



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:06 AM UTC

PDB ID : 3X07 / pdb_00003x07
Title : Crystal structure of PIP4KIIBETA N203A complex with AMP
Authors : Takeuchi, K.; Lo, Y.H.; Sumita, K.; Senda, M.; Terakawa, J.; Dimitoris, A.; Locasale, J.W.; Sasaki, M.; Yoshino, H.; Zhang, Y.; Kahoud, E.R.; Takano, T.; Yokota, T.; Emerling, B.; Asara, J.A.; Ishida, T.; Shimada, I.; Daikoku, T.; Cantley, L.C.; Senda, T.; Sasaki, A.T.
Deposited on : 2014-10-09
Resolution : 2.60 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](#) ①) 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

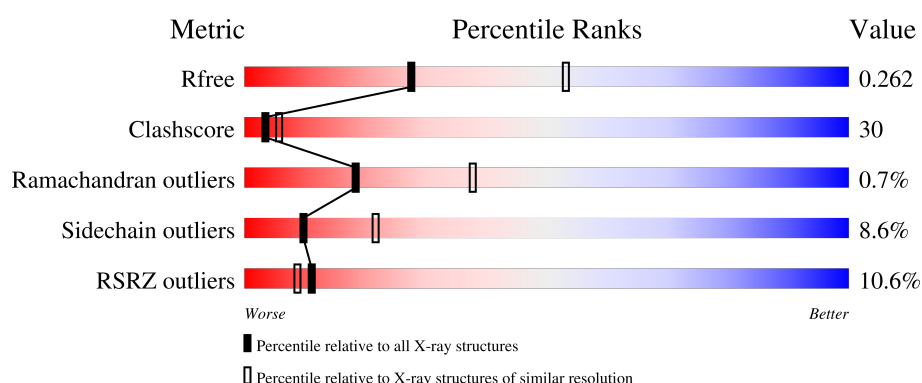
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	393	6% 46% 31% • 20%
1	B	393	11% 42% 26% 5% 26%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5102 atoms, of which 36 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.

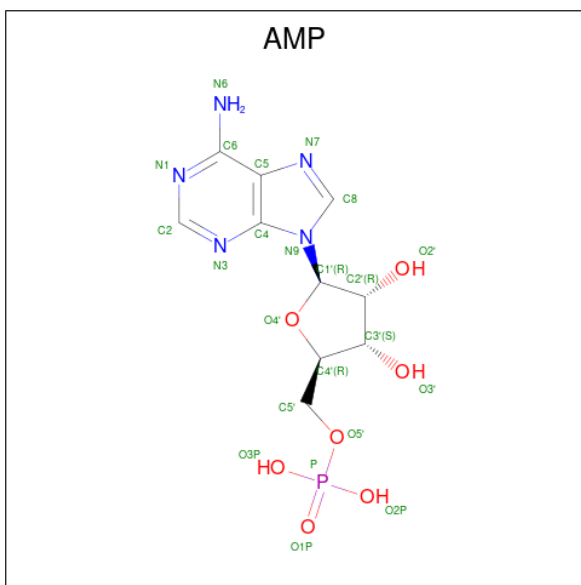
- Molecule 1 is a protein called Phosphatidylinositol 5-phosphate 4-kinase type-2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2577	1642	438	483	14			
1	B	292	Total	C	N	O	S	0	0	0
			2403	1544	409	437	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP P78356
A	25	PRO	-	expression tag	UNP P78356
A	26	ASN	-	expression tag	UNP P78356
A	27	CYS	-	expression tag	UNP P78356
A	28	ALA	-	expression tag	UNP P78356
A	29	PRO	-	expression tag	UNP P78356
A	30	GLY	-	expression tag	UNP P78356
A	203	ALA	ASN	engineered mutation	UNP P78356
B	24	GLY	-	expression tag	UNP P78356
B	25	PRO	-	expression tag	UNP P78356
B	26	ASN	-	expression tag	UNP P78356
B	27	CYS	-	expression tag	UNP P78356
B	28	ALA	-	expression tag	UNP P78356
B	29	PRO	-	expression tag	UNP P78356
B	30	GLY	-	expression tag	UNP P78356
B	203	ALA	ASN	engineered mutation	UNP P78356

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		
2	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		
2	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		

