIS	CG-ND1	-8.54	1.28	1.38
1	B	46	ILE	C-O	-8.34	1.15	1.24
1	B	77	HIS	CG-ND1	-8.11	1.29	1.38
1	A	185	HIS	CG-ND1	-8.10	1.29	1.38
1	B	135	ARG	C-O	-8.10	1.14	1.24
1	A	77	HIS	CG-ND1	-7.92	1.29	1.38
1	B	250	LYS	C-O	-7.91	1.14	1.24
1	B	136	LEU	C-O	-7.91	1.14	1.24
1	B	41	ILE	C-O	-7.87	1.16	1.24
1	A	114	GLN	C-O	-7.77	1.15	1.24
1	B	208[A]	GLU	N-CA	7.70	1.55	1.46
1	B	208[B]	GLU	N-CA	7.70	1.55	1.46
1	B	205	PRO	C-O	-7.66	1.14	1.23
1	B	104	ILE	C-O	-7.65	1.16	1.24
1	B	77	HIS	CD2-NE2	-7.64	1.29	1.37
1	B	185	HIS	CD2-NE2	-7.61	1.29	1.37
1	B	208[A]	GLU	C-O	-7.60	1.14	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208[B]	GLU	C-O	-7.60	1.14	1.24
1	B	330	HIS	CD2-NE2	-7.47	1.29	1.37
1	B	74	VAL	C-O	-7.45	1.15	1.24
1	A	280	ALA	C-O	-7.42	1.15	1.24
1	A	123	LEU	C-O	-7.30	1.15	1.24
1	B	89[A]	ARG	C-O	-7.28	1.15	1.24
1	B	89[B]	ARG	C-O	-7.28	1.15	1.24
1	B	162	VAL	C-O	-7.25	1.15	1.24
1	B	122[A]	GLN	N-CA	7.25	1.55	1.46
1	B	122[B]	GLN	N-CA	7.25	1.55	1.46
1	A	334	VAL	C-O	-7.22	1.16	1.24
1	B	122[A]	GLN	CA-C	7.21	1.61	1.52
1	B	122[B]	GLN	CA-C	7.21	1.61	1.52
1	B	185	HIS	CG-ND1	-7.16	1.30	1.38
1	B	175	HIS	CG-ND1	-7.13	1.30	1.38
1	A	93	LEU	C-O	-7.11	1.15	1.24
1	B	353	VAL	C-O	-7.10	1.15	1.24
1	B	275	ILE	C-O	-7.09	1.15	1.24
1	B	175	HIS	CD2-NE2	-7.09	1.30	1.37
1	B	114	GLN	C-O	-7.08	1.15	1.24
1	B	76	LEU	C-O	-7.08	1.15	1.24
1	B	160	TYR	C-O	-7.03	1.18	1.24
1	A	191	ASP	C-O	-6.99	1.16	1.24
1	A	185	HIS	CD2-NE2	-6.93	1.30	1.37
1	A	120	HIS	CG-ND1	-6.92	1.30	1.38
1	B	72	SER	C-O	-6.92	1.15	1.24
1	A	135	ARG	C-O	-6.90	1.16	1.24
1	B	140	HIS	CG-ND1	-6.88	1.30	1.38
1	B	128	SER	C-O	-6.84	1.15	1.24
1	A	46	ILE	C-O	-6.81	1.15	1.24
1	A	77	HIS	CD2-NE2	-6.80	1.30	1.37
1	A	308	ASP	C-O	-6.79	1.16	1.24
1	A	39	SER	C-O	-6.75	1.15	1.23
1	B	277	ALA	C-O	-6.74	1.16	1.24
1	B	315	ALA	C-O	-6.74	1.18	1.24
1	B	189	VAL	C-O	-6.71	1.16	1.24
1	B	78[A]	SER	CA-C	6.70	1.61	1.52
1	B	78[B]	SER	CA-C	6.70	1.61	1.52
1	A	161	PRO	C-O	-6.66	1.15	1.24
1	B	38	PHE	C-O	-6.64	1.15	1.23
1	A	338	GLY	C-O	-6.63	1.15	1.23
1	A	92	ILE	C-O	-6.62	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	GLN	C-O	-6.58	1.16	1.24
1	A	188	LEU	C-O	-6.51	1.16	1.24
1	B	165	ALA	C-O	-6.49	1.16	1.24
1	A	208	GLU	C-O	-6.46	1.16	1.24
1	A	184	GLN	C-O	-6.46	1.16	1.24
1	A	187	GLU	C-O	-6.44	1.16	1.24
1	B	309	ALA	C-O	-6.43	1.16	1.24
1	A	278	VAL	C-O	-6.42	1.16	1.24
1	A	162	VAL	C-O	-6.42	1.16	1.24
1	A	125	TRP	NE1-CE2	-6.41	1.30	1.37
1	B	342	ALA	C-O	-6.41	1.16	1.24
1	B	127	LEU	C-O	-6.39	1.16	1.24
1	B	191	ASP	C-O	-6.39	1.16	1.24
1	B	37	VAL	C-O	-6.39	1.16	1.24
1	B	187	GLU	C-O	-6.39	1.16	1.24
1	B	164	GLN	C-O	-6.39	1.16	1.24
1	A	250	LYS	C-O	-6.38	1.16	1.24
1	B	196	PHE	C-O	-6.38	1.16	1.24
1	B	100	LEU	C-O	-6.38	1.16	1.24
1	A	312	GLU	C-O	-6.37	1.16	1.24
1	B	50	GLY	C-O	-6.37	1.16	1.23
1	B	39	SER	C-O	-6.36	1.16	1.23
1	A	260	SER	C-O	-6.36	1.16	1.24
1	B	168	ILE	C-O	-6.34	1.17	1.24
1	A	133	LEU	C-O	-6.34	1.18	1.24
1	B	105	ASN	C-O	-6.33	1.17	1.24
1	A	175	HIS	CG-ND1	-6.31	1.31	1.38
1	B	80	THR	C-O	-6.30	1.15	1.24
1	B	126	ILE	C-O	-6.29	1.16	1.24
1	A	164	GLN	C-O	-6.25	1.16	1.24
1	B	71	TYR	C-O	-6.24	1.17	1.24
1	A	165	ALA	C-O	-6.24	1.16	1.24
1	B	140	HIS	CD2-NE2	-6.23	1.31	1.37
1	B	157	LEU	C-O	-6.21	1.16	1.24
1	B	216	LYS	C-O	-6.20	1.15	1.23
1	A	36	ARG	C-O	-6.19	1.16	1.23
1	A	281	ALA	C-O	-6.18	1.17	1.24
1	B	305	ALA	C-O	-6.18	1.16	1.24
1	A	138	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	351	GLN	C-O	-6.17	1.17	1.24
1	B	53	LEU	C-O	-6.16	1.16	1.24
1	A	140	HIS	CG-ND1	-6.15	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	GLU	C-O	-6.13	1.17	1.24
1	A	137	GLN	C-O	-6.13	1.16	1.24
1	B	163	LEU	C-O	-6.12	1.17	1.24
1	B	82	PRO	C-O	-6.12	1.16	1.23
1	A	313	LYS	C-O	-6.11	1.17	1.24
1	B	273	SER	C-O	-6.10	1.16	1.24
1	B	188	LEU	C-O	-6.09	1.16	1.24
1	A	330	HIS	CD2-NE2	-6.09	1.31	1.37
1	B	55	ALA	C-O	-6.07	1.16	1.24
1	B	307	ALA	C-O	-6.06	1.17	1.24
1	A	189	VAL	C-O	-6.05	1.17	1.24
1	B	208[A]	GLU	CA-C	6.03	1.59	1.52
1	B	208[B]	GLU	CA-C	6.03	1.59	1.52
1	A	76	LEU	C-O	-6.01	1.17	1.24
1	B	186	MET	C-O	-6.01	1.17	1.24
1	A	197	ASN	C-O	-6.01	1.17	1.24
1	B	54	GLY	C-O	-6.00	1.16	1.23
1	A	302	TYR	C-O	-5.99	1.17	1.24
1	B	81	VAL	C-O	-5.99	1.18	1.23
1	B	117	VAL	C-O	-5.97	1.17	1.24
1	B	338	GLY	C-O	-5.97	1.16	1.23
1	A	247	ILE	C-O	-5.97	1.17	1.24
1	A	168	ILE	C-O	-5.97	1.17	1.24
1	B	271	GLY	C-O	-5.95	1.16	1.23
1	B	330	HIS	C-O	-5.94	1.17	1.24
1	A	265	ASP	C-O	-5.94	1.16	1.24
1	B	88	LEU	C-O	-5.94	1.17	1.24
1	B	77	HIS	C-O	-5.94	1.17	1.24
1	B	320	GLU	C-O	-5.93	1.17	1.24
1	A	246	GLU	C-O	-5.93	1.17	1.24
1	B	68	SER	C-O	-5.93	1.17	1.24
1	B	111	LEU	C-O	-5.92	1.17	1.24
1	A	175	HIS	CD2-NE2	-5.91	1.31	1.37
1	B	310	VAL	C-O	-5.90	1.17	1.24
1	B	356	LEU	C-O	-5.90	1.17	1.24
1	A	345	LEU	C-O	-5.90	1.17	1.24
1	A	79	ILE	C-O	-5.89	1.17	1.24
1	B	319	ARG	C-O	-5.89	1.17	1.24
1	B	70	LEU	C-O	-5.89	1.17	1.24
1	A	55	ALA	C-O	-5.88	1.16	1.24
1	A	131	VAL	C-O	-5.88	1.17	1.24
1	B	78[A]	SER	C-O	-5.88	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78[B]	SER	C-O	-5.88	1.16	1.24
1	A	304	LEU	C-O	-5.87	1.16	1.24
1	A	344	GLU	C-O	-5.87	1.17	1.24
1	B	156	GLY	C-O	-5.84	1.16	1.23
1	A	279	HIS	CG-ND1	-5.84	1.31	1.38
1	B	120	HIS	CD2-NE2	-5.84	1.31	1.37
1	B	237	THR	C-O	-5.83	1.17	1.24
1	A	355	LYS	C-O	-5.83	1.17	1.24
1	B	337	ILE	C-O	-5.83	1.17	1.24
