



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:55 am BST

PDB ID : 3DWL
Title : Crystal Structure of Fission Yeast Arp2/3 Complex Lacking the Arp2 Subunit
Authors : Nolen, B.J.; Pollard, T.D.
Deposited on : 2008-07-22
Resolution : 3.78 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

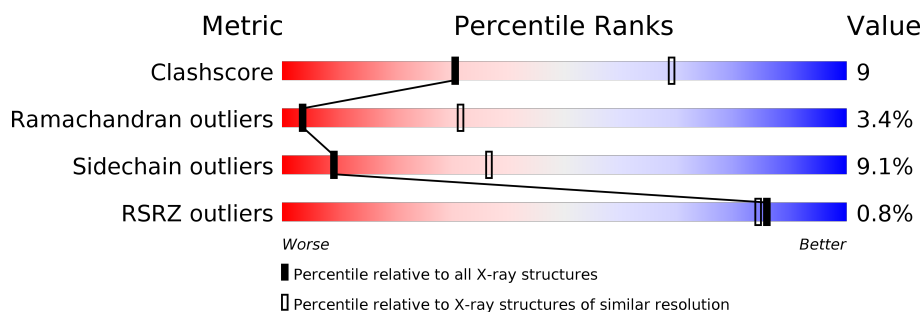
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.78 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1100 (3.96-3.60)
Ramachandran outliers	138981	1062 (3.96-3.60)
Sidechain outliers	138945	1058 (3.96-3.60)
RSRZ outliers	127900	1009 (3.98-3.58)

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 on 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	427	<div> <div>62%</div> <div>19%</div> <div>•</div> <div>17%</div> </div>
1	B	427	<div> <div>65%</div> <div>16%</div> <div>•</div> <div>17%</div> </div>
2	C	377	<div> <div>64%</div> <div>21%</div> <div>•</div> <div>11%</div> </div>
2	H	377	<div> <div>2%</div> <div>67%</div> <div>20%</div> <div>•</div> <div>11%</div> </div>
3	D	317	<div> <div>65%</div> <div>18%</div> <div>•</div> <div>14%</div> </div>
3	I	317	<div> <div>%</div> <div>65%</div> <div>18%</div> <div>•</div> <div>14%</div> </div>
4	E	174	<div> <div>%</div> <div>28%</div> <div>8%</div> <div>64%</div> </div>

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Mol	Chain	Length	Quality of chain
4	J	174	<div><div></div><div>28%8%64%</div></div>
5	F	168	<div>%<div><div></div><div>75%21%..</div></div></div>
5	K	168	<div>2%<div><div></div><div>73%23%..</div></div></div>
6	G	152	<div><div></div><div>56%18%.25%</div></div>
6	L	152	<div>%<div><div></div><div>55%20%.25%</div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18705 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	1	0	0
			2555	1617	432	496	10			
1	B	355	Total	C	N	O	S	1	0	0
			2556	1617	432	497	10			

- Molecule 2 is a protein called Actin-related protein 2/3 complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	336	Total	C	N	O	S	0	0	0
			2252	1413	402	432	5			
2	H	337	Total	C	N	O	S	0	0	0
			2262	1418	403	436	5			

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	272	Total	C	N	O	S	0	0	0
			2028	1302	350	368	8			
3	I	272	Total	C	N	O	S	0	0	0
			2028	1302	350	368	8			

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	63	Total	C	N	O	S	0	0	0
			397	249	71	73	4			
4	J	63	Total	C	N	O	S	0	0	0
			397	249	71	73	4			

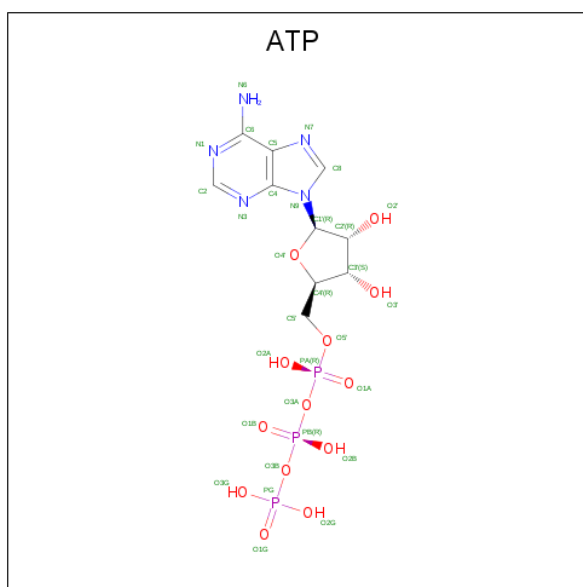
- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	166	Total	C	N	O	S	1	0	0
			1294	825	215	247	7			
5	K	166	Total	C	N	O	S	1	0	0
			1294	825	215	247	7			

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	114	Total	C	N	O	S	0	0	0
			790	497	136	155	2			
6	L	114	Total	C	N	O	S	0	0	0
			790	497	136	155	2			

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

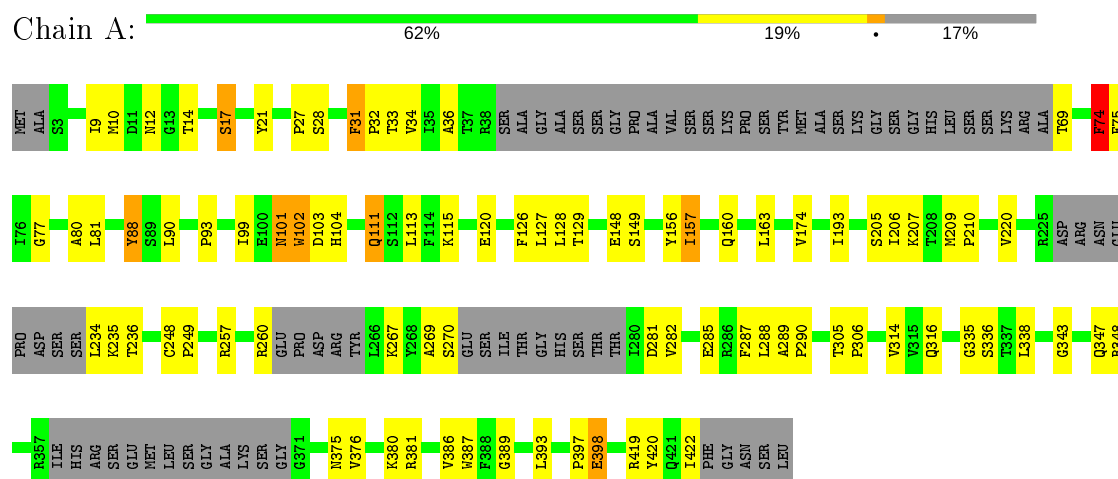


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

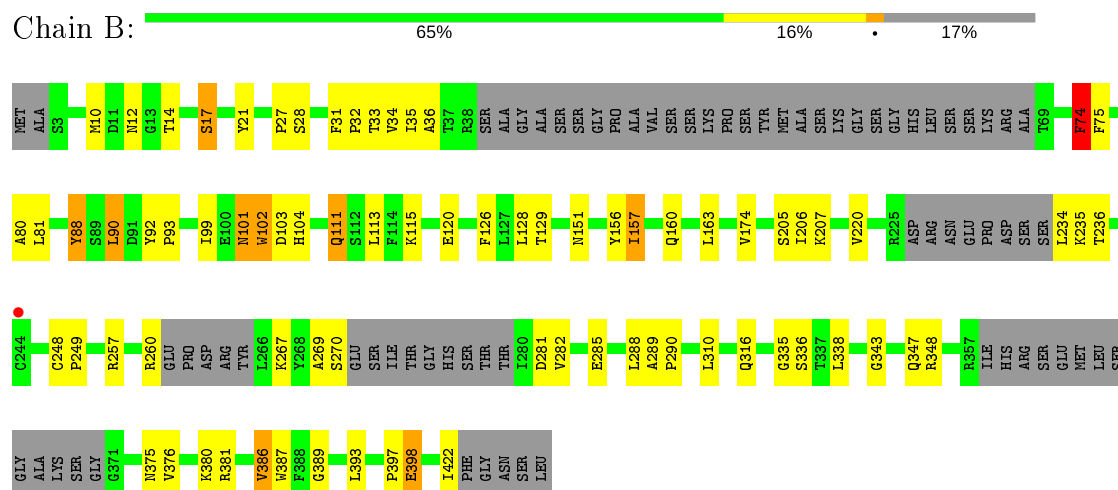
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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-related protein 3