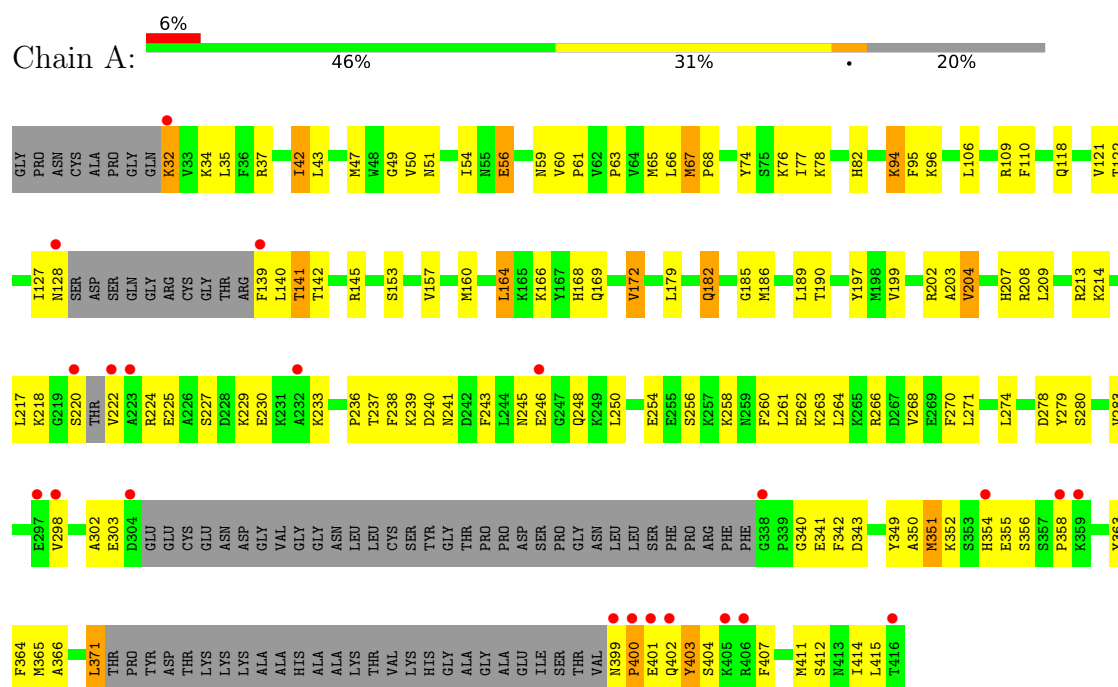
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	8	Total	O	0	0
			8	8		

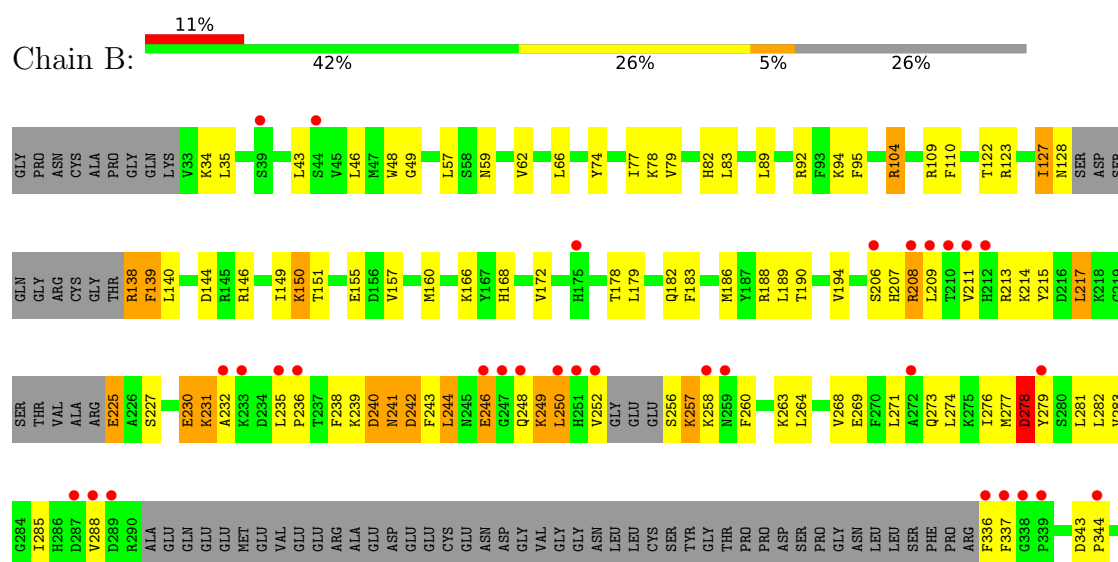
3 Residue-property plots [i](#)

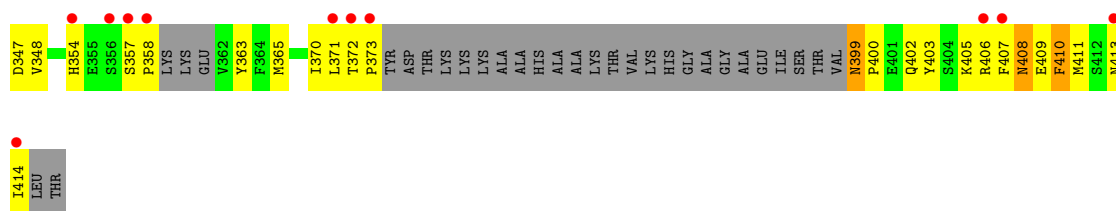
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta



- Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.12Å 185.07Å 107.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.56 – 2.60 53.56 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (53.56-2.60) 98.7 (53.56-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.62Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.223 , 0.270 0.213 , 0.262	Depositor DCC
R_{free} test set	1650 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.019 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5102	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: AMP

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	0.51	0/2629	0.88	2/3533 (0.1%)
1	B	0.62	1/2455 (0.0%)	0.90	5/3303 (0.2%)
All	All	0.57	1/5084 (0.0%)	0.89	7/6836 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	HIS	CG-ND1	-5.45	1.32	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	LEU	N-CA-C	-7.08	100.00	110.48
1	B	194	VAL	N-CA-C	5.96	116.51	108.17
1	B	278	ASP	O-C-N	5.64	127.91	121.88
1	A	164	LEU	N-CA-C	5.54	117.32	111.28
1	A	204	VAL	N-CA-C	-5.40	106.42	111.45
1	B	62	VAL	CA-C-N	5.23	125.21	120.03
1	B	62	VAL	C-N-CA	5.23	125.21	120.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2577	0	2540	145	0
1	B	2403	0	2382	165	0
2	A	69	36	36	2	0
3	A	9	0	0	1	0
3	B	8	0	0	1	0
All	All	5066	36	4958	299	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 30.