1	A	88	LEU	C-O	-5.81	1.17	1.24
1	B	357	VAL	C-O	-5.81	1.16	1.24
1	A	74	VAL	C-O	-5.81	1.16	1.23
1	A	206	VAL	N-CA	-5.80	1.42	1.46
1	B	280	ALA	C-O	-5.80	1.17	1.24
1	A	142	TRP	NE1-CE2	-5.79	1.31	1.37
1	A	226	LYS	C-O	-5.79	1.16	1.23
1	A	342	ALA	C-O	-5.79	1.17	1.24
1	B	238	VAL	C-O	-5.79	1.16	1.23
1	A	57	GLU	C-O	-5.78	1.17	1.24
1	A	176	VAL	C-O	-5.77	1.17	1.24
1	B	190	GLN	C-O	-5.76	1.17	1.24
1	A	41	ILE	C-O	-5.75	1.18	1.24
1	B	134	PRO	C-O	-5.75	1.17	1.24
1	A	68	SER	C-O	-5.75	1.17	1.24
1	B	183	VAL	C-O	-5.74	1.17	1.24
1	A	170	LEU	C-O	-5.74	1.17	1.24
1	B	48	HIS	CD2-NE2	-5.74	1.31	1.37
1	B	329	ASP	C-O	-5.74	1.17	1.24
1	B	142	TRP	NE1-CE2	-5.74	1.31	1.37
1	A	335	LEU	C-O	-5.72	1.17	1.24
1	A	70	LEU	C-O	-5.71	1.17	1.24
1	A	227	MET	C-O	-5.70	1.17	1.23
1	A	357	VAL	C-O	-5.69	1.17	1.24
1	B	166	ALA	C-O	-5.69	1.17	1.24
1	A	52	TYR	C-O	-5.66	1.17	1.24
1	A	167	ASP	C-O	-5.66	1.17	1.24
1	B	92	ILE	C-O	-5.65	1.17	1.24
1	A	186	MET	C-O	-5.65	1.17	1.24
1	B	102	CYS	C-O	-5.65	1.16	1.24
1	A	163	LEU	C-O	-5.64	1.17	1.24
1	B	155	VAL	C-O	-5.64	1.17	1.24
1	B	59	TRP	NE1-CE2	-5.62	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	226	LYS	C-O	-5.62	1.16	1.23
1	B	304	LEU	C-O	-5.61	1.17	1.24
1	A	330	HIS	CG-ND1	-5.61	1.32	1.38
1	A	276	VAL	C-O	-5.61	1.17	1.24
1	A	38	PHE	C-O	-5.60	1.17	1.23
1	B	206	VAL	N-CA	-5.59	1.42	1.46
1	A	199	LYS	C-O	-5.59	1.17	1.24
1	B	42	GLN	C-O	-5.57	1.16	1.24
1	B	301	ARG	C-O	-5.56	1.17	1.24
1	B	334	VAL	C-O	-5.55	1.17	1.24
1	A	60	VAL	C-O	-5.55	1.17	1.24
1	B	87	VAL	C-O	-5.55	1.17	1.24
1	A	303	LYS	C-O	-5.54	1.17	1.24
1	B	123	LEU	C-O	-5.54	1.17	1.24
1	B	312	GLU	C-O	-5.53	1.17	1.24
1	A	71	TYR	C-O	-5.52	1.17	1.24
1	A	183	VAL	C-O	-5.52	1.17	1.24
1	A	113	GLN	C-O	-5.52	1.17	1.24
1	B	91	SER	C-O	-5.52	1.17	1.24
1	A	86	ALA	C-O	-5.51	1.17	1.24
1	B	346	ALA	C-O	-5.50	1.17	1.24
1	A	353	VAL	C-O	-5.49	1.17	1.24
1	B	67	ASP	C-O	-5.49	1.17	1.24
1	B	306	VAL	C-O	-5.48	1.17	1.24
1	B	220	LEU	C-O	-5.47	1.17	1.24
1	B	354	LYS	C-O	-5.46	1.17	1.24
1	A	238	VAL	CA-C	-5.46	1.47	1.53
1	B	333	LYS	C-O	-5.46	1.17	1.24
1	B	124	SER	C-O	-5.45	1.17	1.24
1	A	196	PHE	C-O	-5.45	1.17	1.24
1	A	59	TRP	NE1-CE2	-5.45	1.31	1.37
1	A	100	LEU	C-O	-5.44	1.17	1.24
1	A	171	TYR	C-O	-5.44	1.16	1.24
1	B	222	ASP	C-O	-5.44	1.18	1.24
1	B	107	GLU	C-O	-5.42	1.16	1.24
1	A	255	VAL	C-O	-5.41	1.18	1.24
1	B	85	PRO	C-O	-5.41	1.17	1.24
1	A	77	HIS	CE1-NE2	-5.40	1.27	1.32
1	A	111	LEU	C-O	-5.40	1.17	1.24
1	B	177	PRO	C-O	-5.39	1.18	1.23
1	B	278	VAL	C-O	-5.39	1.17	1.24
1	B	40	GLY	C-O	-5.39	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	GLU	C-O	-5.38	1.17	1.24
1	A	125	TRP	C-O	-5.37	1.18	1.24
1	A	203	PHE	C-O	-5.37	1.17	1.24
1	A	138	HIS	CG-ND1	-5.37	1.32	1.38
1	B	314	PHE	C-O	-5.37	1.17	1.24
1	A	205	PRO	C-O	-5.36	1.17	1.23
1	A	314	PHE	C-O	-5.36	1.17	1.24
1	A	104	ILE	C-O	-5.36	1.18	1.24
1	B	247	ILE	C-O	-5.36	1.18	1.24
1	A	217	VAL	C-O	-5.35	1.18	1.24
1	B	204	PHE	C-O	-5.35	1.17	1.24
1	B	52	TYR	C-O	-5.34	1.18	1.24
1	B	209	SER	C-O	-5.34	1.17	1.23
1	A	341	LYS	C-O	-5.34	1.18	1.24
1	A	306	VAL	C-O	-5.33	1.18	1.24
1	B	313	LYS	C-O	-5.33	1.18	1.24
1	B	219	SER	C-O	-5.32	1.17	1.23
1	A	136	LEU	C-O	-5.32	1.17	1.24
1	B	175	HIS	C-O	-5.31	1.18	1.24
1	B	321	ILE	C-O	-5.31	1.18	1.24
1	A	271	GLY	C-O	-5.30	1.17	1.23
1	B	131	VAL	C-O	-5.30	1.18	1.23
1	B	33	SER	C-O	-5.30	1.18	1.24
1	B	167	ASP	C-O	-5.29	1.18	1.24
1	B	279	HIS	CG-ND1	-5.29	1.32	1.38
1	A	207	PRO	C-O	-5.29	1.17	1.23
1	A	156	GLY	C-O	-5.28	1.17	1.23
1	A	295	ALA	C-O	-5.28	1.17	1.23
1	A	291	VAL	C-O	-5.27	1.17	1.24
1	A	192	LEU	C-O	-5.26	1.18	1.24
1	A	117	VAL	C-O	-5.25	1.18	1.24
1	A	321	ILE	C-O	-5.24	1.18	1.24
1	A	90	GLN	C-O	-5.24	1.18	1.24
1	B	203	PHE	C-O	-5.24	1.17	1.24
1	A	124	SER	C-O	-5.24	1.18	1.24
1	B	158	LEU	C-O	-5.23	1.18	1.24
1	A	336	GLN	C-O	-5.22	1.18	1.24
1	A	254	ALA	C-O	-5.21	1.17	1.23
1	A	320	GLU	C-O	-5.20	1.18	1.24
1	B	206	VAL	C-N	5.20	1.39	1.33
1	B	172	LYS	C-O	-5.20	1.17	1.23
1	A	103	GLY	C-O	-5.18	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	266	PRO	C-O	-5.17	1.17	1.24
1	A	297	MET	C-O	-5.17	1.17	1.24
1	B	359	PHE	C-O	-5.17	1.17	1.24
1	B	69	VAL	C-O	-5.16	1.18	1.24
1	A	211	LEU	C-O	-5.16	1.17	1.23
1	B	272	VAL	C-O	-5.16	1.18	1.24
1	B	79	ILE	C-O	-5.13	1.18	1.24
1	A	157	LEU	C-O	-5.13	1.18	1.24
1	A	228	SER	C-O	-5.12	1.17	1.23
1	A	331	LEU	C-O	-5.12	1.18	1.24
1	B	120	HIS	CG-ND1	-5.11	1.32	1.38
1	B	324	LEU	C-O	-5.11	1.17	1.24
1	B	352	GLU	C-O	-5.10	1.18	1.24
1	A	310	VAL	C-O	-5.09	1.18	1.24
1	B	245	GLU	C-O	-5.09	1.18	1.24
1	A	122	GLN	C-O	-5.09	1.18	1.24
1	B	345	LEU	C-O	-5.09	1.18	1.24
1	A	50	GLY	C-O	-5.08	1.17	1.23
1	A	173	SER	C-O	-5.07	1.17	1.23
1	B	84	ASP	C-O	-5.07	1.17	1.24
1	A	118	SER	C-O	-5.07	1.17	1.24
1	A	354	LYS	C-O	-5.07	1.18	1.24
1	A	169	LEU	C-O	-5.06	1.17	1.24
1	B	355	LYS	C-O	-5.05	1.18	1.24
1	A	143	LYS	C-O	-5.05	1.17	1.24
1	A	48	HIS	CD2-NE2	-5.04	1.32	1.37
1	B	343	LYS	C-O	-5.04	1.18	1.24
1	B	138	HIS	CD2-NE2	-5.04	1.32	1.37
1	A	285	LEU	C-O	-5.04	1.17	1.23
1	A	61	ARG	C-O	-5.04	1.18	1.24
1	A	153	GLY	C-O	-5.04	1.16	1.23
1	A	305	ALA	C-O	-5.03	1.18	1.24
1	A	69	VAL	C-O	-5.02	1.19	1.24
1	A	337	ILE	C-O	-5.02	1.18	1.24
1	B	113	GLN	C-O	-5.02	1.18	1.24
1	B	228	SER	C-O	-5.02	1.18	1.23
1	A	201	GLY	C-O	-5.01	1.17	1.23
1	B	311	ILE	C-O	-5.01	1.18	1.24
1	B	207	PRO	N-CD	5.00	1.54	1.47

