



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 07:33 AM EDT

PDB ID : 1PKX / pdb_00001pkx
Title : Crystal Structure of human ATIC in complex with XMP
Authors : Wolan, D.W.; Cheong, C.G.; Greasley, S.E.; Wilson, I.A.
Deposited on : 2003-06-06
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

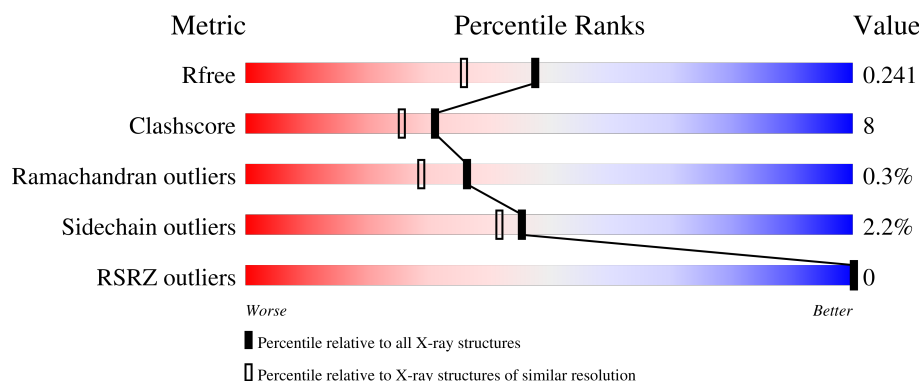
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	592	80% 18% ..
1	B	592	80% 18% ..
1	C	592	78% 19% ..
1	D	592	82% 17% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18791 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.

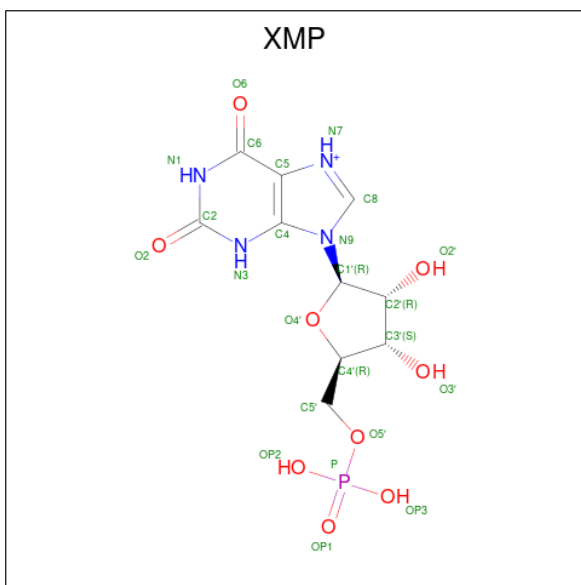
- Molecule 1 is a protein called Bifunctional purine biosynthesis protein PURH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4428	2799	769	842	18			
1	B	589	Total	C	N	O	S	0	0	0
			4462	2818	778	848	18			
1	C	587	Total	C	N	O	S	0	0	0
			4422	2793	771	840	18			
1	D	589	Total	C	N	O	S	0	0	0
			4450	2810	776	846	18			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 3 is XANTHOSINE-5'-MONOPHOSPHATE (CCD ID: XMP) (formula: C₁₀H₁₄N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 24	C 10	N 4	O 9	P 1	0	0
3	C	1	Total 24	C 10	N 4	O 9	P 1	0	0

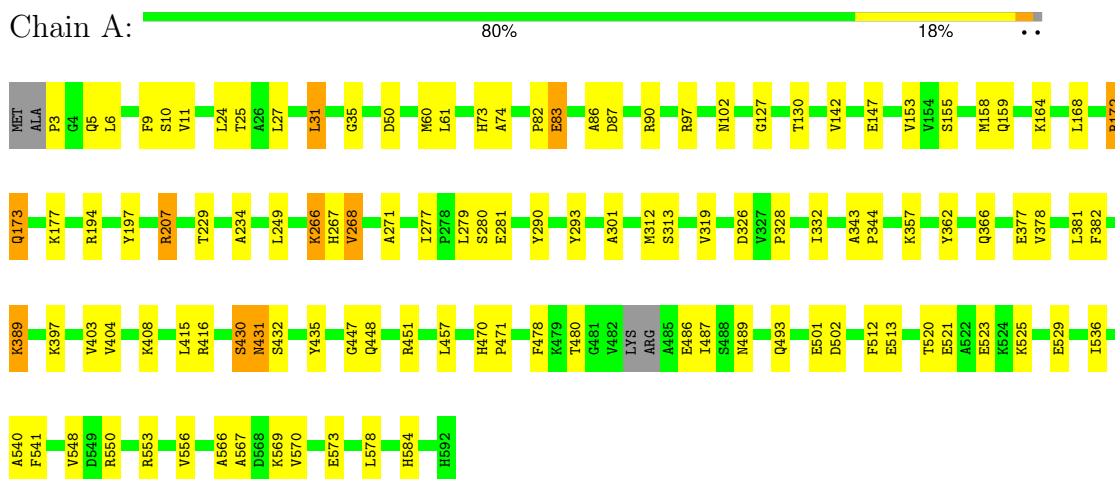
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	210	Total O 210 210	0	0
4	B	278	Total O 278 278	0	0
4	C	209	Total O 209 209	0	0
4	D	280	Total O 280 280	0	0

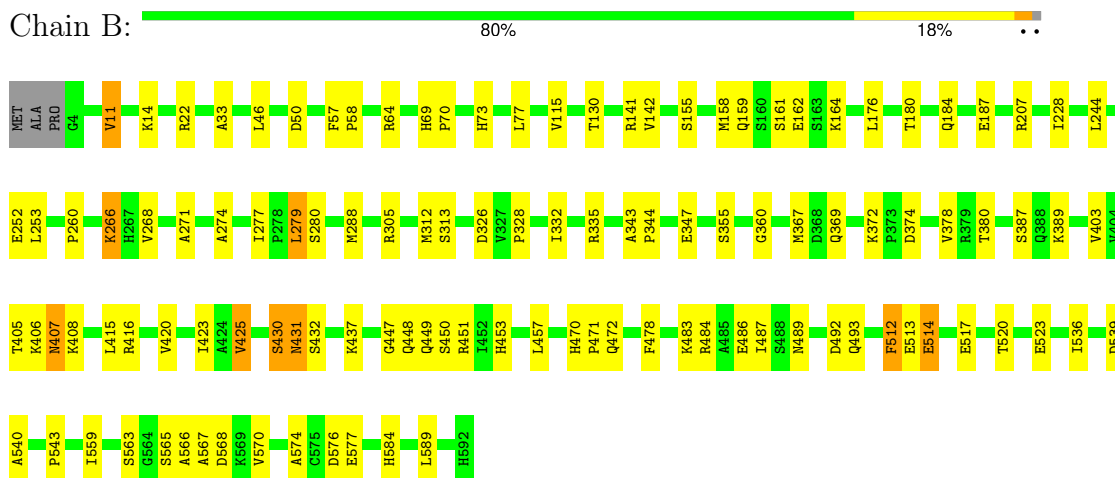
3 Residue-property plots

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.