All (299) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:GLU:HG2	1:B:241:ASN:HB2	1.35	1.08
1:A:42:ILE:HD12	1:A:42:ILE:H	1.11	1.07
1:B:250:LEU:HD22	1:B:414:ILE:HG22	1.41	1.02
1:B:241:ASN:HA	1:B:244:LEU:HD12	1.41	1.01
1:B:243:PHE:HE2	1:B:414:ILE:CG1	1.72	1.01
1:B:243:PHE:HE2	1:B:414:ILE:HG13	1.23	1.00
1:A:77:ILE:HD11	1:B:77:ILE:HD11	1.42	0.99
1:B:217:LEU:CB	1:B:411:MET:HE1	1.93	0.98
1:B:243:PHE:CE2	1:B:414:ILE:HG13	1.98	0.98
1:A:278:ASP:H	1:A:403:TYR:HE2	1.13	0.97
1:B:252:VAL:CG1	1:B:256:SER:HB2	1.95	0.96
1:A:67:MET:HE2	1:A:67:MET:HA	1.47	0.96
1:B:250:LEU:HD22	1:B:414:ILE:CG2	1.96	0.94
1:B:225:GLU:HG2	1:B:241:ASN:CB	1.96	0.94
1:B:78:LYS:HD2	1:B:94:LYS:HE2	1.51	0.93
1:B:277:MET:O	1:B:278:ASP:HB2	1.71	0.88
1:A:141:THR:HG22	1:A:142:THR:O	1.73	0.88
1:A:278:ASP:N	1:A:403:TYR:HE2	1.71	0.88
1:B:260:PHE:CE2	1:B:365:MET:HE3	2.10	0.87
1:B:264:LEU:HD11	1:B:407:PHE:HE2	1.40	0.87
1:A:42:ILE:H	1:A:42:ILE:CD1	1.84	0.86
1:A:32:LYS:HB2	1:A:32:LYS:NZ	1.91	0.85
1:B:217:LEU:HB2	1:B:411:MET:HE1	1.58	0.85
1:B:225:GLU:HA	1:B:239:LYS:HB2	1.59	0.84
1:B:243:PHE:CE2	1:B:414:ILE:CG1	2.60	0.83
1:B:78:LYS:HD2	1:B:94:LYS:CE	2.07	0.83
1:A:42:ILE:HD12	1:A:42:ILE:N	1.92	0.83
1:B:408:ASN:HD22	1:B:408:ASN:C	1.87	0.82
1:A:77:ILE:HD11	1:B:77:ILE:CD1	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ILE:CD1	1:B:77:ILE:HD11	2.11	0.80
1:B:278:ASP:HB2	1:B:372:THR:HG21	1.61	0.80
1:B:217:LEU:HB3	1:B:411:MET:HE1	1.65	0.77
1:B:278:ASP:CB	1:B:372:THR:HG21	2.14	0.77
1:A:218:LYS:HD2	1:A:224:ARG:NH1	1.99	0.77
1:B:94:LYS:HB2	1:B:190:THR:HB	1.66	0.76
1:A:399:ASN:HB3	1:A:402:GLN:HB2	1.68	0.76
1:B:410:PHE:CD1	1:B:410:PHE:C	2.64	0.76
1:B:243:PHE:CE2	1:B:414:ILE:CD1	2.68	0.75
1:B:407:PHE:O	1:B:411:MET:HG2	1.86	0.75
1:A:109:ARG:CZ	1:A:172:VAL:HG13	2.18	0.74
1:B:243:PHE:CE2	1:B:414:ILE:HD12	2.23	0.73
1:B:252:VAL:HG12	1:B:256:SER:HB2	1.69	0.73
1:B:214:LYS:HE3	1:B:235:LEU:HB3	1.69	0.73
1:A:270:PHE:CZ	1:A:274:LEU:HD11	2.24	0.72
1:A:67:MET:HA	1:A:67:MET:CE	2.19	0.72
1:A:67:MET:HE2	1:A:68:PRO:HD3	1.72	0.71
1:B:405:LYS:O	1:B:409:GLU:HB2	1.91	0.71
1:A:268:VAL:CG1	1:A:404:SER:HA	2.20	0.70
1:B:249:LYS:HA	1:B:414:ILE:HG23	1.74	0.69
1:B:271:LEU:HD13	1:B:279:TYR:CE2	2.27	0.69
1:B:243:PHE:CZ	1:B:414:ILE:HG21	2.28	0.69
1:B:138:ARG:NH1	1:B:138:ARG:HG3	2.08	0.69
1:A:51:ASN:HB2	1:A:122:THR:HG21	1.75	0.69
1:B:127:ILE:CG2	1:B:128:ASN:N	2.56	0.68
1:B:257:LYS:HD3	1:B:258:LYS:N	2.08	0.68
1:B:138:ARG:HG3	1:B:138:ARG:HH11	1.59	0.68
1:B:243:PHE:CE2	1:B:414:ILE:HG21	2.29	0.68
1:B:269:GLU:O	1:B:273:GLN:HG3	1.94	0.68
1:A:241:ASN:O	1:A:245:ASN:HB2	1.94	0.68
1:A:169:GLN:O	1:A:172:VAL:HG23	1.94	0.68
1:A:127:ILE:O	1:A:128:ASN:HB2	1.94	0.67
1:A:160:MET:HG2	1:A:371:LEU:HD21	1.74	0.67
1:B:110:PHE:CE1	1:B:182:GLN:HG2	2.29	0.67
1:B:264:LEU:HD11	1:B:407:PHE:CE2	2.27	0.67
1:A:208:ARG:HH22	1:A:342:PHE:HA	1.60	0.67
1:B:410:PHE:C	1:B:410:PHE:HD1	2.03	0.67
1:B:225:GLU:HB3	1:B:242:ASP:OD1	1.96	0.66
1:A:214:LYS:HE3	1:A:237:THR:OG1	1.96	0.66
1:B:271:LEU:HD12	1:B:279:TYR:CZ	2.30	0.66
1:A:77:ILE:CG1	1:B:77:ILE:HD11	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASP:N	1:A:403:TYR:CE2	2.52	0.65
1:B:250:LEU:CD2	1:B:414:ILE:HG22	2.22	0.65
1:B:277:MET:O	1:B:278:ASP:CB	2.45	0.65
1:B:276:ILE:HA	1:B:373:PRO:HG3	1.78	0.65
1:B:243:PHE:HE2	1:B:414:ILE:CD1	2.06	0.64
