



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:16 AM UTC

PDB ID : 8K6F / pdb_00008k6f
Title : LnaB-Actin-PRUb ternary complex
Authors : Chen, T.T.; Ouyang, S.Y.
Deposited on : 2023-07-25
Resolution : 3.41 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

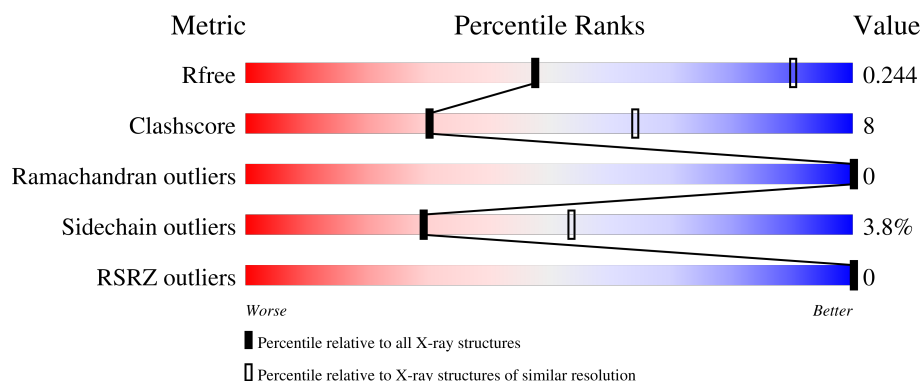
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	375	 67% 28% . .
1	B	375	 66% 30% . .
2	C	352	 73% 22% . .
2	D	352	 69% 26% . .
3	E	76	 71% 20% 9%

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Mol	Chain	Length	Quality of chain
3	F	76	 72% 28%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12736 atoms, of which 33 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 Actin gamma 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2886	1828	486	550	22			
1	B	371	Total	C	N	O	S	0	0	0
			2894	1834	487	551	22			

- Molecule 2 is a protein called Legionella effector LnaB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	347	Total	C	N	O	S	0	0	0
			2817	1798	462	552	5			
2	D	348	Total	C	N	O	S	0	0	0
			2826	1804	464	553	5			

- Molecule 3 is a protein called Ubiquitin.

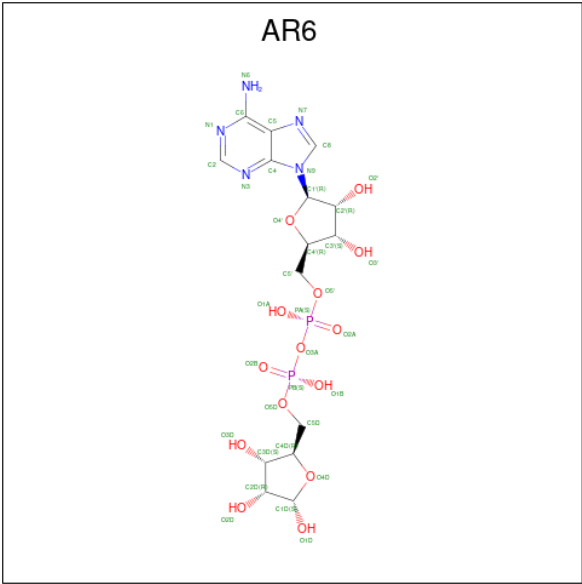
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	76	Total	C	N	O	S	0	0	0
			602	378	105	118	1			
3	F	76	Total	C	N	O	S	0	0	0
			602	378	105	118	1			

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-Y L]METHYL[HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHIDROXYOXOLAN-2-YL]METHOX Y]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂) (labeled as "Ligand of Interest" by depositor).