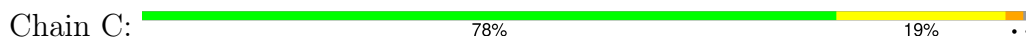
- Molecule 1: Bifunctional purine biosynthesis protein PURH

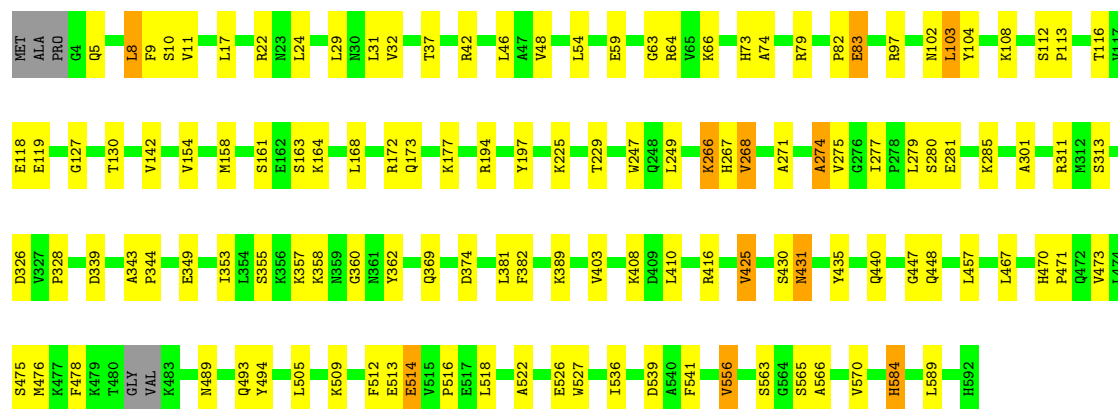


- Molecule 1: Bifunctional purine biosynthesis protein PURH



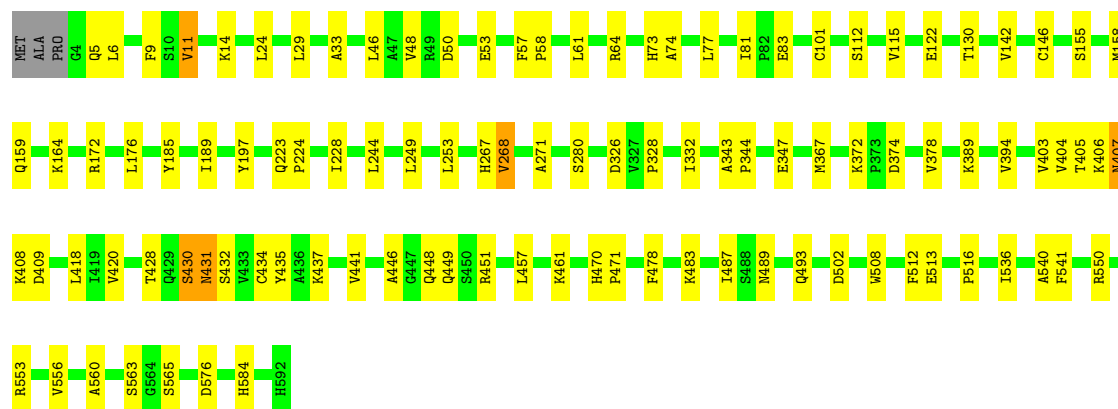
- Molecule 1: Bifunctional purine biosynthesis protein PURH





- Molecule 1: Bifunctional purine biosynthesis protein PURH

Chain D: 82% 17% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.52Å 93.56Å 179.88Å 90.00° 91.09° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.90) 79.3 (50.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.249 0.204 , 0.241	Depositor DCC
R_{free} test set	8882 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.246 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18791	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: K, XMP

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	0.55	0/4510	0.99	15/6135 (0.2%)
1	B	0.57	0/4545	0.98	21/6176 (0.3%)
1	C	0.55	0/4503	0.98	16/6122 (0.3%)
1	D	0.57	0/4533	0.97	18/6163 (0.3%)
All	All	0.56	0/18091	0.98	70/24596 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	271	ALA	N-CA-C	-9.29	100.73	112.90
1	B	271	ALA	N-CA-C	-8.97	101.15	112.90
1	A	271	ALA	N-CA-C	-8.96	100.67	111.69
1	D	271	ALA	N-CA-C	-8.46	102.75	113.23
1	C	513	GLU	N-CA-C	-8.28	103.28	112.72
1	A	513	GLU	N-CA-C	-7.82	103.63	113.02
1	C	566	ALA	N-CA-C	-7.39	104.26	113.20
1	A	566	ALA	N-CA-C	-7.31	103.02	112.23
1	B	77	LEU	N-CA-C	7.05	121.88	113.28
1	B	374	ASP	N-CA-C	-6.86	100.83	110.50
1	C	410	LEU	CA-C-N	6.86	126.84	119.78
1	C	410	LEU	C-N-CA	6.86	126.84	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	563	SER	N-CA-C	-6.75	99.97	110.17
1	B	280	SER	N-CA-C	-6.70	101.88	110.53
1	D	513	GLU	N-CA-C	-6.63	103.98	111.14
1	A	280	SER	N-CA-C	-6.62	101.99	110.53
1	D	74	ALA	N-CA-C	-6.60	104.17	111.36
1	A	486	GLU	N-CA-C	-6.45	104.34	111.82
1	B	277	ILE	N-CA-C	-6.40	103.13	108.63
1	D	347	GLU	N-CA-C	-6.34	100.89	110.28
1	B	566	ALA	N-CA-C	-6.28	104.88	112.54
1	A	3	PRO	N-CA-CB	6.18	109.80	103.00
1	B	513	GLU	N-CA-C	-6.16	104.82	113.20
1	D	374	ASP	N-CA-C	-6.15	101.83	110.50
1	D	280	SER	N-CA-C	-6.11	102.65	110.53
1	C	280	SER	N-CA-C	-6.10	102.66	110.53
1	A	430	SER	N-CA-C	6.06	118.73	110.55
1	D	430	SER	N-CA-C	5.94	118.57	110.55
1	C	74	ALA	N-CA-C	-5.87	104.96	111.36
1	A	6	LEU	N-CA-C	5.84	119.57	110.17
1	C	589	LEU	N-CA-C	5.82	117.42	110.44
1	B	430	SER	N-CA-C	5.64	118.16	110.55
1	D	77	LEU	N-CA-C	5.62	120.14	113.28
1	A	404	VAL	N-CA-C	5.61	118.29	112.90
1	B	372	LYS	CA-C-N	5.59	125.56	120.03
1	B	372	LYS	C-N-CA	5.59	125.56	120.03
1	A	541	PHE	N-CA-C	5.57	117.73	110.43
1	C	103	LEU	N-CA-C	5.57	119.06	110.42
1	C	563	SER	N-CA-C	-5.53	101.78	110.36
1	B	347	GLU	N-CA-C	-5.49	102.16	110.28
1	D	11	VAL	N-CA-C	5.48	116.37	108.48
1	B	11	VAL	N-CA-C	5.47	116.36	108.48
1	D	394	VAL	N-CA-C	5.47	116.46	108.58
1	C	142	VAL	N-CA-C	5.46	117.17	108.87
1	A	319	VAL	N-CA-C	5.44	117.14	108.87
1	B	483	LYS	N-CA-C	5.42	117.52	110.53
1	A	389	LYS	N-CA-C	-5.40	102.28	110.28
1	D	389	LYS	N-CA-C	-5.40	101.67	110.20
1	B	389	LYS	N-CA-C	-5.40	101.67	110.20
1	C	389	LYS	N-CA-C	-5.37	102.33	110.28
1	D	142	VAL	N-CA-C	5.36	117.02	108.87
1	D	502	ASP	CB-CA-C	-5.34	109.96	117.23
1	C	556	VAL	N-CA-C	5.33	115.88	108.84
1	C	311	ARG	N-CA-C	5.30	117.80	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	LEU	N-CA-C	5.29	116.79	110.44
1	A	74	ALA	N-CA-C	-5.25	105.72	111.82
1	D	563	SER	N-CA-C	-5.25	102.23	110.36
1	D	223	GLN	N-CA-C	-5.23	104.11	110.13
1	B	512	PHE	N-CA-C	5.21	118.12	109.46
1	C	374	ASP	N-CA-C	-5.20	103.67	110.53
1	D	372	LYS	CA-C-N	5.18	125.08	119.85
1	D	372	LYS	C-N-CA	5.18	125.08	119.85
1	A	142	VAL	N-CA-C	5.10	116.62	108.87
1	A	502	ASP	CB-CA-C	-5.08	110.73	116.63
1	B	407	ASN	N-CA-C	-5.08	99.97	110.80
1	B	142	VAL	N-CA-C	5.08	116.59	108.87
1	B	274	ALA	N-CA-C	5.05	115.82	108.14
1	D	6	LEU	N-CA-C	5.05	118.34	110.32
1	C	274	ALA	N-CA-C	5.04	115.96	108.60
1	B	187	GLU	N-CA-C	-5.01	105.89	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	TYR	Sidechain

