



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:00 AM UTC

PDB ID : 6ITO / pdb_00006ito
Title : Crystal structure of pyruvate kinase (PYK) from Mycobacterium tuberculosis
in complex with Oxalate, AMP and inhibitor Ribose 5-Phosphate
Authors : Zhong, W.; Cai, Q.; El Sahili, A.; Mu, Y.; Lescar, J.; Dedon, P.C.
Deposited on : 2018-11-24
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

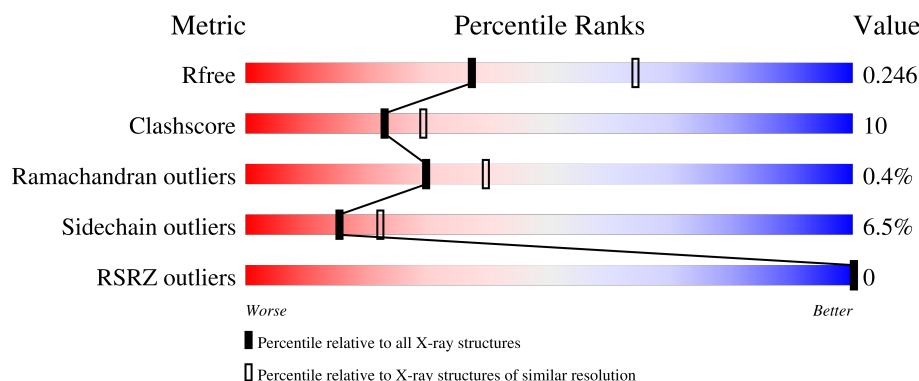
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

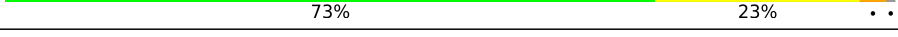
The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	 72% 24% ..
1	B	475	 76% 21% ..
1	C	475	 76% 22% ..
1	D	475	 73% 23% ..

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	502	-	X	-	-
3	OXL	B	502	-	X	-	-
3	OXL	D	502	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14921 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	1	0
			3554	2212	644	680	18			
1	B	471	Total	C	N	O	S	0	0	0
			3543	2206	640	679	18			
1	C	471	Total	C	N	O	S	0	0	0
			3543	2206	640	679	18			
1	D	471	Total	C	N	O	S	0	2	0
			3565	2218	648	681	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P9WKE5
A	-1	GLY	-	expression tag	UNP P9WKE5
A	0	HIS	-	expression tag	UNP P9WKE5
B	-2	GLY	-	expression tag	UNP P9WKE5
B	-1	GLY	-	expression tag	UNP P9WKE5
B	0	HIS	-	expression tag	UNP P9WKE5
C	-2	GLY	-	expression tag	UNP P9WKE5
C	-1	GLY	-	expression tag	UNP P9WKE5
C	0	HIS	-	expression tag	UNP P9WKE5
D	-2	GLY	-	expression tag	UNP P9WKE5
D	-1	GLY	-	expression tag	UNP P9WKE5
D	0	HIS	-	expression tag	UNP P9WKE5

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

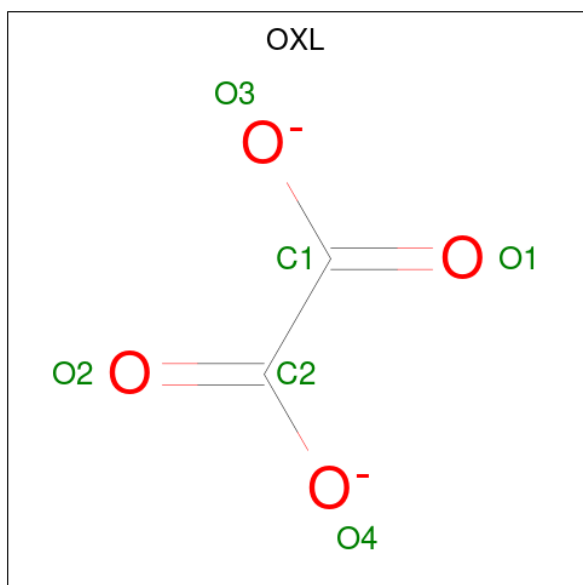
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

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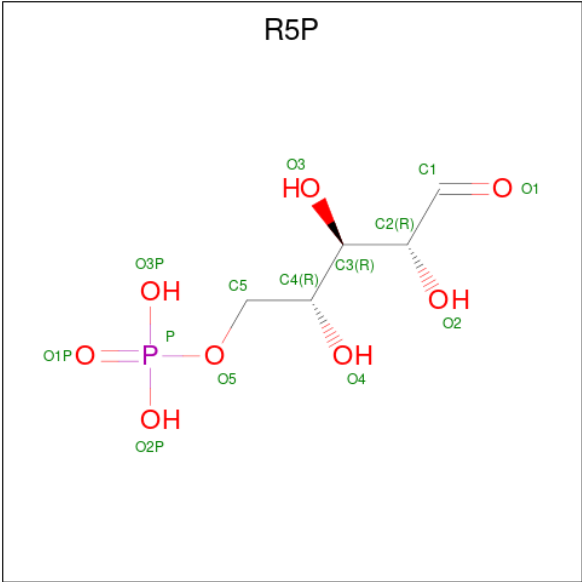
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



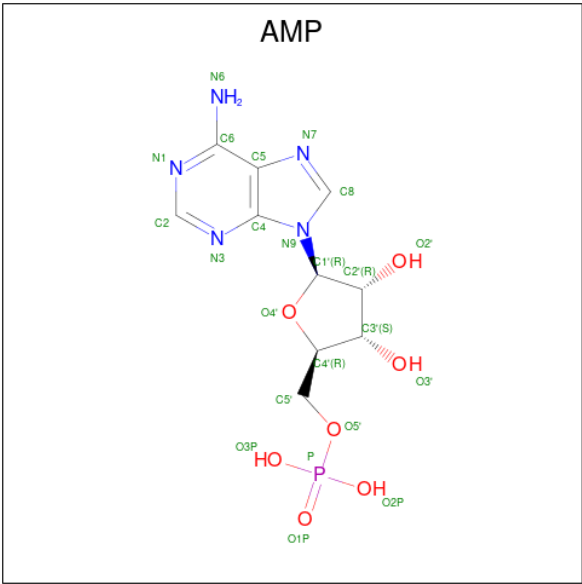
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is RIBOSE-5-PHOSPHATE (CCD ID: R5P) (formula: $C_5H_{11}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			14	5	8	1		
4	B	1	Total	C	O	P	0	0
			14	5	8	1		
4	C	1	Total	C	O	P	0	0
			14	5	8	1		
4	D	1	Total	C	O	P	0	0
			14	5	8	1		

- Molecule 5 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
5	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
5	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
5	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

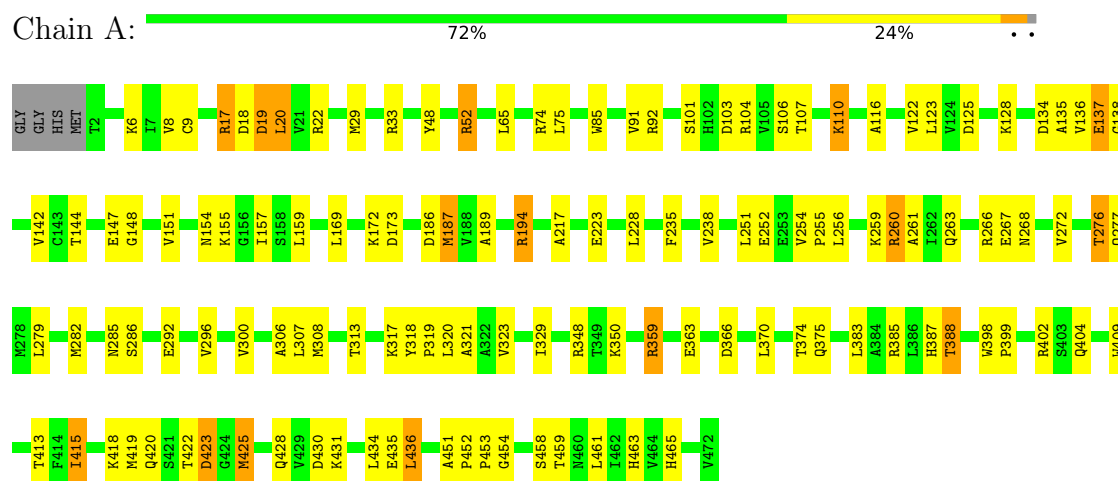
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total	O	0	0
			147	147		
6	B	111	Total	O	0	0
			111	111		
6	C	152	Total	O	0	0
			152	152		
6	D	130	Total	O	0	0
			130	130		

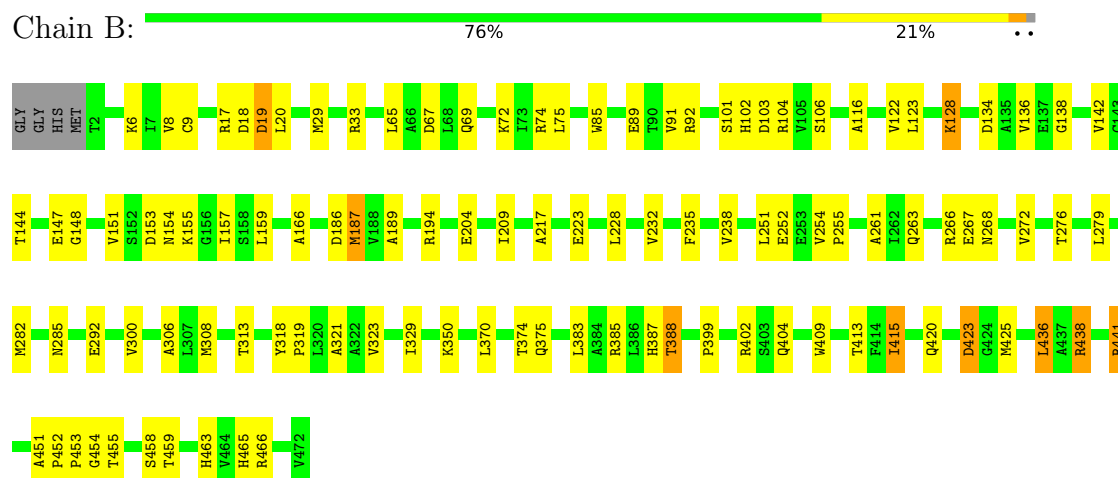
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pyruvate kinase