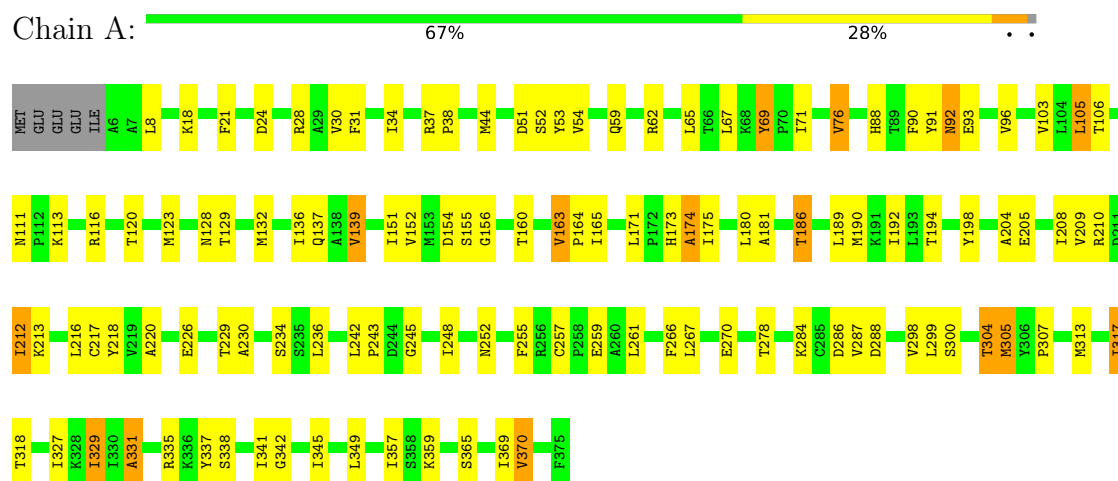


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	H	O	P	0	0
			23	5	9	8	1		

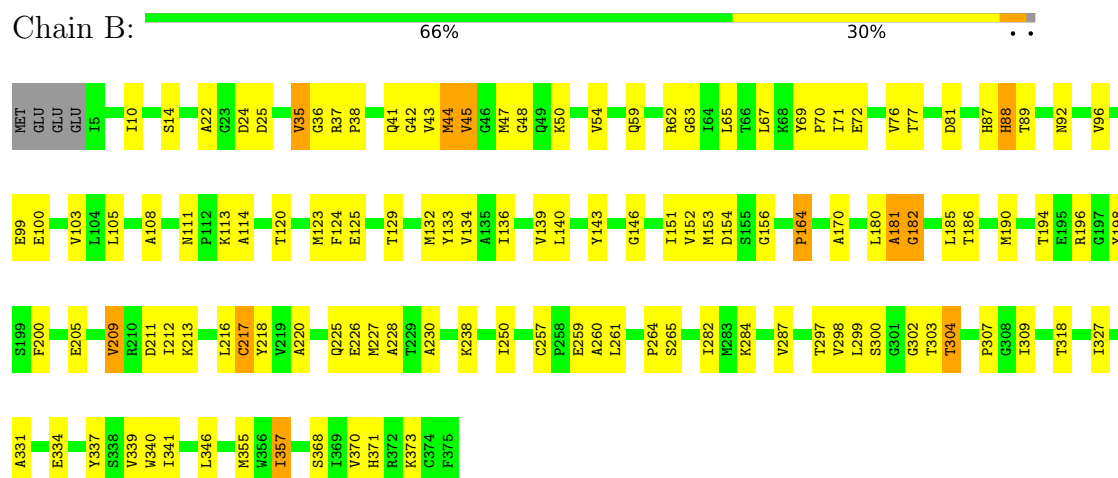
3 Residue-property plots

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: Actin gamma 1

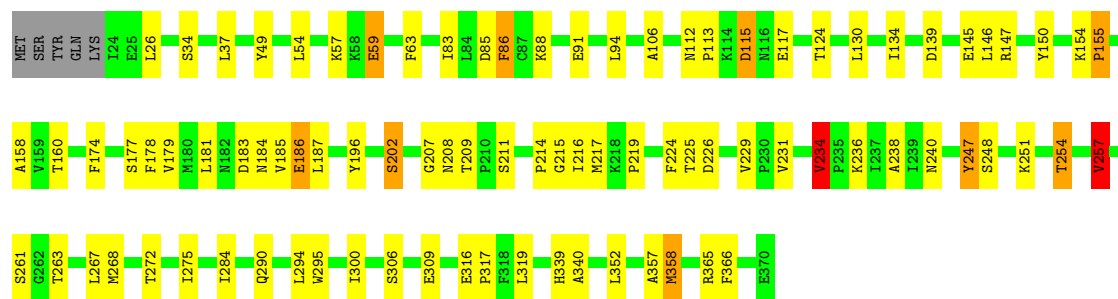


• Molecule 1: Actin gamma 1



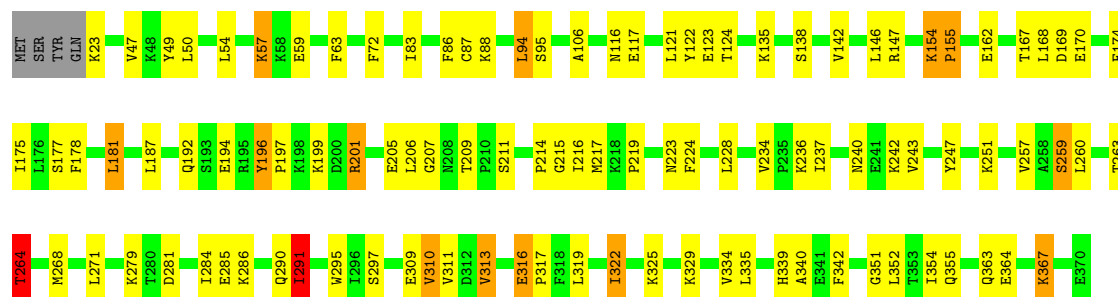
• Molecule 2: Legionella effector LnaB





• Molecule 2: Legionella effector LnaB

Chain D: 69% 26%



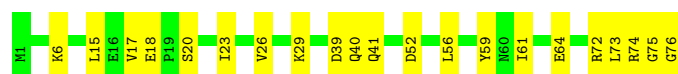
• Molecule 3: Ubiquitin

Chain E: 71% 20% 9%



• Molecule 3: Ubiquitin

Chain F: 72% 28%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.69Å 214.23Å 79.56Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	37.29 – 3.41 37.29 – 3.41	Depositor EDS
% Data completeness (in resolution range)	97.0 (37.29-3.41) 95.6 (37.29-3.41)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.41Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.222 , 0.243 0.222 , 0.244	Depositor DCC
R_{free} test set	1971 reflections (7.94%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.825	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.368 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12736	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: AR6, ATP

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	1.42	3/2949 (0.1%)	1.28	44/3992 (1.1%)
1	B	1.36	4/2957 (0.1%)	1.24	39/4003 (1.0%)
2	C	1.34	5/2872 (0.2%)	1.29	46/3876 (1.2%)
2	D	1.31	5/2881 (0.2%)	1.32	49/3887 (1.3%)
3	E	1.32	3/608 (0.5%)	1.45	14/816 (1.7%)
3	F	1.11	0/608	1.36	9/816 (1.1%)
All	All	1.34	20/12875 (0.2%)	1.30	201/17390 (1.2%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	261	SER	CA-C	-6.93	1.44	1.52
3	E	64	GLU	CA-C	-6.60	1.44	1.52
2	C	202	SER	CA-C	-6.48	1.44	1.52
1	B	181	ALA	CA-CB	-6.27	1.46	1.54
2	D	205	GLU	CA-C	-6.20	1.46	1.53
1	A	213	LYS	CA-C	-5.97	1.47	1.52
2	D	316	GLU	CA-C	-5.89	1.47	1.53
1	A	286	ASP	CA-C	-5.67	1.45	1.52
2	C	267	LEU	CA-C	-5.63	1.45	1.52
2	C	150	TYR	CA-C	-5.44	1.46	1.52
2	D	297	SER	CA-C	-5.25	1.46	1.52
1	B	170	ALA	CA-C	-5.18	1.46	1.52
2	C	49	TYR	CA-C	-5.09	1.46	1.52
2	D	286	LYS	CA-C	-5.09	1.46	1.52
2	D	285	GLU	CA-C	-5.07	1.46	1.52
1	A	91	TYR	CA-C	-5.04	1.48	1.53
3	E	71	LEU	CA-C	-5.04	1.46	1.52
3	E	62	GLN	CA-C	-5.04	1.48	1.53
1	B	108	ALA	CA-C	-5.02	1.46	1.52
1	B	88	HIS	CA-C	-5.00	1.46	1.52