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ASP	N-CA-C	9.20	122.49	111.82
1	B	89[A]	ARG	CA-C-O	8.12	129.59	120.90
1	B	89[B]	ARG	CA-C-O	8.12	129.59	120.90
1	A	268	GLY	N-CA-C	7.70	122.62	112.77
1	A	74	VAL	N-CA-C	7.63	114.37	106.21
1	B	78[A]	SER	N-CA-C	6.92	119.67	111.71
1	B	78[B]	SER	N-CA-C	6.92	119.67	111.71
1	B	122[A]	GLN	N-CA-C	6.60	118.13	111.07
1	B	122[B]	GLN	N-CA-C	6.60	118.13	111.07
1	B	199	LYS	N-CA-C	6.55	118.50	111.36
1	B	206	VAL	CA-C-N	-6.29	113.80	120.03
1	B	206	VAL	C-N-CA	-6.29	113.80	120.03
1	B	206	VAL	CA-C-O	6.24	122.61	119.12
1	B	283	THR	N-CA-C	6.23	118.15	111.36
1	B	289	GLU	N-CA-C	6.02	117.84	111.28
1	A	199	LYS	N-CA-C	5.89	117.50	111.14
1	B	237	THR	N-CA-C	5.88	118.10	108.52
1	B	154	THR	N-CA-C	5.64	118.77	110.59
1	B	208[A]	GLU	N-CA-C	5.63	118.65	109.59
1	B	208[B]	GLU	N-CA-C	5.63	118.65	109.59
1	B	206	VAL	O-C-N	5.53	125.47	121.55
1	A	168	ILE	N-CA-C	5.45	115.65	110.53
1	B	271	GLY	N-CA-C	5.33	118.94	112.49
1	A	260	SER	N-CA-C	5.33	116.90	111.14
1	B	112	PHE	N-CA-C	5.32	117.07	109.14
1	B	136	LEU	N-CA-C	5.16	116.99	111.36
1	B	89[A]	ARG	N-CA-C	5.11	117.25	111.11
1	B	89[B]	ARG	N-CA-C	5.11	117.25	111.11
1	A	206	VAL	CA-C-O	5.07	121.96	119.12
1	B	168	ILE	N-CA-C	5.01	115.24	110.53