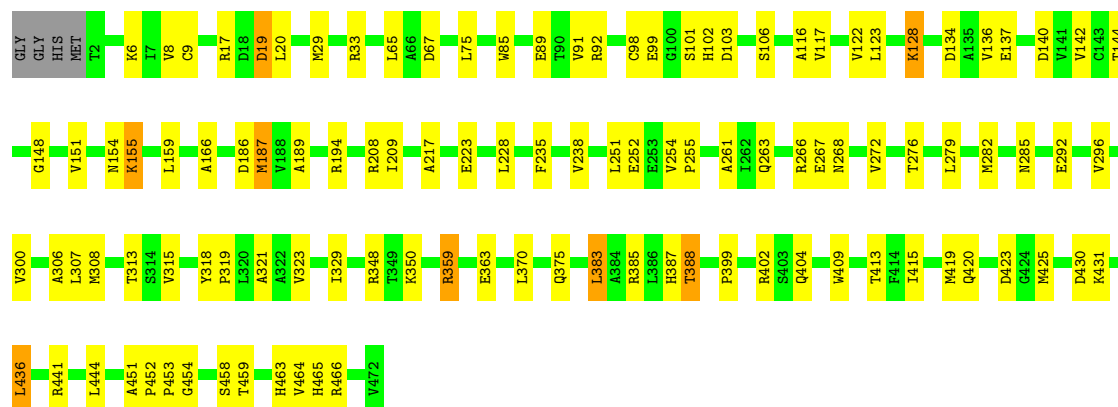


• Molecule 1: Pyruvate kinase

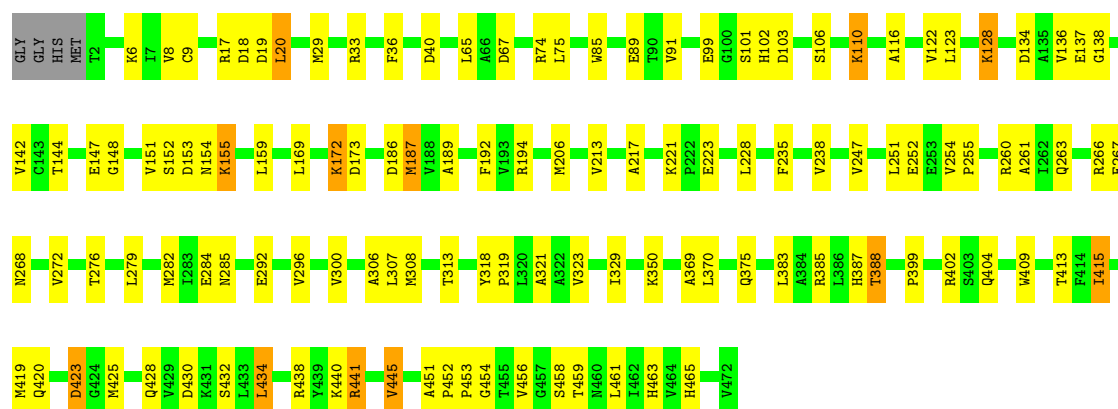


• Molecule 1: Pyruvate kinase





• Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	125.55Å 125.55Å 143.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.77 – 2.55 62.77 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.77-2.55) 100.0 (62.77-2.55)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.206 , 0.248 0.208 , 0.246	Depositor DCC
R_{free} test set	4108 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.762	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 25.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.468 for -h,-k,l 0.477 for h,-h-k,-l 0.469 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14921	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AMP, OXL, R5P

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.12	0/3604	1.40	0/4895
1	B	1.11	0/3593	1.41	1/4881 (0.0%)
1	C	1.10	1/3593 (0.0%)	1.41	0/4881
1	D	1.11	0/3615	1.41	0/4909
All	All	1.11	1/14405 (0.0%)	1.40	1/19566 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	315	VAL	N-CA	5.00	1.50	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	ASP	CA-CB-CG	6.07	118.67	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3554	0	3620	84	2
1	B	3543	0	3608	69	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3543	0	3608	72	2
1	D	3565	0	3632	84	2
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	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
4	A	14	0	9	1	0
4	B	14	0	9	1	0
4	C	14	0	9	1	0
4	D	14	0	9	1	0
5	A	23	0	12	2	0
5	B	23	0	12	3	0
5	C	23	0	12	1	0
5	D	23	0	12	1	0
6	A	147	0	0	9	0
6	B	111	0	0	7	0
6	C	152	0	0	12	0
6	D	130	0	0	11	0
All	All	14921	0	14552	302	4

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 10.