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	257	VAL	N-CA-C	-15.32	77.48	109.34
1	A	212	ILE	N-CA-C	-12.38	100.65	112.29
2	C	290	GLN	N-CA-C	-12.07	99.03	113.88
2	D	169	ASP	N-CA-C	-11.18	99.66	113.97
1	B	22	ALA	N-CA-C	10.60	122.83	111.28
2	C	59	GLU	N-CA-C	-10.18	100.12	112.54
2	C	178	PHE	N-CA-C	-9.92	101.19	113.20
2	C	26	LEU	N-CA-C	-9.85	100.11	112.72
2	C	257	VAL	N-CA-C	-9.54	104.08	111.62
2	C	224	PHE	N-CA-C	9.30	124.36	112.92
2	C	49	TYR	N-CA-C	-9.07	101.36	111.07
1	A	318	THR	N-CA-C	-9.00	102.31	113.38
3	F	40	GLN	N-CA-C	-8.94	101.19	112.90
2	C	117	GLU	N-CA-C	8.89	120.97	111.28
1	B	92	ASN	N-CA-C	8.77	120.84	111.28
2	D	154	LYS	CA-C-N	-8.61	111.88	120.31
2	D	154	LYS	C-N-CA	-8.61	111.88	120.31
1	A	51	ASP	N-CA-C	-8.44	102.70	113.16
1	A	331	ALA	CA-C-N	-8.35	113.65	119.66
1	A	331	ALA	C-N-CA	-8.35	113.65	119.66
1	A	270	GLU	N-CA-C	-8.28	103.29	112.72
2	C	365	ARG	N-CA-C	-8.27	103.71	113.88
1	B	196	ARG	N-CA-C	-8.15	102.36	112.88
2	C	263	THR	N-CA-C	-7.92	103.51	113.01
1	B	318	THR	N-CA-C	-7.73	103.85	113.28
2	D	313	VAL	N-CA-C	-7.68	105.68	111.90
1	B	103	VAL	N-CA-C	7.61	119.38	107.28
2	D	259	SER	N-CA-C	7.60	119.57	111.28
1	A	163	VAL	N-CA-C	7.58	116.25	107.77
2	D	86	PHE	N-CA-C	-7.51	103.10	111.28
2	D	310	VAL	N-CA-C	-7.44	105.16	111.56
2	C	295	TRP	N-CA-C	-7.38	103.18	111.07
2	D	209	THR	CA-C-N	-7.32	113.14	120.31
2	D	209	THR	C-N-CA	-7.32	113.14	120.31
3	F	75	GLY	N-CA-C	-7.29	106.16	115.42
1	A	216	LEU	N-CA-C	7.28	120.65	111.69
1	B	25	ASP	N-CA-C	-7.28	104.42	112.72
2	D	167	THR	N-CA-C	7.27	122.33	113.38
2	D	201	ARG	N-CA-C	-7.23	99.11	109.96
3	E	36	ILE	CA-C-N	-7.21	114.39	119.66
3	E	36	ILE	C-N-CA	-7.21	114.39	119.66
1	A	204	ALA	N-CA-C	-7.17	103.54	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	LYS	N-CA-C	-7.16	102.81	112.26
2	D	177	SER	N-CA-C	-7.14	103.67	112.88
2	C	226	ASP	N-CA-C	-7.11	105.23	114.04
2	D	215	GLY	N-CA-C	7.07	124.16	111.02
2	D	138	SER	N-CA-C	7.06	120.75	109.24
2	C	207	GLY	N-CA-C	7.05	122.19	112.52
2	D	234	VAL	CA-C-N	-7.04	112.98	120.66
2	D	234	VAL	C-N-CA	-7.04	112.98	120.66
2	D	178	PHE	N-CA-C	-7.02	104.69	113.18
2	C	154	LYS	CA-C-N	-6.95	112.77	120.14
2	C	154	LYS	C-N-CA	-6.95	112.77	120.14
3	F	41	GLN	N-CA-C	6.94	121.16	110.20
2	D	290	GLN	N-CA-C	-6.89	105.00	113.41
2	C	272	THR	N-CA-C	-6.86	103.82	111.71
3	E	29	LYS	N-CA-C	-6.86	104.38	112.89
1	B	217	CYS	N-CA-C	6.86	119.15	110.24
1	B	303	THR	N-CA-C	-6.83	105.02	113.15
2	D	364	GLU	N-CA-C	-6.83	104.56	113.17
1	A	93	GLU	N-CA-C	6.82	118.51	111.14
1	A	24	ASP	N-CA-C	-6.81	100.72	110.59
1	B	265	SER	N-CA-C	-6.76	104.89	113.01
2	C	146	LEU	N-CA-C	-6.76	104.51	112.89
2	C	34	SER	CA-C-N	-6.75	112.96	120.45
2	C	34	SER	C-N-CA	-6.75	112.96	120.45
2	C	86	PHE	N-CA-C	-6.73	103.87	111.07
1	A	92	ASN	N-CA-C	6.72	118.40	111.14
1	A	242	LEU	CA-C-N	-6.71	113.00	120.45
1	A	242	LEU	C-N-CA	-6.71	113.00	120.45
2	D	57	LYS	N-CA-C	-6.67	98.02	108.90
2	D	263	THR	N-CA-C	-6.66	105.12	113.18
2	C	209	THR	CA-C-N	-6.63	113.81	120.31
2	C	209	THR	C-N-CA	-6.63	113.81	120.31
2	C	294	LEU	N-CA-C	-6.60	105.38	113.50
2	D	206	LEU	N-CA-C	-6.50	100.81	110.23
1	B	146	GLY	N-CA-C	-6.49	105.36	116.01
3	E	71	LEU	N-CA-C	-6.48	99.89	109.81
1	A	69	TYR	CA-C-N	-6.45	113.04	119.56
1	A	69	TYR	C-N-CA	-6.45	113.04	119.56
2	D	251	LYS	CA-C-N	-6.43	112.98	120.12
2	D	251	LYS	C-N-CA	-6.43	112.98	120.12
3	F	18	GLU	CA-C-N	-6.43	114.27	120.83
3	F	18	GLU	C-N-CA	-6.43	114.27	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	254	THR	CA-C-N	-6.43	113.35	119.85
2	C	254	THR	C-N-CA	-6.43	113.35	119.85
1	A	304	THR	N-CA-C	-6.42	105.40	112.72
2	D	117	GLU	N-CA-C	6.37	118.22	111.28
3	E	18	GLU	N-CA-C	-6.36	100.37	110.10
2	D	242	LYS	N-CA-C	-6.33	104.12	113.61
1	A	111	ASN	CA-C-N	-6.31	113.17	119.92
1	A	111	ASN	C-N-CA	-6.31	113.17	119.92
2	D	196	TYR	CA-C-N	-6.31	113.12	120.12
2	D	196	TYR	C-N-CA	-6.31	113.12	120.12
2	C	145	GLU	N-CA-C	-6.29	106.14	113.88
3	F	29	LYS	N-CA-C	-6.24	104.92	112.54
2	D	207	GLY	N-CA-C	6.22	122.73	112.66
2	D	264	THR	N-CA-C	-6.20	104.60	111.36
2	D	322	ILE	N-CA-C	-6.17	104.73	110.53
1	A	37	ARG	CA-C-N	-6.16	113.33	119.92
1	A	37	ARG	C-N-CA	-6.16	113.33	119.92
1	A	103	VAL	N-CA-C	6.16	116.74	107.75
1	A	111	ASN	N-CA-C	-6.15	102.30	109.93
2	D	367	LYS	N-CA-C	-6.14	105.44	113.17
1	A	37	ARG	N-CA-C	-6.12	98.76	109.48
1	B	339	VAL	N-CA-C	-6.12	104.55	110.42
2	C	215	GLY	N-CA-C	6.09	122.09	111.50
1	B	284	LYS	N-CA-C	-6.07	103.32	111.87
2	C	202	SER	N-CA-C	-6.04	101.54	110.48
1	A	217	CYS	N-CA-C	5.99	118.43	110.53
1	B	72	GLU	N-CA-C	-5.99	99.94	109.76
2	C	240	ASN	N-CA-C	-5.99	100.24	109.76
2	D	49	TYR	N-CA-C	-5.98	104.76	111.28
1	B	260	ALA	N-CA-C	-5.98	105.09	112.38
3	F	6	LYS	N-CA-C	5.97	118.47	108.73
1	A	266	PHE	N-CA-C	-5.96	104.90	111.82
1	B	114	ALA	N-CA-C	5.96	117.86	111.36
2	C	208	ASN	N-CA-C	5.94	119.16	109.59
2	C	106	ALA	N-CA-C	5.89	121.53	113.16
1	B	65	LEU	N-CA-C	5.89	118.81	109.50
1	B	304	THR	N-CA-C	-5.89	105.28	112.88
2	C	366	PHE	N-CA-C	-5.84	106.16	113.28
1	A	342	GLY	N-CA-C	-5.79	105.36	112.77
3	E	67	LEU	N-CA-C	-5.79	101.11	110.32
1	B	88	HIS	N-CA-C	-5.79	104.97	111.28
3	E	63	LYS	N-CA-C	5.78	120.90	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	329	LYS	N-CA-C	-5.77	99.83	109.24
2	C	357	ALA	N-CA-C	5.77	117.65	111.36
2	D	106	ALA	CA-C-N	-5.74	113.70	119.56
2	D	106	ALA	C-N-CA	-5.74	113.70	119.56
1	B	111	ASN	CA-C-N	-5.72	113.89	119.78
1	B	111	ASN	C-N-CA	-5.72	113.89	119.78
1	A	210	ARG	N-CA-C	-5.71	105.42	112.90
1	B	44	MET	N-CA-C	-5.66	106.23	113.02
2	D	155	PRO	N-CA-C	-5.62	103.02	111.57
3	E	65	SER	N-CA-C	-5.60	99.30	108.76
1	B	209	VAL	N-CA-C	-5.59	105.40	113.07
1	B	227	MET	N-CA-C	-5.56	105.37	111.82
2	D	146	LEU	N-CA-C	-5.56	106.50	113.28
2	D	194	GLU	N-CA-C	-5.55	105.87	113.30
2	C	139	ASP	N-CA-C	-5.53	106.39	113.02
2	D	291	ILE	CB-CA-C	-5.52	104.81	112.04
1	B	37	ARG	CA-C-N	-5.51	114.08	119.76
1	B	37	ARG	C-N-CA	-5.51	114.08	119.76
1	A	234	SER	N-CA-C	-5.50	105.88	112.59
2	C	155	PRO	N-CA-C	-5.50	102.50	111.68
2	C	196	TYR	CA-C-N	-5.50	113.95	119.56
2	C	196	TYR	C-N-CA	-5.50	113.95	119.56
1	A	65	LEU	N-CA-C	5.47	117.57	109.69
2	C	247	TYR	N-CA-C	-5.43	105.36	111.28
1	A	359	LYS	N-CA-C	-5.42	105.54	111.82
1	B	69	TYR	CA-C-N	-5.41	113.08	119.84
1	B	69	TYR	C-N-CA	-5.41	113.08	119.84
1	A	52	SER	N-CA-C	5.40	117.22	108.26
2	C	115	ASP	N-CA-C	5.39	116.93	109.54
3	E	42	ARG	N-CA-C	-5.38	99.51	108.34
1	A	31	PHE	CA-C-N	-5.37	114.39	119.76
1	A	31	PHE	C-N-CA	-5.37	114.39	119.76
3	E	41	GLN	N-CA-C	5.36	118.67	110.20
3	E	63	LYS	CA-C-N	-5.36	115.44	123.00
3	E	63	LYS	C-N-CA	-5.36	115.44	123.00
1	A	365	SER	N-CA-C	5.34	120.46	113.30
1	B	357	ILE	CB-CA-C	-5.34	104.99	111.88
1	A	53	TYR	N-CA-C	-5.33	100.49	109.07
1	B	125	GLU	N-CA-C	5.33	116.95	111.03
3	F	39	ASP	N-CA-C	-5.31	106.48	113.17
1	A	186	THR	N-CA-C	-5.30	105.67	111.82
1	A	174	ALA	N-CA-C	5.29	119.88	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	358	MET	N-CA-C	-5.28	105.42	111.07
2	D	247	TYR	N-CA-C	-5.28	105.64	111.71
2	D	309	GLU	N-CA-C	-5.27	106.90	113.38
1	B	63	GLY	N-CA-C	-5.26	106.32	113.37
1	B	331	ALA	CA-C-N	-5.26	114.97	120.38
1	B	331	ALA	C-N-CA	-5.26	114.97	120.38
2	D	106	ALA	N-CA-C	5.25	119.88	112.75
1	B	59	GLN	N-CA-C	-5.24	107.06	113.50
2	C	158	ALA	N-CA-C	5.24	118.23	110.48
2	C	186	GLU	N-CA-C	5.23	116.98	111.28
1	A	88	HIS	N-CA-C	-5.20	105.61	111.28
1	A	229	THR	N-CA-C	-5.19	105.62	111.28
3	E	44	ILE	N-CA-C	5.18	115.58	108.12
2	D	116	ASN	N-CA-C	-5.13	99.88	110.80
1	A	257	CYS	CA-C-N	-5.12	114.43	120.12
1	A	257	CYS	C-N-CA	-5.12	114.43	120.12
2	D	352	LEU	N-CA-C	-5.11	105.83	111.71
3	F	20	SER	N-CA-C	-5.11	106.89	112.72
2	C	187	LEU	N-CA-C	5.10	120.40	113.16
2	D	334	VAL	N-CA-C	-5.10	102.29	109.63
2	D	187	LEU	N-CA-C	5.08	120.51	113.45
2	C	234	VAL	CA-C-N	-5.07	114.12	120.51
2	C	234	VAL	C-N-CA	-5.07	114.12	120.51
1	B	182	GLY	N-CA-C	5.06	118.80	112.73
2	C	94	LEU	N-CA-C	5.05	117.06	109.23
3	E	40	GLN	N-CA-C	-5.05	106.38	112.54
1	B	41	GLN	N-CA-C	5.04	119.28	113.38
1	B	257	CYS	CA-C-N	-5.02	114.49	119.56
1	B	257	CYS	C-N-CA	-5.02	114.49	119.56
2	D	170	GLU	N-CA-C	-5.02	105.89	111.36
1	B	129	THR	CA-C-N	-5.01	113.49	119.05
1	B	129	THR	C-N-CA	-5.01	113.49	119.05
1	A	139	VAL	N-CA-C	-5.00	105.52	110.62