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	4428	0	4367	81	0
1	B	4462	0	4425	68	0
1	C	4422	0	4367	89	0
1	D	4450	0	4400	68	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	24	0	12	2	0
3	C	24	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	210	0	0	4	0
4	B	278	0	0	7	0
4	C	209	0	0	9	0
4	D	280	0	0	2	0
All	All	18791	0	17583	291	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (291) 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:C:5:GLN:HE22	1:C:97:ARG:HD3	1.35	0.90
1:B:312:MET:HE2	1:B:492:ASP:HB3	1.58	0.84
1:C:172:ARG:HD3	1:D:197:TYR:CD1	2.15	0.82
1:A:431:ASN:C	1:A:431:ASN:HD22	1.88	0.81
1:B:11:VAL:O	1:B:14:LYS:HE2	1.79	0.81
1:B:431:ASN:C	1:B:431:ASN:HD22	1.88	0.81
1:A:168:LEU:O	1:A:172:ARG:HG2	1.81	0.80
1:D:431:ASN:HD22	1:D:431:ASN:C	1.93	0.76
1:A:431:ASN:HD21	1:A:448:GLN:HB2	1.51	0.76
1:C:83:GLU:CD	1:C:83:GLU:H	1.94	0.76
1:D:155:SER:O	1:D:159:GLN:HG2	1.87	0.75
1:C:229:THR:HG23	4:C:2183:HOH:O	1.91	0.70
1:D:431:ASN:HD21	1:D:448:GLN:HB2	1.57	0.69
1:D:437:LYS:HE3	4:D:2269:HOH:O	1.93	0.69
1:D:536:ILE:CD1	1:D:556:VAL:HG21	2.22	0.69
1:A:266:LYS:HB3	1:B:449:GLN:HB3	1.76	0.68
1:B:425:VAL:HG13	1:B:539:ASP:HB3	1.74	0.68
1:A:83:GLU:CD	1:A:83:GLU:H	2.00	0.68
1:C:5:GLN:NE2	1:C:97:ARG:HD3	2.08	0.68
1:D:536:ILE:HD11	1:D:556:VAL:HG21	1.77	0.67
1:C:32:VAL:HG11	1:C:54:LEU:HD12	1.76	0.67
4:C:2117:HOH:O	1:D:378:VAL:HG12	1.95	0.67
1:B:536:ILE:CG2	1:B:559:ILE:HG12	2.24	0.66
1:D:403:VAL:HG11	1:D:408:LYS:HA	1.77	0.66
1:A:25:THR:OG1	1:A:31:LEU:HD11	1.95	0.65
1:C:435:TYR:CE2	1:C:536:ILE:HD11	2.31	0.65
1:C:457:LEU:HD23	1:C:457:LEU:C	2.22	0.65
1:C:64:ARG:HG3	4:C:2156:HOH:O	1.96	0.65
1:A:31:LEU:HD12	1:A:31:LEU:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:ASN:ND2	1:D:409:ASP:OD1	2.31	0.63
1:C:489:ASN:O	1:C:493:GLN:HG3	1.98	0.63
1:A:266:LYS:HG3	1:A:313:SER:O	1.99	0.63
1:B:207:ARG:HG2	4:B:2047:HOH:O	1.99	0.62
1:A:435:TYR:CE2	1:A:536:ILE:HD11	2.35	0.62
1:A:31:LEU:HD12	1:A:31:LEU:H	1.65	0.62
1:A:403:VAL:HG11	1:A:408:LYS:HA	1.82	0.62
1:B:266:LYS:HG3	1:B:313:SER:O	1.99	0.62
1:B:431:ASN:C	1:B:431:ASN:ND2	2.57	0.61
1:D:435:TYR:CE2	1:D:536:ILE:HD11	2.35	0.61
1:A:147:GLU:OE1	1:A:177:LYS:HD3	2.00	0.61
1:A:389:LYS:HE2	4:A:2107:HOH:O	2.01	0.60
1:A:431:ASN:ND2	1:A:448:GLN:HB2	2.17	0.60
1:B:328:PRO:O	1:B:332:ILE:HG13	2.02	0.60
1:A:207:ARG:NH1	1:A:234:ALA:O	2.34	0.60
1:C:431:ASN:HB2	1:C:448:GLN:O	2.01	0.59
1:B:335:ARG:CZ	1:B:484:ARG:HH11	2.15	0.59
1:B:335:ARG:NH2	1:B:484:ARG:HH11	1.99	0.59
1:B:180:THR:HG22	1:B:184:GLN:HE21	1.66	0.59
1:A:158:MET:O	1:A:164:LYS:HA	2.02	0.58
1:C:8:LEU:C	1:C:8:LEU:HD13	2.28	0.58
1:B:406:LYS:N	1:B:576:ASP:OD1	2.32	0.58
1:A:73:HIS:CE1	1:A:130:THR:HG22	2.39	0.57
1:C:403:VAL:HG11	1:C:408:LYS:HA	1.86	0.57
1:C:79:ARG:NE	4:C:2194:HOH:O	2.37	0.57
1:C:116:THR:OG1	1:C:119:GLU:HG3	2.04	0.57
1:C:5:GLN:NE2	1:C:97:ARG:HB2	2.20	0.57
1:B:470:HIS:HD2	1:B:472:GLN:H	1.51	0.57
1:C:63:GLY:HA2	1:C:66:LYS:HD3	1.86	0.57
1:C:339:ASP:HA	1:C:358:LYS:NZ	2.20	0.57
1:A:5:GLN:HE22	1:A:97:ARG:HD3	1.71	0.56
1:D:489:ASN:O	1:D:493:GLN:HG3	2.04	0.56
1:B:536:ILE:HG22	1:B:559:ILE:HG12	1.87	0.56
1:D:253:LEU:HD21	1:D:420:VAL:HA	1.87	0.56
1:A:478:PHE:CZ	1:A:487:ILE:HG23	2.41	0.56
1:A:569:LYS:O	1:A:573:GLU:HG3	2.06	0.56
1:C:473:VAL:O	1:C:476:MET:HG3	2.06	0.56
1:A:457:LEU:C	1:A:457:LEU:HD23	2.31	0.56
1:C:522:ALA:O	1:C:526:GLU:HG3	2.05	0.55
1:C:168:LEU:HD21	1:C:172:ARG:NH2	2.21	0.55
1:A:277:ILE:HD11	1:A:416:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:PHE:HA	1:C:512:PHE:HA	1.88	0.55
1:C:194:ARG:HG3	1:D:176:LEU:HD11	1.87	0.55
1:B:451:ARG:NH2	1:B:540:ALA:HB3	2.22	0.55
1:B:512:PHE:C	1:B:514:GLU:H	2.15	0.55
1:D:451:ARG:NH2	1:D:540:ALA:HB3	2.22	0.54
1:A:520:THR:OG1	1:A:523:GLU:HG3	2.07	0.54
1:C:247:TRP:HH2	1:C:369:GLN:HE21	1.53	0.54
1:B:403:VAL:HG11	1:B:408:LYS:HA	1.90	0.54
1:B:574:ALA:O	1:B:577:GLU:HB3	2.08	0.54
1:A:87:ASP:HA	1:A:90:ARG:HD3	1.90	0.54
1:B:279:LEU:HD12	1:B:305:ARG:CZ	2.38	0.54
1:B:288:MET:O	1:B:484:ARG:NH1	2.39	0.54
1:A:326:ASP:CG	1:A:328:PRO:HD2	2.33	0.54
1:A:536:ILE:CD1	1:A:556:VAL:HG21	2.38	0.53
1:A:382:PHE:HE2	1:B:367:MET:HE3	1.74	0.53
1:B:14:LYS:HD2	1:B:14:LYS:N	2.24	0.53
1:C:10:SER:OG	3:C:1903:XMP:H8	2.08	0.53
1:D:457:LEU:O	1:D:457:LEU:HD23	2.09	0.53
1:A:281:GLU:HG2	1:A:290:TYR:HE1	1.74	0.53
1:B:457:LEU:C	1:B:457:LEU:HD23	2.33	0.52
1:D:478:PHE:CZ	1:D:487:ILE:HG23	2.44	0.52
1:D:61:LEU:O	1:D:64:ARG:HG3	2.09	0.52
1:A:290:TYR:O	1:A:293:TYR:HB2	2.09	0.52
