



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:21 pm BST

PDB ID : 2PC9
Title : Crystal Structure Of ATP-Dependent Phosphoenolpyruvate Carboxykinase From *Thermus thermophilus* HB8
Authors : Sugahara, M.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-03-29
Resolution : 2.40 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

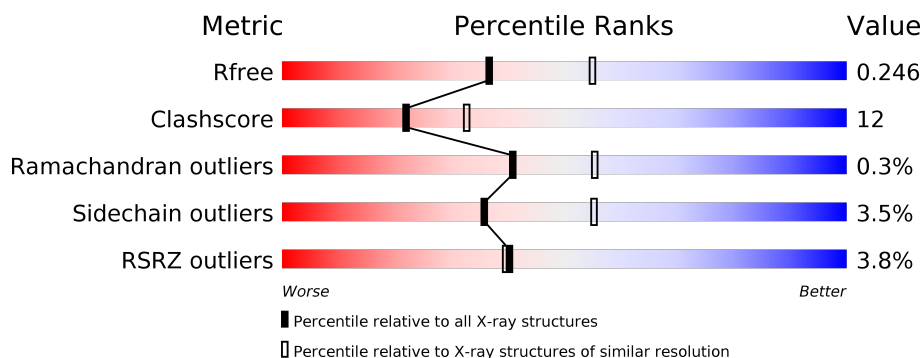
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	529	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> % 79% 17% .. </div> </div>
1	B	529	<div> <div style="width: 10%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> 10% 66% 29% .. </div> </div>
1	C	529	<div> <div style="width: 3%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> 3% 77% 20% .. </div> </div>
1	D	529	<div> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> 2% 71% 24% .. </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	B	3013	-	X	-	-
3	PO4	C	3014	-	X	-	-
3	PO4	C	3016	-	X	-	-
3	PO4	C	3017	-	X	-	-
3	PO4	D	3015	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17321 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.

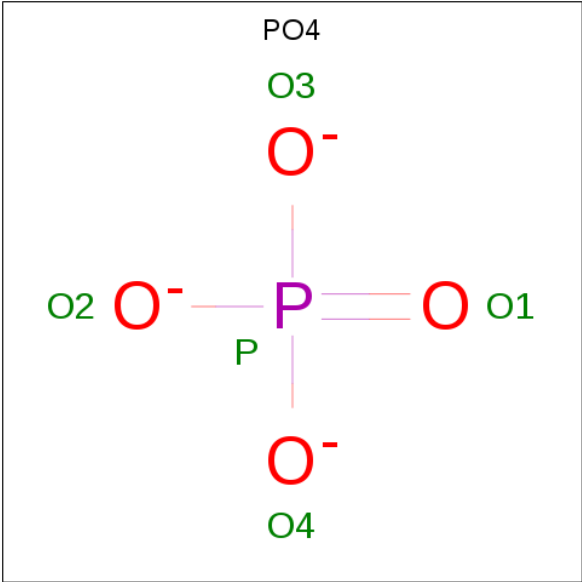
- Molecule 1 is a protein called Phosphoenolpyruvate carboxykinase [ATP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			4096	2637	716	733	10			
1	B	511	Total	C	N	O	S	0	0	0
			4071	2622	711	729	9			
1	C	517	Total	C	N	O	S	0	0	0
			4112	2646	717	740	9			
1	D	512	Total	C	N	O	S	0	0	0
			4071	2623	712	727	9			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



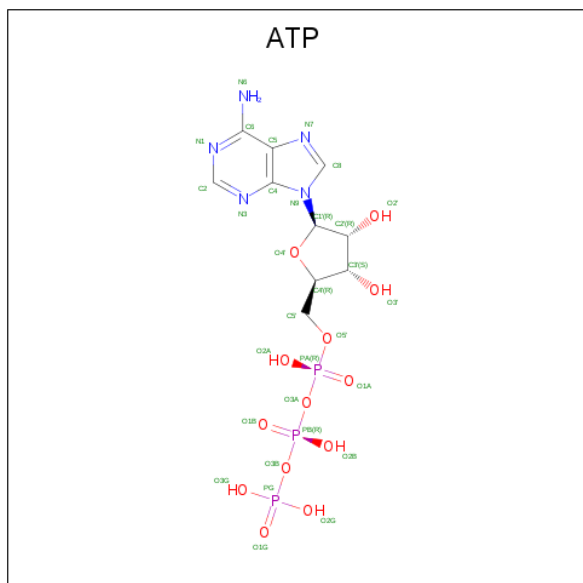
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	241	Total	O	0	0
			241	241		
5	B	95	Total	O	0	0
			95	95		
5	C	207	Total	O	0	0
			207	207		

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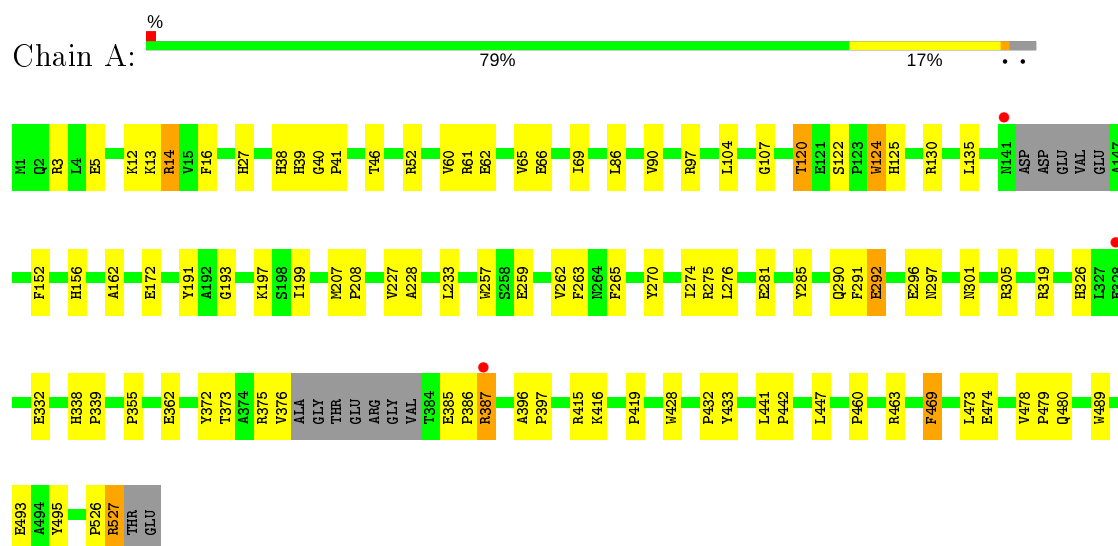
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	220	Total 220	O 220	0	0

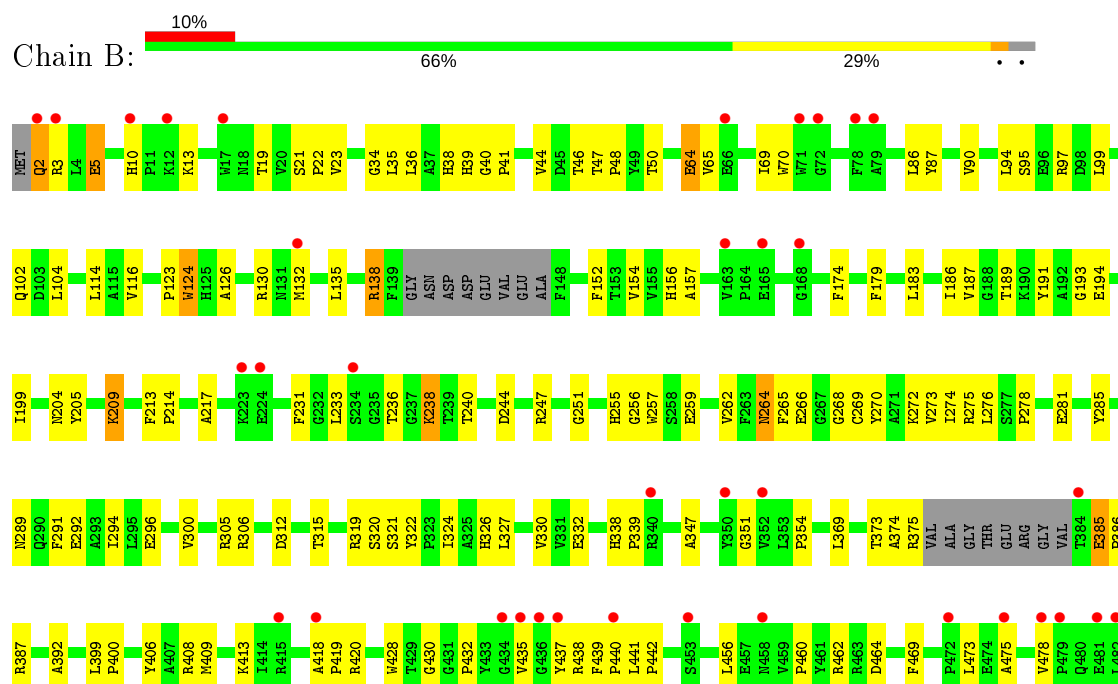
3 Residue-property plots

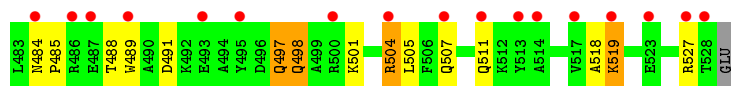
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Phosphoenolpyruvate carboxykinase [ATP]

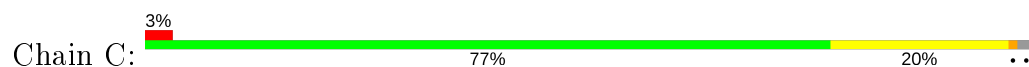


• Molecule 1: Phosphoenolpyruvate carboxykinase [ATP]

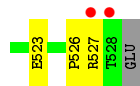
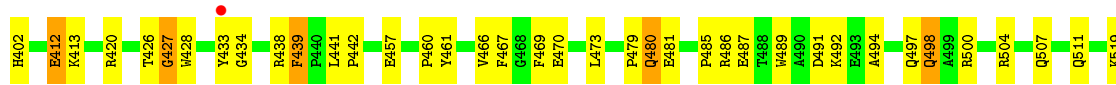
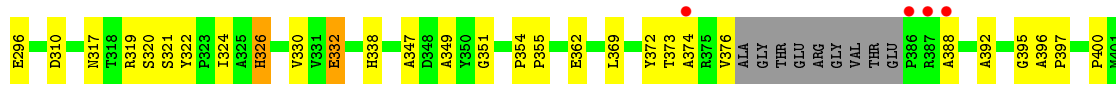
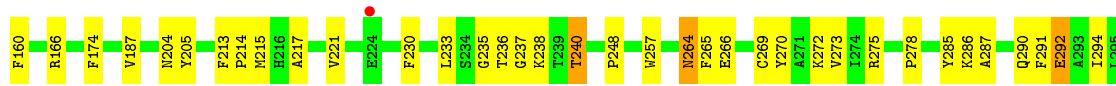
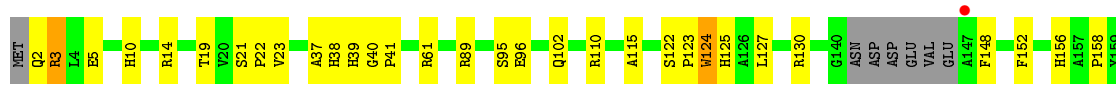