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	2886	0	2858	60	0
1	B	2894	0	2869	65	0
2	C	2817	0	2821	29	0
2	D	2826	0	2834	44	0
3	E	602	0	629	11	0
3	F	602	0	629	8	0
4	A	31	12	12	0	0
4	B	31	12	12	1	0
5	D	14	9	9	0	0
All	All	12703	33	12673	213	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 (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:PRO:HD3	2:D:181:LEU:HD23	1.29	1.09
1:A:105:LEU:HD21	1:A:123:MET:HE3	1.65	0.78
1:B:153:MET:HE2	1:B:299:LEU:HD22	1.66	0.78
2:D:211:SER:HB2	2:D:219:PRO:HB3	1.66	0.77
1:B:186:THR:HG22	1:B:213:LYS:HE2	1.69	0.74
1:A:156:GLY:O	1:A:181:ALA:HB1	1.88	0.73
1:B:156:GLY:O	1:B:181:ALA:HB1	1.89	0.72
2:C:316:GLU:HG3	2:C:317:PRO:HD2	1.71	0.71
1:A:120:THR:HG21	1:A:370:VAL:HB	1.72	0.70
3:F:23:ILE:HB	3:F:52:ASP:HA	1.72	0.70
2:C:216:ILE:HD12	2:C:257:VAL:HG21	1.74	0.70
1:B:186:THR:HG22	1:B:213:LYS:CE	2.23	0.69
1:B:123:MET:HB2	1:B:132:MET:HE2	1.77	0.67
3:F:74:ARG:C	3:F:76:GLY:H	2.03	0.66
2:D:268:MET:HE2	2:D:319:LEU:HD22	1.78	0.65
1:A:331:ALA:HB1	1:A:335:ARG:NH1	2.12	0.64
1:B:10:ILE:CG2	1:B:105:LEU:HD23	2.28	0.64
1:B:47:MET:HB3	1:B:50:LYS:HB3	1.79	0.64
2:D:123:GLU:HB2	2:D:216:ILE:HD11	1.79	0.63
1:B:156:GLY:HA3	4:B:401:ATP:O1B	1.98	0.63
2:D:135:LYS:HG2	2:D:168:LEU:HD23	1.81	0.63
3:E:42:ARG:HD3	3:E:72:ARG:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ILE:HG23	1:B:216:LEU:HD12	1.81	0.62
1:A:120:THR:HG22	1:A:132:MET:HE1	1.83	0.61
1:A:305:MET:HE2	1:A:335:ARG:H	1.65	0.61
1:A:139:VAL:HG12	1:A:165:ILE:HG12	1.81	0.61
1:A:230:ALA:HB2	1:A:236:LEU:HD12	1.81	0.61
1:A:220:ALA:HB1	1:A:226:GLU:HG3	1.81	0.61
2:D:175:ILE:HG22	2:D:295:TRP:HE3	1.65	0.60
1:A:155:SER:OG	1:A:304:THR:HG23	2.02	0.59
2:C:113:PRO:HG3	2:C:248:SER:HB3	1.83	0.59
1:A:136:ILE:HD12	1:A:136:ILE:H	1.68	0.58
2:D:316:GLU:HG3	2:D:317:PRO:HD2	1.84	0.58
2:D:47:VAL:HG21	2:D:342:PHE:HE2	1.67	0.58
2:C:306:SER:HB2	2:C:309:GLU:HG3	1.87	0.57
3:F:59:TYR:HB2	3:F:61:ILE:HG13	1.86	0.57
1:A:208:ILE:O	1:A:212:ILE:HG13	2.04	0.57
2:D:201:ARG:HG3	2:D:237:ILE:CG2	2.35	0.57
1:B:337:TYR:O	1:B:341:ILE:HG12	2.05	0.56
1:B:132:MET:HG2	1:B:133:TYR:N	2.21	0.56
1:B:120:THR:HA	1:B:132:MET:HE1	1.88	0.56
1:A:71:ILE:HD13	1:A:76:VAL:HG22	1.88	0.55
1:B:225:GLN:HE21	3:F:73:LEU:HD21	1.71	0.55
1:B:35:VAL:HG11	1:B:81:ASP:HB3	1.89	0.55
1:B:340:TRP:HE3	1:B:341:ILE:HD13	1.72	0.54
2:D:154:LYS:HA	2:D:181:LEU:CD2	2.38	0.53
1:A:212:ILE:HD13	1:A:248:ILE:HD11	1.90	0.53
1:B:304:THR:O	1:B:309:ILE:HG21	2.09	0.53
2:C:63:PHE:HZ	2:C:83:ILE:HA	1.74	0.53
2:D:199:LYS:HE3	2:D:260:LEU:H	1.74	0.53
1:B:154:ASP:HA	1:B:300:SER:O	2.08	0.52
3:E:1:MET:HB3	3:E:17:VAL:O	2.10	0.52
1:A:205:GLU:O	1:A:209:VAL:HG23	2.10	0.52
1:A:34:ILE:HD11	1:A:59:GLN:HG2	1.91	0.52
1:A:218:TYR:HA	1:A:307:PRO:HD2	1.91	0.52
1:A:154:ASP:HA	1:A:300:SER:O	2.10	0.52
2:D:264:THR:HG21	2:D:313:VAL:HG23	1.91	0.52
2:C:214:PRO:HG3	2:C:229:VAL:HG13	1.90	0.52
2:D:310:VAL:O	2:D:313:VAL:HG22	2.09	0.52
2:D:63:PHE:HZ	2:D:83:ILE:HA	1.74	0.51
2:D:351:GLY:HA2	2:D:354:ILE:HG12	1.91	0.51
2:C:147:ARG:HA	2:C:174:PHE:CZ	2.45	0.51
1:B:14:SER:HA	1:B:71:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:GLU:C	1:B:261:LEU:N	2.67	0.51
1:A:21:PHE:HD2	1:A:28:ARG:HG3	1.75	0.51
2:C:268:MET:HE2	2:C:319:LEU:HD22	1.92	0.51
1:A:62:ARG:HG2	1:A:67:LEU:HD21	1.92	0.51
1:A:335:ARG:HA	1:A:338:SER:HB2	1.93	0.51
2:C:275:ILE:HA	2:C:284:ILE:HD11	1.93	0.51
1:B:182:GLY:O	1:B:186:THR:HG23	2.11	0.50
1:B:153:MET:CE	1:B:299:LEU:HD22	2.39	0.50
1:B:180:LEU:CD1	1:B:264:PRO:HB3	2.42	0.50
1:A:38:PRO:HG2	1:A:44:MET:HG2	1.93	0.50
1:A:152:VAL:HA	1:A:298:VAL:O	2.12	0.49
2:D:316:GLU:CG	2:D:317:PRO:HD2	2.42	0.49
2:C:177:SER:C	2:C:179:VAL:H	2.20	0.49
3:F:74:ARG:C	3:F:76:GLY:N	2.69	0.49
1:A:18:LYS:HD2	1:A:337:TYR:HD1	1.77	0.49
1:A:171:LEU:O	1:A:175:ILE:HG13	2.13	0.49
2:C:211:SER:HB3	2:C:234:VAL:HG11	1.94	0.49
2:D:175:ILE:HG22	2:D:295:TRP:CE3	2.46	0.49
1:B:340:TRP:CE3	1:B:341:ILE:HD13	2.48	0.49
1:A:337:TYR:O	1:A:341:ILE:HG13	2.13	0.49
1:A:92:ASN:ND2	1:B:48:GLY:HA2	2.28	0.49
1:B:186:THR:CG2	1:B:213:LYS:HE2	2.39	0.49
2:D:217:MET:HE1	2:D:223:ASN:HB3	1.94	0.49
1:B:355:MET:HG2	2:D:354:ILE:HD12	1.95	0.48
1:A:357:ILE:HD13	1:A:369:ILE:HG23	1.94	0.48
1:A:92:ASN:HD21	1:B:48:GLY:HA2	1.79	0.48
2:D:57:LYS:C	2:D:59:GLU:H	2.20	0.48
3:F:17:VAL:HG21	3:F:26:VAL:HG22	1.94	0.48
1:B:370:VAL:HG13	1:B:371:HIS:CD2	2.49	0.48
1:A:21:PHE:HE1	1:A:96:VAL:HG11	1.78	0.48
2:C:57:LYS:C	2:C:59:GLU:H	2.22	0.47
2:D:201:ARG:HG3	2:D:237:ILE:HG23	1.95	0.47
1:B:220:ALA:HB1	1:B:226:GLU:HG3	1.95	0.47
2:D:50:LEU:HD21	2:D:87:CYS:SG	2.53	0.47
1:B:99:GLU:HG3	1:B:100:GLU:HG3	1.97	0.47
2:D:47:VAL:HG21	2:D:342:PHE:CE2	2.48	0.47
2:D:124:THR:HG21	2:D:214:PRO:HB2	1.97	0.47
2:D:142:VAL:HG21	2:D:291:ILE:HD11	1.95	0.47
3:E:4:PHE:HB3	3:E:12:THR:OG1	2.15	0.47
1:B:194:THR:HA	1:B:198:TYR:O	2.14	0.47
1:A:71:ILE:HG13	1:A:71:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:LEU:HD21	2:D:224:PHE:CE2	2.50	0.46
1:A:151:ILE:HD13	1:A:278:THR:HG23	1.96	0.46
1:A:180:LEU:HD11	1:A:267:LEU:HD12	1.98	0.46
1:A:8:LEU:HD11	1:A:90:PHE:CE1	2.51	0.46
1:B:43:VAL:C	1:B:45:VAL:H	2.24	0.46
2:D:240:ASN:HB3	2:D:243:VAL:HG23	1.98	0.46