All (302) 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:D:441[A]:ARG:HB3	1:D:441[A]:ARG:HH11	1.29	0.97
1:D:441[A]:ARG:H	1:D:441[A]:ARG:HD2	1.39	0.84
1:D:350:LYS:HE3	1:D:459:THR:O	1.78	0.84
1:A:350:LYS:HE3	1:A:459:THR:O	1.77	0.84
1:B:350:LYS:HE3	1:B:459:THR:O	1.77	0.84
1:C:350:LYS:HE3	1:C:459:THR:O	1.78	0.84
1:C:128:LYS:HB3	6:C:684:HOH:O	1.80	0.81
1:D:441[A]:ARG:HH11	1:D:441[A]:ARG:CB	1.94	0.80
1:A:134:ASP:OD2	1:A:144:THR:OG1	2.02	0.77
1:D:441[A]:ARG:H	1:D:441[A]:ARG:CD	1.97	0.76
1:C:458:SER:OG	5:C:504:AMP:O3'	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:PRO:HA	1:A:415:ILE:HD12	1.69	0.75
1:B:399:PRO:HA	1:B:415:ILE:HD12	1.69	0.75
1:A:194:ARG:HG2	1:A:194:ARG:HH11	1.53	0.73
1:C:399:PRO:HA	1:C:415:ILE:HD12	1.69	0.73
1:A:256:LEU:O	1:A:260[B]:ARG:HG3	1.89	0.72
1:D:399:PRO:HA	1:D:415:ILE:HD12	1.70	0.72
1:C:383:LEU:HD12	1:C:383:LEU:O	1.92	0.70
1:A:107:THR:O	1:A:110:LYS:NZ	2.22	0.70
1:D:153:ASP:O	6:D:601:HOH:O	2.09	0.69
1:D:441[A]:ARG:HD2	1:D:441[A]:ARG:N	2.07	0.68
1:B:187:MET:HE2	1:B:404:GLN:HA	1.75	0.67
1:D:440:LYS:HE2	1:D:441[B]:ARG:HH12	1.59	0.66
1:D:440:LYS:HE2	1:D:441[B]:ARG:NH1	2.11	0.66
1:B:153:ASP:O	6:B:601:HOH:O	2.14	0.65
1:A:419:MET:HE3	1:A:419:MET:HA	1.79	0.65
1:D:192:PHE:O	1:D:194:ARG:NH2	2.29	0.65
1:B:19:ASP:HA	6:B:686:HOH:O	1.97	0.65
1:A:52:ARG:NH1	1:A:186:ASP:OD2	2.30	0.64
1:B:134:ASP:OD2	1:B:144:THR:OG1	2.17	0.63
1:A:52:ARG:HH12	1:A:186:ASP:CG	2.07	0.62
1:B:423:ASP:OD1	1:B:423:ASP:N	2.32	0.62
1:D:134:ASP:OD2	1:D:144:THR:OG1	2.16	0.62
1:A:85:TRP:CE3	1:A:151:VAL:HG11	2.35	0.62
1:C:134:ASP:OD2	1:C:144:THR:OG1	2.17	0.61
1:C:166:ALA:O	1:C:194:ARG:NH1	2.33	0.61
1:A:148:GLY:HA3	6:A:642:HOH:O	2.00	0.61
1:A:423:ASP:OD1	1:A:423:ASP:N	2.34	0.61
1:D:425:MET:CE	1:D:453:PRO:HB3	2.32	0.60
1:D:148:GLY:HA3	6:D:621:HOH:O	2.01	0.60
1:B:74:ARG:HG2	1:B:74:ARG:HH21	1.67	0.59
1:B:374:THR:HA	5:B:504:AMP:H5'2	1.84	0.59
1:A:92:ARG:HH22	1:A:137:GLU:HG3	1.66	0.59
1:C:425:MET:CE	1:C:453:PRO:HB3	2.33	0.59
1:D:423:ASP:OD1	1:D:423:ASP:N	2.33	0.59
1:D:65:LEU:HD11	1:D:189:ALA:HB2	1.85	0.59
1:B:85:TRP:CE3	1:B:151:VAL:HG11	2.38	0.58
1:C:85:TRP:CE3	1:C:151:VAL:HG11	2.38	0.58
1:D:155:LYS:HD2	6:D:627:HOH:O	2.03	0.58
1:D:441[A]:ARG:HH11	1:D:441[A]:ARG:CG	2.15	0.58
1:C:122:VAL:HG22	1:C:159:LEU:CD1	2.34	0.58
1:B:166:ALA:O	1:B:194:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:PHE:O	1:D:172:LYS:NZ	2.36	0.58
1:D:463:HIS:HD2	1:D:465:HIS:HB2	1.69	0.57
1:A:286:SER:OG	1:B:147:GLU:OE2	2.18	0.57
1:C:65:LEU:HD11	1:C:189:ALA:HB2	1.87	0.57
1:D:85:TRP:CE3	1:D:151:VAL:HG11	2.39	0.57
1:A:398:TRP:NE1	6:A:606:HOH:O	2.38	0.57
1:A:458:SER:OG	5:A:504:AMP:O3'	2.21	0.57
1:C:463:HIS:HD2	1:C:465:HIS:HB2	1.69	0.57
1:A:374:THR:HA	5:A:504:AMP:H5'2	1.86	0.57
1:B:122:VAL:HG22	1:B:159:LEU:CD1	2.35	0.57
1:A:300:VAL:HG13	6:A:614:HOH:O	2.05	0.57
1:D:128:LYS:HB3	6:D:712:HOH:O	2.03	0.57
1:B:425:MET:CE	1:B:453:PRO:HB3	2.35	0.56
1:D:458:SER:OG	5:D:504:AMP:O3'	2.24	0.56
1:C:122:VAL:HG22	1:C:159:LEU:HD11	1.87	0.56
1:A:65:LEU:HD11	1:A:189:ALA:HB2	1.86	0.56
1:A:463:HIS:HD2	1:A:465:HIS:HB2	1.70	0.56
1:B:458:SER:OG	5:B:504:AMP:O3'	2.21	0.55
1:A:122:VAL:HG22	1:A:159:LEU:CD1	2.37	0.55
1:B:65:LEU:HD11	1:B:189:ALA:HB2	1.87	0.55
1:C:148:GLY:HA3	6:C:663:HOH:O	2.05	0.55
1:C:430:ASP:OD2	6:C:601:HOH:O	2.17	0.55
1:B:463:HIS:HD2	1:B:465:HIS:HB2	1.70	0.55
1:D:99:GLU:HG3	6:D:691:HOH:O	2.05	0.55
1:D:441[A]:ARG:HB3	1:D:441[A]:ARG:NH1	2.10	0.55
1:C:444:LEU:HD11	1:C:464:VAL:CG1	2.38	0.54
1:D:17:ARG:HB3	1:D:20:LEU:HD12	1.88	0.54
1:D:387:HIS:HE1	6:D:616:HOH:O	1.90	0.54
1:D:122:VAL:HG22	1:D:159:LEU:CD1	2.38	0.54
1:D:194:ARG:HB2	1:D:223:GLU:HB2	1.90	0.53
1:B:441:ARG:NH1	6:B:609:HOH:O	2.42	0.53
1:B:436:LEU:HD13	1:B:436:LEU:N	2.23	0.53
1:C:436:LEU:N	1:C:436:LEU:HD13	2.24	0.53
1:A:85:TRP:CZ2	1:A:91:VAL:HG11	2.44	0.53
1:A:282:MET:HA	1:A:285:ASN:O	2.09	0.53
1:B:122:VAL:HG22	1:B:159:LEU:HD11	1.91	0.53
1:B:148:GLY:HA3	6:B:636:HOH:O	2.08	0.53
1:D:75:LEU:O	1:D:154:ASN:HA	2.09	0.53
1:B:300:VAL:HG13	6:B:611:HOH:O	2.08	0.53
1:C:444:LEU:HD11	1:C:464:VAL:HG13	1.91	0.53
1:A:48:TYR:OH	1:A:52:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:HG22	1:A:159:LEU:HD11	1.91	0.53
1:A:135:ALA:HB3	1:A:142:VAL:CG1	2.39	0.53
1:A:123:LEU:HD23	1:A:123:LEU:N	2.23	0.53
1:B:75:LEU:O	1:B:154:ASN:HA	2.09	0.52
1:C:75:LEU:O	1:C:154:ASN:HA	2.09	0.52
1:A:75:LEU:O	1:A:154:ASN:HA	2.09	0.52
1:D:122:VAL:HG22	1:D:159:LEU:HD11	1.92	0.52
1:C:92:ARG:NH2	1:C:137:GLU:OE1	2.39	0.52
1:B:282:MET:HA	1:B:285:ASN:O	2.10	0.52
1:D:402:ARG:HG3	1:D:413:THR:HB	1.92	0.52
1:D:152:SER:OG	1:D:155:LYS:HE2	2.09	0.52
1:C:300:VAL:HG13	6:C:614:HOH:O	2.10	0.51
1:C:387:HIS:HE1	6:C:621:HOH:O	1.93	0.51
1:C:318:TYR:HB3	1:C:321:ALA:HB3	1.93	0.51
1:D:9:CYS:HB2	1:D:29:MET:SD	2.51	0.51
1:D:300:VAL:HG13	6:D:619:HOH:O	2.11	0.51
1:D:419:MET:CE	6:D:716:HOH:O	2.58	0.51
1:D:33:ARG:NH2	1:D:67:ASP:OD2	2.41	0.51
1:D:430:ASP:O	1:D:434:LEU:HD12	2.11	0.51
1:B:455:THR:O	5:B:504:AMP:H4'	2.10	0.51
1:C:187:MET:HE2	1:C:404:GLN:HA	1.93	0.51
1:A:251:LEU:C	1:A:251:LEU:HD12	2.36	0.51
1:A:318:TYR:HB3	1:A:321:ALA:HB3	1.93	0.51
1:B:9:CYS:HB2	1:B:29:MET:SD	2.51	0.51
1:B:228:LEU:HD21	1:B:261:ALA:HA	1.93	0.51
1:C:9:CYS:HB2	1:C:29:MET:SD	2.51	0.51
1:A:9:CYS:HB2	1:A:29:MET:SD	2.51	0.50
1:B:33:ARG:NH2	1:B:67:ASP:OD2	2.42	0.50
1:A:187:MET:HE2	1:A:404:GLN:HA	1.93	0.50
1:B:370:LEU:HD12	1:B:388:THR:HG21	1.91	0.50
1:C:33:ARG:NH2	1:C:67:ASP:OD2	2.42	0.50
1:D:370:LEU:HD12	1:D:388:THR:HG21	1.92	0.50
1:A:228:LEU:HD21	1:A:261:ALA:HA	1.94	0.50
1:C:402:ARG:HG3	1:C:413:THR:HB	1.94	0.50
1:B:251:LEU:C	1:B:251:LEU:HD12	2.36	0.50
1:C:370:LEU:HD12	1:C:388:THR:HG21	1.93	0.50
1:B:69:GLN:O	6:B:602:HOH:O	2.20	0.50
1:D:282:MET:HA	1:D:285:ASN:O	2.10	0.50
1:D:318:TYR:HB3	1:D:321:ALA:HB3	1.94	0.50
1:A:402:ARG:HG3	1:A:413:THR:HB	1.93	0.49
1:B:402:ARG:HG3	1:B:413:THR:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:MET:HA	1:C:285:ASN:O	2.10	0.49
1:D:251:LEU:C	1:D:251:LEU:HD12	2.36	0.49
1:C:228:LEU:HD21	1:C:261:ALA:HA	1.92	0.49
1:C:251:LEU:HD12	1:C:251:LEU:C	2.37	0.49
1:B:318:TYR:HB3	1:B:321:ALA:HB3	1.94	0.49
1:D:187:MET:HE2	1:D:404:GLN:HA	1.94	0.49
1:B:85:TRP:CZ2	1:B:91:VAL:HG11	2.47	0.49
1:C:98:CYS:HA	6:C:715:HOH:O	2.13	0.49
1:D:85:TRP:CZ2	1:D:91:VAL:HG11	2.48	0.49
1:C:155:LYS:HD3	1:C:155:LYS:HA	1.62	0.49
1:D:221:LYS:NZ	6:D:610:HOH:O	2.45	0.48
1:A:387:HIS:HE1	6:A:632:HOH:O	1.96	0.48
1:D:74:ARG:HG2	1:D:74:ARG:HH21	1.79	0.48
1:A:19:ASP:O	1:A:22:ARG:HB3	2.14	0.48
1:A:263:GLN:O	1:A:267:GLU:HG2	2.14	0.48
1:B:186:ASP:C	1:B:187:MET:HG3	2.39	0.48
1:C:268:ASN:OD1	6:C:602:HOH:O	2.20	0.48
1:D:228:LEU:HD21	1:D:261:ALA:HA	1.94	0.48