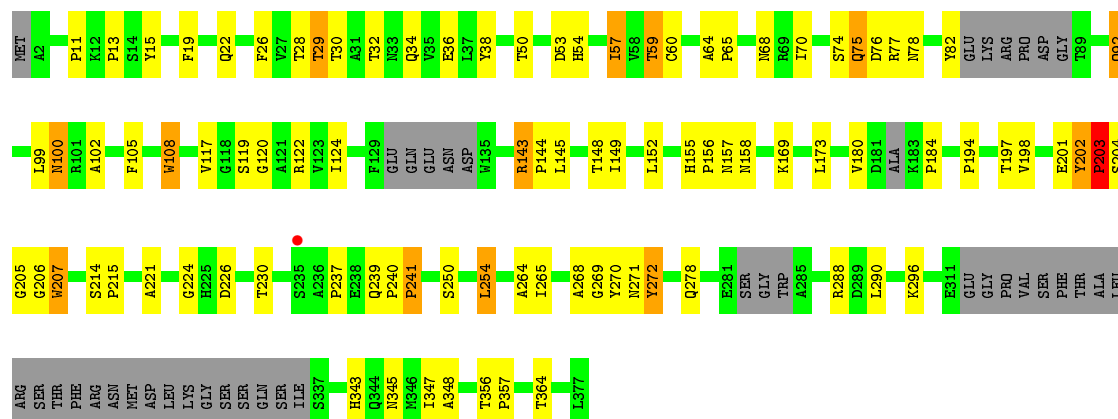


• Molecule 1: Actin-related protein 3

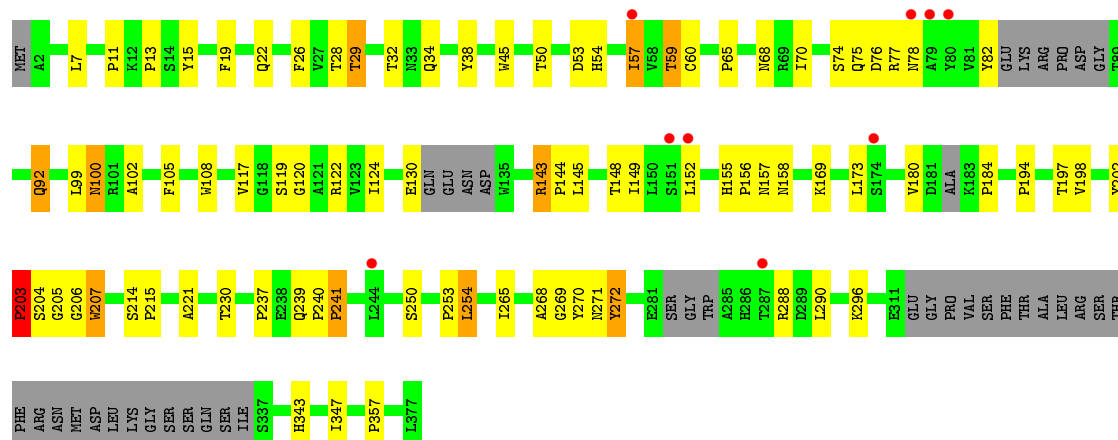


• Molecule 2: Actin-related protein 2/3 complex subunit 1

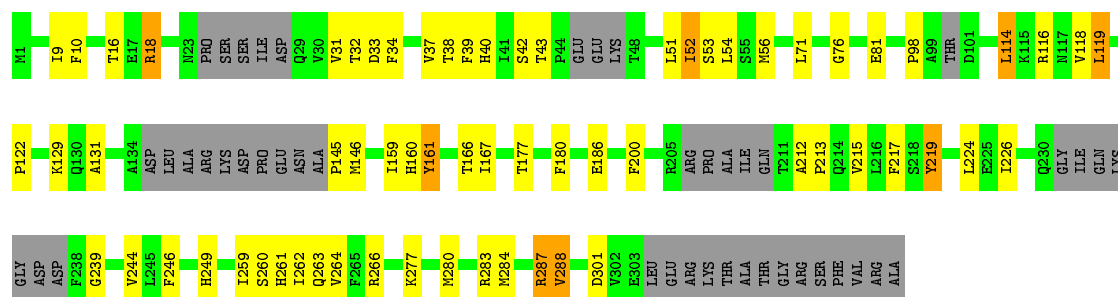




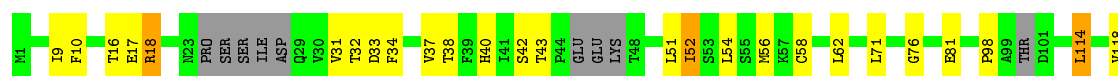
• Molecule 2: Actin-related protein 2/3 complex subunit 1

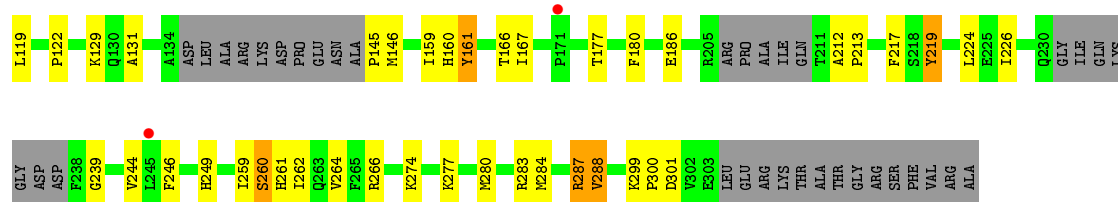


• Molecule 3: Actin-related protein 2/3 complex subunit 2

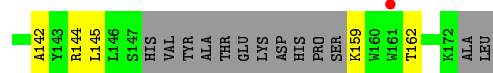
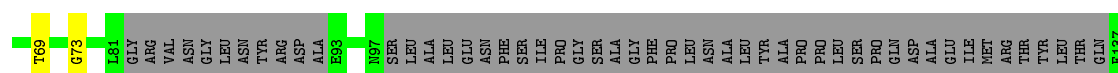
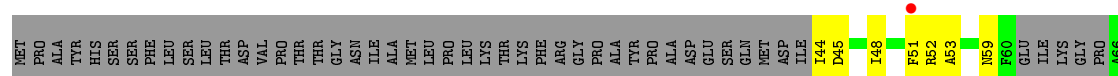


• Molecule 3: Actin-related protein 2/3 complex subunit 2

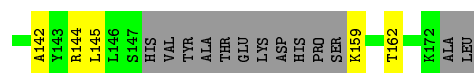
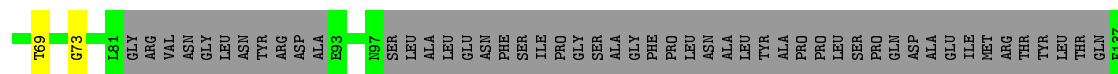
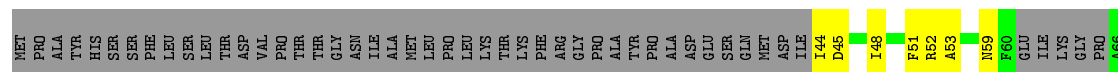




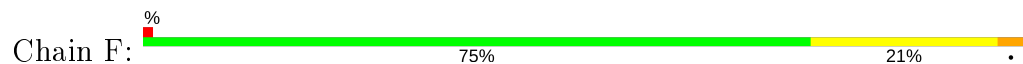
• Molecule 4: Actin-related protein 2/3 complex subunit 3



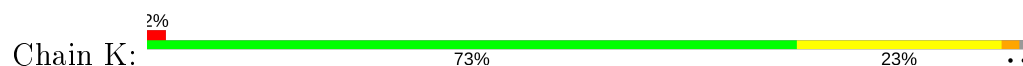
• Molecule 4: Actin-related protein 2/3 complex subunit 3