1:A:264:LEU:HD11	1:A:407:PHE:HE2	1.62	0.64
1:A:217:LEU:HD13	1:A:414:ILE:HD11	1.79	0.64
1:A:349:TYR:CD1	1:A:366:ALA:HB2	2.33	0.63
1:B:243:PHE:CE2	1:B:414:ILE:CG2	2.82	0.63
1:A:66:LEU:HD12	1:A:168:HIS:CE1	2.34	0.62
1:A:218:LYS:HG2	1:A:403:TYR:OH	1.98	0.62
1:B:277:MET:HE1	1:B:399:ASN:C	2.23	0.62
1:A:246:GLU:O	1:A:246:GLU:HG2	1.97	0.62
1:A:278:ASP:CA	1:A:403:TYR:HE2	2.13	0.62
1:A:56:GLU:OE2	1:B:48:TRP:NE1	2.26	0.62
1:B:127:ILE:HG23	1:B:128:ASN:N	2.14	0.61
1:A:264:LEU:HD21	1:A:411:MET:HB2	1.81	0.61
1:A:32:LYS:HB2	1:A:32:LYS:HZ2	1.61	0.61
1:B:281:LEU:HD22	1:B:283:VAL:HG23	1.82	0.60
1:B:225:GLU:HG2	1:B:241:ASN:HB3	1.83	0.60
1:B:281:LEU:C	1:B:281:LEU:HD23	2.27	0.60
1:B:166:LYS:HD2	1:B:274:LEU:HD21	1.84	0.59
1:A:65:MET:HE2	1:A:67:MET:HE3	1.84	0.59
1:B:238:PHE:HD2	1:B:242:ASP:HB3	1.66	0.59
1:B:271:LEU:CD1	1:B:279:TYR:CZ	2.86	0.59
1:A:260:PHE:CD2	1:A:415:LEU:HD11	2.38	0.59
1:B:217:LEU:H	1:B:217:LEU:HD22	1.69	0.58
1:A:220:SER:CB	1:A:222:VAL:N	2.67	0.58
1:B:230:GLU:C	1:B:232:ALA:H	2.11	0.58
1:A:250:LEU:HG	1:A:414:ILE:HG22	1.86	0.58
1:A:139:PHE:CE2	2:A:501:AMP:O4'	2.56	0.57
1:A:141:THR:CG2	1:A:145:ARG:HA	2.35	0.57
1:B:281:LEU:HB2	1:B:407:PHE:CZ	2.39	0.57
1:A:208:ARG:NH2	1:A:342:PHE:HA	2.18	0.57
1:B:144:ASP:OD2	1:B:146:ARG:HD2	2.03	0.57
1:A:145:ARG:HH21	1:A:207:HIS:C	2.11	0.57
1:A:139:PHE:CD1	1:A:139:PHE:C	2.81	0.57
1:B:215:TYR:CD1	1:B:238:PHE:HB2	2.40	0.57
1:A:399:ASN:HA	1:A:402:GLN:HG3	1.87	0.57
1:B:189:LEU:HD12	1:B:189:LEU:N	2.20	0.57
1:B:139:PHE:CD1	1:B:139:PHE:C	2.82	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:PHE:CE1	1:B:411:MET:HE3	2.40	0.56
1:A:110:PHE:CZ	1:A:182:GLN:HB3	2.40	0.56
1:A:169:GLN:C	1:A:172:VAL:HG23	2.30	0.56
1:B:46:LEU:HD21	1:B:149:ILE:HD13	1.88	0.56
1:B:260:PHE:CE2	1:B:365:MET:CE	2.88	0.55
1:A:241:ASN:O	1:A:245:ASN:CB	2.55	0.55
1:B:240:ASP:O	1:B:244:LEU:HG	2.07	0.55
1:A:32:LYS:HB2	1:A:32:LYS:HZ3	1.71	0.55
1:B:252:VAL:HG13	1:B:256:SER:HB2	1.83	0.55
1:A:127:ILE:O	1:A:128:ASN:CB	2.53	0.55
1:A:186:MET:HG3	1:A:199:VAL:HG22	1.88	0.55
1:B:140:LEU:HB2	1:B:149:ILE:HB	1.89	0.55
1:B:243:PHE:HE2	1:B:414:ILE:CG2	2.19	0.55
1:B:240:ASP:HB3	1:B:410:PHE:CE2	2.41	0.55
1:B:276:ILE:HD13	1:B:370:ILE:O	2.07	0.55
1:B:281:LEU:HD22	1:B:283:VAL:CG2	2.37	0.55
1:A:202:ARG:HG3	1:A:203:ALA:N	2.22	0.55
1:B:138:ARG:HH11	1:B:138:ARG:CG	2.20	0.54
1:B:78:LYS:HD2	1:B:94:LYS:HE3	1.88	0.54
1:A:283:VAL:HG22	1:A:365:MET:HG2	1.90	0.54
1:B:236:PRO:HB2	1:B:238:PHE:CE1	2.42	0.54
1:B:243:PHE:CZ	1:B:414:ILE:CG2	2.91	0.54
1:A:169:GLN:HA	1:A:172:VAL:HG23	1.91	0.53
1:A:208:ARG:HB3	1:A:208:ARG:NH1	2.24	0.53
1:B:403:TYR:N	1:B:406:ARG:HH21	2.07	0.53
1:A:109:ARG:NH1	1:A:109:ARG:HG2	2.24	0.53
1:A:160:MET:O	1:A:164:LEU:HB2	2.08	0.53
1:A:208:ARG:NH2	1:A:341:GLU:O	2.30	0.53
1:A:256:SER:HB3	1:A:351:MET:HE2	1.91	0.52
1:B:127:ILE:HG22	1:B:128:ASN:HB3	1.90	0.52
1:B:157:VAL:HG13	1:B:186:MET:HE3	1.90	0.52
1:A:139:PHE:C	1:A:139:PHE:HD1	2.16	0.52
1:A:278:ASP:HA	1:A:403:TYR:CE2	2.45	0.52
1:A:168:HIS:O	1:A:172:VAL:HG22	2.09	0.52
1:B:250:LEU:CD2	1:B:414:ILE:CG2	2.78	0.52
1:A:54:ILE:HG21	1:A:118:GLN:HB2	1.91	0.52
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.75	0.51
1:B:271:LEU:HD13	1:B:279:TYR:CD2	2.45	0.51
1:A:278:ASP:CA	1:A:403:TYR:CE2	2.93	0.51
1:B:217:LEU:HB2	1:B:411:MET:CE	2.36	0.51