• Molecule 1: Phosphoenolpyruvate carboxykinase [ATP]



• Molecule 1: Phosphoenolpyruvate carboxykinase [ATP]



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.69Å 128.55Å 178.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 2.40 39.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.91-2.40) 99.9 (39.91-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.250 0.207 , 0.246	Depositor DCC
R_{free} test set	4919 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17321	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: PO4, CA, 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	0.53	2/4215 (0.0%)	0.76	0/5731
1	B	0.53	3/4190 (0.1%)	0.73	0/5698
1	C	0.52	1/4231 (0.0%)	0.76	1/5753 (0.0%)
1	D	0.51	2/4190 (0.0%)	0.72	1/5697 (0.0%)
All	All	0.52	8/16826 (0.0%)	0.74	2/22879 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	TRP	NE1-CE2	8.84	1.49	1.37
1	D	489	TRP	NE1-CE2	8.79	1.49	1.37
1	B	489	TRP	NE1-CE2	8.76	1.49	1.37
1	D	124	TRP	NE1-CE2	8.76	1.49	1.37
1	A	428	TRP	NE1-CE2	8.74	1.49	1.37
1	C	124	TRP	NE1-CE2	8.73	1.49	1.37
1	B	70	TRP	NE1-CE2	8.64	1.48	1.37
1	B	124	TRP	NE1-CE2	8.61	1.48	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	272	LYS	O-C-N	-5.58	113.78	122.70
1	C	486	ARG	CD-NE-CZ	-5.29	116.20	123.60

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	4096	0	4026	72	0
1	B	4071	0	3998	123	0
1	C	4112	0	4034	82	0
1	D	4071	0	4003	109	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	15	0	0	1	0
3	B	15	0	0	0	0
3	C	30	0	0	1	0
3	D	20	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	1	0
4	C	31	0	12	3	0
4	D	31	0	12	6	0
5	A	241	0	0	2	0
5	B	95	0	0	5	0
5	C	207	0	0	6	0
5	D	220	0	0	10	0
All	All	17321	0	16109	384	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 12.

