Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:34 PM GMT

PDB ID	:	1PKX
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

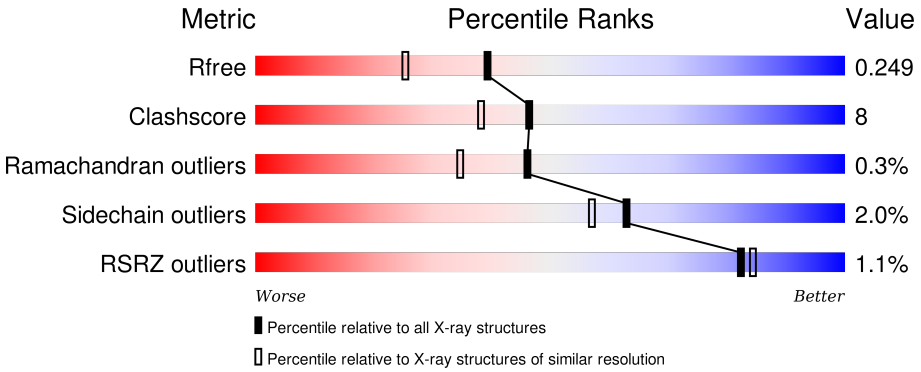
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	82% 16%
1	B	592	83% 16%
1	C	592	81% 18%
1	D	592	85% 14%

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.

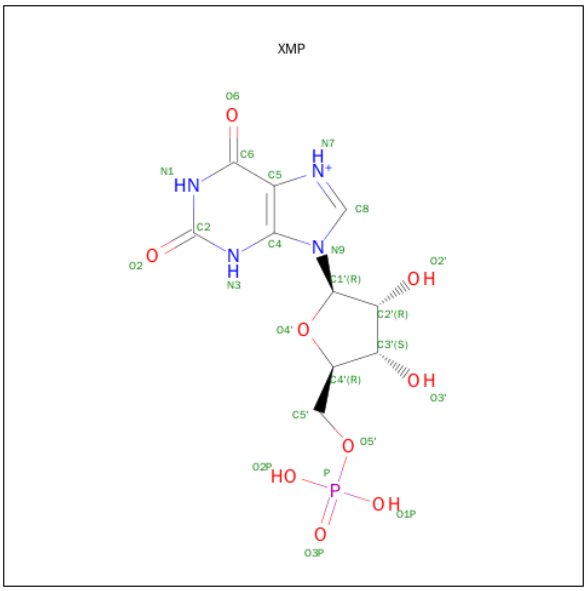
- Molecule 1 is a protein called Bifunctional purine biosynthesis protein PURH.

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 (three-letter code: K) (formula: K).

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

- Molecule 3 is XANTHOSINE-5'-MONOPHOSPHATE (three-letter code: XMP) (formula: $C_{10}H_{14}N_4O_9P$).



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

- Molecule 4 is water.

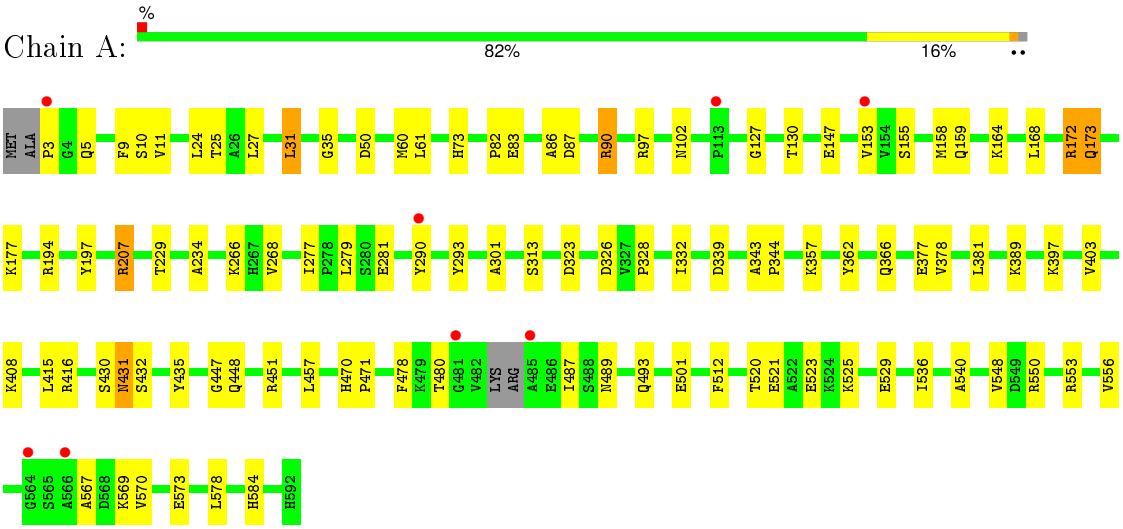
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	210	Total	O	0	0
			210	210		
4	B	278	Total	O	0	0
			278	278		
4	C	209	Total	O	0	0
			209	209		
4	D	280	Total	O	0	0
			280	280		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