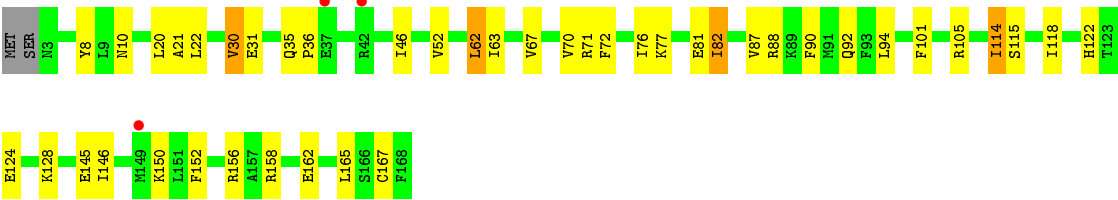


• Molecule 5: Actin-related protein 2/3 complex subunit 4



• Molecule 5: Actin-related protein 2/3 complex subunit 4

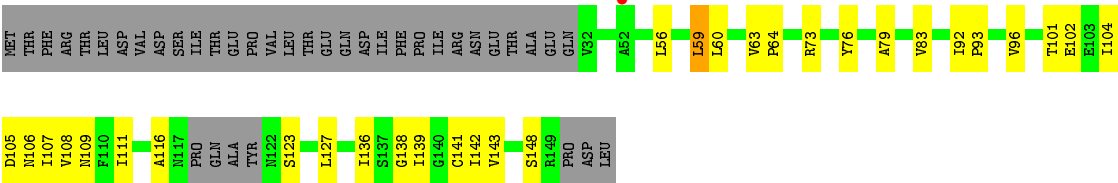




● Molecule 6: Actin-related protein 2/3 complex subunit 5



● Molecule 6: Actin-related protein 2/3 complex subunit 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	218.97Å 218.97Å 315.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 3.78 49.05 – 3.79	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.00-3.78) 85.8 (49.05-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.324 , 0.344 0.301 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	83.8	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 106.2	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	0.79	EDS
Total number of atoms	18705	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	1/2610 (0.0%)	0.56	2/3567 (0.1%)
1	B	0.41	1/2611 (0.0%)	0.56	2/3569 (0.1%)
2	C	0.37	0/2300	0.61	8/3170 (0.3%)
2	H	0.37	1/2310 (0.0%)	0.61	8/3184 (0.3%)
3	D	0.39	0/2072	0.56	3/2816 (0.1%)
3	I	0.39	0/2072	0.56	3/2816 (0.1%)
4	E	0.35	0/399	0.45	0/540
4	J	0.39	0/399	0.45	0/540
5	F	0.37	0/1314	0.54	0/1777
5	K	0.43	1/1314 (0.1%)	0.54	1/1777 (0.1%)
6	G	0.38	0/799	0.53	0/1097
6	L	0.35	0/799	0.51	0/1097
All	All	0.40	4/18999 (0.0%)	0.56	27/25950 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
5	F	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	TYR	C-O	12.02	1.46	1.23
5	K	167	CYS	C-O	-9.32	1.05	1.23
1	B	88	TYR	C-O	8.89	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	130	GLU	C-O	5.62	1.34	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	TYR	CA-C-O	-12.76	93.31	120.10
1	B	88	TYR	O-C-N	-12.05	103.42	122.70
1	B	88	TYR	CA-C-O	-8.63	101.97	120.10
1	A	88	TYR	O-C-N	-8.15	109.67	122.70
2	C	241	PRO	N-CA-CB	6.19	110.72	103.30
2	C	184	PRO	N-CA-CB	6.08	110.59	103.30
2	H	241	PRO	N-CA-CB	6.06	110.57	103.30
2	H	184	PRO	N-CA-CB	6.05	110.56	103.30
3	D	213	PRO	N-CA-CB	6.04	110.55	103.30
2	H	357	PRO	N-CA-CB	6.00	110.49	103.30
2	C	357	PRO	N-CA-CB	5.90	110.38	103.30
2	H	237	PRO	N-CA-CB	5.89	110.37	103.30
3	I	213	PRO	N-CA-CB	5.84	110.31	103.30
3	D	98	PRO	N-CA-CB	5.83	110.29	103.30
3	I	145	PRO	N-CA-CB	5.78	110.24	103.30
2	C	237	PRO	N-CA-CB	5.76	110.21	103.30
2	H	11	PRO	N-CA-CB	5.74	110.19	103.30
2	C	11	PRO	N-CA-CB	5.74	110.19	103.30
2	C	240	PRO	N-CA-CB	5.73	110.18	103.30
2	H	240	PRO	N-CA-CB	5.69	110.13	103.30
3	D	145	PRO	N-CA-CB	5.68	110.11	103.30
3	I	98	PRO	N-CA-CB	5.66	110.09	103.30
2	C	203	PRO	N-CA-CB	5.57	109.99	103.30
2	H	203	PRO	N-CA-CB	5.52	109.93	103.30
2	H	13	PRO	N-CA-CB	5.48	109.88	103.30
5	K	167	CYS	O-C-N	5.41	131.35	122.70
2	C	13	PRO	N-CA-CB	5.40	109.78	103.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	TYR	Mainchain
1	B	88	TYR	Mainchain
5	F	167	CYS	Mainchain

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	2555	0	2244	47	0
1	B	2556	0	2244	44	0
2	C	2252	0	1845	43	0
2	H	2262	0	1851	38	0
3	D	2028	0	1774	39	0
3	I	2028	0	1774	42	0
4	E	397	0	275	4	0
4	J	397	0	275	4	0
5	F	1294	0	1260	27	0
5	K	1294	0	1260	27	0
6	G	790	0	717	17	0
6	L	790	0	717	19	0
7	A	31	0	12	0	0
7	B	31	0	12	0	0
All	All	18705	0	16260	322	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 9.