1:D:279:LEU:HD23	1:D:292:GLU:HB3	1.96	0.48
1:D:441[B]:ARG:NH2	6:D:606:HOH:O	2.39	0.48
1:C:263:GLN:O	1:C:267:GLU:HG2	2.14	0.47
1:D:451:ALA:HA	1:D:452:PRO:C	2.38	0.47
1:B:268:ASN:HA	4:B:503:R5P:O4	2.14	0.47
1:C:268:ASN:HA	4:C:503:R5P:O4	2.14	0.47
1:A:399:PRO:HA	1:A:415:ILE:CD1	2.42	0.47
1:A:451:ALA:HA	1:A:452:PRO:C	2.39	0.47
1:A:194:ARG:HG2	1:A:194:ARG:NH1	2.26	0.47
1:B:451:ALA:HA	1:B:452:PRO:C	2.39	0.47
1:A:20:LEU:HD22	1:A:20:LEU:HA	1.69	0.47
1:A:260[A]:ARG:NE	6:A:603:HOH:O	2.35	0.47
1:B:399:PRO:HA	1:B:415:ILE:CD1	2.43	0.47
1:C:387:HIS:HA	1:C:409:TRP:CZ3	2.50	0.47
1:C:451:ALA:HA	1:C:452:PRO:C	2.39	0.47
1:C:19:ASP:HA	6:C:711:HOH:O	2.15	0.47
1:A:122:VAL:C	1:A:123:LEU:HD23	2.40	0.47
1:A:238:VAL:O	1:A:272:VAL:HA	2.15	0.47
1:B:74:ARG:HG2	1:B:74:ARG:NH2	2.28	0.47
1:B:238:VAL:O	1:B:272:VAL:HA	2.15	0.47
1:B:263:GLN:O	1:B:267:GLU:HG2	2.15	0.47
1:D:155:LYS:HA	1:D:155:LYS:HD3	1.65	0.47
1:C:85:TRP:CZ2	1:C:91:VAL:HG11	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:HIS:HA	1:D:409:TRP:CZ3	2.50	0.46
1:B:313:THR:HA	1:B:319:PRO:HB3	1.98	0.46
1:C:99:GLU:HG3	6:C:679:HOH:O	2.16	0.46
1:C:279:LEU:HD23	1:C:292:GLU:HB3	1.97	0.46
1:C:238:VAL:O	1:C:272:VAL:HA	2.15	0.46
1:D:116:ALA:O	1:D:136:VAL:HG21	2.14	0.46
1:D:266:ARG:O	1:D:385:ARG:HD2	2.16	0.46
1:B:387:HIS:HA	1:B:409:TRP:CZ3	2.50	0.46
1:A:387:HIS:HA	1:A:409:TRP:CZ3	2.50	0.46
1:C:128:LYS:CA	1:C:128:LYS:HE3	2.46	0.46
1:C:266:ARG:O	1:C:385:ARG:HD2	2.16	0.46
1:D:194:ARG:HD2	6:D:678:HOH:O	2.16	0.46
1:D:238:VAL:O	1:D:272:VAL:HA	2.15	0.46
1:D:169:LEU:HD22	1:D:173:ASP:HB3	1.97	0.46
1:A:17:ARG:HH11	1:A:17:ARG:HB3	1.81	0.46
1:A:92:ARG:HB3	1:A:104:ARG:HG3	1.99	0.46
1:A:279:LEU:HD23	1:A:292:GLU:HB3	1.97	0.46
1:A:125:ASP:O	1:A:128:LYS:HE3	2.16	0.45
1:C:266:ARG:NH1	6:C:609:HOH:O	2.35	0.45
1:C:313:THR:HA	1:C:319:PRO:HB3	1.98	0.45
1:C:359:ARG:HD3	1:C:363:GLU:CD	2.41	0.45
1:A:313:THR:HA	1:A:319:PRO:HB3	1.99	0.45
1:B:116:ALA:O	1:B:136:VAL:HG21	2.16	0.45
1:A:135:ALA:O	1:A:142:VAL:HG12	2.16	0.45
1:B:128:LYS:CA	1:B:128:LYS:HE3	2.46	0.45
1:B:463:HIS:CD2	1:B:465:HIS:HB2	2.52	0.45
1:D:263:GLN:O	1:D:267:GLU:HG2	2.16	0.45
1:A:116:ALA:O	1:A:136:VAL:HG21	2.16	0.45
1:A:186:ASP:C	1:A:187:MET:HG3	2.42	0.45
1:B:8:VAL:HB	1:B:308:MET:HG3	1.97	0.45
1:B:17:ARG:HH11	1:B:17:ARG:HG2	1.81	0.45
1:C:116:ALA:O	1:C:136:VAL:HG21	2.16	0.45
1:D:313:THR:HA	1:D:319:PRO:HB3	1.98	0.45
1:A:370:LEU:HD12	1:A:388:THR:HG21	1.97	0.45
1:C:186:ASP:C	1:C:187:MET:HG3	2.41	0.45
1:C:194:ARG:HB2	1:C:223:GLU:HB2	1.98	0.45
1:A:259:LYS:NZ	6:A:610:HOH:O	2.46	0.45
1:A:359:ARG:HD3	1:A:363:GLU:CD	2.41	0.45
1:B:438:ARG:H	1:B:438:ARG:HG2	1.40	0.45
1:B:463:HIS:ND1	1:D:461:LEU:HD12	2.32	0.45
1:A:461:LEU:HD12	1:C:463:HIS:ND1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:GLN:OE1	1:D:454:GLY:HA2	2.17	0.44
1:D:463:HIS:CD2	1:D:465:HIS:HB2	2.51	0.44
1:D:186:ASP:C	1:D:187:MET:HG3	2.41	0.44
1:B:266:ARG:O	1:B:385:ARG:HD2	2.17	0.44
1:A:194:ARG:HB2	1:A:223:GLU:HB2	2.00	0.44
1:A:268:ASN:HA	4:A:503:R5P:O4	2.18	0.44
1:C:399:PRO:HA	1:C:415:ILE:CD1	2.43	0.44
1:A:329:ILE:HA	1:B:252:GLU:HB2	2.00	0.44
1:C:375:GLN:OE1	1:C:454:GLY:C	2.60	0.44
1:C:419:MET:HE3	6:C:728:HOH:O	2.16	0.44
1:D:440:LYS:HG2	1:D:441[B]:ARG:NH2	2.31	0.44
1:A:266:ARG:O	1:A:385:ARG:HD2	2.17	0.44
1:B:279:LEU:HD23	1:B:292:GLU:HB3	1.98	0.44
1:A:366:ASP:OD1	6:A:601:HOH:O	2.21	0.44
1:B:128:LYS:HE3	1:B:128:LYS:HA	2.00	0.44
1:C:217:ALA:HB2	1:C:235:PHE:CG	2.53	0.44
1:D:217:ALA:HB2	1:D:235:PHE:CG	2.53	0.44
1:C:463:HIS:CD2	1:C:465:HIS:HB2	2.52	0.44
1:A:375:GLN:OE1	1:A:454:GLY:C	2.61	0.44
1:D:8:VAL:HB	1:D:308:MET:HG3	2.00	0.44
1:C:254:VAL:N	1:C:255:PRO:CD	2.81	0.43
1:B:9:CYS:SG	1:B:323:VAL:HG22	2.59	0.43
1:B:436:LEU:N	1:B:436:LEU:CD1	2.81	0.43
1:D:110:LYS:HD3	1:D:110:LYS:HA	1.71	0.43
1:D:254:VAL:N	1:D:255:PRO:CD	2.82	0.43
1:D:375:GLN:OE1	1:D:454:GLY:C	2.61	0.43
1:B:254:VAL:N	1:B:255:PRO:CD	2.81	0.43
1:B:375:GLN:OE1	1:B:454:GLY:C	2.61	0.43
1:A:217:ALA:HB2	1:A:235:PHE:CG	2.53	0.43
1:B:217:ALA:HB2	1:B:235:PHE:CG	2.53	0.43
1:A:276:THR:HG22	1:A:277:GLN:HG3	2.00	0.43
1:B:89:GLU:OE1	1:B:102:HIS:NE2	2.46	0.43
1:D:369:ALA:HB3	1:D:445:VAL:HG22	2.01	0.43
1:D:399:PRO:HA	1:D:415:ILE:CD1	2.43	0.43
1:A:9:CYS:SG	1:A:323:VAL:HG22	2.59	0.43
1:D:9:CYS:SG	1:D:323:VAL:HG22	2.59	0.43
1:B:194:ARG:HB2	1:B:223:GLU:HB2	2.01	0.43
1:A:17:ARG:HH11	1:A:17:ARG:CG	2.32	0.43
1:C:92:ARG:HG2	1:C:140:ASP:HB3	2.01	0.43
1:C:117:VAL:HG22	6:C:745:HOH:O	2.19	0.43
1:A:74:ARG:HG2	1:A:74:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:HD3	1:A:128:LYS:N	2.33	0.42
1:B:6:LYS:O	1:B:306:ALA:HA	2.20	0.42
1:C:252:GLU:HB2	1:D:329:ILE:HA	2.00	0.42
1:A:17:ARG:HH11	1:A:17:ARG:CB	2.33	0.42
1:C:329:ILE:HA	1:D:252:GLU:HB2	2.00	0.42
1:A:254:VAL:N	1:A:255:PRO:CD	2.82	0.42
1:C:8:VAL:HB	1:C:308:MET:HG3	2.01	0.42
1:D:268:ASN:HA	4:D:503:R5P:O4	2.19	0.42
1:C:194:ARG:HG2	1:C:194:ARG:HH21	1.85	0.42
1:A:6:LYS:O	1:A:306:ALA:HA	2.20	0.42
1:C:9:CYS:SG	1:C:323:VAL:HG22	2.60	0.42
1:A:107:THR:O	1:A:110:LYS:CE	2.67	0.42
1:D:128:LYS:H	1:D:128:LYS:HG2	1.51	0.42
1:D:441[A]:ARG:CG	1:D:441[A]:ARG:NH1	2.78	0.42
1:B:375:GLN:OE1	1:B:454:GLY:HA2	2.20	0.41
1:D:296:VAL:HG13	1:D:307:LEU:CD1	2.50	0.41
1:A:8:VAL:HB	1:A:308:MET:HG3	2.01	0.41
1:A:422:THR:HA	1:A:425:MET:HG3	2.02	0.41
1:C:128:LYS:HE3	1:C:128:LYS:HA	2.01	0.41
1:C:296:VAL:HG13	1:C:307:LEU:CD1	2.51	0.41
1:D:6:LYS:O	1:D:306:ALA:HA	2.20	0.41
1:A:436:LEU:HD13	1:A:436:LEU:N	2.34	0.41
1:D:440:LYS:CE	1:D:441[B]:ARG:HH12	2.28	0.41
1:A:430:ASP:O	1:A:434:LEU:HD12	2.21	0.41
1:B:92:ARG:HB3	1:B:104:ARG:HG3	2.02	0.41
1:C:6:LYS:O	1:C:306:ALA:HA	2.20	0.41
1:C:89:GLU:OE1	1:C:102:HIS:NE2	2.45	0.41
1:A:33:ARG:NH1	6:A:622:HOH:O	2.53	0.41
1:A:169:LEU:HD22	1:A:173:ASP:HB3	2.01	0.41
1:C:436:LEU:N	1:C:436:LEU:CD1	2.83	0.41
1:D:74:ARG:HG2	1:D:74:ARG:NH2	2.35	0.41
1:A:296:VAL:HG13	1:A:307:LEU:CD1	2.51	0.41
1:A:375:GLN:OE1	1:A:454:GLY:HA2	2.21	0.41
1:C:17:ARG:HH21	1:C:17:ARG:HG2	1.86	0.41
1:D:123:LEU:HD12	1:D:247:VAL:HB	2.02	0.41
1:D:206:MET:HE2	1:D:213:VAL:HG22	2.02	0.41
1:A:452:PRO:HA	1:A:453:PRO:HD3	1.96	0.41
1:B:232:VAL:HG22	1:B:238:VAL:HG11	2.02	0.40
1:C:375:GLN:OE1	1:C:454:GLY:HA2	2.22	0.40
1:D:89:GLU:OE1	1:D:102:HIS:NE2	2.46	0.40
1:A:266:ARG:NH1	6:A:609:HOH:O	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LYS:H	1:B:128:LYS:HG2	1.73	0.40
1:A:252:GLU:HB2	1:B:329:ILE:HA	2.04	0.40
1:B:423:ASP:HB3	6:B:662:HOH:O	2.20	0.40
1:B:452:PRO:HA	1:B:453:PRO:HD3	1.95	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:SER:OG	1:D:103:ASP:OD2[1_655]	1.33	0.87
1:B:103:ASP:OD2	1:C:101:SER:OG[1_655]	1.80	0.40
1:B:101:SER:OG	1:C:103:ASP:OD1[1_655]	2.04	0.16
1:A:103:ASP:OD2	1:D:101:SER:OG[1_655]	2.11	0.09