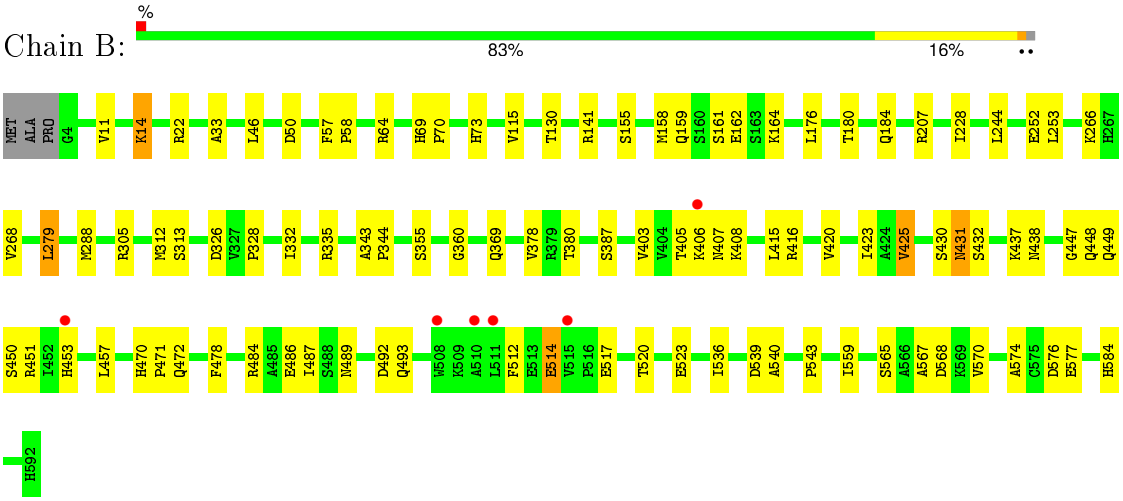
- Molecule 1: Bifunctional purine biosynthesis protein PURH

Chain A:



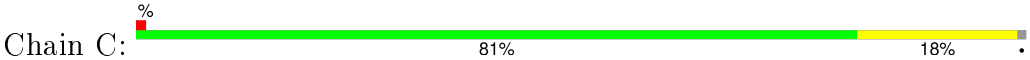
- Molecule 1: Bifunctional purine biosynthesis protein PURH

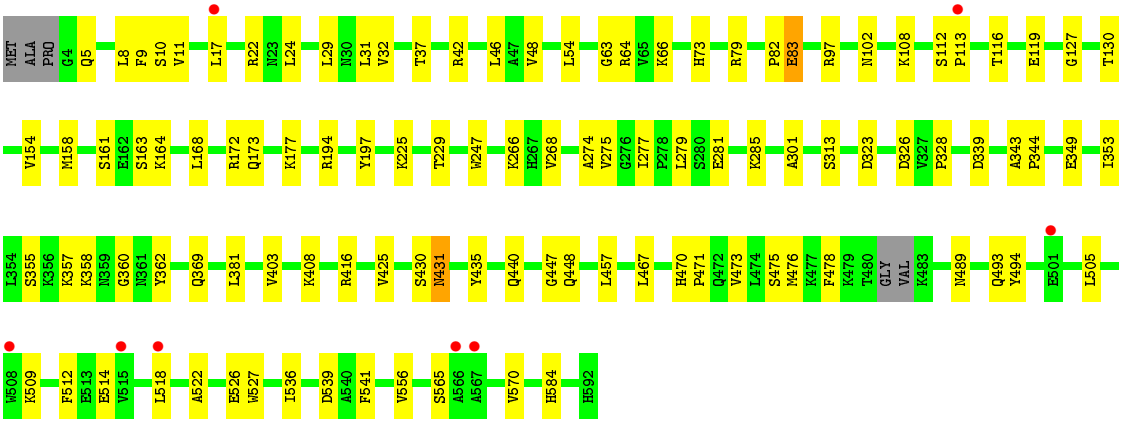
Chain B:



- Molecule 1: Bifunctional purine biosynthesis protein PURH

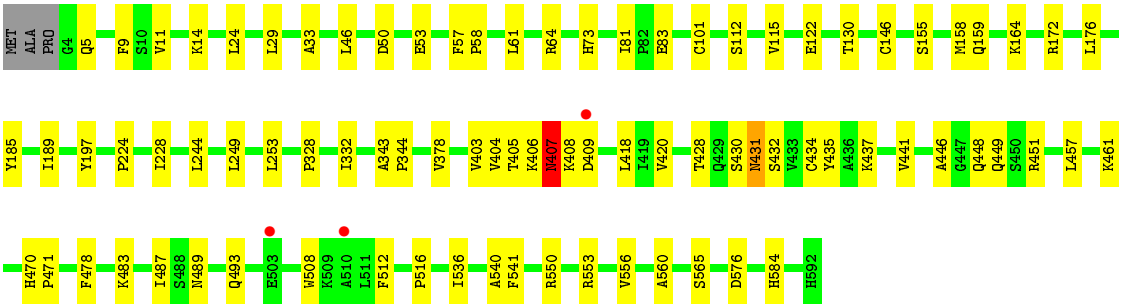
Chain C:





• Molecule 1: Bifunctional purine biosynthesis protein PURH

Chain D:



4 Data and refinement statistics (i)

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 49.40 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.90) 79.3 (49.40-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.249 0.211 , 0.249	Depositor DCC
R_{free} test set	8497 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.5	EDS
Estimated twinning fraction	0.246 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 177117 reflections	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.44	0/4510	0.65	1/6135 (0.0%)
1	B	0.47	0/4545	0.66	0/6176
1	C	0.44	0/4503	0.65	0/6122
1	D	0.46	0/4533	0.65	0/6163
All	All	0.45	0/18091	0.65	1/24596 (0.0%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3	PRO	N-CA-CB	5.41	109.80	103.30