All (322) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:177:THR:HG22	3:D:244:VAL:HG12	1.58	0.86
1:B:21:TYR:CE1	3:I:32:THR:HG22	2.13	0.83
3:I:177:THR:HG22	3:I:244:VAL:HG12	1.59	0.83
1:B:31:PHE:HB2	1:B:32:PRO:HD2	1.61	0.82
3:D:18:ARG:CG	3:D:18:ARG:HH11	1.94	0.81
1:A:21:TYR:CE1	3:D:32:THR:HG22	2.16	0.81
1:A:31:PHE:HB2	1:A:32:PRO:HD2	1.63	0.80
3:I:18:ARG:CG	3:I:18:ARG:HH11	1.95	0.79
2:H:254:LEU:HA	2:H:269:GLY:HA3	1.68	0.74
5:F:8:TYR:HA	6:G:127:LEU:HD21	1.70	0.73
2:H:143:ARG:CB	2:H:144:PRO:HD3	2.18	0.73
2:H:144:PRO:HG2	2:H:198:VAL:CG2	2.18	0.73
2:C:144:PRO:HG2	2:C:198:VAL:CG2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:71:LEU:HD11	3:D:118:VAL:HG12	1.70	0.73
2:C:32:THR:HA	2:C:57:ILE:HG22	1.72	0.72
2:C:143:ARG:CB	2:C:144:PRO:HD3	2.20	0.71
2:H:32:THR:HA	2:H:57:ILE:HG22	1.72	0.71
2:C:254:LEU:HA	2:C:269:GLY:HA3	1.73	0.70
3:I:71:LEU:HD11	3:I:118:VAL:HG12	1.74	0.70
5:K:8:TYR:HA	6:L:127:LEU:HD21	1.76	0.68
5:F:87:VAL:HG12	5:F:146:ILE:HG12	1.76	0.68
2:C:143:ARG:HB2	2:C:144:PRO:HD3	1.76	0.68
5:K:87:VAL:HG12	5:K:146:ILE:HG12	1.75	0.68
2:H:143:ARG:HB2	2:H:144:PRO:HD3	1.74	0.68
2:C:144:PRO:HG2	2:C:198:VAL:HG21	1.79	0.65
3:D:259:ILE:C	3:D:261:HIS:H	2.02	0.64
3:I:18:ARG:HH11	3:I:18:ARG:HG3	1.64	0.63
4:E:44:ILE:HG23	4:E:45:ASP:H	1.63	0.63
5:F:88:ARG:O	5:F:92:GLN:HB2	1.99	0.63
2:H:144:PRO:HG2	2:H:198:VAL:HG21	1.79	0.62
6:G:139:ILE:HD12	6:G:139:ILE:H	1.64	0.62
3:I:259:ILE:C	3:I:261:HIS:H	2.03	0.62
6:L:96:VAL:HG23	6:L:104:ILE:HD12	1.82	0.61
6:G:96:VAL:HG23	6:G:104:ILE:HD12	1.81	0.61
2:C:100:ASN:HD22	2:C:100:ASN:H	1.46	0.61
4:J:48:ILE:HD11	4:J:145:LEU:HA	1.83	0.61
6:L:139:ILE:H	6:L:139:ILE:HD12	1.65	0.61
2:H:100:ASN:HD22	2:H:100:ASN:H	1.47	0.60
3:I:287:ARG:HH11	5:K:145:GLU:HB2	1.66	0.60
5:F:52:VAL:HG12	5:F:62:LEU:HB2	1.82	0.60
1:B:129:THR:HB	1:B:160:GLN:HG3	1.84	0.60
2:C:270:TYR:CD2	5:F:21:ALA:HB1	2.36	0.60
5:K:52:VAL:HG12	5:K:62:LEU:HB2	1.83	0.60
3:D:18:ARG:HG3	3:D:18:ARG:HH11	1.64	0.60
2:C:74:SER:C	2:C:76:ASP:H	2.05	0.60
1:A:129:THR:HB	1:A:160:GLN:HG3	1.83	0.59
1:B:335:GLY:O	1:B:338:LEU:HB2	2.01	0.59
3:D:18:ARG:HH11	3:D:18:ARG:HG2	1.66	0.59
2:H:250:SER:HB2	6:L:138:GLY:HA3	1.84	0.59
1:B:111:GLN:O	1:B:115:LYS:HB2	2.03	0.59
6:G:96:VAL:HG23	6:G:104:ILE:CD1	2.33	0.59
2:H:74:SER:C	2:H:76:ASP:H	2.06	0.58
3:D:122:PRO:HG2	3:D:159:ILE:HD11	1.84	0.58
3:D:287:ARG:HH11	5:F:145:GLU:HB2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:270:TYR:CD2	5:K:21:ALA:HB1	2.39	0.58
6:L:104:ILE:HA	6:L:107:ILE:HG22	1.83	0.58
6:L:96:VAL:HG23	6:L:104:ILE:CD1	2.33	0.58
1:A:111:GLN:O	1:A:115:LYS:HB2	2.04	0.58
1:A:289:ALA:HB3	1:A:290:PRO:HD3	1.85	0.58
3:I:18:ARG:HH11	3:I:18:ARG:HG2	1.68	0.58
3:D:287:ARG:NH1	5:F:145:GLU:HB2	2.19	0.58
6:G:104:ILE:HA	6:G:107:ILE:HG22	1.84	0.58
1:B:129:THR:HB	1:B:160:GLN:CG	2.35	0.57
6:G:59:LEU:O	6:G:76:TYR:OH	2.21	0.57
3:I:40:HIS:CD2	3:I:42:SER:HB2	2.39	0.57
4:J:44:ILE:HG23	4:J:45:ASP:H	1.68	0.57
1:A:248:CYS:HB2	1:A:249:PRO:HD2	1.87	0.57
3:D:51:LEU:HG	3:D:52:ILE:H	1.69	0.57
4:E:48:ILE:HD11	4:E:145:LEU:HA	1.87	0.56
1:B:248:CYS:HB2	1:B:249:PRO:HD2	1.87	0.56
3:I:122:PRO:HG2	3:I:159:ILE:HD11	1.86	0.56
3:D:40:HIS:CD2	3:D:42:SER:HB2	2.40	0.56
2:H:119:SER:H	2:H:149:ILE:HD12	1.71	0.56
2:C:250:SER:HB2	6:G:138:GLY:HA3	1.87	0.56
5:K:88:ARG:O	5:K:92:GLN:HB2	2.05	0.55
1:A:129:THR:HB	1:A:160:GLN:CG	2.36	0.55
1:B:234:LEU:N	1:B:236:THR:HG1	2.04	0.55
3:D:18:ARG:NH1	3:D:18:ARG:HG2	2.22	0.55
6:L:92:ILE:O	6:L:96:VAL:HG12	2.07	0.55
3:I:51:LEU:HG	3:I:52:ILE:H	1.72	0.54
1:A:220:VAL:HG23	1:A:285:GLU:HB2	1.90	0.54
3:I:287:ARG:NH1	5:K:145:GLU:HB2	2.21	0.54
6:L:63:VAL:HG12	6:L:76:TYR:OH	2.07	0.54
3:I:219:TYR:HA	3:I:239:GLY:HA2	1.90	0.54
1:B:220:VAL:HG23	1:B:285:GLU:HB2	1.90	0.54
6:G:108:VAL:HA	6:G:111:ILE:HD12	1.90	0.54
6:G:92:ILE:O	6:G:96:VAL:HG12	2.08	0.53
3:I:18:ARG:CG	3:I:18:ARG:NH1	2.62	0.53
2:C:119:SER:H	2:C:149:ILE:HD12	1.74	0.53
1:B:269:ALA:O	1:B:270:SER:HB2	2.09	0.53
2:H:19:PHE:CD2	2:H:26:PHE:HB3	2.44	0.53
6:G:63:VAL:HG12	6:G:76:TYR:OH	2.09	0.52
3:I:18:ARG:HG2	3:I:18:ARG:NH1	2.23	0.52
2:H:124:ILE:HG13	2:H:145:LEU:HD21	1.92	0.52
1:A:234:LEU:N	1:A:236:THR:HG1	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ALA:HB3	1:B:290:PRO:HD3	1.90	0.52
3:D:219:TYR:HA	3:D:239:GLY:HA2	1.91	0.52
6:L:59:LEU:O	6:L:76:TYR:OH	2.23	0.51
1:A:343:GLY:O	1:A:376:VAL:HG11	2.10	0.51
2:C:19:PHE:CD2	2:C:26:PHE:HB3	2.46	0.51
5:K:20:LEU:HD11	5:K:118:ILE:HG21	1.92	0.51
1:A:101:ASN:HB3	1:A:104:HIS:HB2	1.93	0.51
3:I:54:LEU:HD21	3:I:56:MET:HG3	1.93	0.51
3:D:18:ARG:NH1	3:D:18:ARG:CG	2.61	0.51
2:H:26:PHE:CE1	2:H:38:TYR:HB2	2.46	0.50
1:A:335:GLY:O	1:A:338:LEU:HB2	2.11	0.50
1:B:343:GLY:O	1:B:376:VAL:HG11	2.12	0.50
2:C:26:PHE:CE1	2:C:38:TYR:HB2	2.46	0.50
1:B:267:LYS:O	1:B:282:VAL:HB	2.12	0.50
1:B:398:GLU:H	1:B:398:GLU:CD	2.15	0.50
3:I:33:ASP:OD1	3:I:34:PHE:N	2.40	0.49
2:C:169:LYS:HA	2:C:203:PRO:CB	2.42	0.49
6:L:56:LEU:O	6:L:60:LEU:HB2	2.12	0.49
1:A:269:ALA:O	1:A:270:SER:HB2	2.13	0.49
1:B:347:GLN:HB2	1:B:376:VAL:HG12	1.95	0.49
2:C:124:ILE:HG13	2:C:145:LEU:HD21	1.94	0.49
1:B:10:MET:HB2	1:B:128:LEU:CD2	2.43	0.49
2:H:169:LYS:HA	2:H:203:PRO:CB	2.42	0.49
3:D:54:LEU:HD21	3:D:56:MET:HG3	1.94	0.48
5:K:70:VAL:HG12	5:K:118:ILE:HB	1.95	0.48
3:D:259:ILE:O	3:D:261:HIS:N	2.45	0.48
1:A:163:LEU:O	1:A:389:GLY:HA3	2.13	0.48
1:B:101:ASN:HB3	1:B:104:HIS:HB2	1.94	0.48
3:I:280:MET:O	3:I:284:MET:HB2	2.14	0.48
5:F:70:VAL:HG12	5:F:118:ILE:HB	1.95	0.48
5:F:8:TYR:CA	6:G:127:LEU:HD21	2.41	0.48
6:G:56:LEU:O	6:G:60:LEU:HB2	2.14	0.48
1:A:398:GLU:H	1:A:398:GLU:CD	2.17	0.48
3:D:51:LEU:HG	3:D:52:ILE:N	2.28	0.48
1:B:34:VAL:HG21	1:B:81:LEU:CD2	2.44	0.48
1:A:126:PHE:O	1:A:156:TYR:N	2.46	0.48
2:H:92:GLN:HE21	2:H:92:GLN:H	1.61	0.48
1:B:115:LYS:O	3:I:9:ILE:HD13	2.13	0.48
2:H:214:SER:HB2	2:H:215:PRO:HD2	1.96	0.47
1:A:34:VAL:HG21	1:A:81:LEU:CD2	2.44	0.47
2:C:214:SER:HB2	2:C:215:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PRO:HG3	1:A:387:TRP:CD2	2.50	0.47
2:H:15:TYR:H	2:H:29:THR:HG23	1.80	0.47
3:I:37:VAL:HG22	3:I:56:MET:HG2	1.96	0.47
6:L:108:VAL:HA	6:L:111:ILE:HD12	1.96	0.47
3:I:259:ILE:O	3:I:261:HIS:N	2.47	0.47
6:G:64:PRO:HB2	6:G:73:ARG:HG2	1.97	0.47
2:C:271:ASN:O	5:F:128:LYS:NZ	2.48	0.47
2:H:268:ALA:HB1	2:H:347:ILE:HG13	1.96	0.47
5:K:87:VAL:CG1	5:K:146:ILE:HG12	2.44	0.47
5:K:114:ILE:HD13	5:K:115:SER:H	1.80	0.47
5:F:20:LEU:HD11	5:F:118:ILE:HG21	1.96	0.47
1:A:74:PHE:CZ	1:A:111:GLN:HG3	2.50	0.46
1:A:347:GLN:HB2	1:A:376:VAL:HG12	1.97	0.46
2:C:343:HIS:CD2	2:C:347:ILE:HD11	2.50	0.46
1:B:157:ILE:HD13	1:B:157:ILE:N	2.30	0.46
2:C:155:HIS:O	2:C:157:ASN:N	2.46	0.46
3:D:180:PHE:HZ	3:D:262:ILE:O	1.98	0.46
3:I:288:VAL:HG13	5:K:94:LEU:HD22	1.96	0.46
2:C:70:ILE:HG12	2:C:82:TYR:HB2	1.97	0.46
1:B:163:LEU:O	1:B:389:GLY:HA3	2.15	0.46
6:L:64:PRO:HB2	6:L:73:ARG:HG2	1.97	0.46
1:A:267:LYS:O	1:A:282:VAL:HB	2.16	0.46
3:D:280:MET:O	3:D:284:MET:HB2	2.15	0.46
2:C:30:THR:HG23	2:C:36:GLU:HG2	1.98	0.46
1:B:10:MET:HE3	1:B:128:LEU:HD21	1.99	0.45
2:C:59:THR:HB	2:C:60:CYS:H	1.59	0.45
2:C:92:GLN:H	2:C:92:GLN:HE21	1.63	0.45
2:C:76:ASP:O	2:C:77:ARG:HB2	2.17	0.45
3:D:244:VAL:HG23	3:D:244:VAL:O	2.17	0.45
2:H:105:PHE:O	2:H:117:VAL:HA	2.16	0.45
2:H:271:ASN:O	5:K:128:LYS:NZ	2.49	0.45
2:C:120:GLY:HA2	2:C:148:THR:HG23	1.98	0.45