All (384) 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:2:GLN:NE2	1:B:2:GLN:HA	1.62	1.13
1:B:373:THR:HG22	1:B:374:ALA:H	1.06	1.10
1:C:291:PHE:O	1:C:292:GLU:HB2	1.50	1.10
1:B:38:HIS:O	1:B:39:HIS:HB2	1.54	1.06
1:B:10:HIS:O	1:B:95:SER:HB3	1.63	0.99
1:B:373:THR:HG22	1:B:374:ALA:N	1.86	0.89
1:D:124:TRP:HD1	5:D:3028:HOH:O	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ALA:H	1:B:373:THR:HG23	1.41	0.86
1:D:257:TRP:HE1	1:D:338:HIS:HD2	1.23	0.86
1:D:507:GLN:HA	1:D:507:GLN:HE21	1.41	0.83
1:A:415:ARG:NH1	5:A:3209:HOH:O	2.03	0.83
1:B:40:GLY:N	1:B:41:PRO:CD	2.42	0.82
1:D:40:GLY:N	1:D:41:PRO:HD2	1.95	0.81
1:B:2:GLN:CA	1:B:2:GLN:NE2	2.43	0.81
1:C:373:THR:HG23	1:C:374:ALA:N	1.96	0.81
1:D:40:GLY:N	1:D:41:PRO:CD	2.44	0.81
1:D:3:ARG:HB2	1:D:3:ARG:HH11	1.44	0.80
1:C:40:GLY:N	1:C:41:PRO:HD2	1.97	0.80
1:D:480:GLN:OE1	1:D:481:GLU:HG3	1.83	0.78
1:C:273:VAL:HG11	1:C:320:SER:HB2	1.64	0.78
1:B:460:PRO:HB2	1:B:473:LEU:HD12	1.65	0.77
1:C:163:VAL:HB	1:C:166:ARG:HB3	1.67	0.77
1:B:2:GLN:HE21	1:B:2:GLN:HA	1.50	0.77
1:B:264:ASN:HD22	1:B:265:PHE:N	1.84	0.76
1:D:124:TRP:CZ2	1:D:125:HIS:CE1	2.73	0.76
1:A:40:GLY:N	1:A:41:PRO:CD	2.48	0.76
1:B:40:GLY:N	1:B:41:PRO:HD2	2.02	0.75
1:B:332:GLU:HG2	5:B:3088:HOH:O	1.85	0.75
1:B:291:PHE:O	1:B:292:GLU:HB2	1.86	0.74
1:C:441:LEU:HB3	1:C:442:PRO:HD3	1.69	0.74
1:B:373:THR:CG2	1:B:374:ALA:H	1.87	0.74
1:A:38:HIS:O	1:A:41:PRO:HD2	1.88	0.74
1:D:217:ALA:HB1	1:D:230:PHE:O	1.87	0.73
1:D:96:GLU:HG2	5:D:3180:HOH:O	1.86	0.73
1:B:264:ASN:ND2	1:B:266:GLU:H	1.87	0.72
1:D:123:PRO:HD2	5:D:3028:HOH:O	1.90	0.71
1:D:38:HIS:O	1:D:39:HIS:HB2	1.88	0.71
1:A:276:LEU:HD21	1:A:285:TYR:HA	1.73	0.70
1:D:89:ARG:CZ	1:D:166:ARG:HD2	2.22	0.70
1:D:507:GLN:HA	1:D:507:GLN:NE2	2.07	0.70
1:D:40:GLY:H	1:D:41:PRO:HD2	1.55	0.69
1:A:291:PHE:O	1:A:292:GLU:HB2	1.93	0.69
1:D:102:GLN:HE22	1:D:130:ARG:HH11	1.41	0.69
1:D:460:PRO:HB2	1:D:473:LEU:HD12	1.74	0.68
1:C:291:PHE:O	1:C:292:GLU:CB	2.33	0.68
1:C:486:ARG:HD3	5:C:3148:HOH:O	1.93	0.68
1:A:14:ARG:CG	1:A:14:ARG:HH11	2.07	0.67
1:B:240:THR:HG22	4:B:1001:ATP:O1A	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:GLY:N	1:C:41:PRO:CD	2.58	0.66
1:A:276:LEU:HD12	1:A:281:GLU:HB2	1.77	0.66
1:D:461:TYR:HB3	1:D:470:GLU:HG3	1.78	0.66
1:C:338:HIS:HE1	5:C:3085:HOH:O	1.79	0.65
1:A:38:HIS:O	1:A:39:HIS:HB2	1.96	0.65
1:A:387:ARG:CG	1:A:387:ARG:O	2.44	0.65
1:A:387:ARG:HG2	1:A:387:ARG:O	1.95	0.65
1:C:415:ARG:HG2	1:C:415:ARG:HH11	1.62	0.65
1:B:40:GLY:H	1:B:41:PRO:HD2	1.60	0.64
1:D:240:THR:HG22	4:D:1004:ATP:O1A	1.97	0.64
1:B:236:THR:HG21	5:B:3018:HOH:O	1.97	0.64
1:B:375:ARG:HH11	1:B:387:ARG:HE	1.46	0.64
1:B:375:ARG:NH1	1:B:387:ARG:HE	1.96	0.64
1:C:38:HIS:O	1:C:39:HIS:HB2	1.97	0.64
1:B:65:VAL:O	1:B:69:ILE:HG12	1.99	0.63
3:C:3016:PO4:O3	4:C:1002:ATP:O1G	2.16	0.63
1:B:13:LYS:HG3	1:B:97:ARG:HA	1.81	0.63
1:A:14:ARG:HG2	1:A:14:ARG:NH1	2.13	0.63
1:C:68:GLU:OE2	1:C:209:LYS:NZ	2.33	0.62
1:A:40:GLY:N	1:A:41:PRO:HD2	2.15	0.62
1:A:14:ARG:CG	1:A:14:ARG:NH1	2.63	0.61
1:B:430:GLY:HA3	1:B:488:THR:HG22	1.81	0.61
1:B:2:GLN:CA	1:B:2:GLN:HE21	2.09	0.61
1:D:412:GLU:HG3	1:D:413:LYS:N	2.14	0.61
1:D:204:ASN:ND2	1:D:214:PRO:HB2	2.15	0.61
1:D:3:ARG:HG3	1:D:5:GLU:OE1	2.00	0.61
1:B:135:LEU:O	1:B:138:ARG:HB2	1.99	0.60
1:C:274:ILE:O	1:C:275:ARG:HB2	2.00	0.60
1:B:475:ALA:HB3	1:B:478:VAL:HB	1.83	0.60
1:A:526:PRO:O	1:A:527:ARG:C	2.39	0.60
1:D:349:ALA:H	1:D:374:ALA:HB3	1.65	0.60
1:B:498:GLN:CA	1:B:498:GLN:HE21	2.15	0.59
1:D:355:PRO:HB3	1:D:439:PHE:CZ	2.37	0.59
1:D:257:TRP:HE1	1:D:338:HIS:CD2	2.13	0.59
1:B:268:GLY:HA2	1:B:324:ILE:HG13	1.83	0.58
1:B:50:THR:HB	1:B:315:THR:HG21	1.85	0.58
1:D:264:ASN:ND2	1:D:266:GLU:H	2.01	0.58
1:D:491:ASP:OD2	1:D:494:ALA:HB2	2.04	0.58
1:D:291:PHE:O	1:D:292:GLU:HB2	2.03	0.57
1:C:273:VAL:CG1	1:C:320:SER:HB2	2.34	0.57
1:A:52:ARG:HD3	1:A:197:LYS:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:TYR:N	1:B:437:TYR:CD1	2.72	0.57
1:C:460:PRO:HB2	1:C:473:LEU:HD12	1.86	0.57
1:B:217:ALA:HB2	1:B:231:PHE:HA	1.87	0.57
1:D:349:ALA:H	1:D:374:ALA:CB	2.17	0.57
1:D:372:TYR:HE1	1:D:388:ALA:HB1	1.70	0.57
1:C:273:VAL:O	1:C:276:LEU:HB2	2.05	0.57
1:B:40:GLY:O	1:B:291:PHE:HA	2.04	0.57
1:C:89:ARG:NE	1:C:166:ARG:HD2	2.19	0.57
1:B:86:LEU:O	1:B:90:VAL:HG23	2.05	0.56
1:A:120:THR:HB	1:A:156:HIS:HB3	1.87	0.56
1:B:430:GLY:CA	1:B:488:THR:HG22	2.35	0.56
1:C:241:LEU:HD13	1:C:448:LEU:HD11	1.88	0.56
1:D:324:ILE:HG22	5:D:3164:HOH:O	2.05	0.56
1:B:204:ASN:ND2	1:B:214:PRO:HB2	2.21	0.56
1:B:3:ARG:HB2	1:B:5:GLU:HG2	1.87	0.56
1:C:408:ARG:HD3	1:D:61:ARG:HH22	1.71	0.56
1:A:276:LEU:CD1	1:A:281:GLU:HB2	2.36	0.56
1:A:60:VAL:HG12	1:A:62:GLU:HG3	1.87	0.56
1:D:102:GLN:HE22	1:D:130:ARG:NH1	2.03	0.56
1:D:347:ALA:HB3	1:D:373:THR:HG23	1.88	0.56
1:D:491:ASP:HB3	1:D:494:ALA:HB3	1.87	0.56
1:A:362:GLU:OE2	1:A:415:ARG:NH2	2.39	0.56
1:B:273:VAL:HG11	1:B:320:SER:HB2	1.87	0.56
1:B:501:LYS:O	1:B:505:LEU:HG	2.06	0.56
1:B:34:GLY:O	1:B:35:LEU:HD23	2.05	0.55
1:D:270:TYR:OH	1:D:296:GLU:OE1	2.22	0.55
1:B:39:HIS:HB3	1:B:289:ASN:O	2.06	0.55
1:B:64:GLU:CD	1:B:64:GLU:H	2.10	0.55
1:D:507:GLN:CA	1:D:507:GLN:HE21	2.14	0.55
1:A:362:GLU:CD	1:A:362:GLU:H	2.09	0.55
1:C:40:GLY:H	1:C:41:PRO:HD2	1.70	0.55
1:C:460:PRO:HG2	1:C:473:LEU:HB2	1.88	0.55
1:B:268:GLY:CA	1:B:324:ILE:HG13	2.36	0.55
1:D:38:HIS:O	1:D:41:PRO:HD2	2.07	0.55
1:A:469:PHE:CD1	1:A:469:PHE:C	2.81	0.54
1:D:204:ASN:HD22	1:D:214:PRO:HB2	1.73	0.54
1:D:233:LEU:HD12	1:D:373:THR:HB	1.89	0.54
1:B:432:PRO:HD2	1:B:435:VAL:HB	1.90	0.54
1:B:498:GLN:HA	1:B:498:GLN:HE21	1.73	0.54
1:B:339:PRO:O	1:B:419:PRO:HB3	2.07	0.54
1:C:21:SER:HB2	1:C:22:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LEU:O	1:B:236:THR:HG23	2.08	0.54
1:A:191:TYR:CE2	1:A:193:GLY:HA3	2.43	0.53
1:A:16:PHE:CZ	1:A:27:HIS:HE1	2.26	0.53
1:B:276:LEU:HD12	1:B:281:GLU:OE1	2.08	0.53
1:B:418:ALA:N	1:B:419:PRO:HD3	2.23	0.53
1:D:233:LEU:O	1:D:236:THR:HG23	2.09	0.53
1:D:37:ALA:O	1:D:38:HIS:C	2.44	0.53
1:A:460:PRO:HD2	1:A:474:GLU:HG2	1.90	0.53
1:B:114:LEU:O	1:B:116:VAL:HG23	2.09	0.53
1:B:123:PRO:O	1:B:126:ALA:HB3	2.09	0.53
1:D:354:PRO:HA	1:D:485:PRO:HG3	1.91	0.53
1:D:264:ASN:HD22	1:D:265:PHE:N	2.07	0.53
1:A:104:LEU:CD2	1:A:135:LEU:HD23	2.39	0.53
1:B:251:GLY:HA3	1:B:255:HIS:NE2	2.23	0.53
1:D:122:SER:HB3	1:D:125:HIS:HB2	1.91	0.53
1:B:375:ARG:O	1:B:386:PRO:HA	2.09	0.53
1:C:30:LEU:HD23	1:C:30:LEU:O	2.09	0.53
1:D:21:SER:HB2	1:D:22:PRO:HD3	1.91	0.53
1:B:456:LEU:HB2	5:B:3095:HOH:O	2.09	0.52
1:D:497:GLN:CD	1:D:500:ARG:HH12	2.12	0.52
1:A:46:THR:HG21	1:A:296:GLU:OE2	2.10	0.52
1:D:124:TRP:CD1	5:D:3028:HOH:O	2.42	0.52
1:D:273:VAL:HG11	1:D:320:SER:HB2	1.91	0.52
1:D:434:GLY:HA2	5:D:3223:HOH:O	2.10	0.52
1:B:130:ARG:HG3	1:B:135:LEU:HD21	1.90	0.51
1:A:469:PHE:HD1	1:A:469:PHE:C	2.13	0.51
1:B:327:LEU:HD11	5:B:3044:HOH:O	2.09	0.51
1:B:439:PHE:CG	1:B:440:PRO:HD2	2.46	0.51
1:B:46:THR:HG21	1:B:296:GLU:OE2	2.10	0.51
1:D:500:ARG:HG2	1:D:504:ARG:NH1	2.25	0.51
1:C:30:LEU:HD23	1:C:30:LEU:C	2.30	0.51
1:A:339:PRO:O	1:A:419:PRO:HB3	2.11	0.51
1:A:460:PRO:HB2	1:A:473:LEU:HD12	1.92	0.51
1:A:493:GLU:HA	1:A:493:GLU:OE1	2.10	0.51
1:B:264:ASN:HD22	1:B:265:PHE:H	1.52	0.51
1:C:38:HIS:O	1:C:41:PRO:HD2	2.11	0.51
1:B:213:PHE:HB3	1:B:257:TRP:HB3	1.93	0.51
1:B:354:PRO:HA	1:B:485:PRO:HG3	1.93	0.51
1:C:269:CYS:HB2	1:C:322:TYR:CE1	2.46	0.51
1:D:441:LEU:HB3	1:D:442:PRO:HD3	1.92	0.51
1:D:519:LYS:O	1:D:523:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:HG21	1:A:433:TYR:CE2	2.46	0.51
1:C:64:GLU:HG3	1:C:180:GLN:HG3	1.93	0.51
1:C:191:TYR:CE2	1:C:193:GLY:HA3	2.46	0.50
1:A:257:TRP:CZ2	1:A:339:PRO:HD2	2.46	0.50
1:B:462:ARG:HB3	1:B:473:LEU:HD21	1.93	0.50
1:D:237:GLY:HA2	1:D:240:THR:CG2	2.40	0.50
1:D:487:GLU:O	1:D:487:GLU:HG2	2.10	0.50
1:A:375:ARG:HB2	1:A:387:ARG:HG2	1.93	0.50
1:C:274:ILE:HG23	1:C:274:ILE:O	2.10	0.50
1:C:339:PRO:O	1:C:419:PRO:HB3	2.12	0.50
1:D:426:THR:HB	4:D:1004:ATP:N1	2.27	0.50
1:D:498:GLN:HA	1:D:498:GLN:HE21	1.77	0.50
1:C:215:MET:HB3	1:C:231:PHE:CE2	2.45	0.50
1:D:275:ARG:HA	1:D:310:ASP:OD1	2.12	0.50
1:B:102:GLN:HE22	1:B:130:ARG:HH11	1.59	0.50
1:B:439:PHE:CD1	1:B:440:PRO:HD2	2.47	0.50
1:B:205:TYR:HB2	1:B:400:PRO:HG3	1.94	0.50
1:B:324:ILE:HG22	1:B:330:VAL:HG21	1.94	0.49
1:C:64:GLU:H	1:C:64:GLU:CD	2.15	0.49
1:D:351:GLY:HA2	1:D:428:TRP:O	2.12	0.49
1:A:291:PHE:O	1:A:292:GLU:CB	2.59	0.49
1:D:2:GLN:O	1:D:2:GLN:HG2	2.12	0.49
1:A:124:TRP:CE3	1:A:124:TRP:O	2.65	0.49
1:B:21:SER:HB2	1:B:22:PRO:HD3	1.94	0.49
1:D:292:GLU:OE1	1:D:326:HIS:HE1	1.96	0.49
1:A:296:GLU:HG2	5:A:3195:HOH:O	2.12	0.49
1:C:338:HIS:CE1	5:C:3085:HOH:O	2.59	0.49
1:B:154:VAL:CG2	1:B:199:ILE:HD11	2.43	0.49
1:D:287:ALA:O	1:D:326:HIS:HD2	1.94	0.49