1:A:147:GLU:CD	1:A:177:LYS:HD3	2.33	0.52
1:A:570:VAL:HG23	4:A:2122:HOH:O	2.10	0.52
1:B:253:LEU:HD21	1:B:420:VAL:HA	1.91	0.52
1:A:493:GLN:HG2	4:A:2171:HOH:O	2.09	0.52
1:C:83:GLU:CD	1:C:83:GLU:N	2.67	0.52
1:C:326:ASP:CG	1:C:328:PRO:HD2	2.35	0.51
1:A:550:ARG:O	1:A:553:ARG:HG2	2.11	0.51
1:D:249:LEU:HD23	1:D:249:LEU:C	2.35	0.51
1:D:5:GLN:O	1:D:29:LEU:HD22	2.10	0.51
1:A:86:ALA:O	1:A:90:ARG:HG2	2.10	0.51
1:C:425:VAL:HG13	1:C:539:ASP:HB3	1.93	0.51
1:B:470:HIS:CD2	1:B:471:PRO:HD2	2.46	0.51
1:B:520:THR:OG1	1:B:523:GLU:HG3	2.10	0.51
1:D:457:LEU:HD23	1:D:457:LEU:C	2.36	0.51
1:B:312:MET:HE2	1:B:492:ASP:CB	2.37	0.51
1:D:57:PHE:CG	1:D:58:PRO:HD2	2.46	0.51
1:D:431:ASN:ND2	1:D:448:GLN:HB2	2.23	0.51
1:A:470:HIS:ND1	1:A:471:PRO:HD2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:LEU:HD23	1:C:457:LEU:O	2.11	0.51
1:C:8:LEU:HD13	1:C:9:PHE:N	2.26	0.50
1:C:369:GLN:NE2	4:C:2140:HOH:O	2.45	0.50
1:C:24:LEU:HD22	1:C:29:LEU:HD12	1.93	0.50
1:A:155:SER:O	1:A:159:GLN:HG3	2.11	0.50
1:B:161:SER:HB3	4:B:2201:HOH:O	2.12	0.50
1:B:158:MET:O	1:B:164:LYS:HA	2.12	0.49
1:C:357:LYS:HB2	1:C:362:TYR:HB2	1.93	0.49
1:B:64:ARG:NH1	4:B:2270:HOH:O	2.44	0.49
1:D:470:HIS:ND1	1:D:471:PRO:HD2	2.27	0.49
1:A:343:ALA:HB1	1:A:344:PRO:HD2	1.93	0.49
1:D:508:TRP:CH2	1:D:516:PRO:HG2	2.47	0.49
1:D:508:TRP:HH2	1:D:516:PRO:HG2	1.78	0.49
1:A:27:LEU:HD21	1:A:158:MET:HB3	1.95	0.49
1:A:229:THR:OG1	1:A:366:GLN:HB3	2.13	0.49
1:B:430:SER:O	1:B:447:GLY:HA2	2.12	0.49
1:C:277:ILE:HD11	1:C:416:ARG:HD2	1.94	0.49
1:D:83:GLU:CD	1:D:83:GLU:H	2.19	0.49
1:C:173:GLN:NE2	1:C:177:LYS:HE3	2.28	0.49
1:A:25:THR:C	1:A:27:LEU:H	2.20	0.48
1:A:279:LEU:CD1	1:A:301:ALA:HB1	2.43	0.48
1:A:357:LYS:HB2	1:A:362:TYR:HB2	1.95	0.48
1:A:536:ILE:HD11	1:A:556:VAL:HG21	1.96	0.48
1:A:194:ARG:HG3	1:B:176:LEU:HD11	1.95	0.48
1:A:525:LYS:O	1:A:529:GLU:HG3	2.14	0.48
1:A:478:PHE:CE1	1:A:487:ILE:HG23	2.48	0.48
1:D:431:ASN:C	1:D:431:ASN:ND2	2.66	0.48
1:A:548:VAL:HG12	1:A:578:LEU:HD12	1.96	0.48
1:B:252:GLU:HB3	1:B:423:ILE:HD13	1.96	0.48
1:C:42:ARG:HG3	1:C:42:ARG:HH11	1.78	0.48
1:D:33:ALA:O	1:D:50:ASP:HA	2.14	0.48
1:D:478:PHE:CE1	1:D:487:ILE:HG23	2.49	0.48
1:D:434:CYS:SG	1:D:441:VAL:HG22	2.54	0.48
1:C:584:HIS:HE1	4:C:2053:HOH:O	1.97	0.47
1:A:10:SER:OG	3:A:1901:XMP:H8	2.15	0.47
1:A:451:ARG:NH2	1:A:540:ALA:HB3	2.29	0.47
1:C:536:ILE:CD1	1:C:556:VAL:HG21	2.43	0.47
1:B:431:ASN:HD21	1:B:448:GLN:HB2	1.79	0.47
1:B:73:HIS:CE1	1:B:130:THR:HG22	2.49	0.47
1:B:343:ALA:HB1	1:B:344:PRO:HD2	1.97	0.47
1:D:11:VAL:HG23	1:D:14:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:550:ARG:HD2	1:D:553:ARG:HD3	1.97	0.47
1:C:161:SER:C	1:C:163:SER:H	2.23	0.46
1:A:60:MET:HG3	1:A:61:LEU:HG	1.97	0.46
1:A:430:SER:O	1:A:447:GLY:HA2	2.16	0.46
1:C:17:LEU:HD21	1:C:37:THR:HG23	1.96	0.46
1:A:457:LEU:HD23	1:A:457:LEU:O	2.15	0.46
1:B:22:ARG:CZ	1:B:46:LEU:HD21	2.46	0.46
1:C:339:ASP:HA	1:C:358:LYS:HZ2	1.80	0.46
1:D:112:SER:HB3	1:D:115:VAL:CG1	2.46	0.46
1:B:279:LEU:HD11	1:B:305:ARG:HG3	1.97	0.46
1:D:50:ASP:O	1:D:53:GLU:HB2	2.16	0.46
1:C:505:LEU:HD11	1:C:509:LYS:HE3	1.98	0.46
1:A:127:GLY:HA3	3:A:1901:XMP:C6	2.46	0.46
1:A:381:LEU:HD23	1:B:244:LEU:HD12	1.98	0.46
1:B:228:ILE:HD11	1:B:244:LEU:HD21	1.98	0.46
1:C:279:LEU:CD1	1:C:301:ALA:HB1	2.45	0.45
1:D:406:LYS:O	1:D:407:ASN:HB2	2.15	0.45
1:A:430:SER:HB3	1:A:431:ASN:HA	1.98	0.45
1:C:177:LYS:HE2	1:D:224:PRO:HG3	1.98	0.45
1:C:266:LYS:HG3	1:C:313:SER:O	2.16	0.45
1:A:489:ASN:O	1:A:493:GLN:HG3	2.16	0.45
1:B:155:SER:O	1:B:159:GLN:HG2	2.16	0.45
1:C:431:ASN:HD22	1:C:431:ASN:HA	1.56	0.45
1:D:430:SER:CB	1:D:431:ASN:HA	2.46	0.45
1:A:377:GLU:HB2	1:B:380:THR:HB	1.99	0.45
1:B:22:ARG:NH2	1:B:46:LEU:CD2	2.79	0.45
1:B:326:ASP:CG	1:B:328:PRO:HD2	2.41	0.45
1:B:489:ASN:O	1:B:493:GLN:HG3	2.17	0.45
1:B:416:ARG:HD3	4:B:2259:HOH:O	2.16	0.45
1:C:355:SER:O	1:C:360:GLY:HA2	2.15	0.45
1:B:57:PHE:CD1	1:B:58:PRO:HD2	2.52	0.45
1:C:467:LEU:HD23	1:C:527:TRP:CD1	2.52	0.45
1:A:521:GLU:O	1:A:525:LYS:HG3	2.17	0.45
1:A:478:PHE:HA	1:A:512:PHE:HA	1.98	0.45
1:B:378:VAL:HG22	1:B:387:SER:HB2	1.98	0.45
1:C:31:LEU:HD12	1:C:31:LEU:N	2.32	0.44
1:C:158:MET:O	1:C:164:LYS:HA	2.17	0.44
1:D:428:THR:CG2	1:D:446:ALA:HB2	2.48	0.44
1:D:9:PHE:HZ	1:D:24:LEU:HD12	1.82	0.44
1:D:73:HIS:CE1	1:D:130:THR:HG22	2.53	0.44
1:A:378:VAL:HG12	4:B:2118:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:ALA:HB1	1:C:344:PRO:HD2	2.00	0.44
1:C:457:LEU:C	1:C:457:LEU:CD2	2.89	0.44
1:D:46:LEU:HD11	4:D:2138:HOH:O	2.18	0.44
1:D:326:ASP:CG	1:D:328:PRO:HD2	2.42	0.44