3:E:15:LEU:HD11	3:E:30:ILE:HG12	1.98	0.46
2:C:130:LEU:O	2:C:134:ILE:HG12	2.16	0.46
2:D:281:ASP:OD2	2:D:284:ILE:HB	2.16	0.46
3:E:17:VAL:HG12	3:E:29:LYS:HE2	1.98	0.46
2:C:183:ASP:H	2:C:186:GLU:HG2	1.81	0.46
1:B:35:VAL:HG23	1:B:54:VAL:HG22	1.97	0.45
3:E:30:ILE:HB	3:E:41:GLN:HE22	1.82	0.45
1:A:189:LEU:HA	1:A:192:ILE:HG12	1.97	0.45
1:B:151:ILE:HG23	1:B:297:THR:HG23	1.98	0.45
3:E:1:MET:HE1	3:E:19:PRO:HG3	1.98	0.45
1:A:34:ILE:HD12	1:A:67:LEU:HG	1.99	0.45
1:B:70:PRO:O	1:B:71:ILE:C	2.57	0.45
1:B:151:ILE:HD12	1:B:164:PRO:HG3	1.98	0.45
1:B:218:TYR:HA	1:B:307:PRO:HD2	1.98	0.45
1:B:259:GLU:O	1:B:259:GLU:HG3	2.15	0.45
2:C:216:ILE:HG12	2:C:300:ILE:HG23	1.99	0.45
1:A:106:THR:HB	1:A:137:GLN:HG2	1.99	0.45
1:B:24:ASP:HB2	1:B:340:TRP:HH2	1.82	0.45
1:B:105:LEU:HD21	1:B:123:MET:HE3	1.98	0.45
1:A:194:THR:HA	1:A:198:TYR:O	2.17	0.44
1:A:313:MET:O	1:A:317:ILE:HG13	2.17	0.44
1:A:105:LEU:HD11	1:A:123:MET:HG3	2.00	0.44
1:B:36:GLY:HA3	1:B:67:LEU:HD23	2.00	0.44
1:B:140:LEU:O	1:B:143:TYR:HB2	2.18	0.44
2:D:236:LYS:HD2	2:D:236:LYS:HA	1.74	0.44
2:C:54:LEU:HD13	2:C:86:PHE:HE2	1.83	0.44
1:A:299:LEU:CD1	1:A:329:ILE:HG23	2.47	0.44
2:C:155:PRO:HD3	2:C:181:LEU:CD2	2.47	0.44
3:F:17:VAL:HG11	3:F:56:LEU:HD11	2.00	0.44
1:A:163:VAL:HG13	1:A:175:ILE:HG12	2.00	0.44
1:A:186:THR:O	1:A:190:MET:HG3	2.18	0.44
1:A:243:PRO:C	1:A:245:GLY:H	2.26	0.44
1:A:313:MET:HB3	1:A:313:MET:HE3	1.68	0.43
1:B:10:ILE:HD12	1:B:89:THR:HG21	1.98	0.43
1:B:136:ILE:HB	1:B:139:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLU:O	1:B:209:VAL:HG23	2.18	0.43
2:C:112:ASN:HB3	2:C:115:ASP:OD1	2.18	0.43
2:C:247:TYR:CE2	2:C:254:THR:HG21	2.54	0.43
2:D:23:LYS:HE2	2:D:23:LYS:HB3	1.68	0.43
1:B:190:MET:HE2	1:B:200:PHE:O	2.18	0.43
1:A:345:ILE:O	1:A:349:LEU:HG	2.19	0.43
2:C:124:THR:HG21	2:C:214:PRO:HB2	2.00	0.43
2:D:147:ARG:HA	2:D:174:PHE:CZ	2.54	0.43
2:D:196:TYR:N	2:D:197:PRO:CD	2.82	0.43
2:D:223:ASN:HD21	2:D:228:LEU:HD23	1.83	0.43
1:A:252:ASN:HA	1:A:255:PHE:CE1	2.54	0.43
1:A:259:GLU:C	1:A:261:LEU:N	2.71	0.43
1:A:299:LEU:HD11	1:A:329:ILE:HG23	2.00	0.43
2:C:251:LYS:O	2:C:254:THR:HG22	2.18	0.43
1:A:154:ASP:O	1:A:160:THR:HG23	2.18	0.43
2:D:57:LYS:C	2:D:59:GLU:N	2.77	0.43
2:D:135:LYS:HE3	2:D:135:LYS:HB3	1.86	0.43
1:A:34:ILE:HG22	1:A:69:TYR:CD2	2.54	0.42
2:C:85:ASP:HA	2:C:88:LYS:HD3	2.01	0.42
2:D:367:LYS:HA	2:D:367:LYS:HD3	1.78	0.42
1:A:21:PHE:CD2	1:A:28:ARG:HG3	2.53	0.42
1:A:113:LYS:HA	1:A:116:ARG:HD3	2.00	0.42
2:C:236:LYS:HD2	2:C:236:LYS:HA	1.85	0.42
2:D:363:GLN:O	2:D:367:LYS:HG2	2.19	0.42
3:F:72:ARG:HE	3:F:72:ARG:HB2	1.60	0.42
1:A:164:PRO:HG2	1:A:174:ALA:HB1	2.02	0.42
1:B:87:HIS:O	1:B:88:HIS:C	2.61	0.42
1:B:213:LYS:O	1:B:217:CYS:HB2	2.20	0.42
1:B:38:PRO:HG2	1:B:44:MET:HG2	2.01	0.42
1:B:186:THR:HG22	1:B:213:LYS:HE3	2.00	0.42
2:C:177:SER:C	2:C:179:VAL:N	2.75	0.42
1:B:151:ILE:HG21	1:B:282:ILE:HD11	2.00	0.42
1:B:185:LEU:HD21	1:B:261:LEU:HG	2.01	0.42
1:A:116:ARG:HH21	1:A:370:VAL:HG22	1.84	0.42
2:C:211:SER:HB2	2:C:219:PRO:HB3	2.01	0.42
2:D:50:LEU:O	2:D:54:LEU:HB2	2.19	0.42
2:C:217:MET:HE2	2:C:217:MET:HB3	1.93	0.41
2:C:339:HIS:O	2:C:340:ALA:C	2.62	0.41
2:C:202:SER:OG	2:C:238:ALA:HB3	2.20	0.41
1:B:10:ILE:HG21	1:B:105:LEU:HD23	2.00	0.41
2:D:94:LEU:HB3	2:D:95:SER:H	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLY:C	1:B:304:THR:H	2.28	0.41
1:B:373:LYS:HE3	1:B:373:LYS:HB3	1.84	0.41
2:D:319:LEU:HD23	2:D:319:LEU:HA	1.82	0.41
3:E:4:PHE:O	3:E:66:THR:HA	2.21	0.41
1:A:136:ILE:O	1:A:139:VAL:HG22	2.20	0.41
1:B:153:MET:HE3	1:B:304:THR:HG22	2.02	0.41
1:B:216:LEU:CD1	1:B:250:ILE:HD13	2.50	0.41
1:A:128:ASN:O	1:A:129:THR:C	2.64	0.41
1:B:211:ASP:O	1:B:212:ILE:C	2.63	0.41
1:B:228:ALA:C	1:B:230:ALA:N	2.76	0.41
2:C:268:MET:HE3	2:C:268:MET:HB3	1.93	0.41
2:D:54:LEU:HG	2:D:94:LEU:HD11	2.03	0.41
3:E:36:ILE:HG21	3:E:71:LEU:HD22	2.03	0.41
1:B:42:GLY:C	1:B:44:MET:H	2.28	0.41
2:D:54:LEU:HD23	2:D:54:LEU:HA	1.86	0.41
3:E:36:ILE:HG21	3:E:71:LEU:CD2	2.51	0.41
1:B:355:MET:HE2	1:B:355:MET:HB3	1.79	0.41
3:E:40:GLN:HG2	3:E:71:LEU:HB3	2.03	0.41
1:A:113:LYS:HB2	1:A:113:LYS:HE3	1.91	0.40
1:B:357:ILE:HD11	1:B:370:VAL:HA	2.02	0.40
2:D:72:PHE:HD1	2:D:122:TYR:HE2	1.70	0.40
2:D:339:HIS:O	2:D:340:ALA:C	2.60	0.40
1:A:259:GLU:O	1:A:259:GLU:HG3	2.20	0.40
1:A:18:LYS:HG2	1:A:30:VAL:HG13	2.02	0.40
1:B:62:ARG:HG3	1:B:67:LEU:HD11	2.04	0.40
1:B:124:PHE:CE2	1:B:132:MET:HE3	2.57	0.40
1:B:152:VAL:HA	1:B:298:VAL:O	2.21	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	368/375 (98%)	356 (97%)	12 (3%)	0	100	100
1	B	369/375 (98%)	354 (96%)	15 (4%)	0	100	100
2	C	345/352 (98%)	331 (96%)	14 (4%)	0	100	100
2	D	346/352 (98%)	335 (97%)	11 (3%)	0	100	100
3	E	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
3	F	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
All	All	1576/1606 (98%)	1520 (96%)	56 (4%)	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	313/318 (98%)	302 (96%)	11 (4%)	32	55
1	B	314/318 (99%)	300 (96%)	14 (4%)	24	50
2	C	321/326 (98%)	310 (97%)	11 (3%)	32	56
2	D	322/326 (99%)	307 (95%)	15 (5%)	23	49
3	E	68/68 (100%)	67 (98%)	1 (2%)	57	69
3	F	68/68 (100%)	66 (97%)	2 (3%)	37	59
All	All	1406/1424 (99%)	1352 (96%)	54 (4%)	29	54