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	2565	2660	2650	19	1
1	B	2583	2678	2677	51	1
2	A	19	0	15	0	0
2	B	19	0	15	0	0
3	A	31	12	12	0	0
3	B	31	12	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	B	12	16	16	2	0
6	A	283	0	0	2	1
6	B	258	0	0	4	1
All	All	5805	5378	5397	70	2

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 7.

All (70) 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:B:130:MET:CE	6:B:526:HOH:O	1.86	1.24
1:B:29:LEU:HD22	1:B:208[B]:GLU:CD	1.67	1.20
1:B:249:GLN:OE1	1:B:252:ARG:NH1	1.88	1.06
1:B:130:MET:HE2	6:B:526:HOH:O	1.56	0.92
1:B:61:ARG:NH1	1:B:65:GLU:OE2	2.14	0.81
1:B:29:LEU:CD2	1:B:208[B]:GLU:CD	2.52	0.80
1:B:61:ARG:NH1	1:B:65:GLU:CD	2.40	0.80
1:B:251:PHE:O	1:B:303:LYS:HE3	1.93	0.69
1:B:141:GLN:O	1:B:145:LYS:HD2	1.93	0.69
1:B:29:LEU:HD22	1:B:208[A]:GLU:HG3	1.75	0.68
1:A:43:PRO:O	1:A:91:SER:HB3	1.95	0.67
1:B:255:VAL:O	1:B:256:THR:HG22	1.97	0.64
1:B:234:LYS:HE3	1:B:250:LYS:NZ	2.14	0.63
1:B:29:LEU:HD22	1:B:208[B]:GLU:OE2	1.98	0.62
1:B:255:VAL:O	1:B:256:THR:CG2	2.46	0.62
1:B:255:VAL:C	1:B:256:THR:HG23	2.24	0.62
1:B:255:VAL:C	1:B:256:THR:CG2	2.73	0.62
1:B:29:LEU:CD2	1:B:208[B]:GLU:OE2	2.47	0.61
1:A:69:VAL:HG12	1:A:109:SER:HB3	1.84	0.60
1:B:234:LYS:HE3	1:B:250:LYS:HZ1	1.68	0.59
1:B:328:LYS:O	1:B:332:GLU:HG3	2.02	0.58
1:A:234:LYS:HD2	1:A:250:LYS:NZ	2.19	0.58
1:B:43:PRO:HD2	1:B:78[B]:SER:OG	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:HD22	1:B:208[B]:GLU:CG	2.32	0.55
1:B:292:ARG:HH11	1:B:292:ARG:HG3	1.73	0.54
1:A:130:MET:HE3	6:A:556:HOH:O	2.08	0.53
1:B:347:TYR:CZ	5:B:406:GOL:H11	2.42	0.53
1:A:46:ILE:HD12	1:A:46:ILE:N	2.24	0.53
1:A:132:ARG:HH11	1:A:132:ARG:HG2	1.74	0.51
1:A:234:LYS:HD2	1:A:250:LYS:HZ3	1.74	0.50
1:B:61:ARG:HH11	1:B:65:GLU:CD	2.09	0.50
1:A:47:LEU:HD11	1:A:56:ILE:HG13	1.93	0.49
1:B:234:LYS:HE3	1:B:250:LYS:CE	2.43	0.49
1:B:249:GLN:CD	1:B:252:ARG:HH11	2.20	0.49
1:B:61:ARG:HH12	1:B:65:GLU:CD	2.12	0.49
1:A:37:VAL:HB	1:A:69:VAL:HG22	1.94	0.48
1:B:214:MET:HE3	1:B:217:VAL:HG22	1.96	0.48
1:B:69:VAL:C	1:B:70:LEU:HD12	2.38	0.48
1:A:231:ASP:OD1	1:A:232:PRO:HD2	2.13	0.48
1:A:113:GLN:HB2	1:A:335:LEU:HD13	1.96	0.47
1:A:160:TYR:N	1:A:161:PRO:CD	2.76	0.47
1:B:141:GLN:HB3	1:B:145:LYS:HE2	1.95	0.47
1:A:55:ALA:O	1:A:58:SER:HB2	2.14	0.46
1:A:234:LYS:HD2	1:A:250:LYS:CE	2.46	0.46
1:B:29:LEU:HB3	1:B:208[A]:GLU:OE2	2.17	0.45
1:B:347:TYR:CE1	5:B:406:GOL:H11	2.52	0.45
1:A:46:ILE:HD12	1:A:46:ILE:H	1.81	0.45
1:B:29:LEU:HD21	1:B:208[B]:GLU:OE2	2.17	0.45
1:B:69:VAL:CG1	1:B:71:TYR:CZ	3.00	0.45
1:B:61:ARG:NH1	1:B:61:ARG:HG2	2.31	0.44
1:B:315:ALA:N	1:B:316:PRO:CD	2.81	0.44
1:B:89[B]:ARG:HA	1:B:89[B]:ARG:HD2	1.87	0.43
1:B:231:ASP:OD1	1:B:232:PRO:HD2	2.18	0.43
1:B:289:GLU:O	1:B:293:ARG:HG3	2.19	0.43
1:B:160:TYR:N	1:B:161:PRO:CD	2.82	0.43
1:B:248:VAL:HG13	1:B:304:LEU:HD22	2.02	0.42
1:B:292:ARG:HG3	1:B:292:ARG:NH1	2.35	0.42
1:B:145:LYS:HD3	1:B:157:LEU:HD21	2.02	0.42
1:B:165:ALA:HB2	1:B:189:VAL:HG22	2.03	0.41
1:A:70:LEU:HG	1:A:110:ILE:HB	2.03	0.41
1:B:105:ASN:HA	1:B:106:PRO:HD2	1.91	0.41
1:B:29:LEU:HD22	1:B:208[B]:GLU:OE1	2.12	0.41
1:B:133:LEU:HB3	1:B:134:PRO:HD3	2.03	0.41
1:B:37:VAL:HB	1:B:69:VAL:HG22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:HB	1:A:77:HIS:HD2	1.84	0.40
1:A:116:GLN:HG3	6:A:595:HOH:O	2.21	0.40
1:B:130:MET:HE3	6:B:526:HOH:O	1.84	0.40
1:B:145:LYS:HE3	1:B:160:TYR:HE2	1.87	0.40
1:A:69:VAL:HG12	1:A:109:SER:CB	2.49	0.40
1:B:145:LYS:NZ	6:B:509:HOH:O	2.48	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:HH11	1:B:33:SER:HG[3_455]	1.21	0.39
6:A:736:HOH:O	6:B:701:HOH:O[3_455]	2.14	0.06