1:A:354:HIS:HD2	1:A:355:GLU:H	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLN:HA	1:A:172:VAL:CG2	2.40	0.51
1:B:78:LYS:CD	1:B:94:LYS:HE2	2.34	0.51
1:A:189:LEU:N	1:A:189:LEU:HD12	2.26	0.51
1:B:241:ASN:HA	1:B:244:LEU:CD1	2.27	0.51
1:A:157:VAL:HG21	1:A:197:TYR:CD2	2.46	0.50
1:A:243:PHE:CE1	1:A:248:GLN:HG2	2.46	0.50
1:B:236:PRO:HG2	1:B:238:PHE:HE1	1.77	0.50
1:B:238:PHE:HD2	1:B:242:ASP:CB	2.24	0.50
1:B:276:ILE:CG2	1:B:277:MET:N	2.74	0.50
1:B:250:LEU:HD22	1:B:414:ILE:HG21	1.89	0.50
1:B:213:ARG:CZ	1:B:238:PHE:CZ	2.94	0.50
1:A:35:LEU:HD13	1:A:37:ARG:HH22	1.77	0.49
1:A:224:ARG:O	1:A:241:ASN:HB2	2.12	0.49
1:B:79:VAL:O	1:B:92:ARG:HA	2.12	0.49
1:A:354:HIS:CD2	1:A:355:GLU:N	2.80	0.49
1:B:277:MET:HE1	1:B:399:ASN:HB3	1.95	0.49
1:B:189:LEU:N	1:B:189:LEU:CD1	2.75	0.49
1:B:227:SER:OG	1:B:230:GLU:HB2	2.12	0.49
1:B:66:LEU:HD12	1:B:168:HIS:CE1	2.47	0.49
1:B:276:ILE:HG22	1:B:277:MET:N	2.27	0.49
1:A:264:LEU:HD11	1:A:407:PHE:CE2	2.44	0.48
1:B:43:LEU:HD21	1:B:140:LEU:HD11	1.95	0.48
1:B:230:GLU:C	1:B:232:ALA:N	2.70	0.48
1:A:250:LEU:HG	1:A:414:ILE:CG2	2.43	0.48
1:B:166:LYS:HD2	1:B:274:LEU:CD2	2.44	0.48
1:B:230:GLU:O	1:B:232:ALA:N	2.46	0.48
1:B:281:LEU:C	1:B:281:LEU:CD2	2.87	0.48
1:B:408:ASN:C	1:B:408:ASN:ND2	2.59	0.48
1:B:225:GLU:CG	1:B:241:ASN:HB2	2.25	0.48
1:A:261:LEU:HD21	1:A:412:SER:HA	1.96	0.48
1:A:264:LEU:CD2	1:A:411:MET:HB2	2.44	0.48
1:A:350:ALA:HA	1:A:363:TYR:O	2.14	0.48
1:A:236:PRO:HB2	1:A:238:PHE:CE2	2.49	0.48
1:B:74:TYR:CD1	1:B:74:TYR:C	2.92	0.48
1:B:236:PRO:CG	1:B:238:PHE:HE1	2.27	0.47
1:A:213:ARG:NH2	1:A:246:GLU:OE1	2.47	0.47
1:A:225:GLU:HG3	1:A:241:ASN:HB2	1.95	0.47
1:B:277:MET:HE3	1:B:400:PRO:HA	1.95	0.47
1:B:109:ARG:CZ	1:B:172:VAL:HG22	2.44	0.47
1:B:188:ARG:C	1:B:189:LEU:HD12	2.39	0.47
1:B:208:ARG:HG2	1:B:209:LEU:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ARG:NH2	1:B:246:GLU:OE2	2.47	0.47
1:A:258:LYS:NZ	1:A:262:GLU:OE2	2.32	0.47
1:A:340:GLY:O	1:A:352:LYS:HE2	2.14	0.47
1:B:271:LEU:CD1	1:B:279:TYR:CE2	2.96	0.47
1:B:277:MET:O	1:B:372:THR:HB	2.13	0.47
1:A:65:MET:HE2	1:A:67:MET:CE	2.45	0.47
1:A:243:PHE:CZ	1:A:414:ILE:HG23	2.50	0.47
1:B:49:GLY:HA3	1:B:95:PHE:CE2	2.50	0.47
1:B:281:LEU:HB2	1:B:407:PHE:HZ	1.80	0.47
1:A:77:ILE:HG22	1:A:95:PHE:HB3	1.97	0.46
1:A:271:LEU:HD13	1:A:279:TYR:CE2	2.50	0.46
1:A:96:LYS:NZ	2:A:503:AMP:O3P	2.47	0.46
1:B:336:PHE:CD2	1:B:337:PHE:O	2.68	0.46
1:A:109:ARG:NH1	1:A:172:VAL:HG13	2.29	0.46
1:A:153:SER:O	1:A:157:VAL:HG23	2.15	0.46
1:B:82:HIS:CE1	1:B:83:LEU:HG	2.49	0.46
1:A:218:LYS:HE2	1:A:278:ASP:O	2.15	0.46
1:A:225:GLU:C	1:A:239:LYS:HG3	2.41	0.46
1:B:277:MET:CE	1:B:400:PRO:HA	2.46	0.46
1:B:410:PHE:CD1	1:B:410:PHE:O	2.68	0.46
1:B:217:LEU:HD22	1:B:217:LEU:N	2.29	0.46
1:A:168:HIS:O	1:A:172:VAL:CG2	2.64	0.46
1:A:160:MET:CG	1:A:371:LEU:HD21	2.45	0.46
1:B:252:VAL:HG12	1:B:257:LYS:H	1.81	0.46
1:A:77:ILE:HD12	1:B:79:VAL:HG22	1.97	0.45
1:A:243:PHE:HZ	1:A:414:ILE:HG23	1.80	0.45
1:A:169:GLN:CA	1:A:172:VAL:HG23	2.46	0.45
1:A:225:GLU:O	1:A:239:LYS:HG3	2.16	0.45
1:A:350:ALA:HB2	1:A:364:PHE:CD1	2.51	0.45
1:B:206:SER:HA	1:B:347:ASP:OD1	2.17	0.45
1:B:399:ASN:HA	1:B:402:GLN:CB	2.47	0.45
1:A:400:PRO:HG2	1:A:401:GLU:H	1.82	0.45
1:A:224:ARG:O	1:A:225:GLU:HG3	2.15	0.45
1:A:243:PHE:CE1	1:A:248:GLN:CG	3.00	0.45
1:A:49:GLY:HA3	1:A:95:PHE:CE1	2.51	0.44
1:A:94:LYS:HB2	1:A:190:THR:HB	1.99	0.44
1:A:166:LYS:HD2	1:A:274:LEU:HD21	1.98	0.44