1:A:11:VAL:HB	1:A:102:ASN:HD22	1.83	0.44
1:D:112:SER:HB3	1:D:115:VAL:HG11	1.98	0.44
1:B:430:SER:HB3	1:B:431:ASN:HA	1.98	0.44
1:C:42:ARG:NH2	1:C:48:VAL:O	2.50	0.44
1:D:267:HIS:C	1:D:268:VAL:HG23	2.42	0.44
1:C:31:LEU:N	1:C:31:LEU:CD1	2.81	0.44
1:C:382:PHE:HE2	1:D:367:MET:HE2	1.83	0.43
1:C:541:PHE:CE1	1:C:565:SER:HB3	2.53	0.43
1:C:570:VAL:HG23	4:C:2154:HOH:O	2.17	0.43
1:D:430:SER:HB3	1:D:431:ASN:HA	1.99	0.43
1:C:197:TYR:CD2	1:D:172:ARG:HB3	2.53	0.43
1:D:158:MET:O	1:D:164:LYS:HA	2.19	0.43
1:A:9:PHE:HZ	1:A:24:LEU:HD12	1.82	0.43
1:A:550:ARG:HA	1:A:553:ARG:NH1	2.34	0.43
1:B:478:PHE:CD2	1:B:487:ILE:HG12	2.53	0.43
1:C:494:TYR:HE1	1:C:518:LEU:HA	1.83	0.43
1:C:118:GLU:N	1:C:118:GLU:CD	2.76	0.43
1:C:467:LEU:HD23	1:C:527:TRP:HD1	1.83	0.43
1:C:470:HIS:ND1	1:C:471:PRO:HD2	2.33	0.43
1:C:475:SER:HB3	4:C:2137:HOH:O	2.19	0.43
1:B:567:ALA:O	1:B:570:VAL:HG22	2.19	0.43
1:C:267:HIS:C	1:C:268:VAL:HG23	2.43	0.43
1:C:281:GLU:O	1:C:285:LYS:HG3	2.19	0.43
1:C:430:SER:O	1:C:447:GLY:HA2	2.19	0.43
1:B:543:PRO:O	1:B:567:ALA:HB3	2.18	0.43
1:C:11:VAL:HB	1:C:102:ASN:HD22	1.84	0.43
1:C:381:LEU:HD21	1:D:244:LEU:HB2	2.00	0.43
1:A:381:LEU:HD21	1:B:244:LEU:HB2	1.99	0.43
1:A:431:ASN:C	1:A:431:ASN:ND2	2.61	0.43
1:B:33:ALA:O	1:B:50:ASP:HA	2.19	0.43
1:C:431:ASN:HB2	1:C:448:GLN:C	2.43	0.43
1:D:328:PRO:O	1:D:332:ILE:HG13	2.19	0.43
1:C:118:GLU:CD	1:C:118:GLU:H	2.27	0.43
1:D:228:ILE:HD11	1:D:244:LEU:HD21	2.01	0.42
1:D:541:PHE:CD1	1:D:565:SER:HB2	2.54	0.42
1:C:494:TYR:CE1	1:C:518:LEU:HA	2.53	0.42
1:A:397:LYS:HA	1:A:415:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ALA:HA	4:A:2122:HOH:O	2.19	0.42
1:C:108:LYS:HG3	4:C:2069:HOH:O	2.19	0.42
1:C:349:GLU:O	1:C:353:ILE:HG13	2.20	0.42
1:D:541:PHE:CD1	1:D:541:PHE:C	2.98	0.42
1:B:425:VAL:CG1	1:B:539:ASP:HB3	2.48	0.42
1:C:249:LEU:C	1:C:249:LEU:HD23	2.45	0.42
1:C:279:LEU:HD13	1:C:301:ALA:HB1	2.01	0.42
1:B:450:SER:HB3	1:B:453:HIS:HB2	2.02	0.42
1:D:81:ILE:HD12	1:D:83:GLU:OE1	2.20	0.42
1:D:457:LEU:HD21	1:D:461:LYS:HE3	2.00	0.42
1:A:173:GLN:HE21	1:A:173:GLN:HB3	1.62	0.42
1:A:249:LEU:C	1:A:249:LEU:HD23	2.45	0.42
1:C:79:ARG:HD3	1:D:122:GLU:OE1	2.19	0.42
1:B:115:VAL:O	1:B:115:VAL:HG13	2.19	0.41
1:D:101:CYS:O	1:D:146:CYS:HA	2.19	0.41
1:A:279:LEU:HD13	1:A:301:ALA:HB1	2.02	0.41
1:C:73:HIS:CE1	1:C:130:THR:HG22	2.55	0.41
1:D:406:LYS:N	1:D:576:ASP:OD1	2.30	0.41
1:A:312:MET:HE2	1:A:312:MET:HB3	1.91	0.41
1:A:5:GLN:NE2	1:A:97:ARG:HD3	2.33	0.41
1:A:31:LEU:H	1:A:31:LEU:CD1	2.31	0.41
1:D:343:ALA:HB1	1:D:344:PRO:HD2	2.02	0.41
1:A:5:GLN:NE2	1:A:97:ARG:HB2	2.35	0.41
1:B:57:PHE:CG	1:B:58:PRO:HD2	2.55	0.41
1:B:161:SER:OG	1:B:162:GLU:N	2.53	0.41
1:C:22:ARG:HG2	1:C:46:LEU:HD21	2.02	0.41
1:C:154:VAL:O	1:C:158:MET:HG3	2.20	0.41
1:C:274:ALA:HB2	1:C:440:GLN:HB2	2.03	0.41
1:B:69:HIS:HA	1:B:70:PRO:HD3	1.93	0.41
1:A:87:ASP:O	1:A:90:ARG:HG3	2.21	0.41
1:A:267:HIS:C	1:A:268:VAL:HG23	2.45	0.41
1:B:437:LYS:HE2	4:B:2277:HOH:O	2.20	0.41
1:C:103:LEU:O	1:C:104:TYR:C	2.64	0.41
1:C:112:SER:HA	1:C:113:PRO:HD3	1.87	0.41
1:C:225:LYS:HZ2	1:C:229:THR:HG22	1.85	0.41
1:D:418:LEU:HD22	1:D:560:ALA:HB2	2.02	0.41
1:B:565:SER:HB3	1:B:568:ASP:OD1	2.21	0.41
1:A:31:LEU:N	1:A:31:LEU:CD1	2.82	0.41
1:C:127:GLY:HA3	3:C:1903:XMP:C6	2.51	0.41
1:C:266:LYS:HB3	1:D:449:GLN:HB3	2.03	0.41
1:C:476:MET:HE2	1:C:516:PRO:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:VAL:O	1:D:115:VAL:HG23	2.21	0.41
1:D:512:PHE:CD1	1:D:512:PHE:N	2.89	0.41
1:A:328:PRO:O	1:A:332:ILE:HG13	2.21	0.41
1:B:141:ARG:HD2	4:B:2139:HOH:O	2.21	0.40
1:B:430:SER:CB	1:B:431:ASN:HA	2.51	0.40
1:C:8:LEU:C	1:C:8:LEU:CD1	2.94	0.40
1:D:249:LEU:HD23	1:D:249:LEU:O	2.21	0.40
1:B:355:SER:O	1:B:360:GLY:HA2	2.21	0.40
1:C:59:GLU:CD	1:C:66:LYS:HD2	2.46	0.40
1:D:483:LYS:O	1:D:487:ILE:HG13	2.22	0.40
1:A:266:LYS:CB	1:B:449:GLN:HB3	2.50	0.40
1:D:409:ASP:CG	1:D:409:ASP:O	2.64	0.40
1:A:457:LEU:C	1:A:457:LEU:CD2	2.95	0.40
1:A:550:ARG:NH1	1:A:553:ARG:HG3	2.35	0.40
1:C:512:PHE:C	1:C:514:GLU:H	2.30	0.40
1:D:185:TYR:CE2	1:D:189:ILE:HD11	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	584/592 (99%)	562 (96%)	19 (3%)	3 (0%)	24	16
1	B	587/592 (99%)	571 (97%)	14 (2%)	2 (0%)	36	29
1	C	583/592 (98%)	561 (96%)	20 (3%)	2 (0%)	36	29
1	D	587/592 (99%)	573 (98%)	13 (2%)	1 (0%)	43	36
All	All	2341/2368 (99%)	2267 (97%)	66 (3%)	8 (0%)	36	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	THR
1	B	514	GLU
1	D	407	ASN
1	B	407	ASN
1	C	514	GLU
1	A	35	GLY
1	A	82	PRO
1	C	82	PRO