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	76	0
1	B	4462	0	4425	67	0
1	C	4422	0	4367	77	0
1	D	4450	0	4400	63	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
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	270	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 (270) 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:C:172:ARG:HD3	1:D:197:TYR:CD1	2.15	0.82
1:B:11:VAL:O	1:B:14:LYS:HE2	1.79	0.81
1:A:168:LEU:O	1:A:172:ARG:HG2	1.81	0.80
1:A:431:ASN:C	1:A:431:ASN:HD22	1.88	0.77
1:A:431:ASN:HD21	1:A:448:GLN:HB2	1.51	0.76
1:B:431:ASN:C	1:B:431:ASN:HD22	1.88	0.75
1:D:155:SER:O	1:D:159:GLN:HG2	1.87	0.75
1:D:431:ASN:HD22	1:D:431:ASN:C	1.93	0.72
1:C:83:GLU:H	1:C:83:GLU:CD	1.94	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:ILE:CD1	1:D:556:VAL:HG21	2.22	0.69
1:B:425:VAL:HG13	1:B:539:ASP:HB3	1.74	0.68
1:A:266:LYS:HB3	1:B:449:GLN:HB3	1.76	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:64:ARG:HG3	4:C:2156:HOH:O	1.96	0.65
1:A:83:GLU:CD	1:A:83:GLU:H	2.00	0.64
1:A:31:LEU:HD12	1:A:31:LEU:N	2.12	0.64
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:H	1:A:31:LEU:HD12	1.65	0.62
1:B:266:LYS:HG3	1:B:313:SER:O	1.99	0.62
1:A:403:VAL:HG11	1:A:408:LYS:HA	1.82	0.62
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:C:457:LEU:C	1:C:457:LEU:HD23	2.22	0.60
1:A:431:ASN:ND2	1:A:448:GLN:HB2	2.17	0.60
1:B:312:MET:HE2	1:B:492:ASP:HB3	1.84	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: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:116:THR:OG1	1:C:119:GLU:HG3	2.04	0.57
1:C:79:ARG:NE	4:C:2194:HOH:O	2.37	0.57
1:C:5:GLN:NE2	1:C:97:ARG:HB2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:ASN:C	1:B:431:ASN:ND2	2.57	0.57
1:B:470:HIS:HD2	1:B:472:GLN:H	1.51	0.57
1:C:339:ASP:HA	1:C:358:LYS:NZ	2.20	0.57
1:C:63:GLY:HA2	1:C:66:LYS:HD3	1.86	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:569:LYS:O	1:A:573:GLU:HG3	2.06	0.56
1:A:478:PHE:CZ	1:A:487:ILE:HG23	2.41	0.56
1:C:473:VAL:O	1:C:476:MET:HG3	2.06	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:C:478:PHE:HA	1:C:512:PHE:HA	1.88	0.55
1:A:277:ILE:HD11	1:A:416:ARG:HD2	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: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:574:ALA:O	1:B:577:GLU:HB3	2.08	0.54
1:B:403:VAL:HG11	1:B:408:LYS:HA	1.90	0.54
1:B:288:MET:O	1:B:484:ARG:NH1	2.39	0.54
1:B:279:LEU:HD12	1:B:305:ARG:CZ	2.38	0.54
1:C:8:LEU:C	1:C:8:LEU:HD13	2.28	0.54
1:A:87:ASP:HA	1:A:90:ARG:HD3	1.90	0.54
1:A:431:ASN:C	1:A:431:ASN:ND2	2.61	0.53
1:A:536:ILE:CD1	1:A:556:VAL:HG21	2.38	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:HD23	1:D:457:LEU:O	2.09	0.53
1:A:281:GLU:HG2	1:A:290:TYR:HE1	1.74	0.53
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: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:A:550:ARG:O	1:A:553:ARG:HG2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:431:ASN:ND2	1:D:448:GLN:HB2	2.23	0.51
1:A:457:LEU:C	1:A:457:LEU:HD23	2.31	0.51
1:D:57:PHE:CG	1:D:58:PRO:HD2	2.46	0.51
1:A:470:HIS:ND1	1:A:471:PRO:HD2	2.25	0.51
1:C:457:LEU:O	1:C:457:LEU:HD23	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:512:PHE:C	1:B:514:GLU:H	2.15	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:326:ASP:CG	1:A:328:PRO:HD2	2.33	0.49
1:A:27:LEU:HD21	1:A:158:MET:HB3	1.95	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:A:229:THR:OG1	1:A:366:GLN:HB3	2.13	0.49
1:A:147:GLU:CD	1:A:177:LYS:HD3	2.33	0.49
1:C:173:GLN:NE2	1:C:177:LYS:HE3	2.28	0.49
1:A:357:LYS:HB2	1:A:362:TYR:HB2	1.95	0.48
1:A:279:LEU:CD1	1:A:301:ALA:HB1	2.43	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:B:457:LEU:C	1:B:457:LEU:HD23	2.33	0.48
1:A:478:PHE:CE1	1:A:487:ILE:HG23	2.48	0.48
1:D:478:PHE:CE1	1:D:487:ILE:HG23	2.49	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:B:252:GLU:HB3	1:B:423:ILE:HD13	1.96	0.48
1:A:548:VAL:HG12	1:A:578:LEU:HD12	1.96	0.48
1:D:434:CYS:SG	1:D:441:VAL:HG22	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:584:HIS:HE1	4:C:2053:HOH:O	1.97	0.47
1:D:431:ASN:C	1:D:431:ASN:ND2	2.66	0.47
1:C:536:ILE:CD1	1:C:556:VAL:HG21	2.43	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:B:431:ASN:HD21	1:B:448:GLN:HB2	1.79	0.47
1:C:339:ASP:HA	1:C:358:LYS:HZ2	1.79	0.47
1:B:73:HIS:CE1	1:B:130:THR:HG22	2.49	0.47
1:C:83:GLU:CD	1:C:83:GLU:N	2.67	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
1:D:249:LEU:HD23	1:D:249:LEU:C	2.35	0.47