1:B:242:ASP:OD1	1:B:242:ASP:N	2.48	0.44
1:A:60:VAL:HA	1:A:61:PRO:HD2	1.88	0.44
1:A:82:HIS:HB2	1:B:74:TYR:CZ	2.53	0.44
1:A:50:VAL:HG21	1:A:121:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PHE:CE1	1:A:182:GLN:HB3	2.53	0.44
1:A:208:ARG:NH1	1:A:208:ARG:CB	2.80	0.44
1:B:150:LYS:HE3	1:B:150:LYS:HB2	1.47	0.44
1:B:104:ARG:HD2	3:B:503:HOH:O	2.17	0.44
1:A:43:LEU:O	1:A:47:MET:HG3	2.18	0.43
1:A:59:ASN:HB3	1:B:34:LYS:O	2.18	0.43
1:A:403:TYR:O	1:A:407:PHE:N	2.40	0.43
1:B:260:PHE:HE2	1:B:365:MET:HE3	1.78	0.43
1:A:128:ASN:HB2	1:A:140:LEU:HA	2.00	0.43
1:B:48:TRP:HB2	1:B:89:LEU:HD21	2.00	0.43
1:A:204:VAL:HA	1:A:349:TYR:CD2	2.53	0.43
1:B:179:LEU:HG	1:B:263:LYS:HG2	2.01	0.43
1:B:414:ILE:HG22	1:B:414:ILE:O	2.19	0.43
1:B:260:PHE:CD1	1:B:260:PHE:C	2.96	0.43
1:A:246:GLU:O	1:A:246:GLU:CG	2.66	0.43
1:B:57:LEU:O	1:B:104:ARG:NH2	2.51	0.43
1:A:350:ALA:HB2	1:A:364:PHE:CE1	2.53	0.43
1:A:185:GLY:HA2	3:A:602:HOH:O	2.19	0.43
1:A:354:HIS:HD2	1:A:355:GLU:N	2.16	0.43
1:B:399:ASN:N	1:B:400:PRO:CD	2.82	0.42
1:B:238:PHE:C	1:B:239:LYS:HG2	2.44	0.42
1:A:34:LYS:O	1:B:59:ASN:HB3	2.18	0.42
1:A:109:ARG:CZ	1:A:172:VAL:CG1	2.93	0.42
1:B:277:MET:HE3	1:B:400:PRO:CA	2.49	0.42
1:A:43:LEU:HD21	1:A:140:LEU:CD1	2.49	0.42
1:B:231:LYS:HE2	1:B:238:PHE:CE2	2.54	0.42
1:A:179:LEU:HG	1:A:263:LYS:HB3	2.01	0.42
1:B:250:LEU:HD22	1:B:250:LEU:H	1.85	0.42
1:B:343:ASP:HA	1:B:344:PRO:HD2	1.92	0.42
1:A:270:PHE:CE1	1:A:274:LEU:CD1	3.03	0.42
1:B:213:ARG:NH2	1:B:238:PHE:CE2	2.87	0.42
1:B:238:PHE:CD2	1:B:242:ASP:HB3	2.52	0.42
1:A:74:TYR:CD1	1:A:74:TYR:C	2.97	0.42
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.89	0.42
1:B:411:MET:C	1:B:413:ASN:H	2.27	0.42
1:A:74:TYR:CZ	1:B:82:HIS:HB2	2.54	0.42
1:A:230:GLU:CD	1:A:233:LYS:HD3	2.44	0.41
1:A:302:ALA:O	1:A:303:GLU:C	2.62	0.41
1:A:354:HIS:C	1:A:356:SER:H	2.28	0.41
1:B:250:LEU:HB3	1:B:363:TYR:CE2	2.55	0.41
1:B:281:LEU:HD23	1:B:282:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:THR:HG23	1:A:145:ARG:HA	2.01	0.41
1:B:144:ASP:OD1	1:B:144:ASP:C	2.61	0.41
1:A:227:SER:C	1:A:229:LYS:N	2.77	0.41
1:A:343:ASP:C	1:A:343:ASP:OD1	2.63	0.41
1:A:78:LYS:HB3	1:B:78:LYS:HB3	2.02	0.41
1:A:407:PHE:CE1	1:A:411:MET:HE3	2.56	0.41
1:B:248:GLN:O	1:B:414:ILE:HD12	2.20	0.41
1:B:399:ASN:HA	1:B:402:GLN:HB3	2.02	0.41
1:A:67:MET:HE2	1:A:68:PRO:CD	2.45	0.41
1:A:49:GLY:HA3	1:A:95:PHE:CZ	2.56	0.41
1:A:208:ARG:HB3	1:A:208:ARG:CZ	2.50	0.41
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.86	0.41
1:B:127:ILE:HG22	1:B:128:ASN:CB	2.51	0.41
1:B:268:VAL:HG13	1:B:279:TYR:OH	2.21	0.41
1:B:365:MET:HE3	1:B:365:MET:HB2	1.85	0.41
1:A:78:LYS:HG3	1:A:94:LYS:CG	2.51	0.41
1:A:166:LYS:HD2	1:A:274:LEU:CD2	2.51	0.41
1:B:160:MET:HE1	1:B:183:PHE:CD1	2.55	0.41
1:A:209:LEU:HD11	1:A:342:PHE:HB3	2.03	0.40
1:B:283:VAL:HG22	1:B:365:MET:HG2	2.02	0.40
1:A:63:PRO:HB2	1:A:65:MET:O	2.22	0.40
1:B:157:VAL:HG13	1:B:186:MET:CE	2.51	0.40
1:B:411:MET:C	1:B:413:ASN:N	2.79	0.40
1:B:357:SER:HB2	1:B:358:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	304/393 (77%)	287 (94%)	15 (5%)	2 (1%)	18 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	278/393 (71%)	260 (94%)	16 (6%)	2 (1%)	18	38
All	All	582/786 (74%)	547 (94%)	31 (5%)	4 (1%)	18	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	231	LYS
1	A	358	PRO
1	A	400	PRO
1	B	354	HIS