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	462/488 (95%)	449 (97%)	13 (3%)	38	32
1	B	469/488 (96%)	456 (97%)	13 (3%)	38	32
1	C	461/488 (94%)	453 (98%)	8 (2%)	53	52
1	D	466/488 (96%)	459 (98%)	7 (2%)	57	56
All	All	1858/1952 (95%)	1817 (98%)	41 (2%)	45	42

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	50	ASP
1	A	83	GLU
1	A	153	VAL
1	A	172	ARG
1	A	173	GLN
1	A	207	ARG
1	A	266	LYS
1	A	268	VAL
1	A	431	ASN
1	A	432	SER
1	A	501	GLU
1	A	584	HIS
1	B	260	PRO

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Mol	Chain	Res	Type
1	B	266	LYS
1	B	268	VAL
1	B	279	LEU
1	B	369	GLN
1	B	405	THR
1	B	415	LEU
1	B	425	VAL
1	B	431	ASN
1	B	432	SER
1	B	486	GLU
1	B	517	GLU
1	B	584	HIS
1	C	8	LEU
1	C	83	GLU
1	C	266	LYS
1	C	268	VAL
1	C	275	VAL
1	C	425	VAL
1	C	431	ASN
1	C	584	HIS
1	D	48	VAL
1	D	268	VAL
1	D	404	VAL
1	D	405	THR
1	D	431	ASN
1	D	432	SER
1	D	584	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	85	ASN
1	A	123	GLN
1	A	173	GLN
1	A	376	ASN
1	A	429	GLN
1	A	431	ASN
1	A	453	HIS
1	A	472	GLN
1	A	493	GLN
1	A	586	ASN

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Mol	Chain	Res	Type
1	B	184	GLN
1	B	196	GLN
1	B	203	GLN
1	B	359	ASN
1	B	376	ASN
1	B	402	ASN
1	B	431	ASN
1	B	449	GLN
1	B	463	ASN
1	B	470	HIS
1	B	586	ASN
1	C	5	GLN
1	C	123	GLN
1	C	159	GLN
1	C	369	GLN
1	C	431	ASN
1	C	449	GLN
1	C	584	HIS
1	C	586	ASN
1	D	184	GLN
1	D	369	GLN
1	D	402	ASN
1	D	407	ASN
1	D	431	ASN
1	D	449	GLN
1	D	469	HIS
1	D	584	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	XMP	A	1901	-	26,26,26	2.11	10 (38%)	34,40,40	1.94	12 (35%)
3	XMP	C	1903	-	26,26,26	2.19	10 (38%)	34,40,40	1.96	12 (35%)

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
3	XMP	A	1901	-	-	5/10/26/26	0/3/3/3
3	XMP	C	1903	-	-	5/10/26/26	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1903	XMP	C2-N1	4.66	1.45	1.37
3	A	1901	XMP	P-OP1	4.29	1.63	1.50
3	A	1901	XMP	C2-N1	4.21	1.44	1.37
3	A	1901	XMP	C2-N3	3.94	1.44	1.37
3	C	1903	XMP	P-OP1	3.86	1.62	1.50
3	C	1903	XMP	C4-N3	3.73	1.43	1.37
3	C	1903	XMP	C2-N3	3.59	1.43	1.37
3	C	1903	XMP	C1'-N9	3.46	1.57	1.47
3	A	1901	XMP	C4-N3	3.38	1.43	1.37
3	A	1901	XMP	C6-N1	3.03	1.44	1.38
3	C	1903	XMP	C6-N1	2.97	1.44	1.38
3	A	1901	XMP	C1'-N9	2.92	1.55	1.47
3	A	1901	XMP	C5-C4	2.59	1.42	1.38
3	C	1903	XMP	P-O5'	2.49	1.68	1.60
3	C	1903	XMP	C5-C4	2.48	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1903	XMP	C5'-C4'	2.39	1.58	1.51
3	C	1903	XMP	C8-N7	2.37	1.39	1.32
3	A	1901	XMP	C8-N7	2.26	1.38	1.32
3	A	1901	XMP	C5'-C4'	2.26	1.58	1.51
3	A	1901	XMP	P-O5'	2.19	1.67	1.60