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	325/343 (95%)	317 (98%)	8 (2%)	0	100	100
1	B	327/343 (95%)	321 (98%)	6 (2%)	0	100	100
All	All	652/686 (95%)	638 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	286/296 (97%)	279 (98%)	7 (2%)	43	27
1	B	290/296 (98%)	276 (95%)	14 (5%)	23	6
All	All	576/592 (97%)	555 (96%)	21 (4%)	30	13

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	SER
1	A	81	VAL
1	A	160	TYR
1	A	234	LYS
1	A	323	LYS
1	A	325	LYS
1	A	328	LYS
1	B	29	LEU
1	B	30	GLN
1	B	31	LYS
1	B	34	LYS
1	B	47	LEU
1	B	58	SER
1	B	63	GLN
1	B	130	MET
1	B	145	LYS
1	B	160	TYR
1	B	234	LYS
1	B	240	ILE
1	B	292	ARG
1	B	323	LYS

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

Mol	Chain	Res	Type
1	A	42	GLN
1	A	141	GLN
1	B	164	GLN
1	B	182	GLN
1	B	330	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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	GOL	B	406	-	5,5,5	0.35	0	5,5,5	0.44	0
3	ATP	B	402	4	32,33,33	1.38	7 (21%)	48,52,52	1.82	10 (20%)
5	GOL	B	405	-	5,5,5	0.47	0	5,5,5	0.15	0
2	5BX	B	401	-	19,21,21	2.66	10 (52%)	20,30,30	3.22	3 (15%)
2	5BX	A	401	-	19,21,21	2.70	11 (57%)	20,30,30	3.21	5 (25%)
3	ATP	A	402	4	32,33,33	1.37	7 (21%)	48,52,52	1.87	11 (22%)

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	GOL	B	406	-	-	2/4/4/4	-
3	ATP	B	402	4	-	4/22/38/38	0/3/3/3
5	GOL	B	405	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5BX	B	401	-	-	0/10/22/22	0/3/3/3
2	5BX	A	401	-	-	0/10/22/22	0/3/3/3
3	ATP	A	402	4	-	4/22/38/38	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	5BX	O08-C03	5.59	1.41	1.36
2	B	401	5BX	O08-C03	5.57	1.41	1.36
2	A	401	5BX	C12-C11	4.48	1.41	1.36
2	B	401	5BX	C12-C11	4.43	1.41	1.36
3	B	402	ATP	C5-C4	4.24	1.46	1.39
3	A	402	ATP	C5-C4	4.18	1.46	1.39
2	B	401	5BX	C03-N04	3.58	1.42	1.33
2	A	401	5BX	C03-N04	3.53	1.42	1.33
2	A	401	5BX	C07-C05	-3.53	1.48	1.52
2	B	401	5BX	C15-C14	3.47	1.45	1.39
2	B	401	5BX	C07-C05	-3.46	1.48	1.52
2	A	401	5BX	C15-C14	3.39	1.45	1.39
2	A	401	5BX	C17-C16	3.31	1.45	1.38
2	B	401	5BX	C17-C16	3.29	1.45	1.38
2	A	401	5BX	C01-N02	2.96	1.50	1.45
2	B	401	5BX	C01-N02	2.89	1.50	1.45
2	A	401	5BX	C09-C07	-2.86	1.51	1.54
2	B	401	5BX	O08-C07	-2.66	1.41	1.45
3	B	402	ATP	PB-O3A	2.64	1.62	1.59
2	A	401	5BX	C18-C19	2.56	1.43	1.39
2	B	401	5BX	C09-C07	-2.54	1.51	1.54
2	A	401	5BX	O08-C07	-2.54	1.41	1.45
3	B	402	ATP	C5-C6	2.47	1.47	1.41
3	A	402	ATP	C5-C6	2.44	1.47	1.41
2	B	401	5BX	C18-C19	2.43	1.43	1.39
3	A	402	ATP	C8-N7	2.28	1.36	1.31
3	A	402	ATP	C5-N7	-2.27	1.34	1.39
3	A	402	ATP	PB-O3B	2.25	1.61	1.59
3	B	402	ATP	C8-N7	2.24	1.36	1.31
3	B	402	ATP	PA-O3A	2.13	1.61	1.59
3	A	402	ATP	PA-O3A	2.12	1.61	1.59
3	B	402	ATP	C4-N9	-2.12	1.33	1.37
3	B	402	ATP	C5-N7	-2.11	1.35	1.39
2	A	401	5BX	C14-N13	2.03	1.41	1.37
3	A	402	ATP	C4-N9	-2.00	1.33	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	5BX	O08-C03-N04	-12.84	108.75	117.73
2	A	401	5BX	O08-C03-N04	-12.40	109.06	117.73
3	A	402	ATP	C5-C4-N3	-5.46	119.19	126.72
3	B	402	ATP	C5-C4-N3	-5.37	119.33	126.72
3	B	402	ATP	N3-C4-N9	4.89	135.49	127.17
3	A	402	ATP	N3-C4-N9	4.83	135.38	127.17
2	A	401	5BX	C10-C09-C07	4.49	117.32	111.66
3	B	402	ATP	C4-N9-C8	4.18	110.12	105.74
3	A	402	ATP	N3-C2-N1	-4.04	122.47	128.58
3	B	402	ATP	N3-C2-N1	-3.98	122.56	128.58
3	A	402	ATP	C2-N3-C4	3.92	121.40	111.83
3	B	402	ATP	C2-N3-C4	3.84	121.21	111.83
3	A	402	ATP	C4-N9-C8	3.79	109.72	105.74
2	B	401	5BX	C10-C09-C07	3.73	116.37	111.66
2	B	401	5BX	C11-C12-N13	-3.13	107.77	110.31
2	A	401	5BX	C11-C12-N13	-2.98	107.89	110.31
3	A	402	ATP	C4-C5-N7	-2.87	107.30	110.58
3	B	402	ATP	C4-C5-N7	-2.86	107.31	110.58
3	B	402	ATP	N9-C8-N7	-2.81	109.95	113.94
3	A	402	ATP	N9-C8-N7	-2.74	110.04	113.94
2	A	401	5BX	C15-C14-C19	-2.63	119.65	122.19
3	A	402	ATP	C5-N7-C8	2.58	107.51	103.45
3	B	402	ATP	C5-N7-C8	2.53	107.43	103.45
3	A	402	ATP	O3A-PB-O1B	-2.33	103.70	110.70
3	B	402	ATP	C6-C5-N7	2.30	136.52	132.09
3	A	402	ATP	C6-C5-N7	2.18	136.29	132.09
2	A	401	5BX	C19-C11-C12	2.11	107.86	106.25
3	B	402	ATP	C2-N1-C6	2.03	122.06	118.73
3	A	402	ATP	O2B-PB-O3A	2.00	112.68	107.27