1:C:470:GLU:OE2	5:C:3196:HOH:O	2.19	0.48
1:D:355:PRO:HB3	1:D:439:PHE:CE2	2.48	0.48
1:B:174:PHE:CD1	1:B:174:PHE:C	2.86	0.48
1:B:191:TYR:CE2	1:B:193:GLY:HA3	2.48	0.48
1:C:369:LEU:O	1:C:392:ALA:HA	2.12	0.48
1:D:481:GLU:HA	1:D:487:GLU:OE2	2.13	0.48
1:C:124:TRP:CZ3	1:C:294:ILE:HG21	2.49	0.48
1:C:415:ARG:NH1	1:C:415:ARG:HG2	2.27	0.48
1:D:127:LEU:HG	1:D:294:ILE:HD11	1.96	0.48
1:D:330:VAL:HG23	1:D:332:GLU:OE1	2.14	0.48
1:D:427:GLY:O	1:D:438:ARG:HG3	2.14	0.48
1:B:441:LEU:HB3	1:B:442:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:THR:HG23	1:C:374:ALA:H	1.75	0.48
1:A:233:LEU:HD12	1:A:373:THR:HG22	1.95	0.47
1:A:469:PHE:HD1	1:A:469:PHE:O	1.95	0.47
1:B:354:PRO:CA	1:B:485:PRO:HG3	2.44	0.47
1:C:124:TRP:O	1:C:124:TRP:CE3	2.67	0.47
1:A:495:TYR:C	1:A:495:TYR:CD1	2.87	0.47
1:B:294:ILE:HB	1:B:321:SER:HB3	1.95	0.47
1:D:110:ARG:HD2	5:D:3199:HOH:O	2.14	0.47
1:A:274:ILE:HG13	1:A:275:ARG:HG3	1.97	0.47
1:D:467:PHE:CD2	1:D:526:PRO:HB3	2.50	0.47
1:C:373:THR:CG2	1:C:374:ALA:N	2.65	0.47
1:B:104:LEU:CD2	1:B:135:LEU:HD23	2.44	0.47
1:D:89:ARG:NH2	1:D:166:ARG:HD2	2.30	0.47
1:D:486:ARG:NH1	1:D:492:LYS:HB3	2.30	0.47
1:C:458:ASN:ND2	5:C:3190:HOH:O	2.48	0.47
1:A:130:ARG:NH1	3:A:3001:PO4:O3	2.48	0.46
1:B:10:HIS:O	1:B:95:SER:CB	2.51	0.46
1:D:376:VAL:HG21	1:D:433:TYR:CE2	2.50	0.46
1:B:504:ARG:HG3	1:B:504:ARG:HH11	1.81	0.46
1:B:189:THR:HG21	1:B:194:GLU:HG3	1.97	0.46
1:C:257:TRP:CZ2	1:C:339:PRO:HD2	2.50	0.46
1:B:157:ALA:HB3	1:B:187:VAL:HG12	1.98	0.46
1:B:420:ARG:NH1	1:B:420:ARG:HB2	2.30	0.46
1:C:37:ALA:HB3	1:C:41:PRO:HG2	1.97	0.46
1:D:10:HIS:O	1:D:95:SER:HB3	2.15	0.46
1:D:369:LEU:O	1:D:392:ALA:HA	2.14	0.46
1:D:291:PHE:O	1:D:292:GLU:CB	2.63	0.46
1:D:2:GLN:HB3	5:D:3188:HOH:O	2.16	0.46
1:B:257:TRP:CZ2	1:B:339:PRO:HD2	2.51	0.46
1:C:3:ARG:HD2	1:C:3:ARG:HH11	1.60	0.46
1:D:115:ALA:HB1	1:D:148:PHE:CZ	2.51	0.46
1:B:269:CYS:HB2	1:B:322:TYR:CE1	2.52	0.45
1:B:498:GLN:HA	1:B:498:GLN:NE2	2.31	0.45
1:C:163:VAL:HG12	1:C:166:ARG:H	1.80	0.45
1:D:294:ILE:HB	1:D:321:SER:HB3	1.98	0.45
1:D:376:VAL:HG21	1:D:433:TYR:CD2	2.51	0.45
1:B:204:ASN:HD22	1:B:214:PRO:HB2	1.80	0.45
1:C:60:VAL:HG12	1:C:62:GLU:HG3	1.97	0.45
1:D:221:VAL:O	1:D:248:PRO:HD2	2.16	0.45
1:D:235:GLY:N	4:D:1004:ATP:O2B	2.49	0.45
1:D:402:HIS:HD2	5:D:3039:HOH:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ARG:NH2	5:C:3113:HOH:O	2.46	0.45
1:C:527:ARG:HG2	1:C:529:GLU:O	2.16	0.45
1:B:270:TYR:O	1:B:319:ARG:NH2	2.49	0.45
1:B:36:LEU:O	1:B:305:ARG:NH1	2.50	0.45
1:B:274:ILE:HG23	1:B:274:ILE:O	2.17	0.45
1:B:156:HIS:HD2	1:B:186:ILE:HB	1.81	0.45
1:C:10:HIS:O	1:C:95:SER:HB3	2.18	0.45
1:D:235:GLY:H	4:D:1004:ATP:PB	2.40	0.45
1:C:238:LYS:HB2	4:C:1002:ATP:O2B	2.17	0.44
1:D:124:TRP:CE2	1:D:125:HIS:CE1	3.05	0.44
1:A:65:VAL:O	1:A:69:ILE:HG12	2.17	0.44
1:B:87:TYR:CE1	1:B:183:LEU:HD13	2.52	0.44
1:C:362:GLU:CD	1:C:362:GLU:H	2.21	0.44
1:C:408:ARG:HD3	1:D:61:ARG:NH2	2.31	0.44
1:B:47:THR:HB	1:B:48:PRO:HA	2.00	0.44
1:C:124:TRP:HE3	1:C:294:ILE:HD13	1.81	0.44
1:B:462:ARG:HG3	1:B:462:ARG:O	2.16	0.44
1:B:94:LEU:O	1:B:99:LEU:HD21	2.17	0.44
1:B:19:THR:CG2	1:B:23:VAL:HB	2.48	0.44
1:D:466:VAL:O	1:D:527:ARG:HG2	2.16	0.44
1:B:217:ALA:HA	1:B:238:LYS:HD2	1.99	0.44
1:C:428:TRP:CE2	1:C:438:ARG:HD2	2.52	0.44
1:C:504:ARG:HA	1:C:507:GLN:HE21	1.81	0.44
1:D:290:GLN:HG3	1:D:326:HIS:CD2	2.53	0.44
1:A:385:GLU:HB2	1:A:386:PRO:HD2	2.00	0.44
1:A:372:TYR:CG	1:A:373:THR:N	2.86	0.44
1:B:497:GLN:HA	1:B:497:GLN:NE2	2.33	0.44
1:D:286:LYS:HB2	1:D:286:LYS:HE3	1.86	0.44
1:D:372:TYR:HE1	1:D:388:ALA:CB	2.31	0.44
1:D:479:PRO:CB	1:D:481:GLU:OE1	2.66	0.44
1:B:418:ALA:N	1:B:419:PRO:CD	2.81	0.43
1:C:279:GLU:CD	1:C:279:GLU:H	2.21	0.43
1:D:14:ARG:HD2	5:D:3136:HOH:O	2.17	0.43
1:D:174:PHE:HB3	1:D:187:VAL:HG22	2.01	0.43
1:D:420:ARG:HD3	1:D:457:GLU:OE2	2.17	0.43
1:A:257:TRP:HE1	1:A:338:HIS:HD2	1.65	0.43
1:B:274:ILE:O	1:B:275:ARG:HB2	2.18	0.43
1:C:274:ILE:CG2	1:C:274:ILE:O	2.66	0.43
1:A:301:ASN:O	1:A:305:ARG:HA	2.18	0.43
1:B:420:ARG:HB2	1:B:420:ARG:HH11	1.82	0.43
1:A:61:ARG:HG3	1:A:66:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LEU:O	1:B:236:THR:CG2	2.67	0.43
1:B:38:HIS:HB2	1:B:306:ARG:HD3	1.99	0.43
1:C:101:VAL:HA	1:C:118:VAL:O	2.19	0.43
1:C:352:VAL:CG2	1:C:498:GLN:HG3	2.48	0.43
1:B:38:HIS:O	1:B:39:HIS:CB	2.37	0.43
1:C:130:ARG:HG3	1:C:135:LEU:HD21	2.00	0.43
1:A:275:ARG:NE	1:C:434:GLY:O	2.47	0.43
1:B:437:TYR:N	1:B:437:TYR:HD1	2.16	0.43
1:D:374:ALA:HA	1:D:388:ALA:HA	2.00	0.43
1:B:244:ASP:HB3	1:B:247:ARG:HB2	2.01	0.43
1:B:399:LEU:HD22	1:B:406:TYR:CE2	2.53	0.43
1:C:527:ARG:O	1:C:528:THR:C	2.57	0.43
1:D:396:ALA:N	1:D:397:PRO:CD	2.82	0.43
1:A:355:PRO:HB2	1:A:447:LEU:CD1	2.49	0.43
1:B:257:TRP:CE2	1:B:413:LYS:HD2	2.54	0.43
1:B:138:ARG:HD2	1:B:138:ARG:HA	1.50	0.42
1:B:205:TYR:O	1:B:209:LYS:HD3	2.19	0.42
1:D:238:LYS:HB3	4:D:1004:ATP:O1B	2.19	0.42
1:C:301:ASN:O	1:C:305:ARG:HA	2.20	0.42
1:D:362:GLU:CD	1:D:362:GLU:H	2.23	0.42
1:A:199:ILE:HD13	1:A:199:ILE:HA	1.94	0.42
1:B:272:LYS:NZ	1:B:272:LYS:HB3	2.34	0.42
1:C:233:LEU:O	1:C:236:THR:HG23	2.19	0.42
1:C:196:LYS:NZ	1:C:254:GLU:OE2	2.51	0.42
1:D:317:ASN:OD1	1:D:319:ARG:HD3	2.19	0.42
1:A:86:LEU:O	1:A:90:VAL:HG23	2.19	0.42
1:C:351:GLY:HA2	1:C:428:TRP:O	2.20	0.42
1:C:84:GLU:HA	1:C:84:GLU:OE1	2.19	0.42
1:D:269:CYS:HB2	1:D:322:TYR:CE1	2.54	0.42
1:A:40:GLY:H	1:A:41:PRO:HD2	1.80	0.42
1:B:2:GLN:HB3	5:B:3055:HOH:O	2.20	0.42
1:B:438:ARG:HH11	1:B:438:ARG:HD3	1.61	0.42
1:C:257:TRP:CE2	1:C:339:PRO:HD2	2.54	0.42
1:C:5:GLU:OE1	1:C:5:GLU:N	2.51	0.42
1:A:40:GLY:N	1:A:41:PRO:HD3	2.32	0.42
1:C:221:VAL:O	1:C:248:PRO:HD2	2.19	0.42
1:D:240:THR:HG21	4:D:1004:ATP:H2'	2.01	0.42
1:D:278:PRO:HG3	1:D:285:TYR:CE1	2.55	0.42
1:B:278:PRO:HG3	1:B:285:TYR:CE2	2.54	0.42
1:B:312:ASP:OD1	1:B:312:ASP:C	2.57	0.42
1:B:507:GLN:HA	1:B:507:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:LYS:NZ	4:C:1002:ATP:O3G	2.41	0.42
1:C:323:PRO:O	1:C:326:HIS:HB2	2.20	0.42
1:D:507:GLN:CA	1:D:507:GLN:NE2	2.77	0.42
1:A:107:GLY:HA2	1:A:265:PHE:HA	2.01	0.42
1:A:270:TYR:O	1:A:319:ARG:NH1	2.53	0.42
1:C:327:LEU:HB3	1:C:330:VAL:CG1	2.49	0.42
1:A:3:ARG:HB2	1:A:5:GLU:OE1	2.20	0.42
1:B:519:LYS:H	1:B:519:LYS:HG2	1.51	0.42
1:C:197:LYS:HA	1:C:197:LYS:HD3	1.75	0.42
1:D:19:THR:HG22	1:D:23:VAL:HB	2.02	0.42
1:A:124:TRP:HE3	1:A:124:TRP:O	2.03	0.41
1:A:162:ALA:O	1:A:172:GLU:HA	2.19	0.41
1:A:432:PRO:HD3	1:A:489:TRP:CH2	2.54	0.41
1:B:369:LEU:O	1:B:392:ALA:HA	2.19	0.41
1:A:441:LEU:HB3	1:A:442:PRO:HD3	2.02	0.41
1:C:63:PRO:HA	1:C:66:GLU:HG3	2.02	0.41
1:A:262:VAL:CG1	1:A:263:PHE:N	2.82	0.41
1:B:351:GLY:HA2	1:B:428:TRP:O	2.21	0.41
1:B:488:THR:HG22	1:B:488:THR:O	2.19	0.41
1:C:355:PRO:HG3	1:C:439:PHE:CE1	2.56	0.41
1:C:312:ASP:C	1:C:312:ASP:OD1	2.59	0.41
1:D:38:HIS:O	1:D:39:HIS:CB	2.62	0.41
1:A:227:VAL:HG12	1:A:228:ALA:N	2.35	0.41
1:A:396:ALA:N	1:A:397:PRO:CD	2.82	0.41
1:C:432:PRO:HD2	1:C:435:VAL:HB	2.01	0.41
1:D:217:ALA:HB1	1:D:230:PHE:C	2.40	0.41
1:A:362:GLU:CD	1:A:362:GLU:N	2.74	0.41
1:D:156:HIS:CE1	1:D:158:PRO:HD3	2.55	0.41
1:A:338:HIS:HA	1:A:339:PRO:HD3	1.94	0.41
1:B:44:VAL:HG21	1:B:124:TRP:CH2	2.55	0.41
1:B:256:GLY:O	1:B:262:VAL:HA	2.20	0.41
1:C:58:PHE:O	1:C:176:GLY:HA2	2.21	0.41
1:D:205:TYR:HB2	1:D:400:PRO:HG3	2.03	0.41
1:B:251:GLY:HA3	1:B:255:HIS:CE1	2.56	0.41
1:B:64:GLU:N	1:B:64:GLU:CD	2.72	0.41
1:A:469:PHE:CD1	1:A:469:PHE:O	2.74	0.40
1:B:300:VAL:O	1:B:300:VAL:HG13	2.21	0.40
1:D:160:PHE:C	1:D:160:PHE:CD1	2.95	0.40
1:A:478:VAL:HA	1:A:479:PRO:HD3	1.97	0.40
1:B:65:VAL:HG11	1:B:179:PHE:HB2	2.04	0.40
1:B:338:HIS:HA	1:B:339:PRO:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:PHE:CE1	1:C:27:HIS:HE1	2.38	0.40
1:A:13:LYS:HG3	1:A:97:ARG:HA	2.02	0.40
1:A:296:GLU:O	1:A:297:ASN:HB2	2.21	0.40
1:C:459:VAL:HB	1:C:460:PRO:HD2	2.03	0.40
1:D:213:PHE:CE2	1:D:215:MET:HG2	2.56	0.40
1:A:124:TRP:CZ2	1:A:125:HIS:CE1	3.09	0.40
1:A:207:MET:HB2	1:A:208:PRO:HD3	2.04	0.40
1:A:290:GLN:HG3	1:A:326:HIS:CE1	2.57	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	509/529 (96%)	495 (97%)	13 (3%)	1 (0%)	47	62
1	B	505/529 (96%)	474 (94%)	29 (6%)	2 (0%)	34	48
1	C	511/529 (97%)	493 (96%)	17 (3%)	1 (0%)	47	62
1	D	506/529 (96%)	490 (97%)	13 (3%)	3 (1%)	25	36
All	All	2031/2116 (96%)	1952 (96%)	72 (4%)	7 (0%)	41	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	518	ALA
1	A	292	GLU
1	D	427	GLY
1	B	385	GLU
1	C	528	THR
1	D	292	GLU
1	D	395	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	427/438 (98%)	414 (97%)	13 (3%)	41	61
1	B	425/438 (97%)	401 (94%)	24 (6%)	21	34
1	C	429/438 (98%)	419 (98%)	10 (2%)	50	70
1	D	424/438 (97%)	412 (97%)	12 (3%)	43	63
All	All	1705/1752 (97%)	1646 (96%)	59 (4%)	36	55