1:C:326:ASP:CG	1:C:328:PRO:HD2	2.35	0.47
1:D:550:ARG:HD2	1:D:553:ARG:HD3	1.97	0.47
1:A:430:SER:O	1:A:447:GLY:HA2	2.16	0.46
1:A:60:MET:HG3	1:A:61:LEU:HG	1.97	0.46
1:D:457:LEU:C	1:D:457:LEU:HD23	2.36	0.46
1:C:17:LEU:HD21	1:C:37:THR:HG23	1.96	0.46
1:A:457:LEU:O	1:A:457:LEU:HD23	2.15	0.46
1:B:22:ARG:CZ	1:B:46:LEU:HD21	2.46	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:B:228:ILE:HD11	1:B:244:LEU:HD21	1.98	0.46
1:A:381:LEU:HD23	1:B:244:LEU:HD12	1.98	0.46
1:D:406:LYS:O	1:D:407:ASN:HB2	2.15	0.45
1:C:279:LEU:CD1	1:C:301:ALA:HB1	2.45	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:D:430:SER:CB	1:D:431:ASN:HA	2.46	0.45
1:C:431:ASN:HA	1:C:431:ASN:HD22	1.56	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:B:22:ARG:NH2	1:B:46:LEU:CD2	2.79	0.45
1:A:377:GLU:HB2	1:B:380:THR:HB	1.99	0.45
1:B:489:ASN:O	1:B:493:GLN:HG3	2.17	0.45
1:C:355:SER:O	1:C:360:GLY:HA2	2.15	0.45
1:B:416:ARG:HD3	4:B:2259:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:312:MET:CE	1:B:492:ASP:HB3	2.47	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:C:31:LEU:N	1:C:31:LEU:HD12	2.32	0.44
1:D:73:HIS:CE1	1:D:130:THR:HG22	2.53	0.44
1:D:9:PHE:HZ	1:D:24:LEU:HD12	1.82	0.44
1:A:378:VAL:HG12	4:B:2118:HOH:O	2.16	0.44
1:C:343:ALA:HB1	1:C:344:PRO:HD2	2.00	0.44
1:D:46:LEU:HD11	4:D:2138:HOH:O	2.18	0.44
1:D:83:GLU:H	1:D:83:GLU:CD	2.19	0.44
1:D:112:SER:HB3	1:D:115:VAL:HG11	1.98	0.44
1:A:11:VAL:HB	1:A:102:ASN:HD22	1.83	0.44
1:B:430:SER:HB3	1:B:431:ASN:HA	1.98	0.44
1:A:25:THR:C	1:A:27:LEU:H	2.20	0.44
1:C:42:ARG:NH2	1:C:48:VAL:O	2.50	0.44
1:C:31:LEU:CD1	1:C:31:LEU:N	2.81	0.44
1:D:430:SER:HB3	1:D:431:ASN:HA	1.99	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:158:MET:O	1:D:164:LYS:HA	2.19	0.43
1:C:197:TYR:CD2	1:D:172:ARG:HB3	2.53	0.43
1:A:550:ARG:HA	1:A:553:ARG:NH1	2.34	0.43
1:C:494:TYR:HE1	1:C:518:LEU:HA	1.83	0.43
1:B:478:PHE:CD2	1:B:487:ILE:HG12	2.53	0.43
1:A:9:PHE:HZ	1:A:24:LEU:HD12	1.82	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:C:430:SER:O	1:C:447:GLY:HA2	2.19	0.43
1:C:281:GLU:O	1:C:285:LYS:HG3	2.19	0.43
1:B:567:ALA:O	1:B:570:VAL:HG22	2.19	0.43
1:B:543:PRO:O	1:B:567:ALA:HB3	2.18	0.43
1:C:381:LEU:HD21	1:D:244:LEU:HB2	2.00	0.43
1:C:11:VAL:HB	1:C:102:ASN:HD22	1.84	0.43
1:A:381:LEU:HD21	1:B:244:LEU:HB2	1.99	0.43
1:D:328:PRO:O	1:D:332:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ALA:O	1:B:50:ASP:HA	2.19	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:C:161:SER:C	1:C:163:SER:H	2.23	0.42
1:A:567:ALA:HA	4:A:2122:HOH:O	2.19	0.42
1:C:349:GLU:O	1:C:353:ILE:HG13	2.20	0.42
1:C:108:LYS:HG3	4:C:2069:HOH:O	2.19	0.42
1:A:397:LYS:HA	1:A:415:LEU:HD11	2.01	0.42
1:B:425:VAL:CG1	1:B:539:ASP:HB3	2.48	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:C:79:ARG:HD3	1:D:122:GLU:OE1	2.19	0.42
1:A:173:GLN:HE21	1:A:173:GLN:HB3	1.62	0.42
1:B:161:SER:OG	1:B:162:GLU:N	2.53	0.41
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:D:406:LYS:N	1:D:576:ASP:OD1	2.30	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:A:31:LEU:CD1	1:A:31:LEU:H	2.31	0.41
1:A:5:GLN:NE2	1:A:97:ARG:HD3	2.33	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:C:154:VAL:O	1:C:158:MET:HG3	2.20	0.41
1:C:22:ARG:HG2	1:C:46:LEU:HD21	2.02	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:D:418:LEU:HD22	1:D:560:ALA:HB2	2.02	0.41
1:C:112:SER:HA	1:C:113:PRO:HD3	1.87	0.41
1:B:437:LYS:HE2	4:B:2277:HOH:O	2.20	0.41
1:B:565:SER:HB3	1:B:568:ASP:OD1	2.21	0.41
1:A:31:LEU:CD1	1:A:31:LEU:N	2.82	0.41
1:C:127:GLY:HA3	3:C:1903:XMP:C6	2.51	0.41
1:D:115:VAL:O	1:D:115:VAL:HG23	2.21	0.41
1:C:266:LYS:HB3	1:D:449:GLN:HB3	2.03	0.41
1:D:512:PHE:CD1	1:D:512:PHE:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:PRO:O	1:A:332:ILE:HG13	2.21	0.41
1:B:430:SER:CB	1:B:431:ASN:HA	2.51	0.40
1:D:249:LEU:HD23	1:D:249:LEU:O	2.21	0.40
1:B:141:ARG:HD2	4:B:2139:HOH:O	2.21	0.40
1:B:326:ASP:CG	1:B:328:PRO:HD2	2.41	0.40
1:D:483:LYS:O	1:D:487:ILE:HG13	2.22	0.40
1:B:355:SER:O	1:B:360:GLY:HA2	2.21	0.40
1:A:266:LYS:CB	1:B:449:GLN:HB3	2.50	0.40
1:A:550:ARG:NH1	1:A:553:ARG:HG3	2.35	0.40
1:C:225:LYS:HZ1	1:C:229:THR:HG22	1.86	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%)	34	21
1	B	587/592 (99%)	571 (97%)	14 (2%)	2 (0%)	46	35
1	C	583/592 (98%)	561 (96%)	20 (3%)	2 (0%)	46	35
1	D	587/592 (99%)	573 (98%)	13 (2%)	1 (0%)	52	42
All	All	2341/2368 (99%)	2267 (97%)	66 (3%)	8 (0%)	46	35