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	470/475 (99%)	455 (97%)	13 (3%)	2 (0%)	30	39
1	B	469/475 (99%)	453 (97%)	14 (3%)	2 (0%)	30	39
1	C	469/475 (99%)	451 (96%)	17 (4%)	1 (0%)	43	56
1	D	471/475 (99%)	456 (97%)	13 (3%)	2 (0%)	30	39
All	All	1879/1900 (99%)	1815 (97%)	57 (3%)	7 (0%)	30	39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	THR
1	B	276	THR
1	C	276	THR

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Mol	Chain	Res	Type
1	D	276	THR
1	D	138	GLY
1	A	138	GLY
1	B	138	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	380/381 (100%)	349 (92%)	31 (8%)	10	14
1	B	379/381 (100%)	358 (94%)	21 (6%)	19	29
1	C	379/381 (100%)	359 (95%)	20 (5%)	20	31
1	D	381/381 (100%)	352 (92%)	29 (8%)	12	17
All	All	1519/1524 (100%)	1418 (93%)	101 (7%)	15	21

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	18	ASP
1	A	19	ASP
1	A	20	LEU
1	A	52	ARG
1	A	106	SER
1	A	110	LYS
1	A	137	GLU
1	A	147	GLU
1	A	155	LYS
1	A	157	ILE
1	A	172	LYS
1	A	187	MET
1	A	194	ARG
1	A	260[A]	ARG
1	A	260[B]	ARG
1	A	317	LYS

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Mol	Chain	Res	Type
1	A	320	LEU
1	A	348	ARG
1	A	359	ARG
1	A	383	LEU
1	A	388	THR
1	A	415	ILE
1	A	418	LYS
1	A	420	GLN
1	A	423	ASP
1	A	425	MET
1	A	428	GLN
1	A	431	LYS
1	A	435	GLU
1	A	436	LEU
1	B	18	ASP
1	B	20	LEU
1	B	72	LYS
1	B	106	SER
1	B	123	LEU
1	B	128	LYS
1	B	142	VAL
1	B	155	LYS
1	B	157	ILE
1	B	187	MET
1	B	204	GLU
1	B	209	ILE
1	B	383	LEU
1	B	388	THR
1	B	415	ILE
1	B	420	GLN
1	B	423	ASP
1	B	436	LEU
1	B	438	ARG
1	B	441	ARG
1	B	466	ARG
1	C	19	ASP
1	C	20	LEU
1	C	106	SER
1	C	123	LEU
1	C	128	LYS
1	C	142	VAL
1	C	155	LYS

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Mol	Chain	Res	Type
1	C	187	MET
1	C	208	ARG
1	C	209	ILE
1	C	348	ARG
1	C	359	ARG
1	C	383	LEU
1	C	388	THR
1	C	420	GLN
1	C	423	ASP
1	C	431	LYS
1	C	436	LEU
1	C	441	ARG
1	C	466	ARG
1	D	18	ASP
1	D	19	ASP
1	D	20	LEU
1	D	40	ASP
1	D	106	SER
1	D	110	LYS
1	D	128	LYS
1	D	137	GLU
1	D	142	VAL
1	D	147	GLU
1	D	155	LYS
1	D	172	LYS
1	D	187	MET
1	D	260[A]	ARG
1	D	260[B]	ARG
1	D	284	GLU
1	D	383	LEU
1	D	388	THR
1	D	415	ILE
1	D	420	GLN
1	D	423	ASP
1	D	428	GLN
1	D	432	SER
1	D	434	LEU
1	D	438	ARG
1	D	441[A]	ARG
1	D	441[B]	ARG
1	D	445	VAL
1	D	456	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	84	HIS
1	A	154	ASN
1	A	387	HIS
1	A	404	GLN
1	B	35	ASN
1	B	44	HIS
1	B	268	ASN
1	B	387	HIS
1	B	404	GLN
1	B	420	GLN
1	B	428	GLN
1	C	35	ASN
1	C	44	HIS
1	C	114	GLN
1	C	387	HIS
1	C	404	GLN
1	C	420	GLN
1	D	35	ASN
1	D	44	HIS
1	D	387	HIS
1	D	404	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	AMP	A	504	-	25,25,25	1.87	9 (36%)	37,38,38	2.14	16 (43%)
4	R5P	B	503	-	12,13,13	2.85	4 (33%)	16,18,18	1.82	5 (31%)
4	R5P	C	503	-	12,13,13	2.71	3 (25%)	16,18,18	1.81	6 (37%)
4	R5P	A	503	-	12,13,13	3.19	5 (41%)	16,18,18	1.75	5 (31%)
3	OXL	A	502	2	5,5,5	1.47	1 (20%)	6,6,6	1.28	2 (33%)
5	AMP	B	504	-	25,25,25	1.86	9 (36%)	37,38,38	2.15	17 (45%)
3	OXL	B	502	2	5,5,5	1.44	1 (20%)	6,6,6	1.93	2 (33%)
3	OXL	C	502	2	5,5,5	1.37	0	6,6,6	1.35	1 (16%)
5	AMP	D	504	-	25,25,25	1.92	8 (32%)	37,38,38	2.18	16 (43%)
5	AMP	C	504	-	25,25,25	1.84	7 (28%)	37,38,38	2.19	17 (45%)
4	R5P	D	503	-	12,13,13	3.39	4 (33%)	16,18,18	1.83	4 (25%)
3	OXL	D	502	2	5,5,5	1.48	1 (20%)	6,6,6	1.92	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AMP	A	504	-	-	5/10/26/26	0/3/3/3
4	R5P	B	503	-	-	1/15/16/16	-
4	R5P	C	503	-	-	6/15/16/16	-
4	R5P	A	503	-	-	3/15/16/16	-
3	OXL	A	502	2	-	4/4/4/4	-
5	AMP	B	504	-	-	1/10/26/26	0/3/3/3
3	OXL	B	502	2	-	4/4/4/4	-
3	OXL	C	502	2	-	4/4/4/4	-
5	AMP	D	504	-	-	0/10/26/26	0/3/3/3
5	AMP	C	504	-	-	0/10/26/26	0/3/3/3
4	R5P	D	503	-	-	3/15/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	D	502	2	-	4/4/4/4	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	R5P	P-O5	8.51	1.87	1.60
4	A	503	R5P	P-O5	7.75	1.84	1.60
4	B	503	R5P	P-O5	6.98	1.82	1.60
4	C	503	R5P	P-O5	6.38	1.80	1.60
4	D	503	R5P	C3-C2	6.24	1.62	1.53
4	A	503	R5P	C3-C2	5.86	1.62	1.53
4	C	503	R5P	C3-C2	5.42	1.61	1.53
4	B	503	R5P	C3-C2	5.35	1.61	1.53
5	C	504	AMP	C2-N1	4.02	1.41	1.33
5	D	504	AMP	C5-N7	-4.00	1.31	1.39
5	D	504	AMP	C2-N1	3.99	1.41	1.33
5	B	504	AMP	C2-N1	3.99	1.41	1.33
5	A	504	AMP	C2-N1	3.89	1.40	1.33
5	B	504	AMP	C5-N7	-3.71	1.32	1.39
5	A	504	AMP	C5-N7	-3.70	1.32	1.39
5	C	504	AMP	C5-N7	-3.52	1.32	1.39
5	C	504	AMP	C2-N3	3.35	1.39	1.33
5	A	504	AMP	C4-N9	-3.35	1.30	1.37
5	D	504	AMP	C2-N3	3.34	1.39	1.33
5	B	504	AMP	C8-N9	-3.34	1.31	1.37
5	D	504	AMP	C8-N9	-3.23	1.32	1.37
5	C	504	AMP	C8-N9	-3.18	1.32	1.37
5	D	504	AMP	C4-N9	-3.01	1.31	1.37
4	D	503	R5P	C5-C4	2.95	1.55	1.51
5	A	504	AMP	C8-N9	-2.94	1.32	1.37
4	D	503	R5P	O5-C5	-2.93	1.33	1.44
4	B	503	R5P	O5-C5	-2.88	1.33	1.44
5	A	504	AMP	C2-N3	2.85	1.39	1.33
5	B	504	AMP	C2-N3	2.79	1.38	1.33
5	B	504	AMP	C4-N9	-2.78	1.31	1.37
5	C	504	AMP	C4-N9	-2.66	1.32	1.37
4	C	503	R5P	O5-C5	-2.61	1.34	1.44
5	B	504	AMP	C2'-C3'	-2.58	1.46	1.53
4	A	503	R5P	O4-C4	-2.55	1.38	1.43
5	A	504	AMP	C5-C6	-2.47	1.34	1.41
3	D	502	OXL	O3-C1	-2.35	1.24	1.30
4	B	503	R5P	O2-C2	-2.35	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	504	AMP	C5-C6	-2.34	1.34	1.41
5	A	504	AMP	C5-C4	-2.31	1.35	1.39
4	A	503	R5P	O5-C5	-2.27	1.36	1.44
4	A	503	R5P	C4-C3	2.24	1.57	1.53
3	B	502	OXL	O3-C1	-2.22	1.24	1.30
5	D	504	AMP	P-O2P	-2.21	1.46	1.54
5	D	504	AMP	P-O3P	-2.19	1.46	1.54
3	A	502	OXL	O3-C1	-2.17	1.24	1.30
5	B	504	AMP	C5-C6	-2.13	1.35	1.41
5	A	504	AMP	O4'-C4'	-2.12	1.40	1.45
5	A	504	AMP	P-O2P	-2.11	1.47	1.54
5	C	504	AMP	C5-C4	-2.09	1.35	1.39
5	C	504	AMP	C5-C6	-2.03	1.35	1.41
5	B	504	AMP	C5-C4	-2.03	1.35	1.39
5	B	504	AMP	P-O3P	-2.01	1.47	1.54