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	ATP	C5'-O5'-PA-O1A
3	B	402	ATP	C5'-O5'-PA-O1A
5	B	405	GOL	C1-C2-C3-O3
5	B	406	GOL	O1-C1-C2-C3
5	B	405	GOL	O2-C2-C3-O3
5	B	406	GOL	O1-C1-C2-O2
3	A	402	ATP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	402	ATP	PB-O3A-PA-O2A
3	A	402	ATP	PG-O3B-PB-O2B
3	A	402	ATP	PB-O3A-PA-O1A
3	B	402	ATP	PG-O3B-PB-O2B
3	B	402	ATP	PB-O3A-PA-O1A

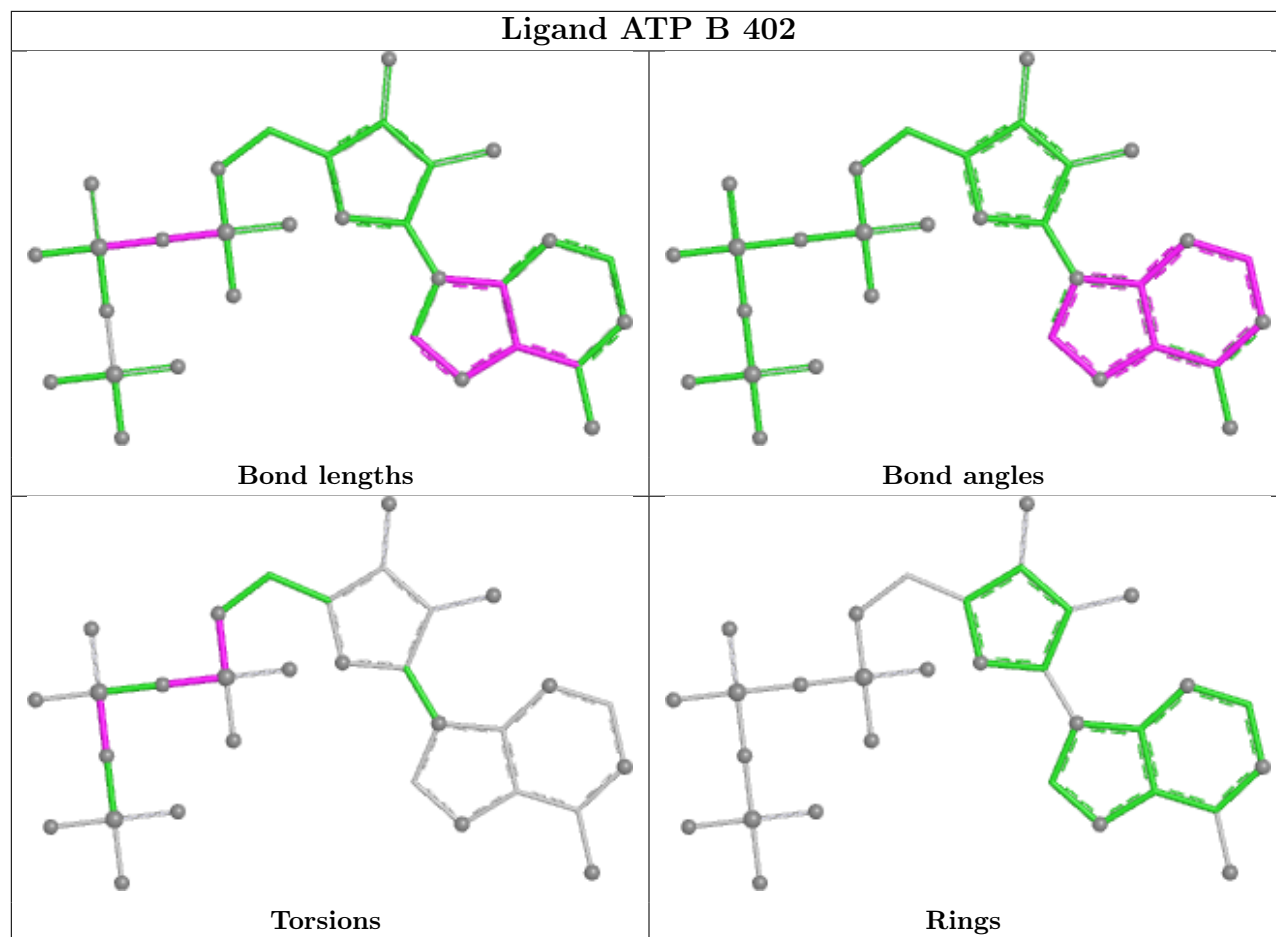
There are no ring outliers.

1 monomer is involved in 2 short contacts:

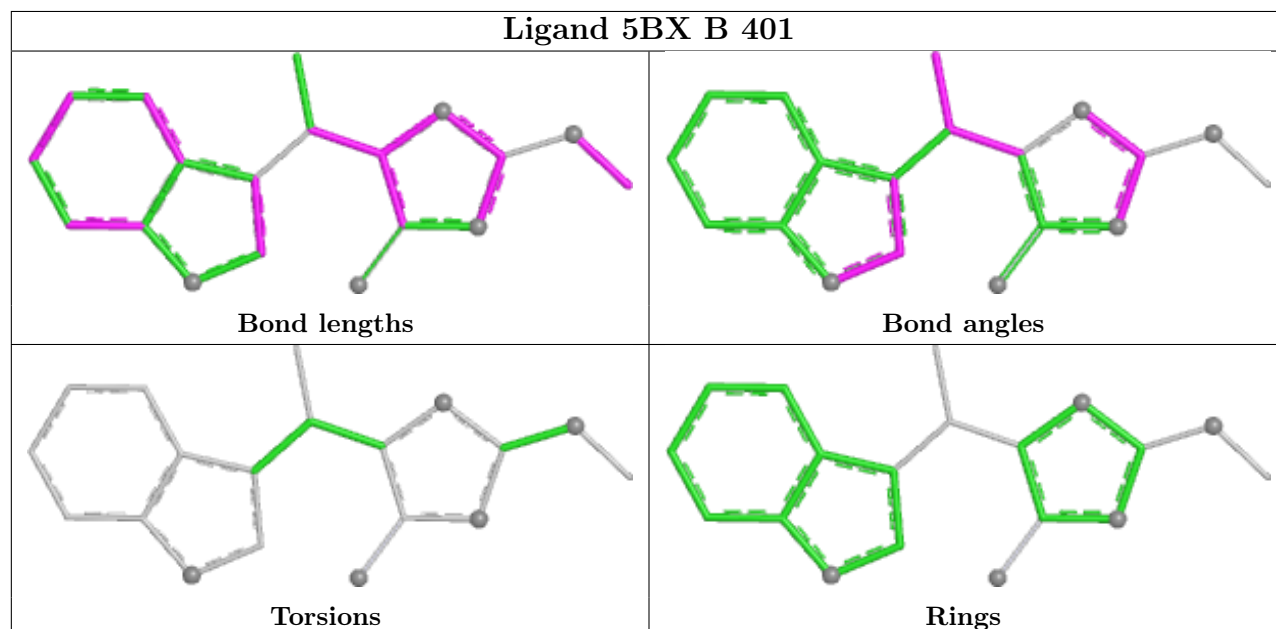
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	406	GOL	2	0