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	14	ARG
1	A	120	THR
1	A	122	SER
1	A	152	PHE
1	A	259	GLU
1	A	332	GLU
1	A	387	ARG
1	A	416	LYS
1	A	463	ARG
1	A	469	PHE
1	A	480	GLN
1	A	527	ARG
1	B	2	GLN
1	B	5	GLU
1	B	64	GLU
1	B	132	MET
1	B	138	ARG
1	B	152	PHE
1	B	209	LYS
1	B	238	LYS
1	B	259	GLU
1	B	264	ASN
1	B	326	HIS

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Mol	Chain	Res	Type
1	B	385	GLU
1	B	408	ARG
1	B	409	MET
1	B	464	ASP
1	B	469	PHE
1	B	484	ASN
1	B	491	ASP
1	B	497	GLN
1	B	498	GLN
1	B	504	ARG
1	B	511	GLN
1	B	519	LYS
1	B	527	ARG
1	C	61	ARG
1	C	64	GLU
1	C	146	GLU
1	C	152	PHE
1	C	259	GLU
1	C	332	GLU
1	C	463	ARG
1	C	469	PHE
1	C	492	LYS
1	C	519	LYS
1	D	3	ARG
1	D	152	PHE
1	D	240	THR
1	D	264	ASN
1	D	326	HIS
1	D	332	GLU
1	D	412	GLU
1	D	439	PHE
1	D	469	PHE
1	D	480	GLN
1	D	498	GLN
1	D	511	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	HIS
1	A	458	ASN
1	A	480	GLN

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Mol	Chain	Res	Type
1	A	511	GLN
1	B	2	GLN
1	B	92	GLN
1	B	102	GLN
1	B	156	HIS
1	B	180	GLN
1	B	204	ASN
1	B	264	ASN
1	B	458	ASN
1	B	497	GLN
1	B	498	GLN
1	B	511	GLN
1	C	92	GLN
1	D	92	GLN
1	D	102	GLN
1	D	204	ASN
1	D	264	ASN
1	D	326	HIS
1	D	329	ASN
1	D	338	HIS
1	D	402	HIS
1	D	458	ASN
1	D	497	GLN
1	D	498	GLN
1	D	507	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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
3	PO4	C	3010	-	4,4,4	1.59	0	6,6,6	0.43	0
3	PO4	C	3017	-	4,4,4	3.01	3 (75%)	6,6,6	1.18	1 (16%)
3	PO4	B	3013	-	4,4,4	3.01	3 (75%)	6,6,6	1.18	1 (16%)
4	ATP	B	1001	-	26,33,33	0.96	1 (3%)	31,52,52	1.58	5 (16%)
3	PO4	A	3001	-	4,4,4	1.78	1 (25%)	6,6,6	0.41	0
3	PO4	B	3006	-	4,4,4	1.63	0	6,6,6	0.44	0
3	PO4	C	3007	-	4,4,4	1.67	0	6,6,6	0.43	0
3	PO4	C	3014	-	4,4,4	3.01	3 (75%)	6,6,6	1.18	1 (16%)
3	PO4	A	3009	-	4,4,4	1.62	0	6,6,6	0.45	0
3	PO4	D	3011	-	4,4,4	1.49	0	6,6,6	0.43	0
4	ATP	A	1003	-	26,33,33	1.11	2 (7%)	31,52,52	1.61	6 (19%)
3	PO4	D	3008	-	4,4,4	1.61	0	6,6,6	0.43	0
3	PO4	D	3015	-	4,4,4	3.01	3 (75%)	6,6,6	1.18	1 (16%)
3	PO4	C	3003	-	4,4,4	1.56	0	6,6,6	0.44	0
3	PO4	C	3016	-	4,4,4	3.00	3 (75%)	6,6,6	1.18	1 (16%)
3	PO4	A	3005	-	4,4,4	1.62	0	6,6,6	0.43	0
4	ATP	D	1004	-	26,33,33	0.96	1 (3%)	31,52,52	1.61	5 (16%)
3	PO4	D	3004	-	4,4,4	1.83	1 (25%)	6,6,6	0.42	0
4	ATP	C	1002	-	26,33,33	1.21	1 (3%)	31,52,52	1.62	5 (16%)
3	PO4	B	3002	-	4,4,4	1.57	0	6,6,6	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	1003	-	-	2/18/38/38	0/3/3/3
4	ATP	D	1004	-	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	B	1001	-	-	1/18/38/38	0/3/3/3
4	ATP	C	1002	-	-	2/18/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1002	ATP	PG-O3G	4.30	1.71	1.54
3	C	3017	PO4	P-O2	-4.02	1.42	1.54
3	C	3014	PO4	P-O2	-4.00	1.42	1.54
3	D	3015	PO4	P-O2	-4.00	1.42	1.54
3	C	3016	PO4	P-O2	-4.00	1.42	1.54
3	B	3013	PO4	P-O2	-3.98	1.42	1.54
3	D	3015	PO4	P-O1	-3.31	1.43	1.50
3	B	3013	PO4	P-O1	-3.30	1.43	1.50
3	C	3016	PO4	P-O1	-3.28	1.43	1.50
3	C	3014	PO4	P-O1	-3.27	1.43	1.50
3	C	3017	PO4	P-O1	-3.26	1.43	1.50
4	A	1003	ATP	PG-O2G	3.07	1.66	1.54
3	B	3013	PO4	P-O4	-3.06	1.45	1.54
3	C	3014	PO4	P-O4	-3.05	1.45	1.54
3	C	3017	PO4	P-O4	-3.05	1.45	1.54
3	C	3016	PO4	P-O4	-3.03	1.45	1.54
3	D	3015	PO4	P-O4	-3.02	1.45	1.54
4	B	1001	ATP	O4'-C1'	2.21	1.44	1.41
3	D	3004	PO4	P-O4	-2.19	1.48	1.54
4	A	1003	ATP	O4'-C1'	2.18	1.44	1.41
3	A	3001	PO4	P-O3	-2.18	1.48	1.54
4	D	1004	ATP	O4'-C1'	2.16	1.44	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1002	ATP	N3-C2-N1	-5.07	120.75	128.68
4	B	1001	ATP	N3-C2-N1	-4.88	121.06	128.68
4	D	1004	ATP	N3-C2-N1	-4.87	121.07	128.68
4	A	1003	ATP	N3-C2-N1	-4.77	121.23	128.68
4	C	1002	ATP	PA-O3A-PB	-4.21	118.39	132.83
4	D	1004	ATP	PB-O3B-PG	-3.70	120.15	132.83
4	D	1004	ATP	PA-O3A-PB	-3.66	120.26	132.83
4	B	1001	ATP	PA-O3A-PB	-3.53	120.73	132.83
4	A	1003	ATP	PA-O3A-PB	-3.51	120.80	132.83
4	B	1001	ATP	PB-O3B-PG	-3.38	121.22	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	ATP	PB-O3B-PG	-3.25	121.67	132.83
4	A	1003	ATP	O4'-C1'-C2'	-3.15	102.33	106.93
4	B	1001	ATP	O4'-C1'-C2'	-2.99	102.56	106.93
4	D	1004	ATP	O4'-C1'-C2'	-2.88	102.72	106.93
4	C	1002	ATP	O4'-C1'-C2'	-2.72	102.94	106.93
4	C	1002	ATP	PB-O3B-PG	-2.53	124.14	132.83
4	A	1003	ATP	C3'-C2'-C1'	-2.45	97.30	100.98
4	C	1002	ATP	C3'-C2'-C1'	-2.36	97.43	100.98
3	C	3016	PO4	O2-P-O1	2.33	119.41	110.89
3	C	3014	PO4	O2-P-O1	2.33	119.41	110.89
3	B	3013	PO4	O2-P-O1	2.32	119.39	110.89
3	C	3017	PO4	O2-P-O1	2.32	119.39	110.89
3	D	3015	PO4	O2-P-O1	2.32	119.37	110.89
4	D	1004	ATP	C3'-C2'-C1'	-2.28	97.55	100.98
4	B	1001	ATP	C3'-C2'-C1'	-2.24	97.61	100.98
4	A	1003	ATP	C4-C5-N7	-2.20	107.11	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1001	ATP	O4'-C4'-C5'-O5'
4	A	1003	ATP	PA-O3A-PB-O1B
4	C	1002	ATP	PB-O3B-PG-O3G
4	D	1004	ATP	O4'-C4'-C5'-O5'
4	D	1004	ATP	PG-O3B-PB-O2B
4	C	1002	ATP	O4'-C4'-C5'-O5'
4	A	1003	ATP	O4'-C4'-C5'-O5'