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	AMP	N3-C2-N1	-6.19	119.22	128.58
5	C	504	AMP	N3-C2-N1	-6.09	119.36	128.58
5	D	504	AMP	N3-C2-N1	-6.05	119.42	128.58
5	B	504	AMP	N3-C2-N1	-6.05	119.43	128.58
5	B	504	AMP	C5-C4-N3	-4.23	120.89	126.72
5	C	504	AMP	C5-C4-N3	-4.23	120.90	126.72
5	D	504	AMP	C5-C4-N3	-4.20	120.93	126.72
5	A	504	AMP	C5-C4-N3	-4.02	121.19	126.72
5	A	504	AMP	N9-C8-N7	-3.82	108.52	113.94
4	D	503	R5P	O2P-P-O5	-3.80	96.75	106.67
5	C	504	AMP	N9-C8-N7	-3.74	108.63	113.94
4	B	503	R5P	O2P-P-O5	-3.71	97.01	106.67
5	B	504	AMP	N9-C8-N7	-3.60	108.83	113.94
5	D	504	AMP	N9-C8-N7	-3.53	108.92	113.94
5	C	504	AMP	C4'-O4'-C1'	-3.22	102.36	109.47
3	B	502	OXL	O4-C2-C1	3.04	118.73	112.83
5	D	504	AMP	C6-C5-C4	3.03	121.32	117.18
4	C	503	R5P	O5-P-O1P	-2.99	98.36	106.44
5	B	504	AMP	C4-C5-N7	-2.97	107.18	110.58
3	D	502	OXL	O4-C2-C1	2.97	118.59	112.83
5	C	504	AMP	C4-C5-N7	-2.96	107.20	110.58
5	C	504	AMP	C2-N3-C4	2.95	119.04	111.83
5	B	504	AMP	C2-N3-C4	2.95	119.03	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	AMP	C2-N3-C4	2.94	119.02	111.83
5	C	504	AMP	C6-C5-C4	2.91	121.15	117.18
5	D	504	AMP	C2-N3-C4	2.90	118.92	111.83
5	C	504	AMP	C5-N7-C8	2.90	108.00	103.45
5	B	504	AMP	C6-C5-C4	2.84	121.06	117.18
5	D	504	AMP	C4-C5-N7	-2.81	107.37	110.58
5	A	504	AMP	C4'-O4'-C1'	-2.81	103.26	109.47
5	D	504	AMP	O2P-P-O5'	-2.80	99.36	106.67
5	B	504	AMP	C5-N7-C8	2.79	107.84	103.45
4	A	503	R5P	O2P-P-O5	-2.78	99.42	106.67
5	B	504	AMP	O4'-C1'-N9	2.77	113.42	108.09
5	A	504	AMP	C6-C5-C4	2.77	120.96	117.18
4	A	503	R5P	O3P-P-O5	-2.76	99.47	106.67
5	D	504	AMP	O4'-C1'-C2'	-2.74	100.76	106.62
3	D	502	OXL	O3-C1-C2	2.70	118.07	112.83
5	D	504	AMP	C5-N7-C8	2.70	107.69	103.45
3	B	502	OXL	O3-C1-C2	2.69	118.04	112.83
5	C	504	AMP	O5'-P-O1P	-2.65	99.28	106.44
5	A	504	AMP	C5-N7-C8	2.61	107.55	103.45
5	A	504	AMP	C4-C5-N7	-2.61	107.60	110.58
5	B	504	AMP	O2P-P-O5'	-2.61	99.88	106.67
4	C	503	R5P	O3P-P-O2P	2.58	117.48	107.80
5	A	504	AMP	C5-C6-N6	-2.57	116.91	123.29
5	D	504	AMP	C4'-O4'-C1'	-2.57	103.79	109.47
5	B	504	AMP	O3P-P-O2P	2.55	117.38	107.80
5	D	504	AMP	O4'-C1'-N9	2.54	112.96	108.09
5	D	504	AMP	C5-C6-N6	-2.52	117.05	123.29
5	D	504	AMP	O3P-P-O2P	2.48	117.11	107.80
4	D	503	R5P	O2-C2-C3	2.48	115.27	109.46
5	C	504	AMP	O4'-C1'-C2'	-2.46	101.35	106.62
5	A	504	AMP	O5'-P-O1P	-2.46	99.80	106.44
4	A	503	R5P	O3-C3-C4	2.44	114.47	108.93
5	C	504	AMP	C5-C6-N6	-2.43	117.26	123.29
5	A	504	AMP	C4-N9-C8	2.36	108.22	105.74
4	D	503	R5P	O3-C3-C4	2.36	114.30	108.93
4	B	503	R5P	O3P-P-O2P	2.35	116.63	107.80
5	A	504	AMP	O3P-P-O5'	-2.35	100.55	106.67
4	A	503	R5P	O3P-P-O2P	2.33	116.54	107.80
4	C	503	R5P	O3P-P-O5	-2.33	100.60	106.67
5	B	504	AMP	C5-C6-N6	-2.31	117.57	123.29
3	C	502	OXL	O3-C1-C2	2.30	117.29	112.83
4	C	503	R5P	O3-C3-C4	2.29	114.14	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	R5P	O3-C3-C4	2.28	114.11	108.93
4	C	503	R5P	O2-C2-C3	2.26	114.76	109.46
5	C	504	AMP	N3-C4-N9	2.26	131.00	127.17
4	C	503	R5P	O2P-P-O5	-2.26	100.79	106.67
5	B	504	AMP	O5'-P-O1P	-2.25	100.36	106.44
4	D	503	R5P	O3P-P-O2P	2.24	116.21	107.80
4	B	503	R5P	O3P-P-O5	-2.24	100.83	106.67
5	D	504	AMP	O5'-P-O1P	-2.24	100.39	106.44
5	B	504	AMP	O4'-C1'-C2'	-2.23	101.85	106.62
5	B	504	AMP	C5-C4-N9	2.22	108.23	105.81
5	C	504	AMP	C4-N9-C8	2.22	108.07	105.74
5	D	504	AMP	C5-C4-N9	2.21	108.22	105.81
4	A	503	R5P	O2-C2-C3	2.20	114.60	109.46
5	C	504	AMP	O3P-P-O5'	-2.19	100.97	106.67
5	B	504	AMP	N3-C4-N9	2.18	130.88	127.17
5	C	504	AMP	O3P-P-O2P	2.17	115.94	107.80
5	D	504	AMP	N3-C4-N9	2.16	130.85	127.17
5	A	504	AMP	O4'-C1'-C2'	-2.14	102.04	106.62
4	B	503	R5P	O2-C2-C3	2.14	114.47	109.46
5	B	504	AMP	O3P-P-O5'	-2.11	101.16	106.67
5	A	504	AMP	C5-C4-N9	2.11	108.11	105.81
5	A	504	AMP	O3P-P-O2P	2.11	115.70	107.80
5	C	504	AMP	C5-C4-N9	2.10	108.10	105.81
3	A	502	OXL	O4-C2-C1	2.09	116.88	112.83
5	A	504	AMP	N3-C4-N9	2.08	130.71	127.17
5	B	504	AMP	C4-N9-C8	2.06	107.91	105.74
3	A	502	OXL	O3-C1-C2	2.05	116.81	112.83
5	C	504	AMP	O4'-C1'-N9	2.02	111.98	108.09

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	R5P	O1-C1-C2-C3
4	B	503	R5P	O1-C1-C2-C3
4	C	503	R5P	O1-C1-C2-C3
4	C	503	R5P	C3-C4-C5-O5
4	C	503	R5P	O4-C4-C5-O5
4	C	503	R5P	C5-O5-P-O1P
4	C	503	R5P	C5-O5-P-O3P
4	D	503	R5P	O1-C1-C2-C3
5	A	504	AMP	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
5	A	504	AMP	C5'-O5'-P-O3P
5	A	504	AMP	C3'-C4'-C5'-O5'
5	A	504	AMP	O4'-C4'-C5'-O5'
3	A	502	OXL	O3-C1-C2-O4
3	C	502	OXL	O3-C1-C2-O4
3	D	502	OXL	O3-C1-C2-O4
3	B	502	OXL	O3-C1-C2-O4
3	A	502	OXL	O1-C1-C2-O2
3	B	502	OXL	O1-C1-C2-O2
3	D	502	OXL	O1-C1-C2-O2
4	A	503	R5P	O4-C4-C5-O5
3	C	502	OXL	O1-C1-C2-O2
4	A	503	R5P	C5-O5-P-O1P
4	D	503	R5P	C5-O5-P-O1P
3	A	502	OXL	O1-C1-C2-O4
3	A	502	OXL	O3-C1-C2-O2
3	B	502	OXL	O1-C1-C2-O4
3	B	502	OXL	O3-C1-C2-O2
3	C	502	OXL	O1-C1-C2-O4
3	C	502	OXL	O3-C1-C2-O2
3	D	502	OXL	O1-C1-C2-O4
3	D	502	OXL	O3-C1-C2-O2
4	C	503	R5P	C5-O5-P-O2P
4	D	503	R5P	C5-O5-P-O3P
5	A	504	AMP	C5'-O5'-P-O1P
5	B	504	AMP	C3'-C4'-C5'-O5'