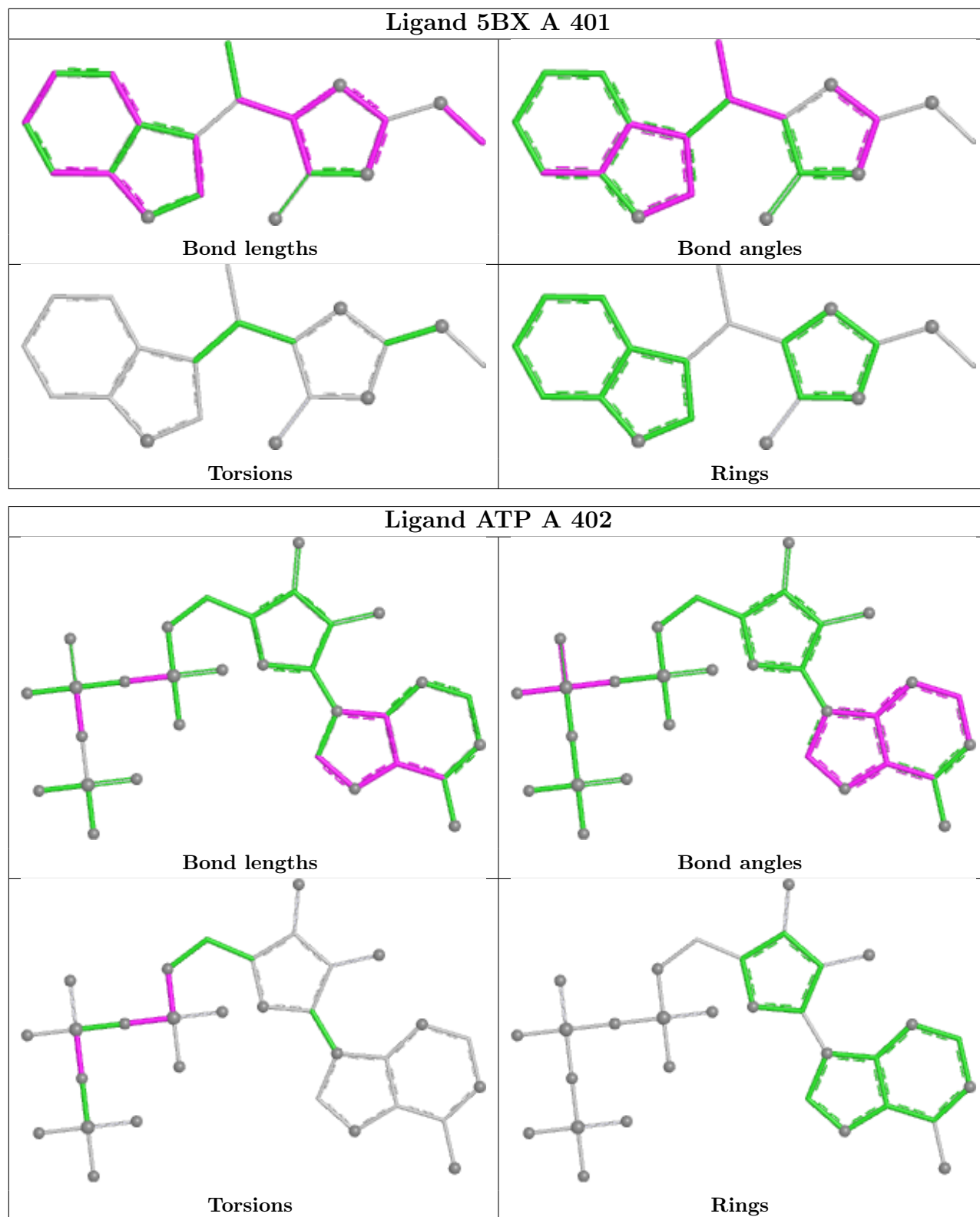
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand ATP B 402



Ligand 5BX B 401





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	327/343 (95%)	-0.36	0	100 100	18, 28, 45, 60	0
1	B	327/343 (95%)	-0.25	3 (0%)	81 85	13, 29, 48, 60	4 (1%)
All	All	654/686 (95%)	-0.30	3 (0%)	87 90	13, 29, 47, 60	4 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	LEU	2.8
1	B	145	LYS	2.7
1	B	147	THR	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
5	GOL	B	406	6/6	0.79	0.12	39,48,58,58	0
5	GOL	B	405	6/6	0.81	0.21	25,32,39,46	14

Continued on next page...

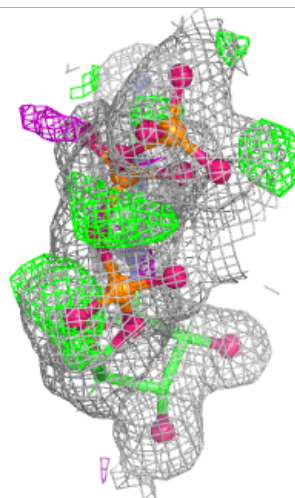
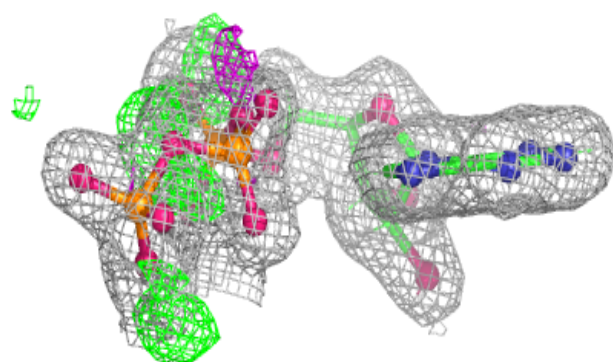
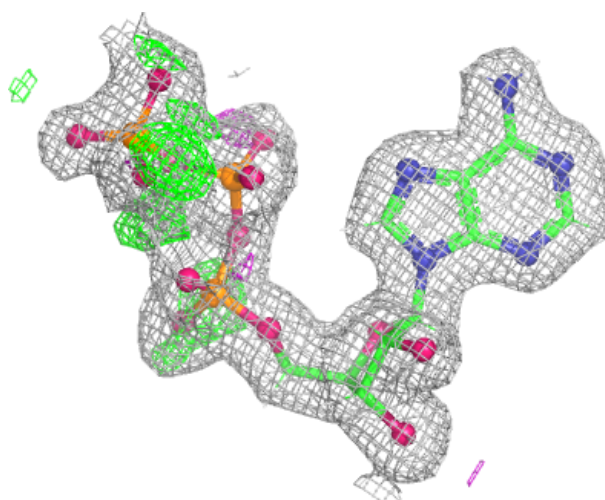
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	B	402	31/31	0.96	0.06	15,20,27,34	0
3	ATP	A	402	31/31	0.97	0.06	13,19,25,40	0
2	5BX	A	401	19/19	0.97	0.06	15,17,21,21	0
2	5BX	B	401	19/19	0.98	0.05	13,17,19,19	0
4	MN	B	404	1/1	0.98	0.04	30,30,30,30	1
4	MN	A	404	1/1	0.99	0.03	25,25,25,25	1
4	MN	B	403	1/1	1.00	0.01	18,18,18,18	0
4	MN	A	403	1/1	1.00	0.01	16,16,16,16	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.