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

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Mol	Chain	Res	Type
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%)	448 (97%)	14 (3%)	48	38
1	B	469/488 (96%)	456 (97%)	13 (3%)	51	41
1	C	461/488 (94%)	456 (99%)	5 (1%)	80	79
1	D	466/488 (96%)	460 (99%)	6 (1%)	76	73
All	All	1858/1952 (95%)	1820 (98%)	38 (2%)	63	57

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	50	ASP
1	A	90	ARG
1	A	153	VAL
1	A	172	ARG
1	A	173	GLN
1	A	207	ARG
1	A	268	VAL
1	A	323	ASP
1	A	339	ASP
1	A	431	ASN
1	A	432	SER
1	A	501	GLU
1	A	584	HIS
1	B	14	LYS
1	B	268	VAL
1	B	279	LEU

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Mol	Chain	Res	Type
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	438	ASN
1	B	486	GLU
1	B	517	GLU
1	B	584	HIS
1	C	83	GLU
1	C	268	VAL
1	C	275	VAL
1	C	323	ASP
1	C	431	ASN
1	D	404	VAL
1	D	405	THR
1	D	407	ASN
1	D	431	ASN
1	D	432	SER
1	D	584	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	85	ASN
1	A	173	GLN
1	A	431	ASN
1	A	449	GLN
1	A	453	HIS
1	A	472	GLN
1	A	586	ASN
1	B	184	GLN
1	B	359	ASN
1	B	431	ASN
1	B	449	GLN
1	B	470	HIS
1	B	586	ASN
1	C	5	GLN
1	C	159	GLN
1	C	173	GLN

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Mol	Chain	Res	Type
1	C	181	HIS
1	C	369	GLN
1	C	431	ASN
1	C	449	GLN
1	C	584	HIS
1	C	586	ASN
1	D	407	ASN
1	D	431	ASN
1	D	449	GLN
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 carbohydrates 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	-	18,26,26	2.37	7 (38%)	22,40,40	2.55	7 (31%)
3	XMP	C	1903	-	18,26,26	2.44	7 (38%)	22,40,40	2.63	8 (36%)