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	288/351 (82%)	271 (94%)	17 (6%)	18	38
1	B	271/351 (77%)	240 (89%)	31 (11%)	5	11
All	All	559/702 (80%)	511 (91%)	48 (9%)	10	22

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	42	ILE
1	A	56	GLU
1	A	67	MET
1	A	76	LYS
1	A	94	LYS
1	A	141	THR
1	A	172	VAL
1	A	182	GLN
1	A	240	ASP
1	A	254	GLU
1	A	266	ARG

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Mol	Chain	Res	Type
1	A	280	SER
1	A	298	VAL
1	A	351	MET
1	A	371	LEU
1	A	403	TYR
1	B	104	ARG
1	B	122	THR
1	B	123	ARG
1	B	127	ILE
1	B	138	ARG
1	B	139	PHE
1	B	150	LYS
1	B	151	THR
1	B	155	GLU
1	B	178	THR
1	B	208	ARG
1	B	211	VAL
1	B	217	LEU
1	B	225	GLU
1	B	230	GLU
1	B	240	ASP
1	B	241	ASN
1	B	242	ASP
1	B	244	LEU
1	B	246	GLU
1	B	249	LYS
1	B	250	LEU
1	B	257	LYS
1	B	278	ASP
1	B	285	ILE
1	B	288	VAL
1	B	348	VAL
1	B	371	LEU
1	B	399	ASN
1	B	408	ASN
1	B	410	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	GLN
1	B	82	HIS