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	76	VAL
1	A	105	LEU
1	A	173	HIS
1	A	287	VAL
1	A	288	ASP
1	A	305	MET

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Mol	Chain	Res	Type
1	A	317	ILE
1	A	327	ILE
1	A	329	ILE
1	A	370	VAL
1	B	35	VAL
1	B	45	VAL
1	B	76	VAL
1	B	77	THR
1	B	96	VAL
1	B	113	LYS
1	B	134	VAL
1	B	164	PRO
1	B	238	LYS
1	B	287	VAL
1	B	327	ILE
1	B	334	GLU
1	B	346	LEU
1	B	368	SER
2	C	37	LEU
2	C	91	GLU
2	C	160	THR
2	C	184	ASN
2	C	185	VAL
2	C	225	THR
2	C	231	VAL
2	C	234	VAL
2	C	257	VAL
2	C	352	LEU
2	C	358	MET
2	D	88	LYS
2	D	94	LEU
2	D	162	GLU
2	D	181	LEU
2	D	192	GLN
2	D	259	SER
2	D	264	THR
2	D	271	LEU
2	D	279	LYS
2	D	291	ILE
2	D	311	VAL
2	D	322	ILE
2	D	325	LYS

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Mol	Chain	Res	Type
2	D	335	LEU
2	D	355	GLN
3	E	66	THR
3	F	15	LEU
3	F	64	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	88	HIS
1	A	92	ASN
1	A	101	HIS
1	A	115	ASN
1	A	161	HIS
1	A	252	ASN
1	A	263	GLN
1	B	88	HIS
1	B	225	GLN
1	B	296	ASN
1	B	371	HIS
2	C	129	HIS
2	C	278	HIS
2	C	293	ASN
2	C	320	GLN
2	C	360	HIS
2	C	368	ASN
2	D	161	HIS
2	D	184	ASN
2	D	192	GLN
2	D	208	ASN
2	D	213	ASN
2	D	220	ASN
2	D	240	ASN
2	D	290	GLN
2	D	293	ASN
2	D	320	GLN
2	D	355	GLN
2	D	368	ASN
3	F	62	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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	AR6	D	401	-	14,14,39	0.75	0	19,21,60	1.12	3 (15%)
4	ATP	A	401	-	32,33,33	1.33	3 (9%)	48,52,52	1.88	7 (14%)
4	ATP	B	401	-	32,33,33	1.34	4 (12%)	48,52,52	1.87	10 (20%)

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	AR6	D	401	-	-	1/6/22/54	0/1/1/4
4	ATP	A	401	-	-	0/22/38/38	0/3/3/3
4	ATP	B	401	-	-	2/22/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	ATP	C5-C4	4.51	1.47	1.39
4	B	401	ATP	C5-C4	4.32	1.46	1.39
4	A	401	ATP	C5-N7	-2.99	1.33	1.39
4	B	401	ATP	C5-N7	-2.96	1.33	1.39
4	A	401	ATP	C5-C6	2.16	1.47	1.41
4	B	401	ATP	C5-C6	2.12	1.46	1.41
4	B	401	ATP	C4-N9	-2.04	1.33	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	ATP	C5-C4-N3	-6.11	118.30	126.72
4	B	401	ATP	C5-C4-N3	-6.06	118.38	126.72
4	B	401	ATP	N3-C4-N9	5.15	135.93	127.17
4	A	401	ATP	N3-C4-N9	5.02	135.71	127.17
4	A	401	ATP	C2-N3-C4	3.68	120.83	111.83
4	B	401	ATP	C2-N3-C4	3.64	120.73	111.83
4	B	401	ATP	O4'-C1'-N9	3.60	115.01	108.09
4	A	401	ATP	N3-C2-N1	-3.38	123.46	128.58
4	B	401	ATP	N3-C2-N1	-3.35	123.52	128.58
4	A	401	ATP	C4-C5-N7	-3.09	107.04	110.58
4	B	401	ATP	C4-C5-N7	-2.77	107.41	110.58
4	B	401	ATP	C4-N9-C8	2.62	108.49	105.74
5	D	401	AR6	C1D-C2D-C3D	2.58	105.47	102.29
4	A	401	ATP	C5-N7-C8	2.53	107.43	103.45
5	D	401	AR6	O1B-PB-O2B	2.42	120.25	110.83
4	B	401	ATP	C5-N7-C8	2.37	107.17	103.45
4	A	401	ATP	C4-N9-C8	2.31	108.17	105.74
4	B	401	ATP	C1'-N9-C8	-2.30	121.99	127.09
5	D	401	AR6	O3A-PB-O5D	-2.11	101.16	106.67
4	B	401	ATP	C2-N1-C6	2.02	122.04	118.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