2:C:32:THR:HG23	2:C:34:GLN:H	1.82	0.45
1:B:31:PHE:HB2	1:B:32:PRO:CD	2.41	0.45
2:C:224:GLY:C	2:C:226:ASP:H	2.21	0.45
2:H:76:ASP:O	2:H:77:ARG:HB2	2.17	0.45
2:C:345:ASN:HA	5:F:128:LYS:HG2	1.99	0.45
3:I:244:VAL:HG23	3:I:244:VAL:O	2.17	0.45
3:I:160:HIS:HA	3:I:166:THR:HG22	1.98	0.45
3:D:54:LEU:HD13	3:D:114:LEU:HD12	1.98	0.44
5:F:158:ARG:O	5:F:162:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:71:ARG:HD2	5:F:105:ARG:NH1	2.32	0.44
2:H:155:HIS:C	2:H:157:ASN:H	2.21	0.44
1:B:21:TYR:CE2	3:I:31:VAL:HA	2.52	0.44
1:B:27:PRO:HG3	1:B:387:TRP:CD2	2.52	0.44
2:H:28:THR:HB	2:H:29:THR:H	1.54	0.44
3:I:51:LEU:HG	3:I:52:ILE:N	2.30	0.44
1:B:126:PHE:O	1:B:156:TYR:N	2.48	0.44
1:B:347:GLN:NE2	1:B:375:ASN:HA	2.32	0.44
2:H:143:ARG:CB	2:H:144:PRO:CD	2.90	0.44
2:H:271:ASN:O	2:H:272:TYR:CB	2.65	0.44
2:C:271:ASN:O	2:C:272:TYR:CB	2.65	0.44
5:F:114:ILE:HD13	5:F:115:SER:H	1.81	0.44
2:H:221:ALA:HA	2:H:230:THR:O	2.17	0.44
2:H:70:ILE:HG12	2:H:82:TYR:HB2	1.98	0.44
1:A:10:MET:HB2	1:A:128:LEU:CD2	2.48	0.44
3:D:33:ASP:OD1	3:D:34:PHE:N	2.46	0.44
2:H:59:THR:HB	2:H:60:CYS:H	1.58	0.44
1:A:248:CYS:SG	1:A:287:PHE:HB2	2.57	0.44
2:C:75:GLN:HA	2:C:102:ALA:HB1	2.00	0.44
3:D:246:PHE:H	3:D:249:HIS:HD2	1.65	0.44
3:D:37:VAL:HG22	3:D:56:MET:HG2	1.99	0.44
5:F:87:VAL:CG1	5:F:146:ILE:HG12	2.46	0.44
5:F:87:VAL:HG23	5:F:88:ARG:N	2.32	0.44
1:B:32:PRO:HB2	1:B:34:VAL:HG13	1.99	0.44
3:I:129:LYS:C	3:I:131:ALA:H	2.21	0.44
3:I:246:PHE:H	3:I:249:HIS:HD2	1.66	0.44
1:B:205:SER:O	1:B:207:LYS:N	2.51	0.44
1:B:99:ILE:O	1:B:99:ILE:HG13	2.18	0.44
2:H:253:PRO:HD3	6:L:143:VAL:HG11	1.99	0.44
1:A:21:TYR:CE2	3:D:31:VAL:HA	2.53	0.43
3:D:51:LEU:O	3:D:52:ILE:HB	2.19	0.43
1:A:10:MET:HE1	1:A:113:LEU:HD11	2.00	0.43
1:A:10:MET:HE3	1:A:128:LEU:HD21	2.00	0.43
1:A:347:GLN:NE2	1:A:375:ASN:HA	2.33	0.43
2:C:15:TYR:H	2:C:29:THR:HG23	1.83	0.43
3:D:122:PRO:CG	3:D:159:ILE:HD11	2.48	0.43
4:E:51:PHE:C	4:E:53:ALA:H	2.21	0.43
3:D:288:VAL:HG13	5:F:94:LEU:HD22	1.99	0.43
1:A:27:PRO:HG3	1:A:387:TRP:CG	2.54	0.43
1:B:93:PRO:HA	1:B:101:ASN:HB2	2.00	0.43
2:C:36:GLU:HB3	2:C:38:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:SER:HB3	3:D:10:PHE:CE1	2.53	0.43
3:I:122:PRO:CG	3:I:159:ILE:HD11	2.48	0.43
3:I:259:ILE:C	3:I:261:HIS:N	2.71	0.43
6:G:105:ASP:O	6:G:109:ASN:HB2	2.19	0.43
3:D:129:LYS:C	3:D:131:ALA:H	2.22	0.43
3:D:186:GLU:OE1	3:D:277:LYS:HE3	2.18	0.43
4:E:142:ALA:C	4:E:144:ARG:H	2.22	0.43
1:A:99:ILE:O	1:A:99:ILE:HG13	2.18	0.43
4:J:51:PHE:C	4:J:53:ALA:H	2.22	0.43
6:G:92:ILE:N	6:G:93:PRO:HD2	2.33	0.43
2:C:347:ILE:CG2	2:C:348:ALA:N	2.82	0.43
1:B:101:ASN:HA	1:B:101:ASN:HD22	1.62	0.42
1:B:28:SER:HB3	3:I:10:PHE:CE1	2.54	0.42
3:D:161:TYR:CE2	3:D:167:ILE:HG13	2.54	0.42
2:H:155:HIS:O	2:H:157:ASN:N	2.48	0.42
5:K:76:ILE:HG22	5:K:77:LYS:N	2.34	0.42
5:K:87:VAL:HG23	5:K:88:ARG:N	2.34	0.42
1:A:157:ILE:N	1:A:157:ILE:HD13	2.33	0.42
1:A:31:PHE:HB2	1:A:32:PRO:CD	2.42	0.42
1:B:151:ASN:HD22	3:I:274:LYS:HE3	1.82	0.42
2:H:32:THR:HG23	2:H:34:GLN:H	1.83	0.42
1:A:205:SER:O	1:A:207:LYS:N	2.52	0.42
5:F:81:GLU:HG3	5:F:82:ILE:H	1.84	0.42
1:B:12:ASN:HA	1:B:17:SER:OG	2.19	0.42
6:L:102:GLU:O	6:L:106:ASN:HB2	2.19	0.42
2:H:343:HIS:CD2	2:H:347:ILE:HD11	2.55	0.42
5:K:90:PHE:HE2	5:K:145:GLU:HG2	1.84	0.42
6:L:79:ALA:O	6:L:83:VAL:HG23	2.19	0.42
2:H:143:ARG:HB3	2:H:144:PRO:HD3	2.01	0.42
1:A:93:PRO:HA	1:A:101:ASN:HB2	2.00	0.42
2:C:155:HIS:C	2:C:157:ASN:H	2.21	0.42
3:I:54:LEU:HD13	3:I:114:LEU:HD12	2.01	0.42
1:A:282:VAL:HA	1:A:285:GLU:OE2	2.20	0.42
3:I:186:GLU:OE1	3:I:277:LYS:HE3	2.19	0.42
5:F:8:TYR:CD2	5:F:55:ARG:HD2	2.55	0.42
5:F:90:PHE:HE2	5:F:145:GLU:HG2	1.84	0.42
3:I:17:GLU:OE2	3:I:18:ARG:HG2	2.19	0.42
3:I:288:VAL:CG1	5:K:94:LEU:HD22	2.49	0.42
4:J:142:ALA:C	4:J:144:ARG:H	2.23	0.42
5:K:158:ARG:O	5:K:162:GLU:HB2	2.19	0.42
6:L:141:CYS:SG	6:L:142:ILE:N	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:MET:HE1	1:B:113:LEU:HD11	2.01	0.42
3:D:39:PHE:HA	3:D:53:SER:O	2.20	0.42
3:I:161:TYR:CE2	3:I:167:ILE:HG13	2.55	0.42
6:L:92:ILE:N	6:L:93:PRO:HD2	2.35	0.42
2:H:75:GLN:HA	2:H:102:ALA:HB1	2.02	0.41
6:L:105:ASP:O	6:L:109:ASN:HB2	2.20	0.41
2:C:105:PHE:O	2:C:117:VAL:HA	2.19	0.41
5:K:71:ARG:HD2	5:K:105:ARG:NH1	2.35	0.41
2:C:64:ALA:HB2	2:C:108:TRP:CE2	2.55	0.41
5:F:63:ILE:HG13	5:F:72:PHE:HD1	1.85	0.41
6:G:79:ALA:O	6:G:83:VAL:HG23	2.19	0.41
1:A:305:THR:HA	1:A:306:PRO:HD3	1.84	0.41
1:B:35:ILE:O	1:B:90:LEU:HA	2.20	0.41
3:D:259:ILE:C	3:D:261:HIS:N	2.70	0.41
5:K:30:VAL:HG21	5:K:35:GLN:HE22	1.85	0.41
1:B:31:PHE:CB	1:B:32:PRO:HD2	2.40	0.41
1:B:36:ALA:HB2	1:B:80:ALA:HB1	2.02	0.41
1:B:92:TYR:HA	1:B:93:PRO:HD3	1.94	0.41
2:C:268:ALA:HB1	2:C:347:ILE:HG13	2.02	0.41
2:C:82:TYR:CE1	2:C:92:GLN:HB3	2.56	0.41
1:A:101:ASN:HD22	1:A:101:ASN:HA	1.61	0.41
1:B:74:PHE:N	1:B:74:PHE:CD2	2.89	0.41
3:I:40:HIS:HD2	3:I:42:SER:HB2	1.86	0.41
5:K:8:TYR:CA	6:L:127:LEU:HD21	2.49	0.41
5:F:46:ILE:HG23	5:F:67:VAL:HG12	2.02	0.41
2:H:269:GLY:C	2:H:271:ASN:H	2.24	0.41
3:I:180:PHE:HZ	3:I:262:ILE:O	2.03	0.41
5:K:122:HIS:C	5:K:124:GLU:H	2.24	0.41
5:K:63:ILE:HG13	5:K:72:PHE:HD1	1.86	0.41
1:A:193:ILE:HB	1:A:314:VAL:HG21	2.03	0.41
1:A:32:PRO:O	1:A:77:GLY:HA2	2.21	0.41
3:D:160:HIS:HA	3:D:166:THR:HG22	2.03	0.41
5:F:114:ILE:CD1	5:F:115:SER:H	2.33	0.41
5:F:150:LYS:C	5:F:152:PHE:H	2.23	0.41
1:A:69:THR:HA	5:F:156:ARG:NH2	2.36	0.41
3:I:58:CYS:O	3:I:62:LEU:HD12	2.20	0.41
1:B:310:LEU:HD12	1:B:310:LEU:HA	1.94	0.41
2:C:201:GLU:O	2:C:202:TYR:C	2.59	0.41
3:I:51:LEU:O	3:I:52:ILE:HB	2.20	0.41
5:K:10:ASN:HA	5:K:10:ASN:HD22	1.66	0.41
2:C:28:THR:HB	2:C:29:THR:H	1.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:150:LYS:C	5:K:152:PHE:H	2.24	0.41
5:K:81:GLU:HG3	5:K:82:ILE:H	1.86	0.41
1:A:12:ASN:HA	1:A:17:SER:OG	2.21	0.41
1:B:386:VAL:HG23	1:B:387:TRP:H	1.85	0.41
1:A:209:MET:HA	1:A:210:PRO:HD3	1.89	0.40
1:A:32:PRO:HB2	1:A:34:VAL:HG13	2.03	0.40
1:A:36:ALA:HB2	1:A:80:ALA:HB1	2.04	0.40
1:B:74:PHE:CZ	1:B:111:GLN:HG3	2.55	0.40
2:C:143:ARG:CB	2:C:144:PRO:CD	2.91	0.40
2:C:264:ALA:HA	2:C:278:GLN:HA	2.04	0.40
3:D:119:LEU:O	3:D:263:GLN:NE2	2.53	0.40
1:A:9:ILE:HD12	1:A:127:LEU:HD22	2.03	0.40
5:F:30:VAL:HG21	5:F:35:GLN:HE22	1.86	0.40
6:G:107:ILE:O	6:G:111:ILE:HG13	2.21	0.40
2:H:7:LEU:HB3	2:H:45:TRP:HE1	1.86	0.40
3:I:299:LYS:HA	3:I:300:PRO:HD3	1.88	0.40
1:A:419:ARG:O	1:A:420:TYR:HB3	2.20	0.40
2:C:221:ALA:HA	2:C:230:THR:O	2.21	0.40
3:D:200:PHE:HD1	3:D:215:VAL:HG21	1.87	0.40
1:A:115:LYS:O	3:D:9:ILE:HD13	2.22	0.40
2:H:120:GLY:HA2	2:H:148:THR:HG23	2.02	0.40
5:K:46:ILE:HG23	5:K:67:VAL:HG12	2.03	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	343/427 (80%)	299 (87%)	36 (10%)	8 (2%)	6	38
1	B	343/427 (80%)	300 (88%)	37 (11%)	6 (2%)	9	43
2	C	324/377 (86%)	245 (76%)	56 (17%)	23 (7%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	325/377 (86%)	245 (75%)	59 (18%)	21 (6%)	1	19
3	D	258/317 (81%)	215 (83%)	35 (14%)	8 (3%)	4	33
3	I	258/317 (81%)	217 (84%)	33 (13%)	8 (3%)	4	33
4	E	53/174 (30%)	40 (76%)	11 (21%)	2 (4%)	3	28
4	J	53/174 (30%)	40 (76%)	11 (21%)	2 (4%)	3	28
5	F	164/168 (98%)	144 (88%)	18 (11%)	2 (1%)	13	49
5	K	164/168 (98%)	143 (87%)	19 (12%)	2 (1%)	13	49
6	G	110/152 (72%)	97 (88%)	11 (10%)	2 (2%)	8	42
6	L	110/152 (72%)	97 (88%)	11 (10%)	2 (2%)	8	42
All	All	2505/3230 (78%)	2082 (83%)	337 (14%)	86 (3%)	3	31