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	-	-	0/6/26/26	0/3/3/3
3	XMP	C	1903	-	-	0/6/26/26	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1901	XMP	C5'-C4'	2.08	1.58	1.51
3	A	1901	XMP	P-O5'	2.08	1.67	1.60
3	C	1903	XMP	C5'-C4'	2.20	1.58	1.51
3	A	1901	XMP	C8-N7	2.23	1.38	1.34
3	C	1903	XMP	P-O5'	2.36	1.68	1.60
3	C	1903	XMP	C8-N7	2.39	1.39	1.34
3	C	1903	XMP	O4'-C1'	2.67	1.44	1.41
3	A	1901	XMP	O4'-C1'	2.69	1.44	1.41
3	C	1903	XMP	P-O3P	3.43	1.62	1.51
3	A	1901	XMP	P-O3P	3.84	1.63	1.51
3	A	1901	XMP	C4-N3	4.54	1.43	1.35
3	C	1903	XMP	C4-N3	4.91	1.43	1.35
3	C	1903	XMP	C6-N1	6.09	1.44	1.33
3	A	1901	XMP	C6-N1	6.15	1.44	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1901	XMP	C4'-O4'-C1'	-4.72	104.53	109.72
3	C	1903	XMP	C4'-O4'-C1'	-4.37	104.92	109.72
3	C	1903	XMP	C5-C6-N1	-2.88	119.65	123.59
3	A	1901	XMP	O3'-C3'-C4'	-2.87	102.44	111.05
3	C	1903	XMP	O3'-C3'-C4'	-2.77	102.75	111.05
3	A	1901	XMP	C5-C6-N1	-2.68	119.92	123.59
3	C	1903	XMP	C4-C5-N7	-2.01	107.63	109.48
3	A	1901	XMP	O2P-P-O5'	2.24	113.01	106.56
3	C	1903	XMP	O2P-P-O5'	2.25	113.03	106.56
3	C	1903	XMP	O3'-C3'-C2'	2.61	120.33	111.83
3	A	1901	XMP	O3'-C3'-C2'	2.94	121.38	111.83
3	A	1901	XMP	C2'-C1'-N9	5.17	122.18	114.29
3	C	1903	XMP	C2'-C1'-N9	5.96	123.39	114.29
3	A	1901	XMP	C6-N1-C2	6.84	121.16	115.25
3	C	1903	XMP	C6-N1-C2	7.13	121.41	115.25

There are no chirality outliers.

There are no torsion outliers.

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.09	8 (1%) 78 80	14, 29, 52, 71	0
1	B	589/592 (99%)	-0.21	6 (1%) 84 86	13, 24, 54, 70	0
1	C	587/592 (99%)	-0.06	8 (1%) 78 80	15, 29, 56, 76	0
1	D	589/592 (99%)	-0.22	3 (0%) 91 92	14, 24, 52, 73	0
All	All	2353/2368 (99%)	-0.15	25 (1%) 82 84	13, 27, 54, 76	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	566	ALA	4.9
1	A	564	GLY	4.3
1	C	113	PRO	4.0
1	D	510	ALA	4.0
1	C	567	ALA	3.5
1	A	113	PRO	3.4
1	B	511	LEU	3.0
1	C	501	GLU	2.9
1	C	508	TRP	2.9
1	A	481	GLY	2.8
1	B	510	ALA	2.7
1	A	566	ALA	2.6
1	B	515	VAL	2.5
1	C	515	VAL	2.5
1	B	406	LYS	2.4
1	B	453	HIS	2.4
1	A	485	ALA	2.3
1	C	518	LEU	2.3
1	C	17	LEU	2.2
1	A	3	PRO	2.2
1	D	503	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	153	VAL	2.1
1	A	290	TYR	2.0
1	B	508	TRP	2.0
1	D	409	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	XMP	C	1903	24/24	0.94	0.12	0.33	28,35,41,43	0
3	XMP	A	1901	24/24	0.92	0.11	0.19	27,32,40,41	0
2	K	B	2002	1/1	0.99	0.08	-0.29	17,17,17,17	0
2	K	A	2001	1/1	1.00	0.06	-0.93	15,15,15,15	0
2	K	D	2004	1/1	1.00	0.06	-2.55	17,17,17,17	0
2	K	C	2003	1/1	1.00	0.04	-2.94	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.