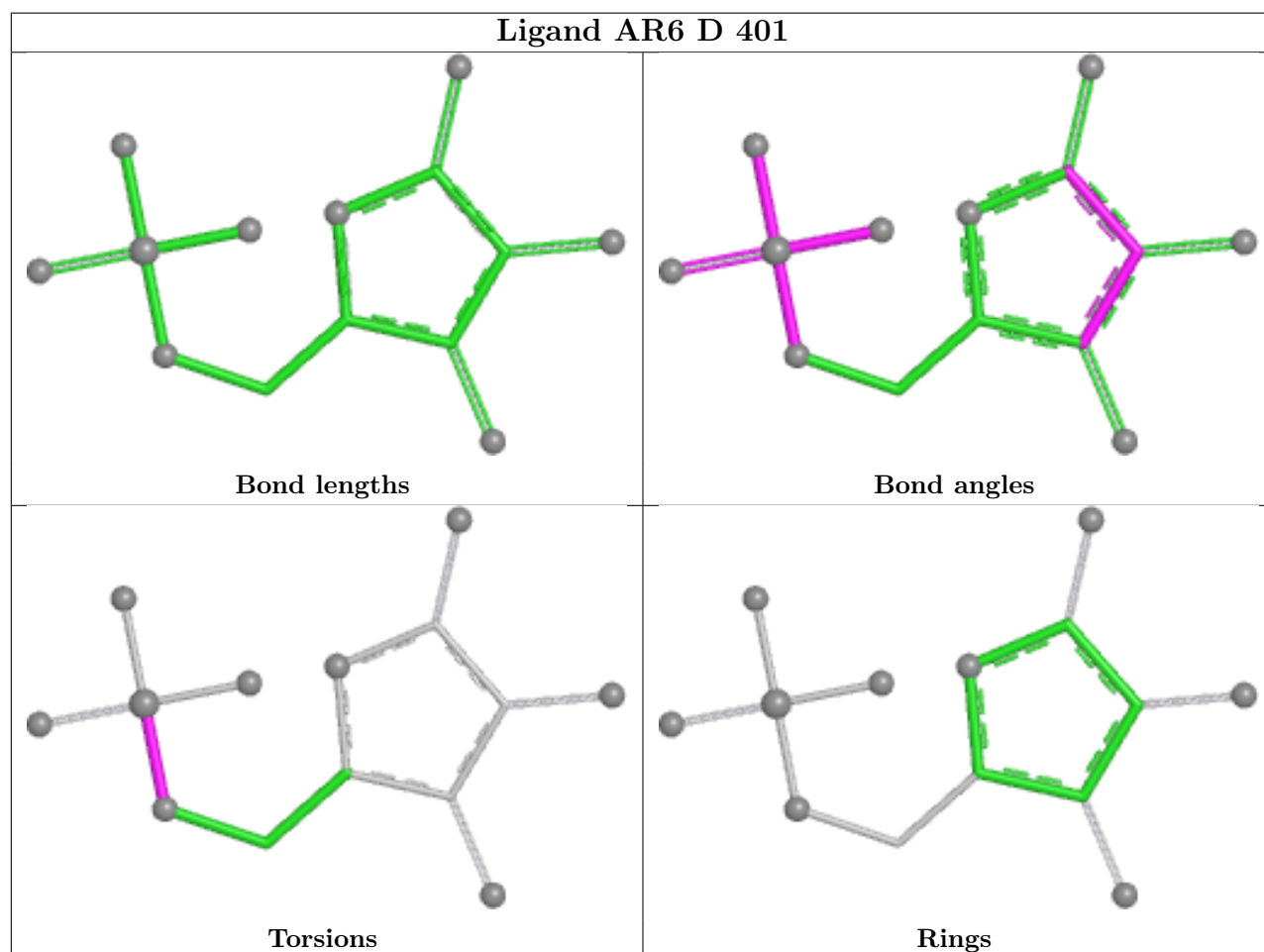
Mol	Chain	Res	Type	Atoms
4	B	401	ATP	PG-O3B-PB-O1B
5	D	401	AR6	C5D-O5D-PB-O1B
4	B	401	ATP	PA-O3A-PB-O2B

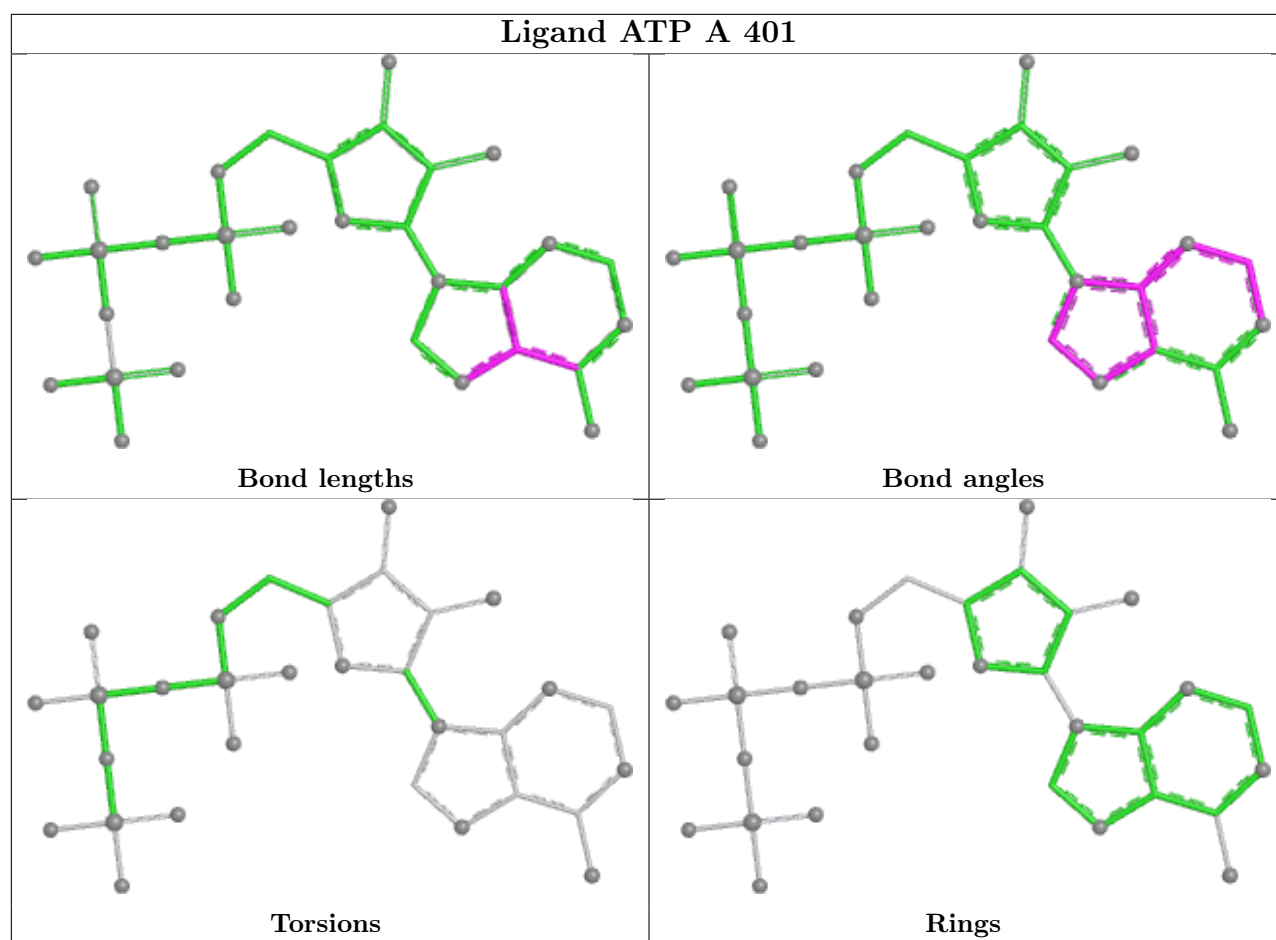
There are no ring outliers.

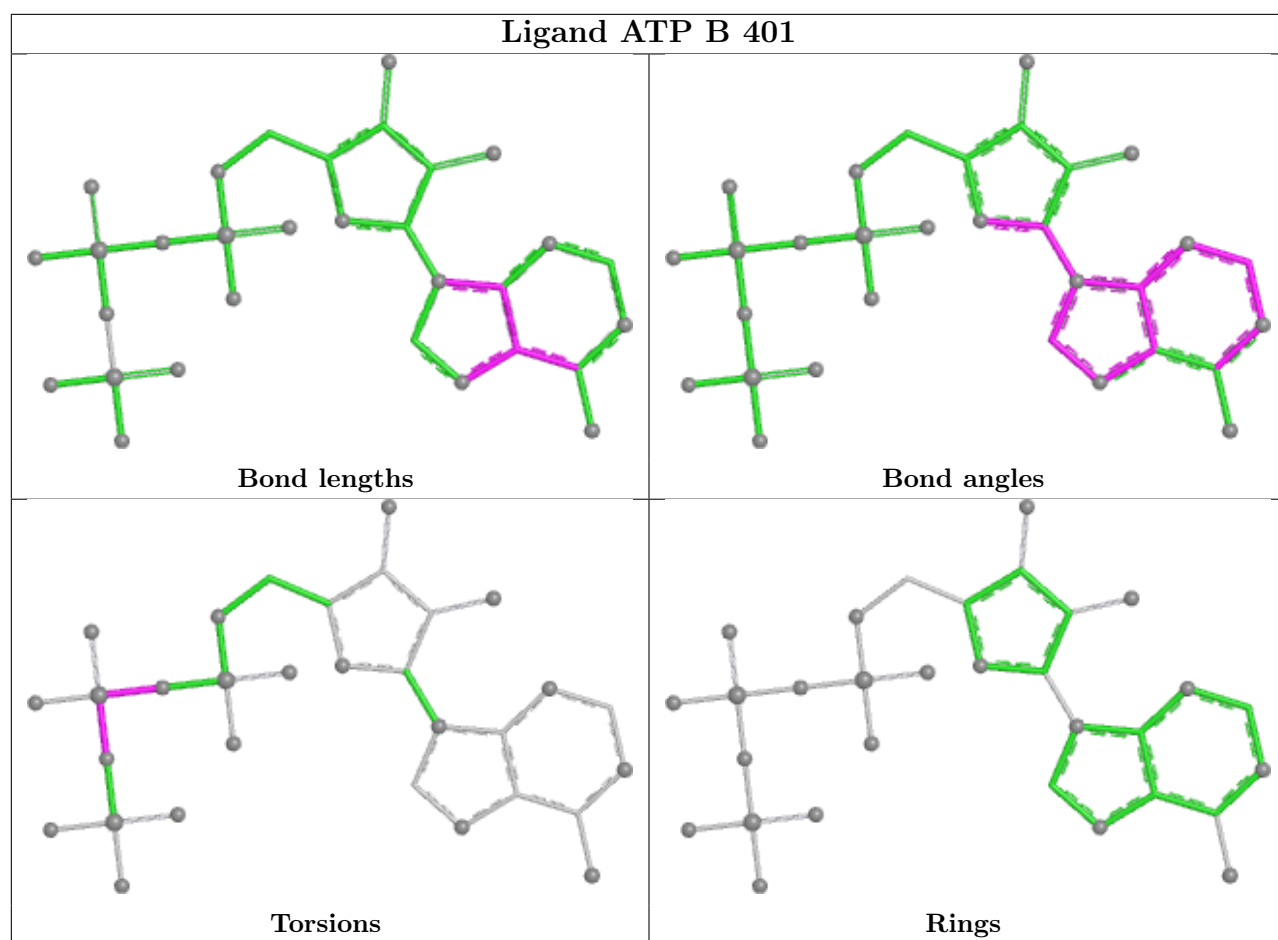
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	ATP	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 [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	370/375 (98%)	-0.89	0 100 100	27, 46, 69, 90	0
1	B	371/375 (98%)	-0.89	0 100 100	30, 46, 70, 90	0
2	C	347/352 (98%)	-0.90	0 100 100	32, 51, 74, 94	0
2	D	348/352 (98%)	-0.89	0 100 100	29, 53, 77, 93	0
3	E	76/76 (100%)	-0.93	0 100 100	45, 66, 86, 99	0
3	F	76/76 (100%)	-0.77	0 100 100	47, 70, 92, 98	0
All	All	1588/1606 (98%)	-0.89	0 100 100	27, 51, 78, 99	0