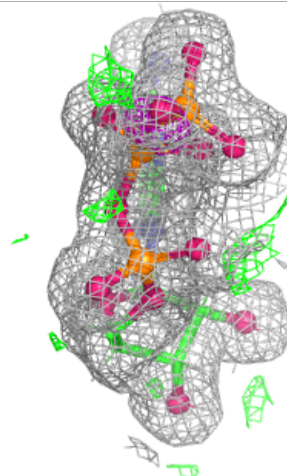
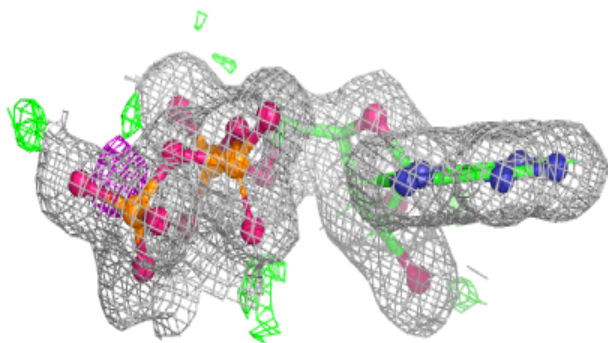
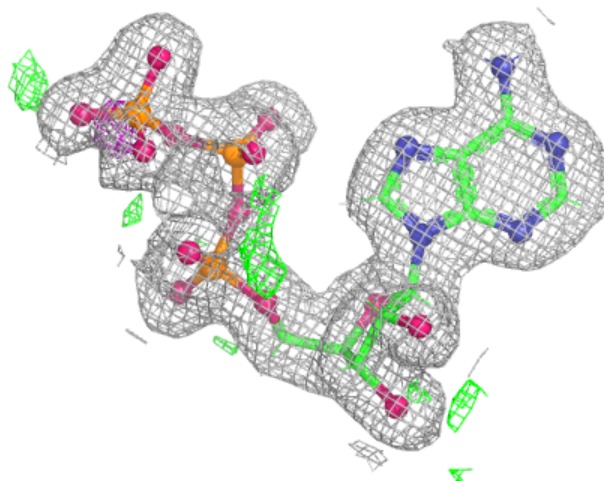
Electron density around ATP B 402:

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



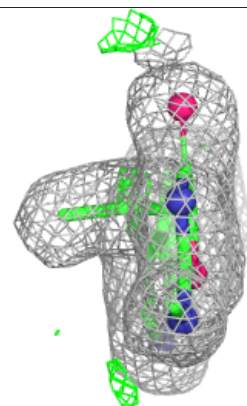
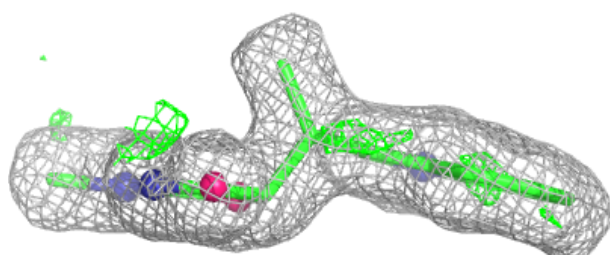
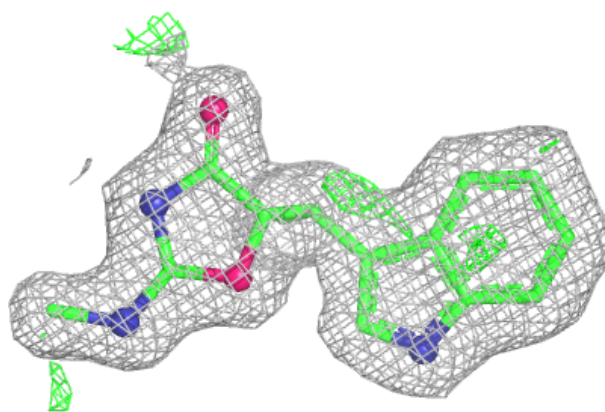
Electron density around ATP A 402:

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

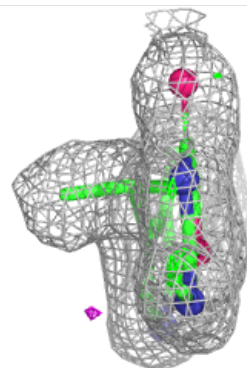
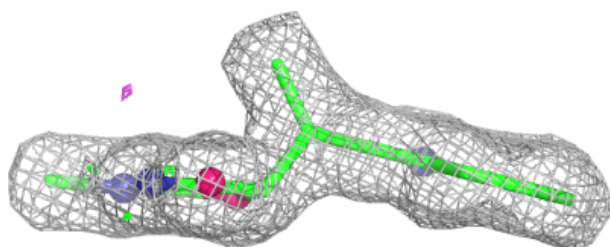
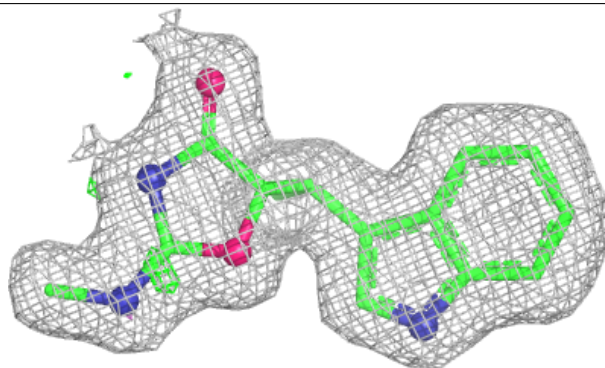


Electron density around 5BX A 401:

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

**Electron density around 5BX B 401:**

$2mF_o-DF_c$ (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.