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1903	XMP	O4'-C1'-C2'	-3.93	98.21	106.62
3	A	1901	XMP	O4'-C1'-C2'	-3.83	98.42	106.62
3	A	1901	XMP	C6-N1-C2	-3.78	121.16	126.37
3	C	1903	XMP	C2'-C1'-N9	3.64	123.39	113.25
3	C	1903	XMP	C6-N1-C2	-3.60	121.41	126.37
3	A	1901	XMP	C8-N9-C4	3.48	109.60	106.67
3	A	1901	XMP	C2'-C1'-N9	3.21	122.18	113.25
3	C	1903	XMP	C8-N9-C4	3.14	109.32	106.67
3	A	1901	XMP	O3'-C3'-C4'	-3.01	102.44	111.08
3	A	1901	XMP	O3'-C3'-C2'	2.98	121.38	111.82
3	C	1903	XMP	O3'-C3'-C4'	-2.90	102.75	111.08
3	C	1903	XMP	C5-C4-N9	2.85	107.56	106.25
3	C	1903	XMP	N9-C8-N7	-2.79	108.22	113.40
3	A	1901	XMP	O6-C6-C5	-2.68	119.47	126.53
3	C	1903	XMP	O3'-C3'-C2'	2.66	120.33	111.82
3	A	1901	XMP	N9-C8-N7	-2.65	108.49	113.40
3	A	1901	XMP	C5-C6-N1	2.62	119.92	113.25
3	C	1903	XMP	O6-C6-C5	-2.53	119.86	126.53
3	C	1903	XMP	C5-C6-N1	2.51	119.65	113.25
3	C	1903	XMP	OP2-P-O5'	2.44	113.03	106.67
3	A	1901	XMP	OP2-P-O5'	2.43	113.01	106.67
3	A	1901	XMP	C4'-O4'-C1'	-2.23	104.53	109.47
3	C	1903	XMP	C4'-O4'-C1'	-2.06	104.92	109.47
3	A	1901	XMP	C5-C4-N9	2.05	107.20	106.25

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1901	XMP	C5'-O5'-P-OP3
3	A	1901	XMP	C5'-O5'-P-OP2
3	A	1901	XMP	C5'-O5'-P-OP1
3	A	1901	XMP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	C	1903	XMP	C5'-O5'-P-OP3
3	C	1903	XMP	C5'-O5'-P-OP2
3	C	1903	XMP	C5'-O5'-P-OP1
3	C	1903	XMP	O4'-C4'-C5'-O5'
3	A	1901	XMP	C3'-C4'-C5'-O5'
3	C	1903	XMP	C3'-C4'-C5'-O5'

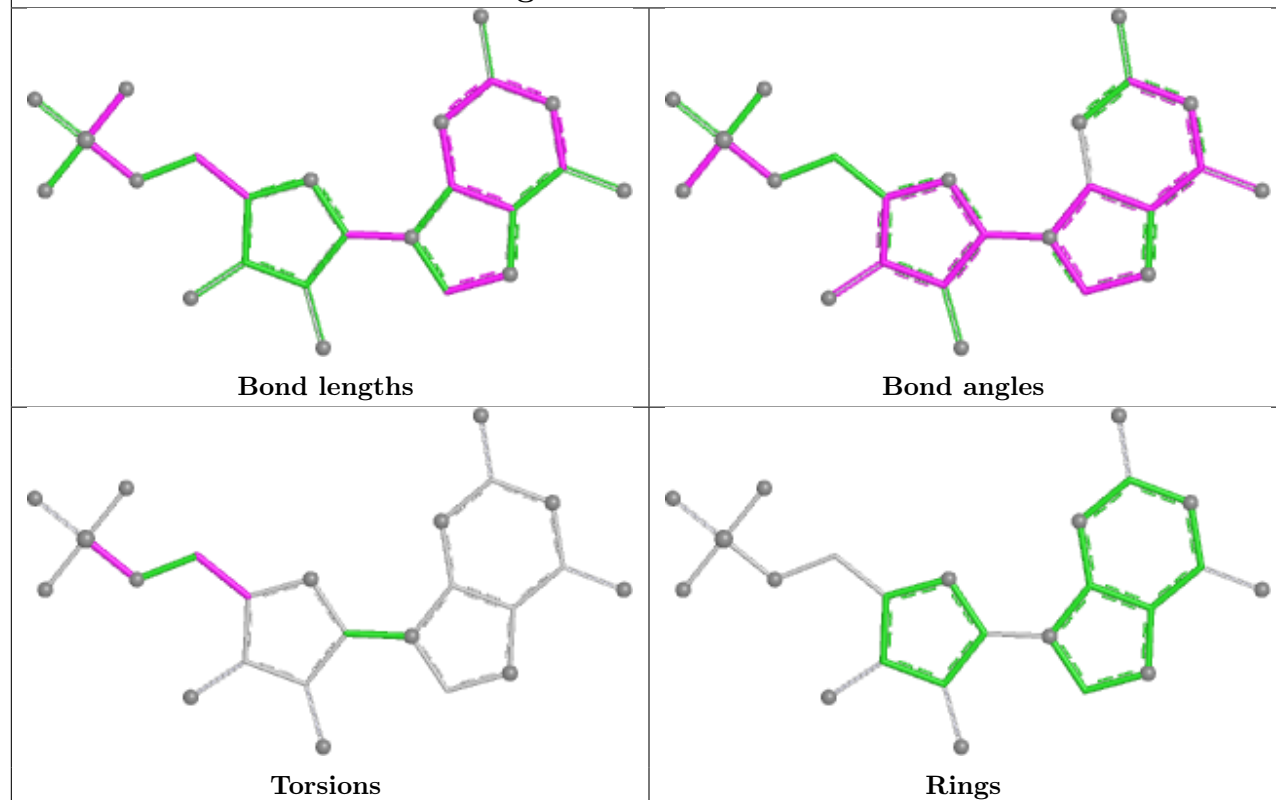
There are no ring outliers.

2 monomers are involved in 4 short contacts:

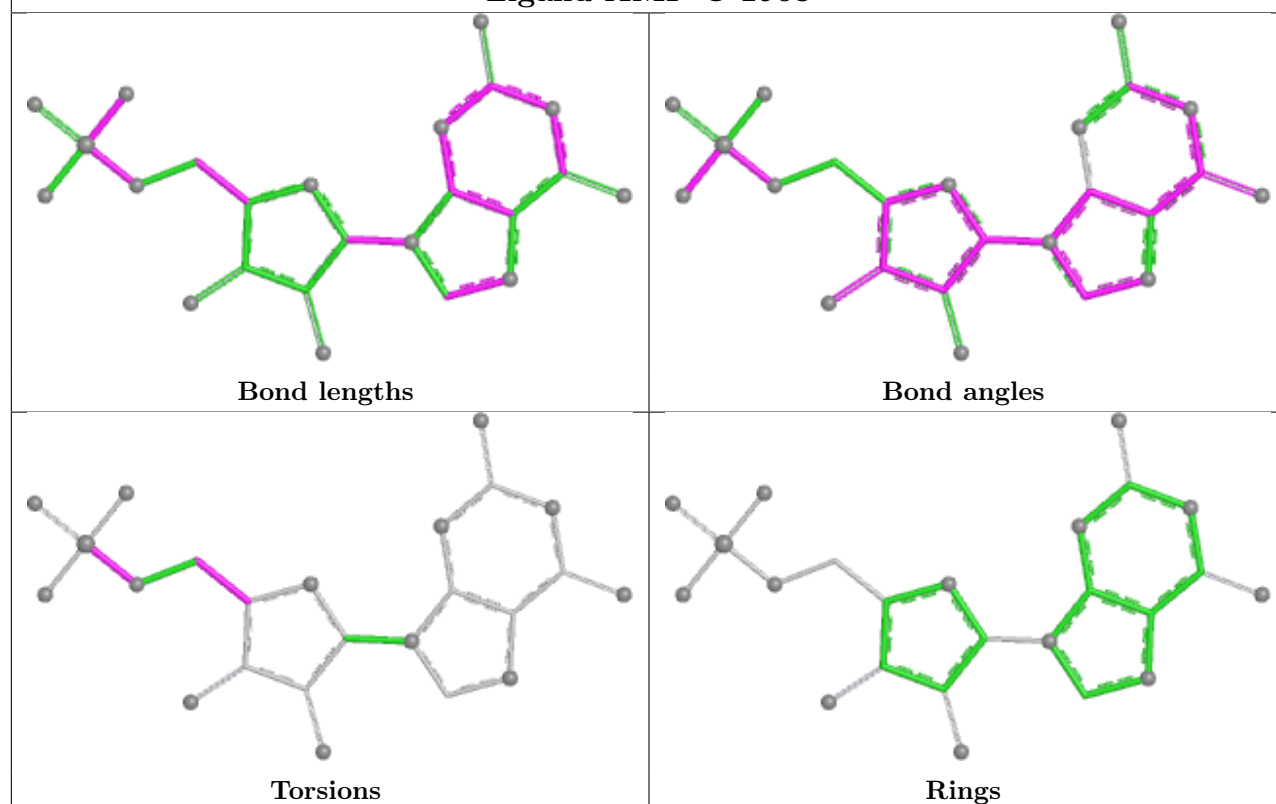
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1901	XMP	2	0
3	C	1903	XMP	2	0

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

Ligand XMP A 1901



Ligand XMP C 1903



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	588/592 (99%)	-1.20	0 100 100	14, 29, 52, 71	0
1	B	589/592 (99%)	-1.27	0 100 100	13, 24, 54, 70	0
1	C	587/592 (99%)	-1.17	0 100 100	15, 29, 56, 76	0
1	D	589/592 (99%)	-1.28	0 100 100	14, 24, 52, 73	0
All	All	2353/2368 (99%)	-1.23	0 100 100	13, 27, 54, 76	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
3	XMP	A	1901	24/24	0.99	0.03	27,32,40,41	0
3	XMP	C	1903	24/24	0.99	0.03	28,35,41,43	0
2	K	C	2003	1/1	1.00	0.01	14,14,14,14	0
2	K	D	2004	1/1	1.00	0.01	17,17,17,17	0

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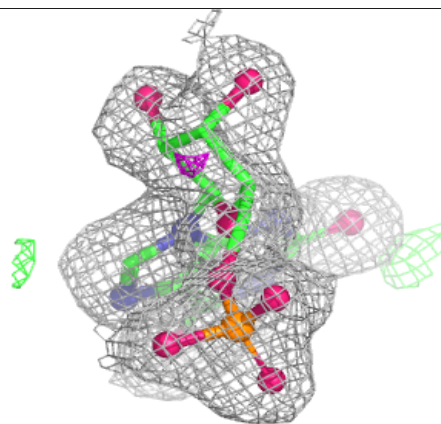
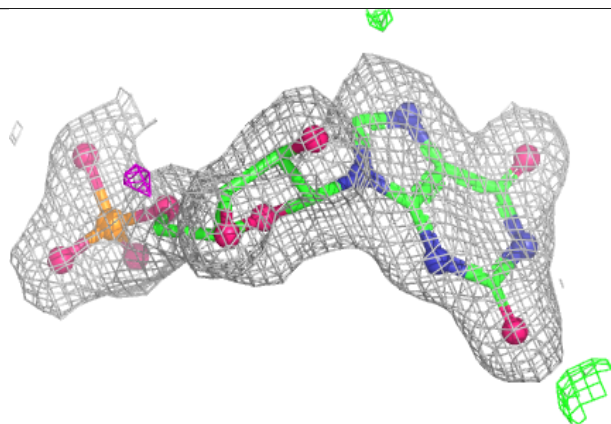
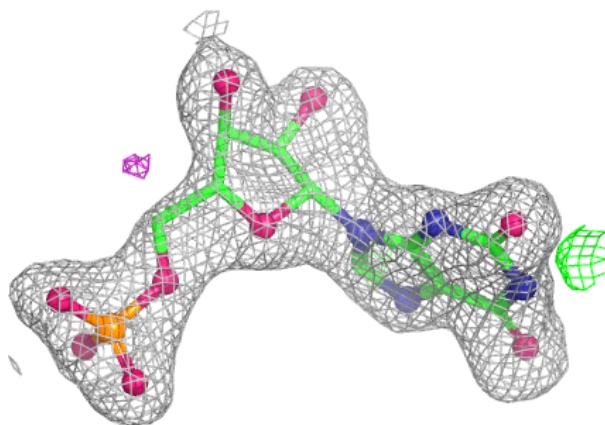
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	K	A	2001	1/1	1.00	0.01	15,15,15,15	0
2	K	B	2002	1/1	1.00	0.01	17,17,17,17	0

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.

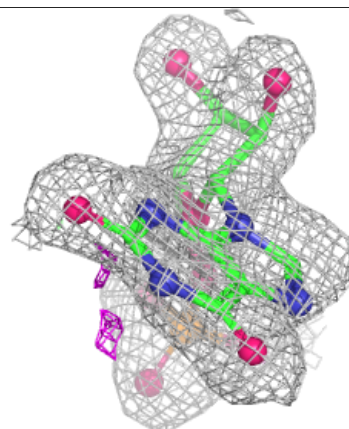
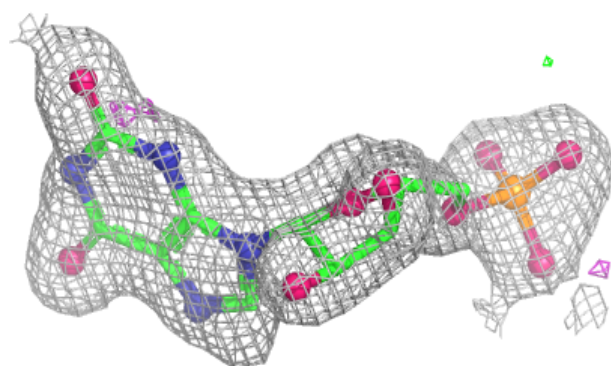
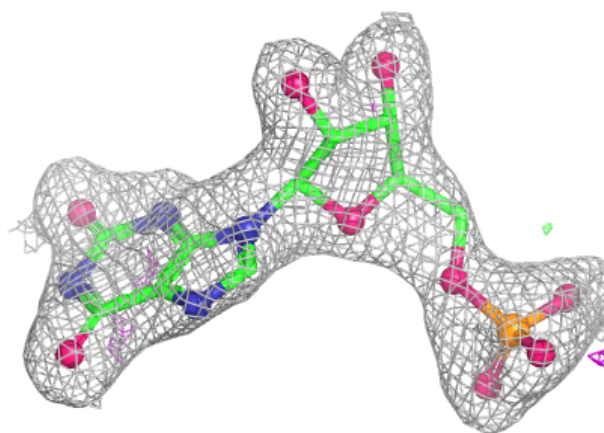
Electron density around XMP A 1901:

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 XMP C 1903:

$2mF_o-DF_c$ (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.