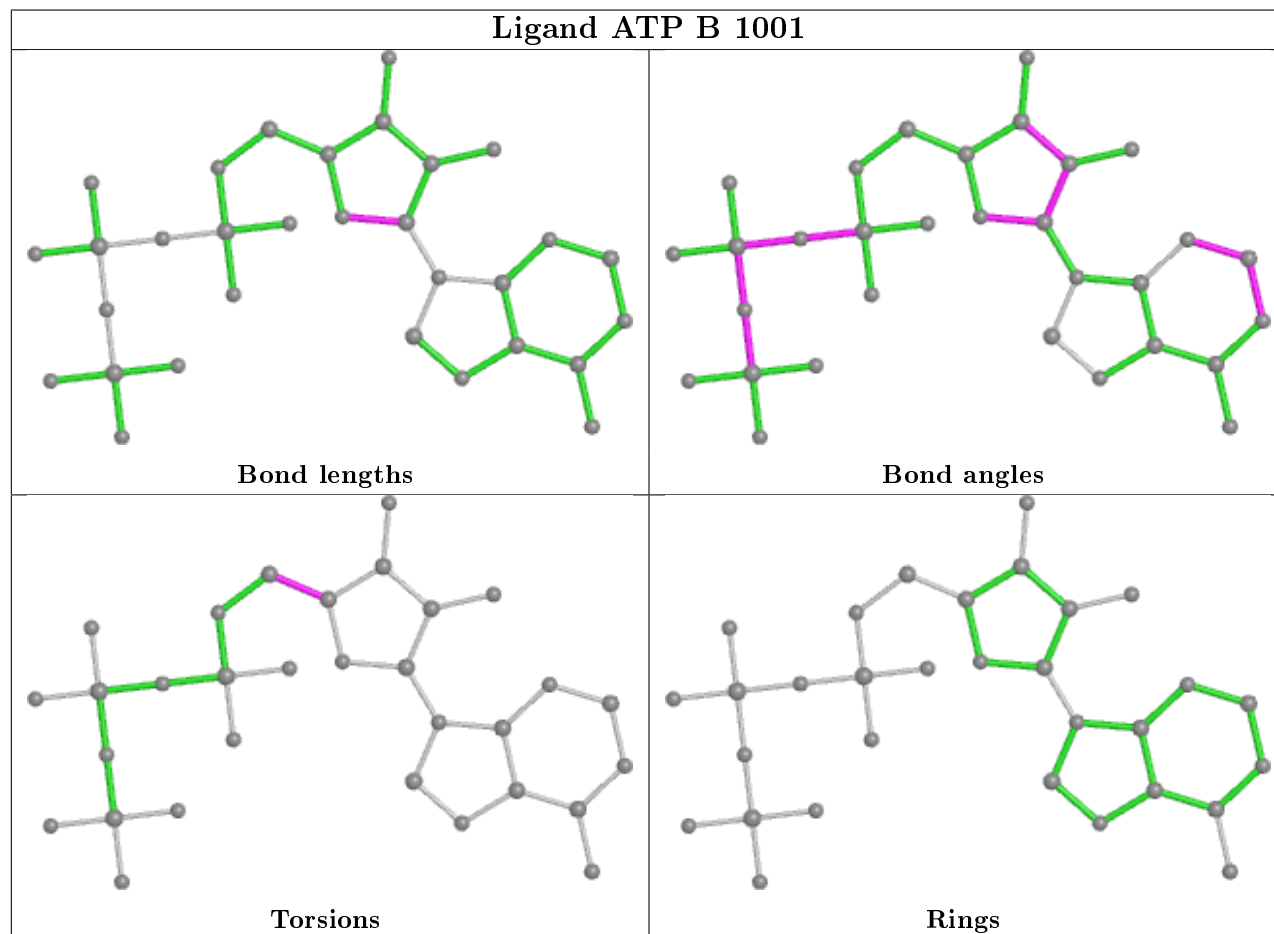
There are no ring outliers.

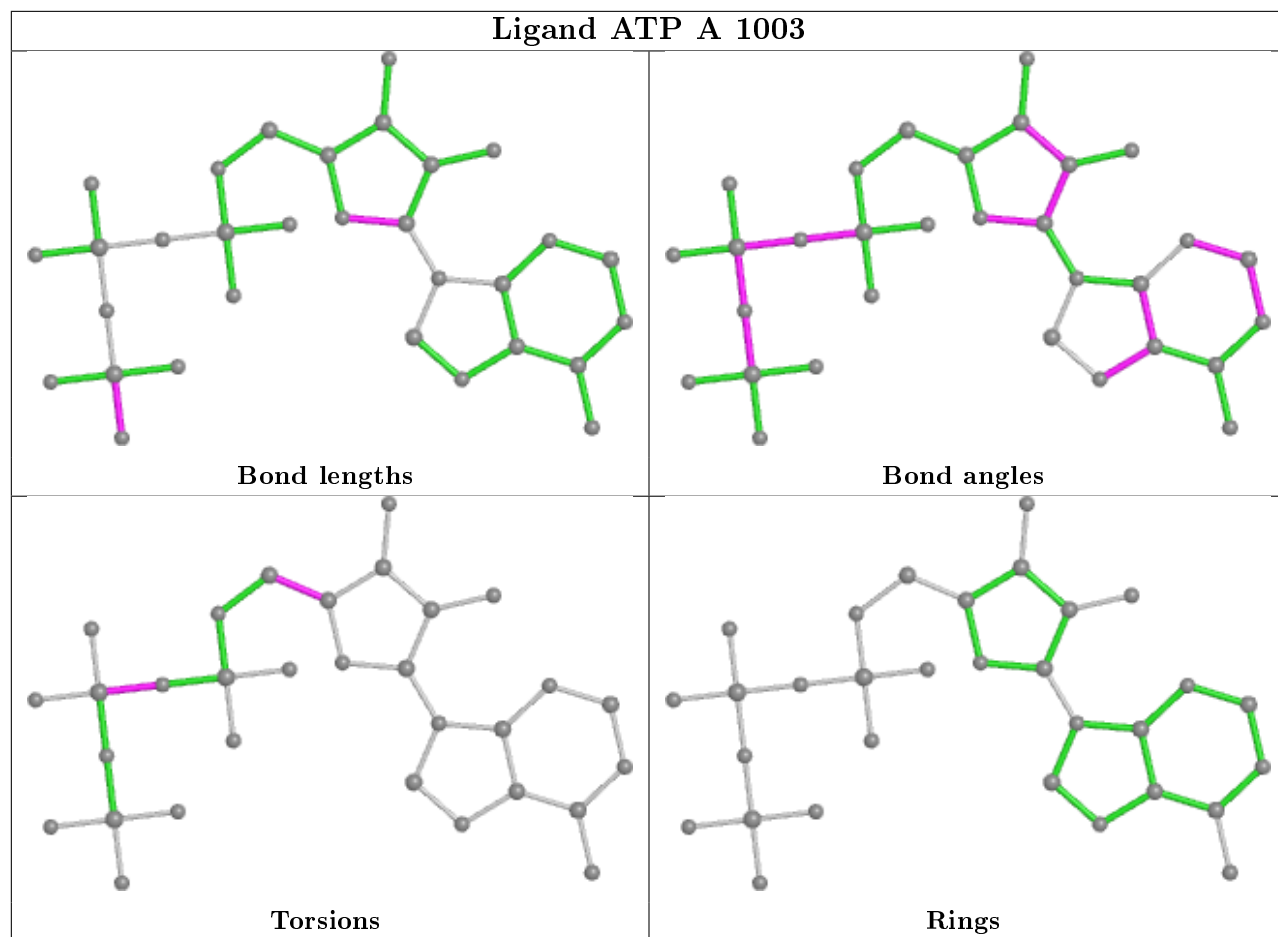
5 monomers are involved in 11 short contacts:

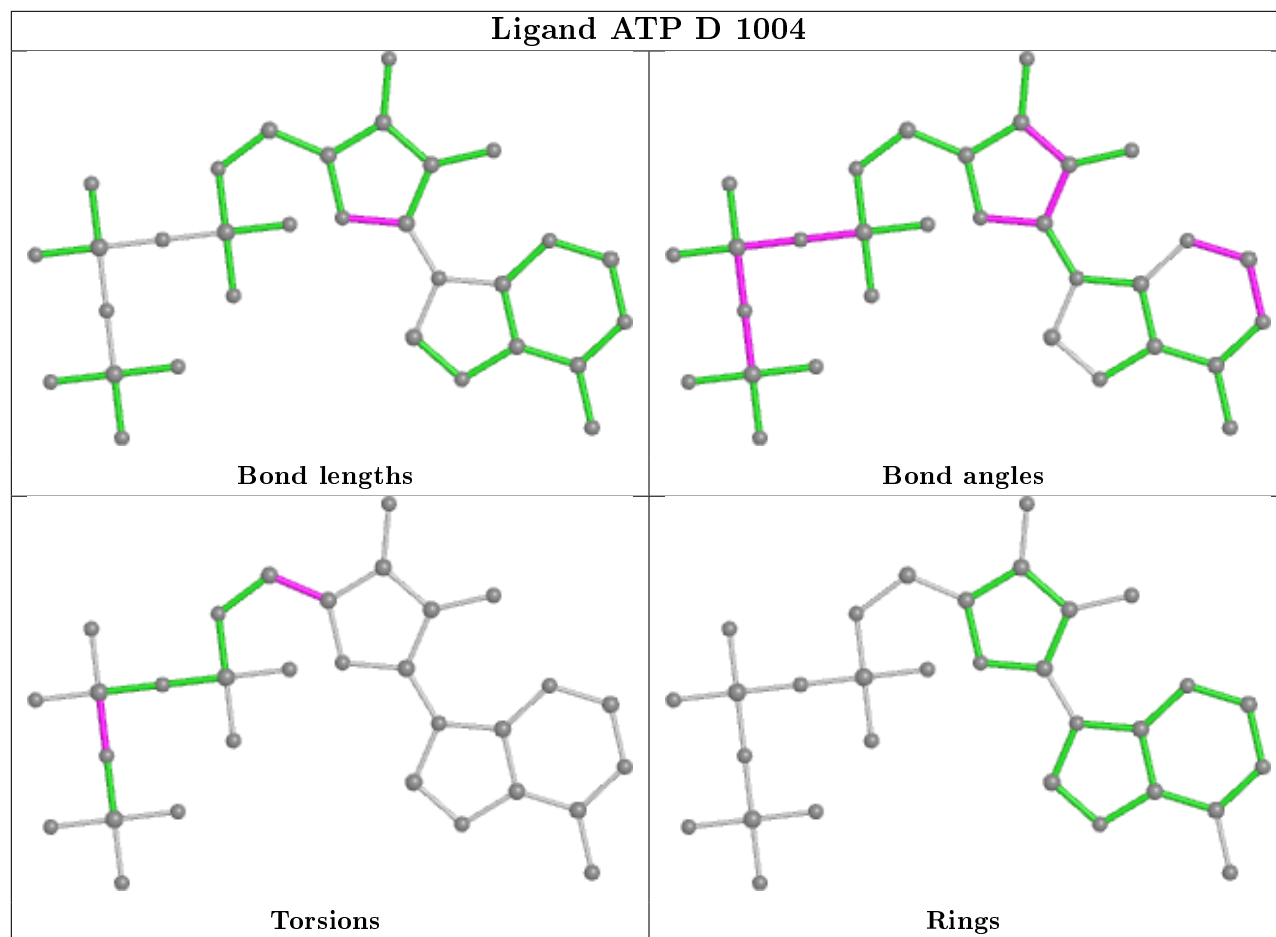
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1001	ATP	1	0
3	A	3001	PO4	1	0
3	C	3016	PO4	1	0
4	D	1004	ATP	6	0
4	C	1002	ATP	3	0

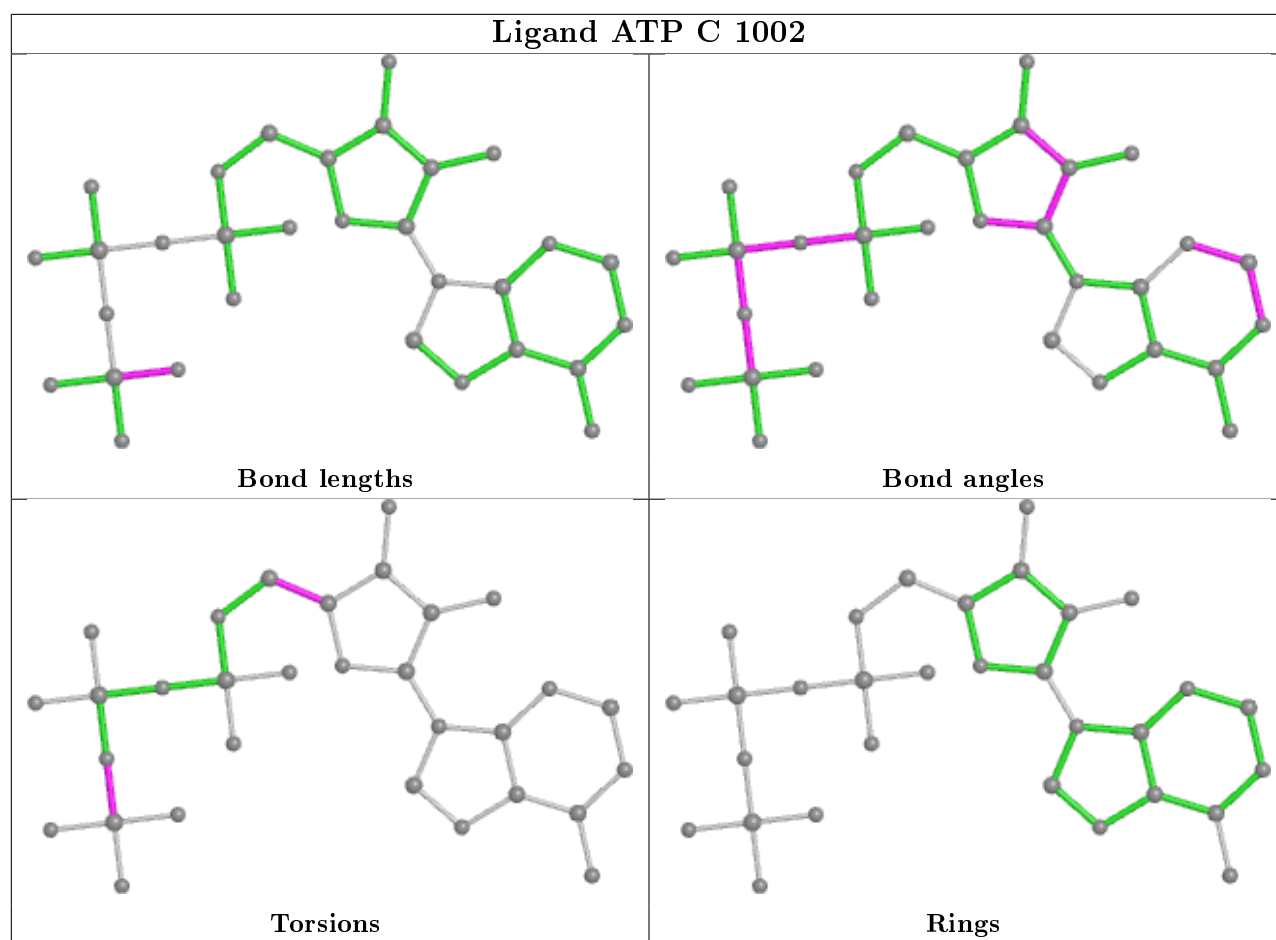
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 ⓘ

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	515/529 (97%)	-0.33	3 (0%) 89 88	22, 35, 54, 76	0
1	B	511/529 (96%)	0.51	53 (10%) 6 6	38, 59, 97, 108	0
1	C	517/529 (97%)	-0.19	14 (2%) 54 52	27, 40, 63, 95	0
1	D	512/529 (96%)	-0.28	9 (1%) 68 66	20, 37, 66, 90	0
All	All	2055/2116 (97%)	-0.07	79 (3%) 40 39	20, 41, 79, 108	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	529	GLU	6.9
1	B	528	THR	6.6
1	B	435	VAL	5.5
1	B	527	ARG	5.5
1	B	384	THR	4.8
1	D	387	ARG	4.5
1	B	223	LYS	4.5
1	C	384	THR	4.4
1	B	2	GLN	4.4
1	C	145	VAL	4.2
1	D	147	ALA	4.2
1	B	479	PRO	3.9
1	C	528	THR	3.9
1	B	511	GLN	3.8
1	B	71	TRP	3.8
1	B	475	ALA	3.8
1	B	224	GLU	3.7
1	B	458	ASN	3.7
1	D	527	ARG	3.7
1	B	340	ARG	3.5
1	B	484	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	527	ARG	3.4
1	B	489	TRP	3.4
1	B	481	GLU	3.3
1	B	12	LYS	3.3
1	B	17	TRP	3.3
1	B	500	ARG	3.2
1	B	478	VAL	3.2
1	B	504	ARG	3.1
1	B	165	GLU	3.1
1	B	482	LEU	3.1
1	B	437	TYR	3.0
1	B	418	ALA	3.0
1	B	486	ARG	3.0
1	B	514	ALA	3.0
1	B	519	LYS	2.9
1	C	146	GLU	2.9
1	B	72	GLY	2.8
1	B	436	GLY	2.7
1	D	388	ALA	2.7
1	D	374	ALA	2.7
1	A	387	ARG	2.7
1	B	66	GLU	2.7
1	B	434	GLY	2.7
1	C	280	HIS	2.7
1	B	513	TYR	2.6
1	B	487	GLU	2.6
1	B	507	GLN	2.6
1	B	10	HIS	2.6
1	C	140	GLY	2.6
1	D	433	TYR	2.6
1	B	163	VAL	2.5
1	B	440	PRO	2.5
1	C	141	ASN	2.5
1	D	224	GLU	2.4
1	B	495	TYR	2.3
1	B	350	TYR	2.3
1	B	79	ALA	2.3
1	A	328	GLU	2.3
1	C	458	ASN	2.3
1	C	12	LYS	2.2
1	B	132	MET	2.2
1	C	139	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	472	PRO	2.2
1	A	141	ASN	2.2
1	B	78	PHE	2.2
1	B	517	VAL	2.1
1	B	168	GLY	2.1
1	B	453	SER	2.1
1	C	96	GLU	2.1
1	D	386	PRO	2.1
1	D	528	THR	2.1
1	B	3	ARG	2.1
1	B	493	GLU	2.1
1	C	415	ARG	2.1
1	B	352	VAL	2.0
1	B	234	SER	2.0
1	B	523	GLU	2.0
1	B	415	ARG	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.