There are no RSRZ outliers to report.

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.

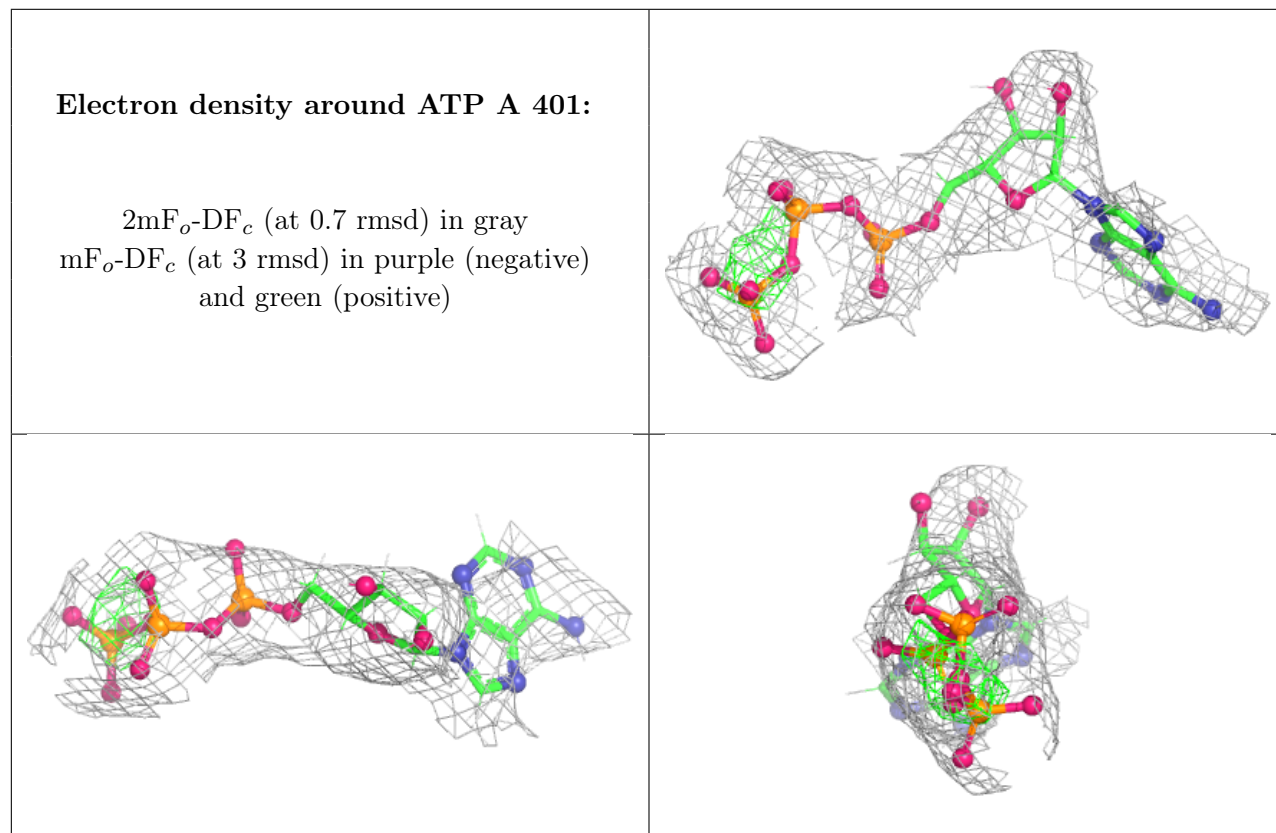
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ATP	A	401	31/31	0.98	0.06	44,58,71,81	0

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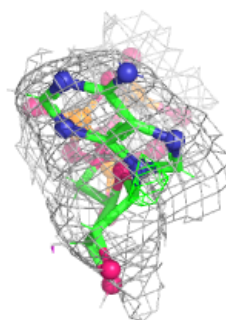
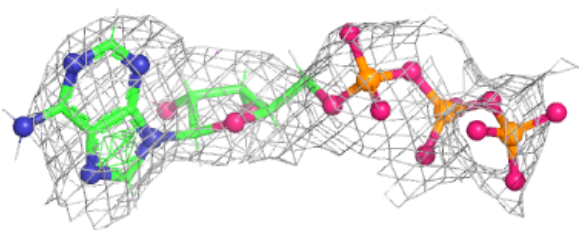
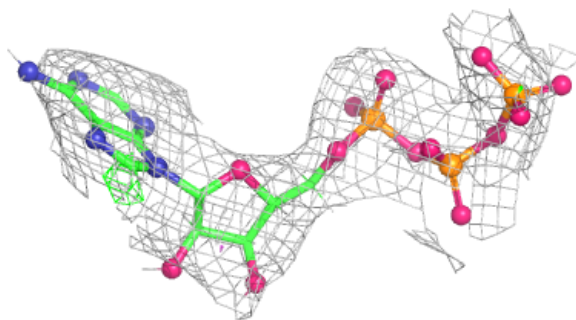
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ATP	B	401	31/31	0.98	0.07	48,59,75,81	0
5	AR6	D	401	14/36	0.98	0.06	49,68,79,85	0

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.

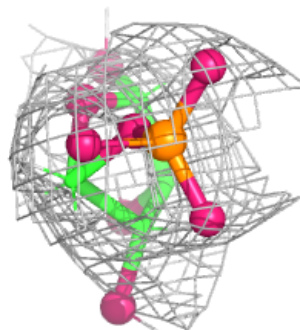
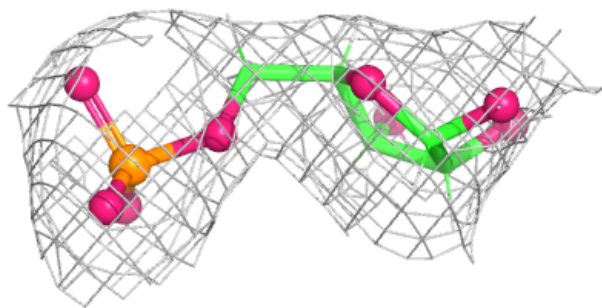
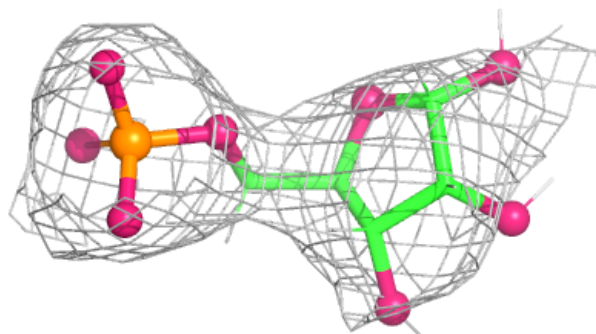


Electron density around ATP B 401:

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

**Electron density around AR6 D 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.