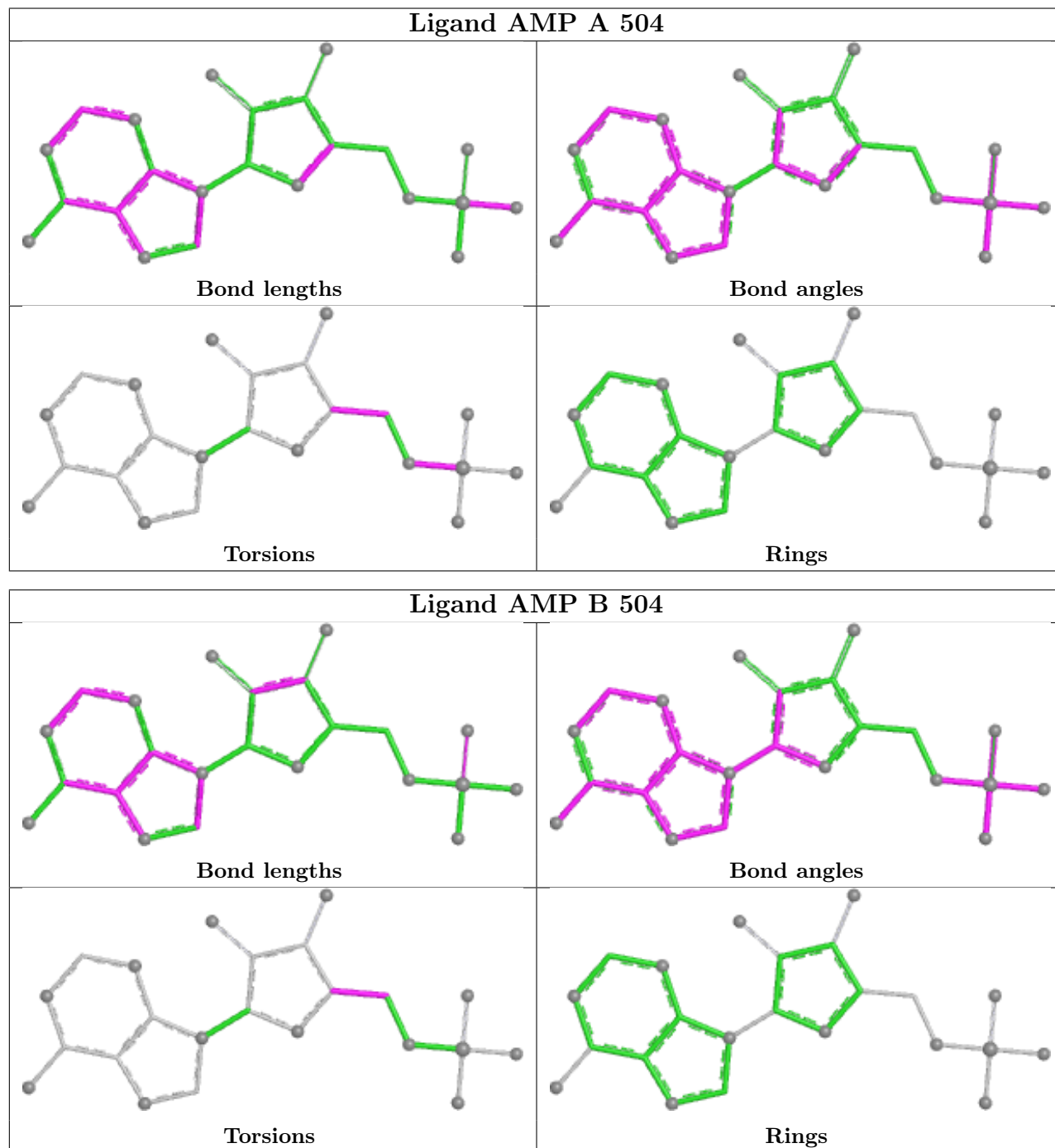
There are no ring outliers.

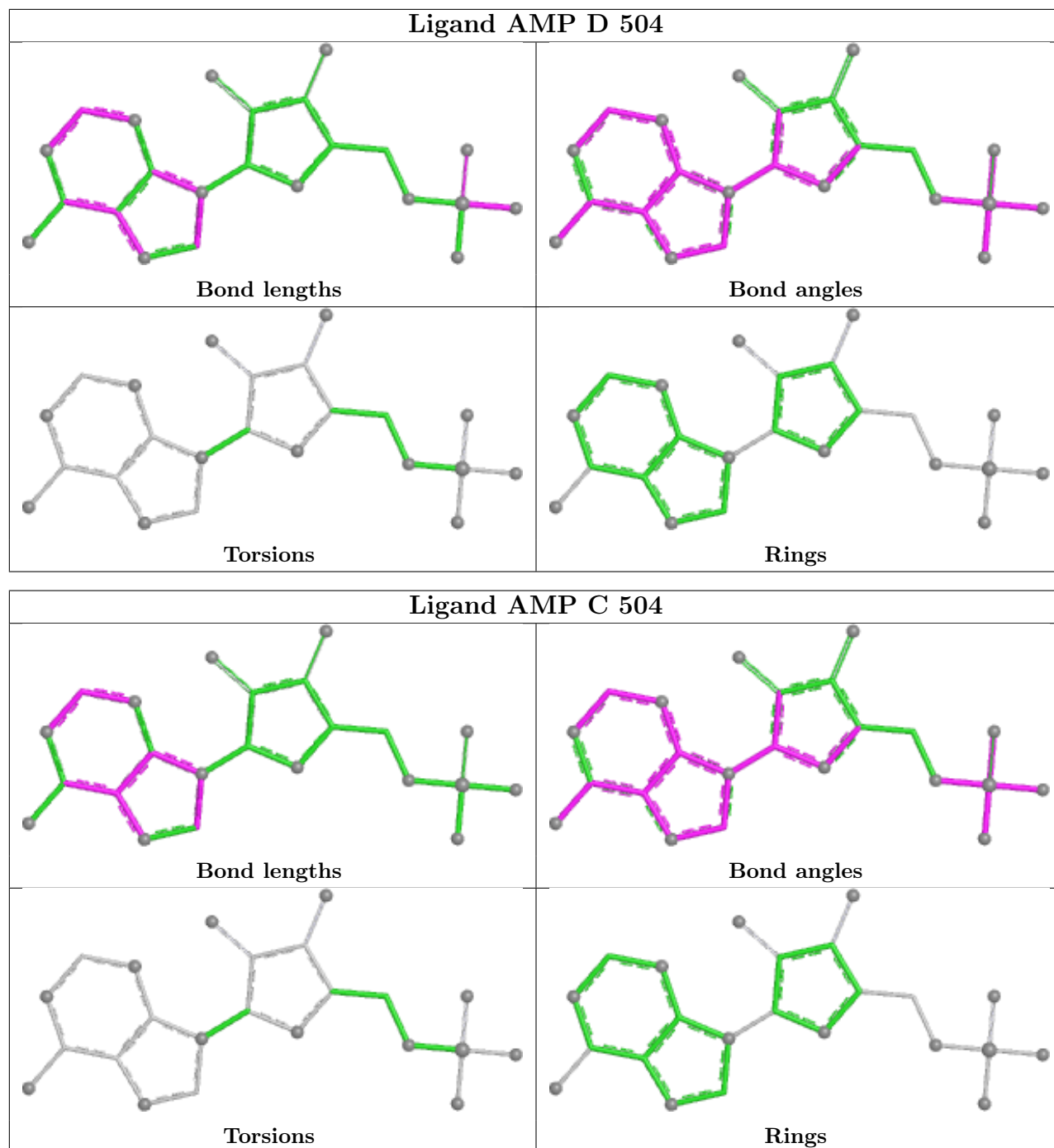
8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	504	AMP	2	0
4	B	503	R5P	1	0
4	C	503	R5P	1	0
4	A	503	R5P	1	0
5	B	504	AMP	3	0
5	D	504	AMP	1	0
5	C	504	AMP	1	0
4	D	503	R5P	1	0

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

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	471/475 (99%)	-1.18	0 100 100	21, 55, 89, 106	1 (0%)
1	B	471/475 (99%)	-1.17	0 100 100	36, 55, 91, 114	0
1	C	471/475 (99%)	-1.16	0 100 100	38, 55, 90, 108	0
1	D	471/475 (99%)	-1.15	0 100 100	22, 55, 89, 110	2 (0%)
All	All	1884/1900 (99%)	-1.17	0 100 100	21, 55, 90, 114	3 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

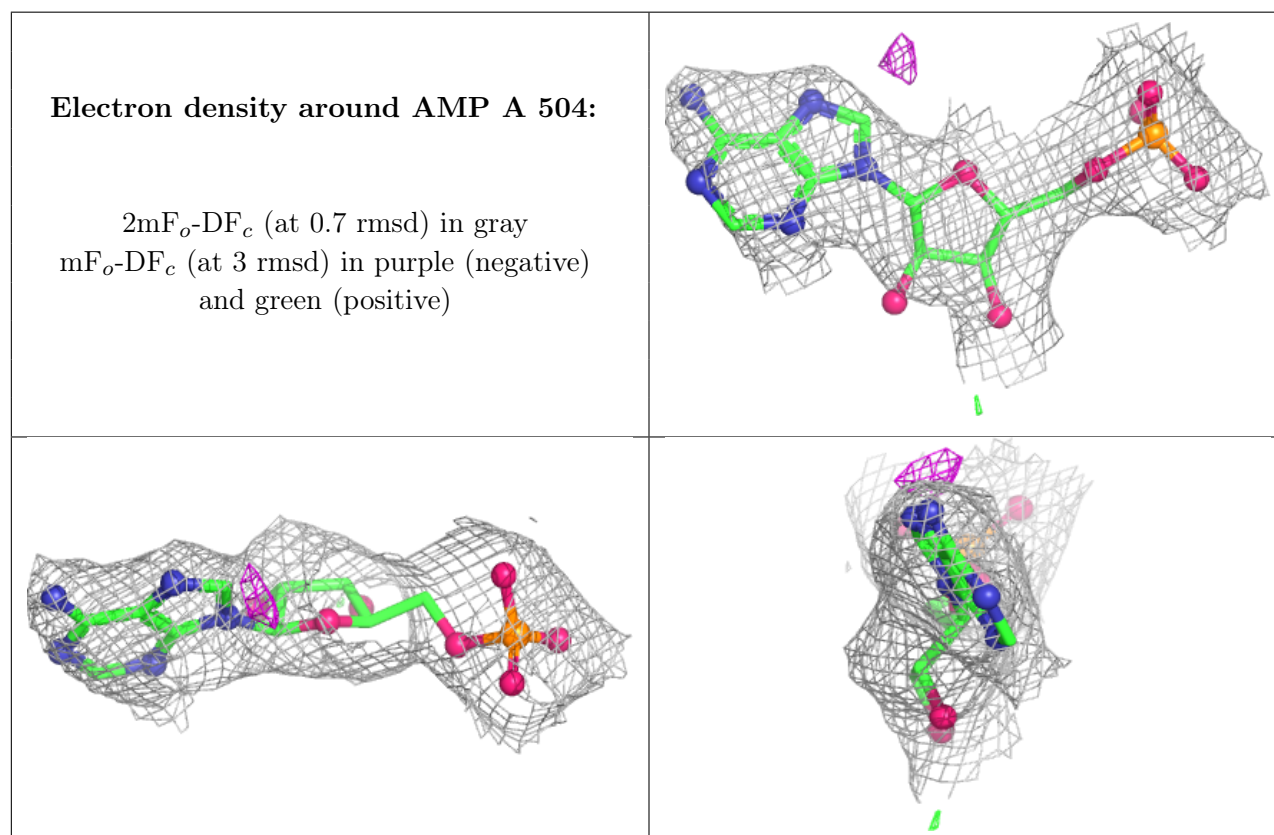
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	501	1/1	0.99	0.03	46,46,46,46	0
2	MG	B	501	1/1	0.99	0.03	41,41,41,41	0
2	MG	C	501	1/1	0.99	0.03	40,40,40,40	0
3	OXL	A	502	6/6	0.99	0.04	43,48,49,52	0