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	TRP
1	A	206	ILE
2	C	54	HIS
2	C	108	TRP
2	C	143	ARG
2	C	203	PRO
2	C	204	SER
2	C	272	TYR
2	C	296	LYS
1	B	102	TRP
1	B	206	ILE
2	H	54	HIS
2	H	143	ARG
2	H	203	PRO
2	H	204	SER
2	H	272	TYR
2	H	296	LYS
1	A	75	PHE
2	C	158	ASN
2	C	194	PRO
2	C	207	TRP
2	C	239	GLN
3	D	76	GLY
3	D	260	SER
6	G	116	ALA

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Mol	Chain	Res	Type
1	B	75	PHE
2	H	108	TRP
2	H	194	PRO
2	H	207	TRP
2	H	239	GLN
2	H	288	ARG
3	I	76	GLY
3	I	260	SER
6	L	116	ALA
2	C	50	THR
2	C	288	ARG
3	D	146	MET
3	D	224	LEU
6	G	148	SER
1	B	174	VAL
2	H	50	THR
2	H	158	ASN
3	I	146	MET
6	L	148	SER
1	A	174	VAL
2	C	180	VAL
2	C	202	TYR
2	C	290	LEU
4	E	52	ARG
5	F	31	GLU
2	H	180	VAL
2	H	202	TYR
2	H	290	LEU
3	I	224	LEU
5	K	31	GLU
1	A	74	PHE
1	A	397	PRO
2	C	241	PRO
3	D	212	ALA
3	D	226	ILE
3	D	283	ARG
1	B	74	PHE
1	B	397	PRO
2	H	241	PRO
3	I	226	ILE
3	I	283	ARG
4	J	52	ARG

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Mol	Chain	Res	Type
1	A	148	GLU
1	A	149	SER
2	C	75	GLN
2	C	156	PRO
3	I	52	ILE
3	I	212	ALA
3	D	52	ILE
5	F	36	PRO
2	H	156	PRO
4	J	73	GLY
2	C	65	PRO
2	C	205	GLY
2	C	206	GLY
4	E	73	GLY
2	H	65	PRO
2	H	206	GLY
5	K	36	PRO
2	C	356	THR
2	H	205	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/364 (66%)	214 (89%)	26 (11%)	6	30
1	B	240/364 (66%)	215 (90%)	25 (10%)	7	31
2	C	181/317 (57%)	163 (90%)	18 (10%)	8	33
2	H	182/317 (57%)	165 (91%)	17 (9%)	9	36
3	D	185/287 (64%)	169 (91%)	16 (9%)	10	40
3	I	185/287 (64%)	169 (91%)	16 (9%)	10	40
4	E	23/150 (15%)	19 (83%)	4 (17%)	2	13
4	J	23/150 (15%)	19 (83%)	4 (17%)	2	13
5	F	140/157 (89%)	131 (94%)	9 (6%)	17	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	K	140/157 (89%)	132 (94%)	8 (6%)	20	52
6	G	74/134 (55%)	67 (90%)	7 (10%)	8	34
6	L	74/134 (55%)	70 (95%)	4 (5%)	22	54
All	All	1687/2818 (60%)	1533 (91%)	154 (9%)	9	36

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	17	SER
1	A	31	PHE
1	A	33	THR
1	A	74	PHE
1	A	90	LEU
1	A	101	ASN
1	A	102	TRP
1	A	103	ASP
1	A	111	GLN
1	A	120	GLU
1	A	157	ILE
1	A	235	LYS
1	A	257	ARG
1	A	260	ARG
1	A	281	ASP
1	A	288	LEU
1	A	316	GLN
1	A	336	SER
1	A	348	ARG
1	A	380	LYS
1	A	381	ARG
1	A	386	VAL
1	A	393	LEU
1	A	398	GLU
1	A	422	ILE
2	C	22	GLN
2	C	29	THR
2	C	53	ASP
2	C	57	ILE
2	C	59	THR
2	C	68	ASN
2	C	78	ASN

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Mol	Chain	Res	Type
2	C	92	GLN
2	C	99	LEU
2	C	100	ASN
2	C	122	ARG
2	C	152	LEU
2	C	173	LEU
2	C	197	THR
2	C	207	TRP
2	C	254	LEU
2	C	265	ILE
2	C	364	THR
3	D	16	THR
3	D	18	ARG
3	D	38	THR
3	D	43	THR
3	D	81	GLU
3	D	114	LEU
3	D	116	ARG
3	D	119	LEU
3	D	161	TYR
3	D	217	PHE
3	D	219	TYR
3	D	264	VAL
3	D	266	ARG
3	D	287	ARG
3	D	288	VAL
3	D	301	ASP
4	E	59	ASN
4	E	69	THR
4	E	159	LYS
4	E	162	THR
5	F	19	SER
5	F	22	LEU
5	F	30	VAL
5	F	62	LEU
5	F	82	ILE
5	F	101	PHE
5	F	114	ILE
5	F	156	ARG
5	F	165	LEU
6	G	59	LEU
6	G	68	ASP