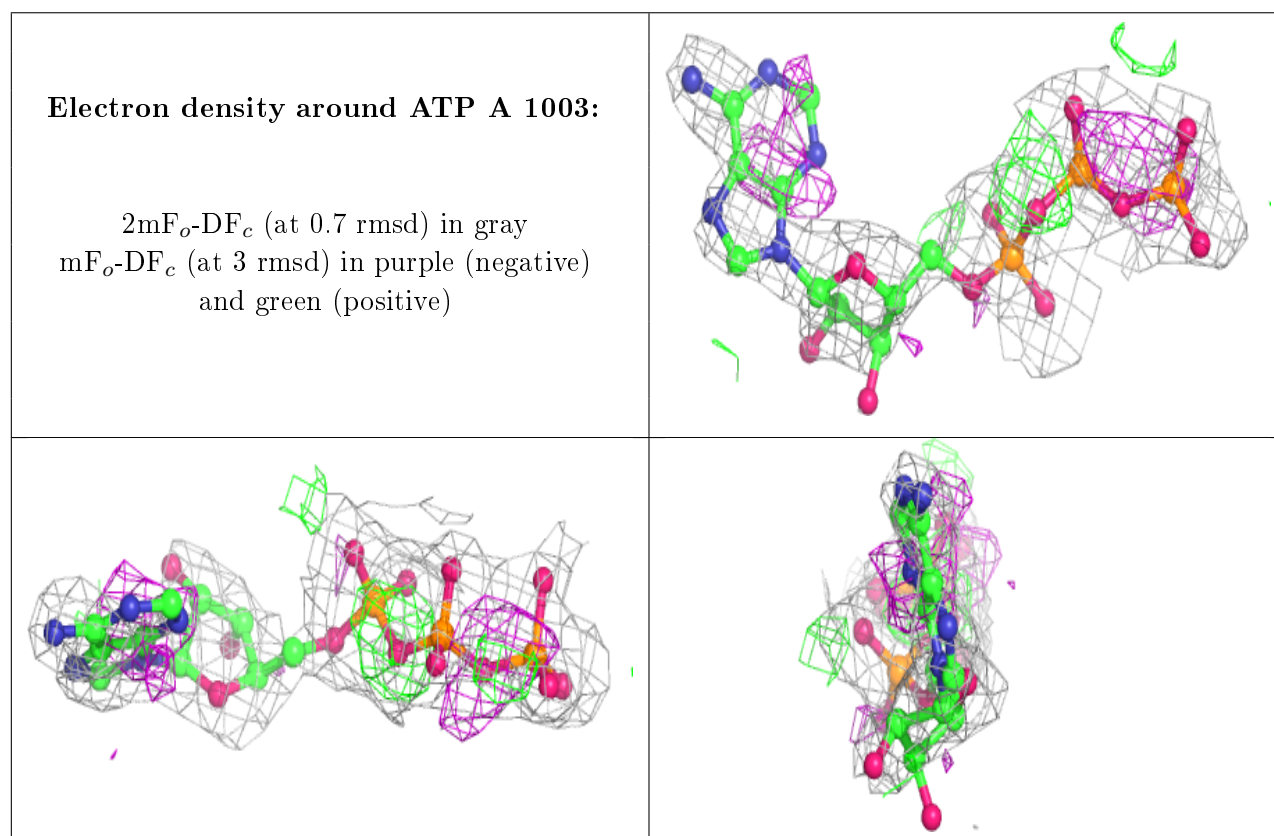
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ATP	A	1003	31/31	0.67	0.31	91,93,103,104	0
4	ATP	D	1004	31/31	0.85	0.24	92,94,107,107	0
4	ATP	B	1001	31/31	0.88	0.19	76,78,88,89	0
3	PO4	A	3009	5/5	0.90	0.16	59,61,62,63	0
4	ATP	C	1002	31/31	0.91	0.15	32,39,65,67	0
2	CA	D	2004	1/1	0.93	0.14	46,46,46,46	0
3	PO4	D	3015	5/5	0.94	0.20	75,76,77,77	0

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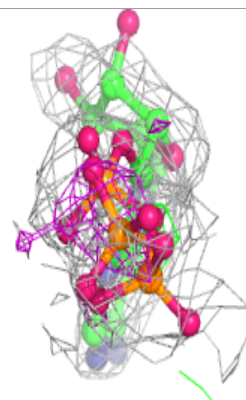
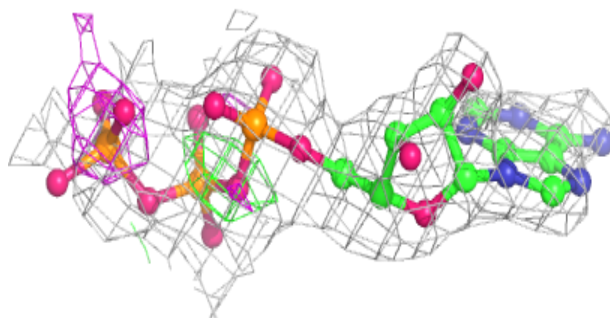
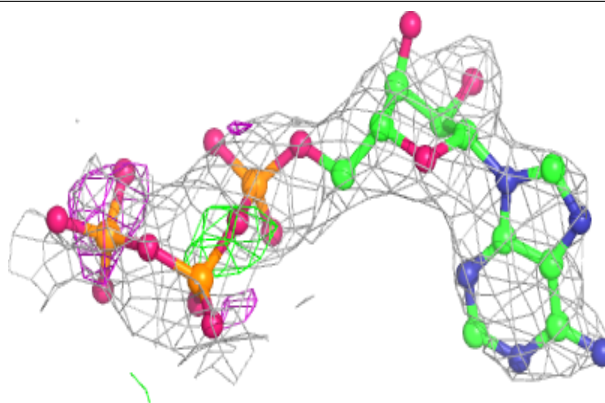
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	B	3013	5/5	0.94	0.31	82,82,83,83	0
3	PO4	B	3006	5/5	0.94	0.15	82,83,83,83	0
2	CA	B	2002	1/1	0.94	0.06	81,81,81,81	0
3	PO4	C	3017	5/5	0.96	0.15	53,56,56,56	0
3	PO4	C	3010	5/5	0.96	0.11	57,58,60,61	0
3	PO4	C	3016	5/5	0.96	0.19	52,52,54,55	0
3	PO4	D	3011	5/5	0.97	0.08	48,50,52,52	0
3	PO4	C	3007	5/5	0.97	0.09	61,62,62,64	0
3	PO4	C	3014	5/5	0.97	0.14	46,46,47,48	0
3	PO4	D	3008	5/5	0.97	0.10	61,62,63,63	0
3	PO4	A	3005	5/5	0.97	0.11	57,59,60,60	0
2	CA	A	2001	1/1	0.98	0.14	43,43,43,43	0
2	CA	C	2003	1/1	0.98	0.05	57,57,57,57	0
3	PO4	A	3001	5/5	0.98	0.14	35,36,38,40	0
3	PO4	B	3002	5/5	0.98	0.11	46,49,49,51	0
3	PO4	C	3003	5/5	0.98	0.08	40,43,44,44	0
3	PO4	D	3004	5/5	0.99	0.12	31,33,33,34	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.

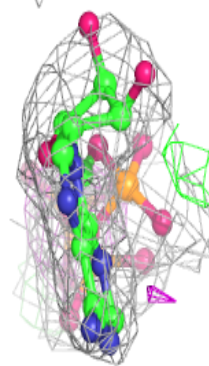
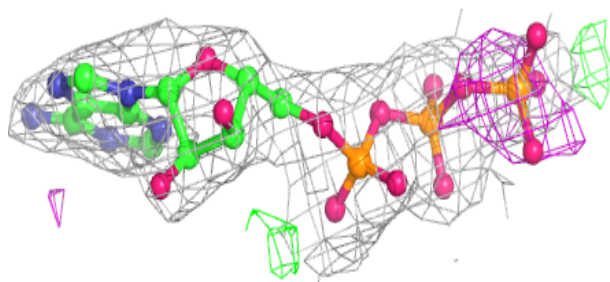
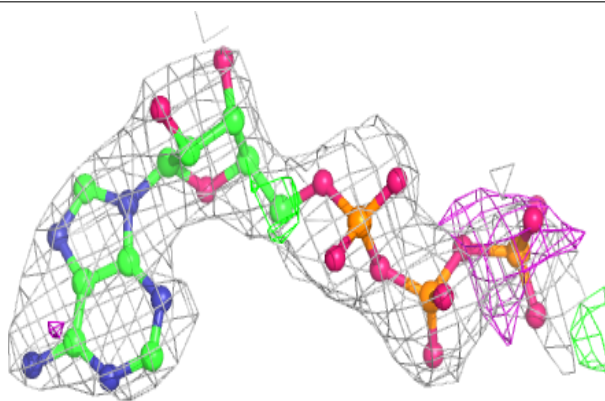


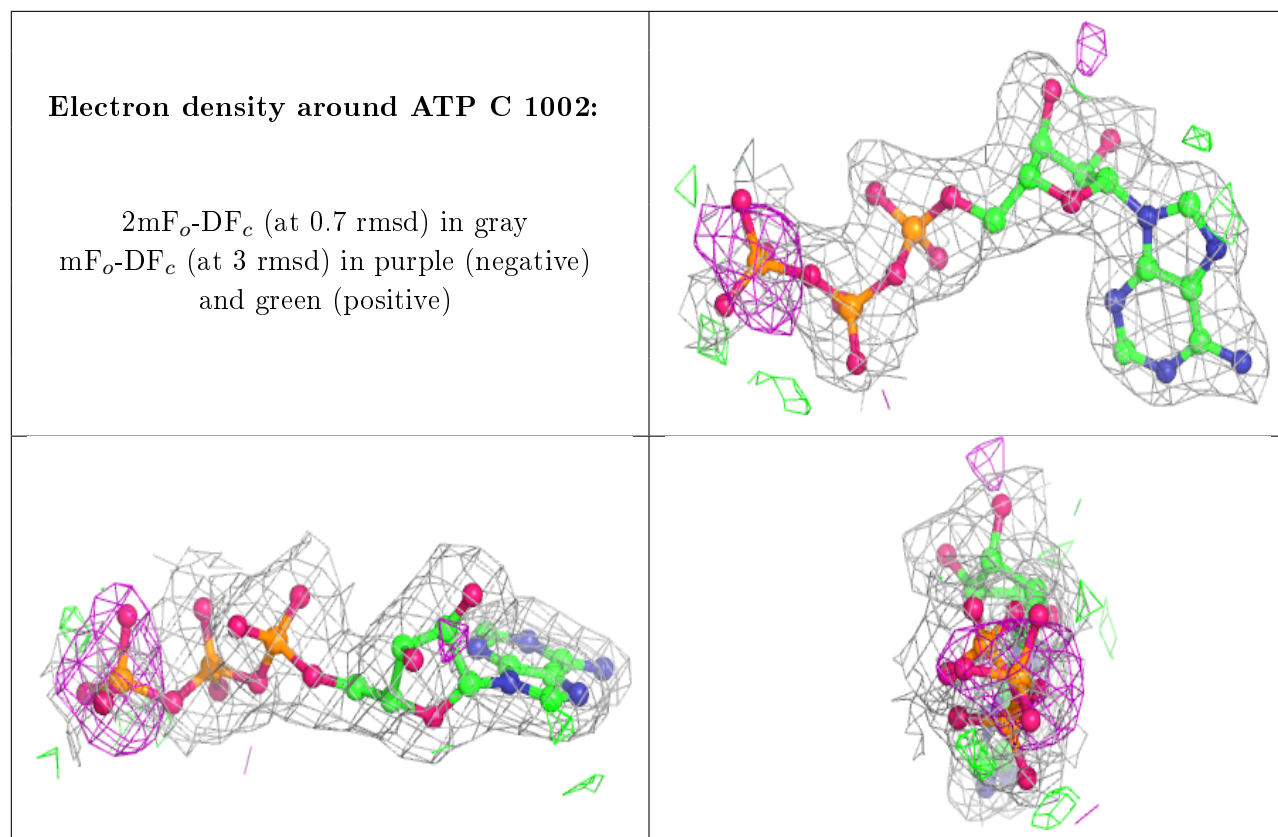
Electron density around ATP D 1004:

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

**Electron density around ATP B 1001:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.