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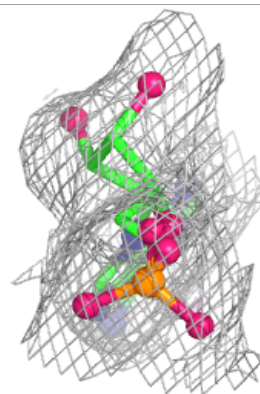
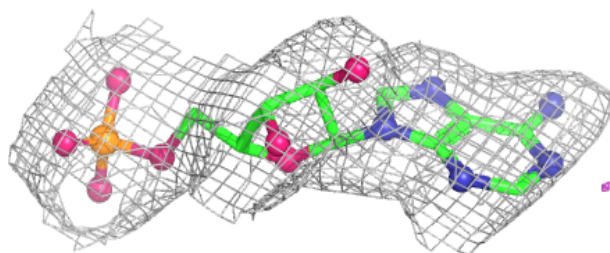
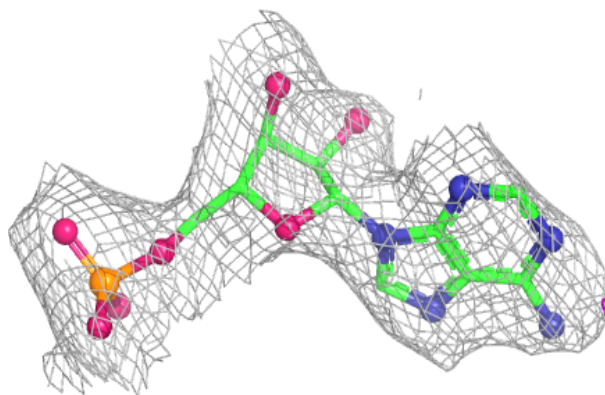
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OXL	B	502	6/6	0.99	0.05	42,51,52,53	0
3	OXL	C	502	6/6	0.99	0.04	42,52,54,56	0
3	OXL	D	502	6/6	0.99	0.04	44,50,51,53	0
4	R5P	A	503	14/14	0.99	0.04	57,70,81,90	0
4	R5P	B	503	14/14	0.99	0.03	51,68,77,82	0
4	R5P	C	503	14/14	0.99	0.03	48,68,79,80	0
4	R5P	D	503	14/14	0.99	0.04	57,73,83,83	0
5	AMP	A	504	23/23	0.99	0.04	45,66,70,79	0
5	AMP	B	504	23/23	0.99	0.04	46,67,71,73	0
5	AMP	C	504	23/23	0.99	0.04	49,67,73,78	0
5	AMP	D	504	23/23	0.99	0.04	48,67,72,77	0
2	MG	D	501	1/1	1.00	0.01	46,46,46,46	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.

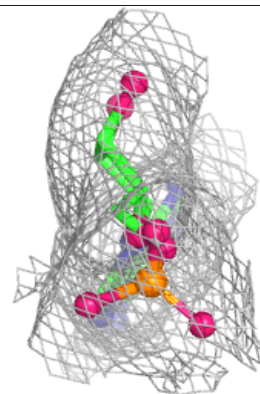
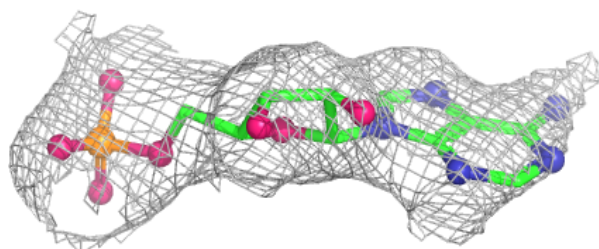
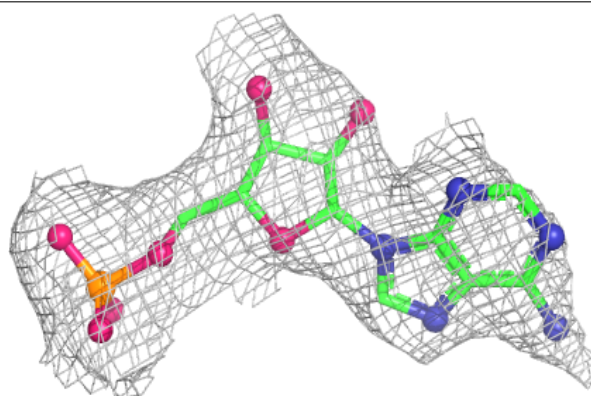


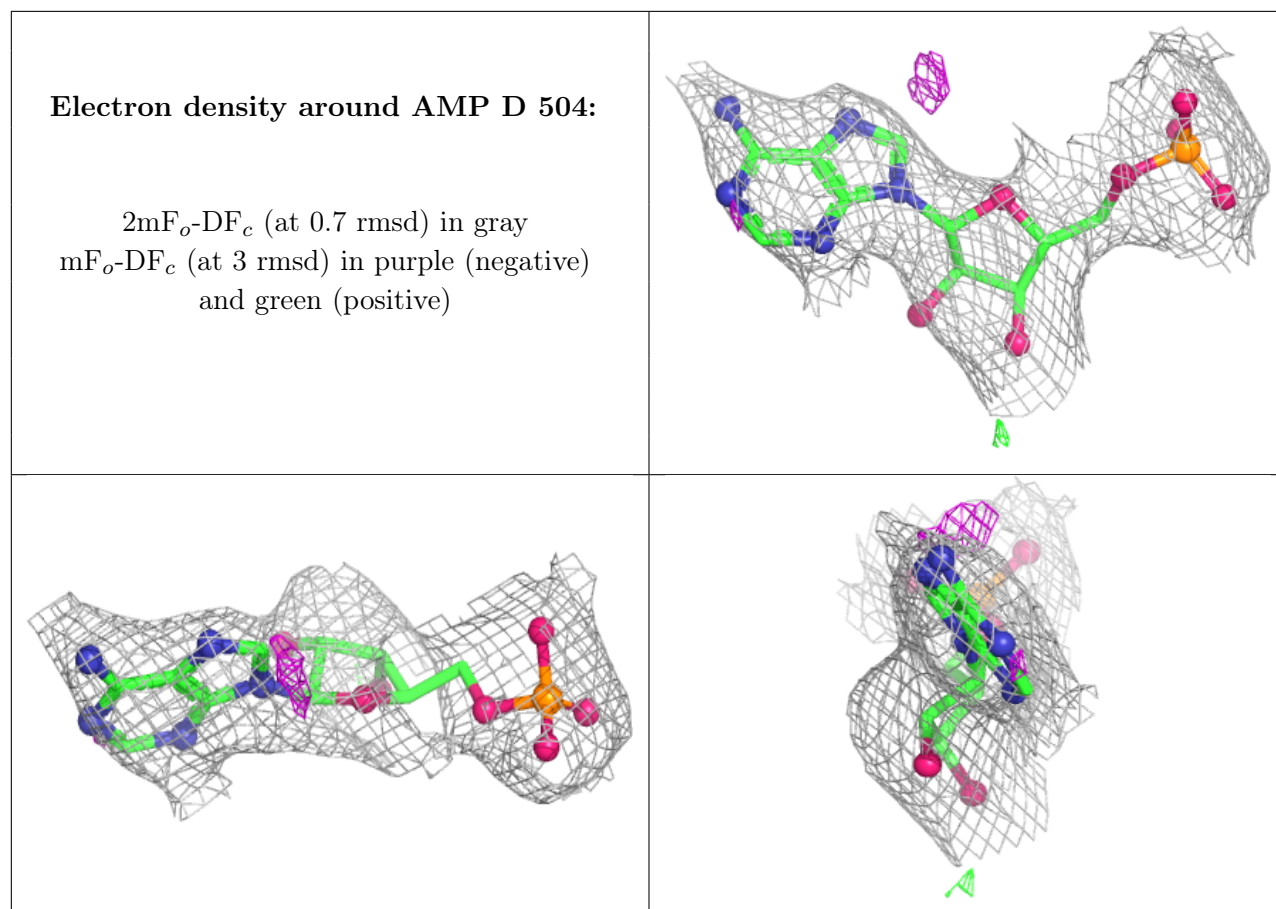
Electron density around AMP B 504:

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

**Electron density around AMP C 504:**

$2mF_o-DF_c$ (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.