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Mol	Chain	Res	Type
6	G	86	ASN
6	G	101	THR
6	G	123	SER
6	G	136	ILE
6	G	137	SER
1	B	14	THR
1	B	17	SER
1	B	33	THR
1	B	74	PHE
1	B	90	LEU
1	B	101	ASN
1	B	102	TRP
1	B	103	ASP
1	B	111	GLN
1	B	120	GLU
1	B	157	ILE
1	B	235	LYS
1	B	257	ARG
1	B	260	ARG
1	B	281	ASP
1	B	288	LEU
1	B	316	GLN
1	B	336	SER
1	B	348	ARG
1	B	380	LYS
1	B	381	ARG
1	B	386	VAL
1	B	393	LEU
1	B	398	GLU
1	B	422	ILE
2	H	22	GLN
2	H	29	THR
2	H	53	ASP
2	H	57	ILE
2	H	59	THR
2	H	68	ASN
2	H	78	ASN
2	H	92	GLN
2	H	99	LEU
2	H	100	ASN
2	H	122	ARG
2	H	152	LEU

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Mol	Chain	Res	Type
2	H	173	LEU
2	H	197	THR
2	H	207	TRP
2	H	254	LEU
2	H	265	ILE
3	I	16	THR
3	I	18	ARG
3	I	38	THR
3	I	43	THR
3	I	81	GLU
3	I	114	LEU
3	I	119	LEU
3	I	161	TYR
3	I	217	PHE
3	I	219	TYR
3	I	260	SER
3	I	264	VAL
3	I	266	ARG
3	I	287	ARG
3	I	288	VAL
3	I	301	ASP
4	J	59	ASN
4	J	69	THR
4	J	159	LYS
4	J	162	THR
5	K	22	LEU
5	K	30	VAL
5	K	62	LEU
5	K	82	ILE
5	K	101	PHE
5	K	114	ILE
5	K	156	ARG
5	K	165	LEU
6	L	59	LEU
6	L	101	THR
6	L	123	SER
6	L	136	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN

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Mol	Chain	Res	Type
1	A	111	GLN
1	A	138	ASN
1	A	192	HIS
1	A	221	GLN
1	A	313	ASN
1	A	316	GLN
1	A	395	GLN
2	C	78	ASN
2	C	92	GLN
2	C	100	ASN
3	D	249	HIS
3	D	253	GLN
5	F	10	ASN
6	G	147	ASN
1	B	12	ASN
1	B	101	ASN
1	B	104	HIS
1	B	111	GLN
1	B	138	ASN
1	B	151	ASN
1	B	192	HIS
1	B	221	GLN
1	B	313	ASN
1	B	316	GLN
1	B	379	HIS
1	B	395	GLN
2	H	43	ASN
2	H	78	ASN
2	H	92	GLN
2	H	100	ASN
2	H	196	ASN
3	I	249	HIS
3	I	253	GLN
5	K	10	ASN
6	L	147	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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$
7	ATP	B	428	-	26,33,33	0.97	2 (7%)	31,52,52	1.53	5 (16%)
7	ATP	A	428	-	26,33,33	0.90	1 (3%)	31,52,52	1.55	4 (12%)

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
7	ATP	B	428	-	-	5/18/38/38	0/3/3/3
7	ATP	A	428	-	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	428	ATP	C5-C4	2.57	1.47	1.40
7	A	428	ATP	C5-C4	2.47	1.47	1.40
7	B	428	ATP	C2-N3	2.08	1.35	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	428	ATP	PA-O3A-PB	-3.82	119.73	132.83
7	B	428	ATP	PB-O3B-PG	-3.74	120.00	132.83
7	A	428	ATP	PB-O3B-PG	-3.64	120.33	132.83
7	B	428	ATP	PA-O3A-PB	-3.25	121.68	132.83
7	B	428	ATP	N3-C2-N1	-3.22	123.64	128.68
7	A	428	ATP	N3-C2-N1	-3.13	123.79	128.68
7	B	428	ATP	C4-C5-N7	-2.99	106.29	109.40
7	A	428	ATP	C4-C5-N7	-2.70	106.59	109.40
7	B	428	ATP	C3'-C2'-C1'	2.20	104.29	100.98

There are no chirality outliers.

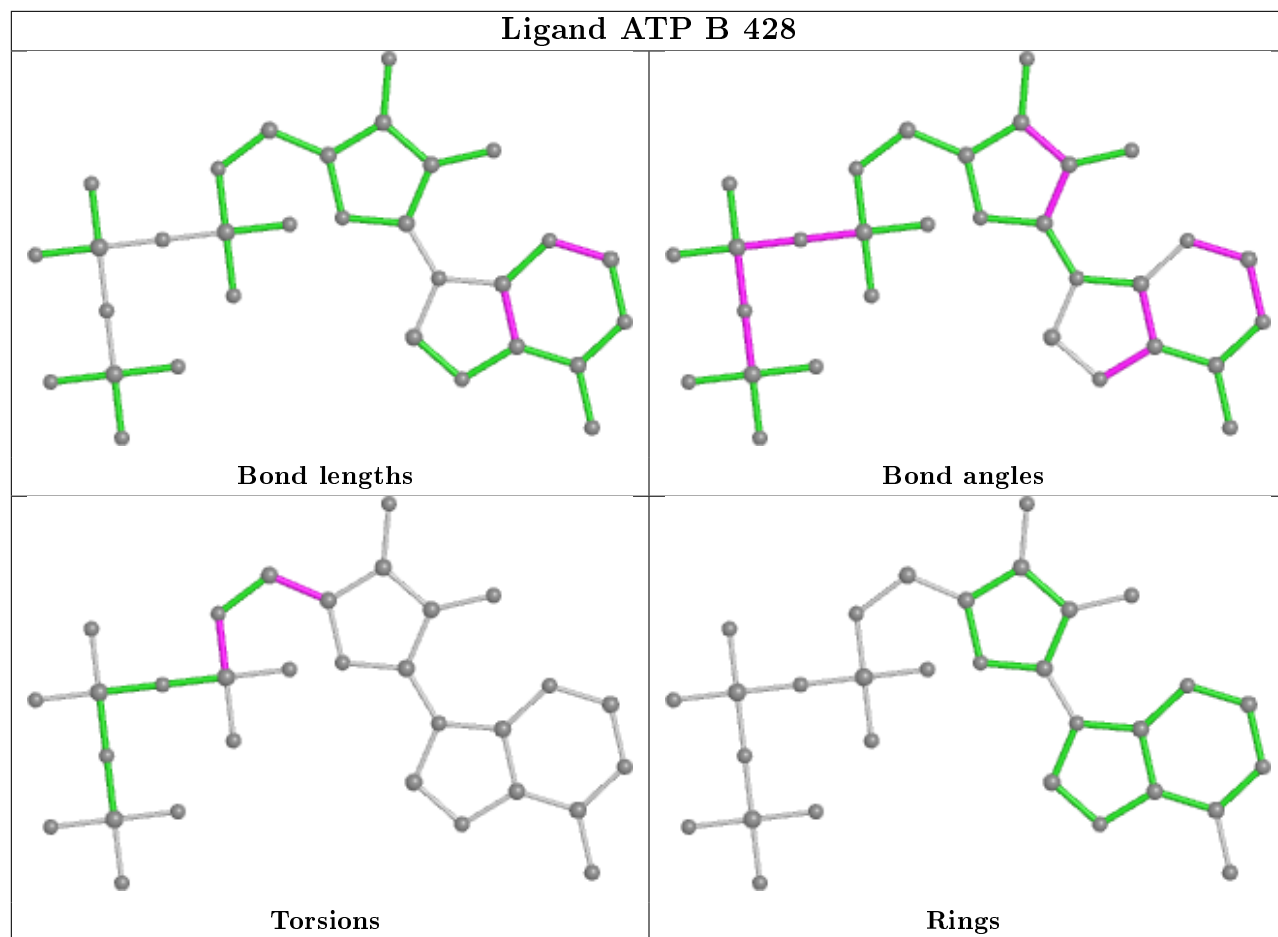
All (9) torsion outliers are listed below:

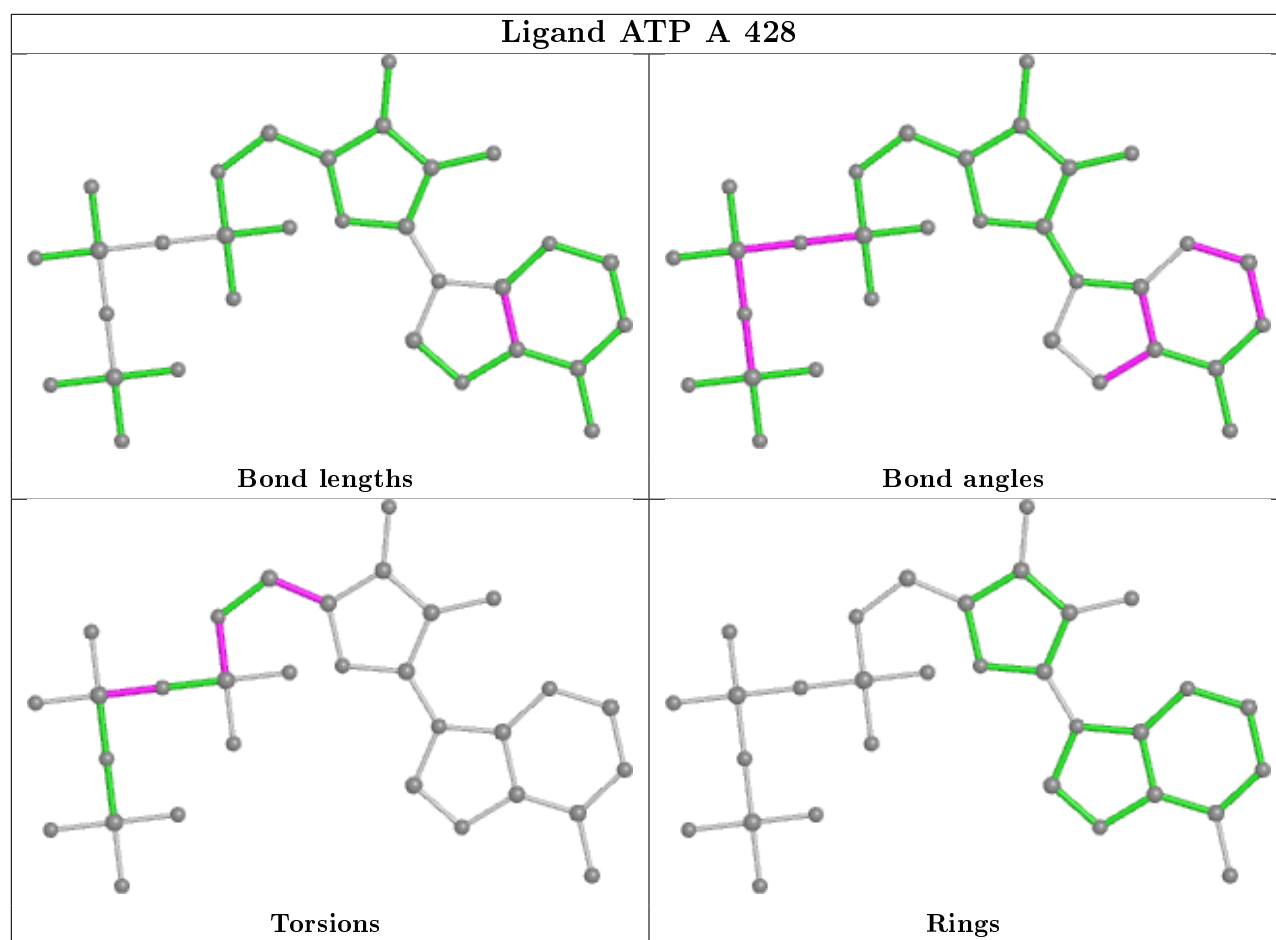
Mol	Chain	Res	Type	Atoms
7	B	428	ATP	C5'-O5'-PA-O3A
7	A	428	ATP	O4'-C4'-C5'-O5'
7	A	428	ATP	C3'-C4'-C5'-O5'
7	B	428	ATP	C3'-C4'-C5'-O5'
7	B	428	ATP	O4'-C4'-C5'-O5'
7	B	428	ATP	C5'-O5'-PA-O1A
7	B	428	ATP	C5'-O5'-PA-O2A
7	A	428	ATP	PA-O3A-PB-O1B
7	A	428	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	355/427 (83%)	-0.24	0 100 100	65, 74, 88, 94	1 (0%)
1	B	355/427 (83%)	-0.23	1 (0%) 94 94	65, 74, 88, 94	1 (0%)
2	C	336/377 (89%)	-0.29	1 (0%) 94 94	65, 76, 86, 95	0
2	H	337/377 (89%)	0.03	9 (2%) 54 48	65, 76, 86, 95	0
3	D	272/317 (85%)	-0.30	0 100 100	65, 72, 86, 96	0
3	I	272/317 (85%)	-0.30	2 (0%) 87 86	65, 72, 86, 96	0
4	E	63/174 (36%)	0.01	2 (3%) 47 41	66, 73, 83, 84	0
4	J	63/174 (36%)	-0.39	0 100 100	66, 73, 83, 84	0
5	F	166/168 (98%)	-0.15	1 (0%) 89 88	65, 74, 84, 99	1 (0%)
5	K	166/168 (98%)	0.05	3 (1%) 68 65	65, 74, 84, 99	1 (0%)
6	G	114/152 (75%)	-0.30	0 100 100	66, 73, 82, 84	0
6	L	114/152 (75%)	-0.04	1 (0%) 84 82	66, 73, 82, 84	0
All	All	2613/3230 (80%)	-0.19	20 (0%) 86 84	65, 74, 86, 99	4 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	287	THR	3.4
4	E	161	TRP	3.0
5	K	42	ARG	2.7
2	H	174	SER	2.5
2	H	151	SER	2.5
1	B	244	CYS	2.4
2	H	79	ALA	2.4
2	C	235	SER	2.4
4	E	51	PHE	2.3
5	K	37	GLU	2.3
2	H	244	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	57	ILE	2.2
6	L	52	ALA	2.1
2	H	80	TYR	2.1
5	K	149	MET	2.1
5	F	58	GLN	2.1
2	H	78	ASN	2.1
2	H	152	LEU	2.0
3	I	245	LEU	2.0
3	I	171	PRO	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 carbohydrates in this entry.

6.4 Ligands [i](#)

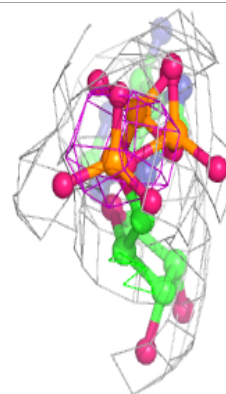
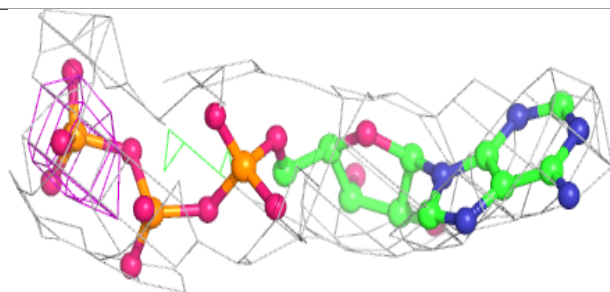
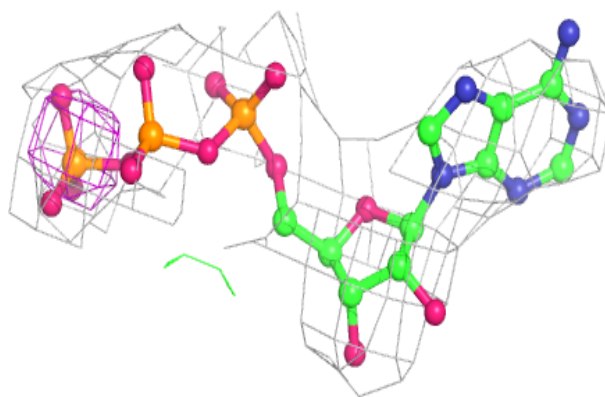
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	ATP	B	428	31/31	0.89	0.27	102,102,108,108	0
7	ATP	A	428	31/31	0.90	0.21	97,98,106,106	0

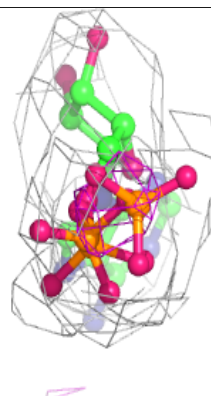
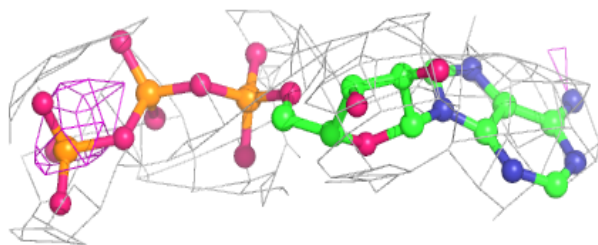
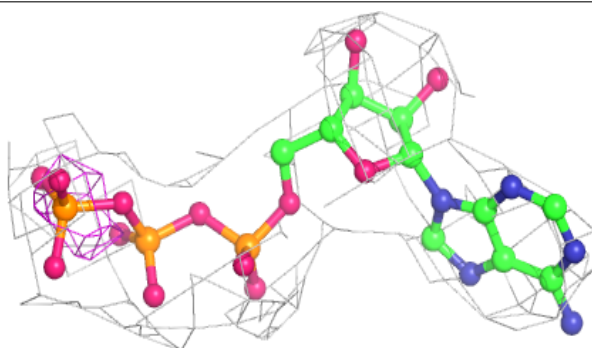
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP B 428:

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

**Electron density around ATP A 428:**

$2mF_o-DF_c$ (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.