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Mol	Chain	Res	Type
1	B	175	HIS
1	B	273	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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	AMP	A	502	-	25,25,25	2.19	10 (40%)	37,38,38	2.00	12 (32%)
2	AMP	A	501	-	25,25,25	1.47	4 (16%)	37,38,38	2.25	10 (27%)
2	AMP	A	503	-	25,25,25	1.36	4 (16%)	37,38,38	1.94	9 (24%)

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
2	AMP	A	502	-	-	3/10/26/26	0/3/3/3
2	AMP	A	501	-	-	5/10/26/26	0/3/3/3
2	AMP	A	503	-	-	3/10/26/26	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	AMP	C5-C4	4.46	1.47	1.39
2	A	502	AMP	C5-N7	-4.29	1.31	1.39
2	A	502	AMP	C8-N9	-3.87	1.31	1.37
2	A	502	AMP	C4-N9	-3.68	1.30	1.37
2	A	501	AMP	C5-N7	-3.47	1.32	1.39
2	A	501	AMP	C5-C4	3.34	1.45	1.39
2	A	502	AMP	P-O3P	-2.96	1.43	1.54
2	A	502	AMP	P-O2P	-2.96	1.43	1.54
2	A	502	AMP	O4'-C4'	-2.82	1.38	1.45
2	A	501	AMP	C8-N9	-2.74	1.32	1.37
2	A	501	AMP	C4-N9	-2.70	1.32	1.37
2	A	503	AMP	C5-C6	2.67	1.48	1.41
2	A	502	AMP	C5-C4	2.46	1.43	1.39
2	A	502	AMP	P-O1P	-2.43	1.42	1.50
2	A	502	AMP	P-O5'	-2.35	1.52	1.60
2	A	503	AMP	C8-N7	2.34	1.36	1.31
2	A	502	AMP	C2'-C3'	-2.30	1.47	1.53
2	A	503	AMP	C4-N9	-2.26	1.33	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	AMP	C5-C4-N3	-6.80	117.35	126.72
2	A	503	AMP	C5-C4-N3	-6.03	118.41	126.72
2	A	502	AMP	C5-C4-N3	-5.76	118.79	126.72
2	A	501	AMP	N3-C4-N9	5.09	135.82	127.17
2	A	502	AMP	N3-C4-N9	4.69	135.14	127.17
2	A	503	AMP	N3-C4-N9	4.42	134.68	127.17
2	A	501	AMP	C2-N3-C4	4.24	122.18	111.83
2	A	503	AMP	C2-N3-C4	3.93	121.42	111.83
2	A	501	AMP	N3-C2-N1	-3.89	122.70	128.58
2	A	501	AMP	C4-C5-N7	-3.85	106.18	110.58
2	A	503	AMP	C4-C5-N7	-3.80	106.24	110.58
2	A	502	AMP	C2-N3-C4	3.67	120.80	111.83
2	A	502	AMP	N3-C2-N1	-3.54	123.22	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	AMP	N3-C2-N1	-3.40	123.43	128.58
2	A	502	AMP	C4-N9-C8	3.02	108.91	105.74
2	A	502	AMP	C4-C5-N7	-3.00	107.15	110.58
2	A	501	AMP	C5-N7-C8	2.81	107.86	103.45
2	A	503	AMP	C4-N9-C8	2.65	108.52	105.74
2	A	503	AMP	C5-N7-C8	2.63	107.58	103.45
2	A	501	AMP	C2'-C1'-N9	2.49	119.48	113.30
2	A	501	AMP	C4-N9-C8	2.49	108.35	105.74
2	A	501	AMP	C3'-C2'-C1'	2.47	106.13	101.46
2	A	502	AMP	O2P-P-O5'	-2.34	100.58	106.67
2	A	503	AMP	C6-C5-N7	2.32	136.56	132.09
2	A	502	AMP	C2-N1-C6	2.27	122.46	118.73
2	A	502	AMP	C2'-C1'-N9	-2.26	107.69	113.30
2	A	503	AMP	N9-C8-N7	-2.26	110.73	113.94
2	A	501	AMP	N9-C8-N7	-2.25	110.75	113.94
2	A	502	AMP	O3P-P-O1P	2.15	119.21	110.83
2	A	502	AMP	C5-N7-C8	2.12	106.79	103.45
2	A	502	AMP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (11) torsion outliers are listed below:

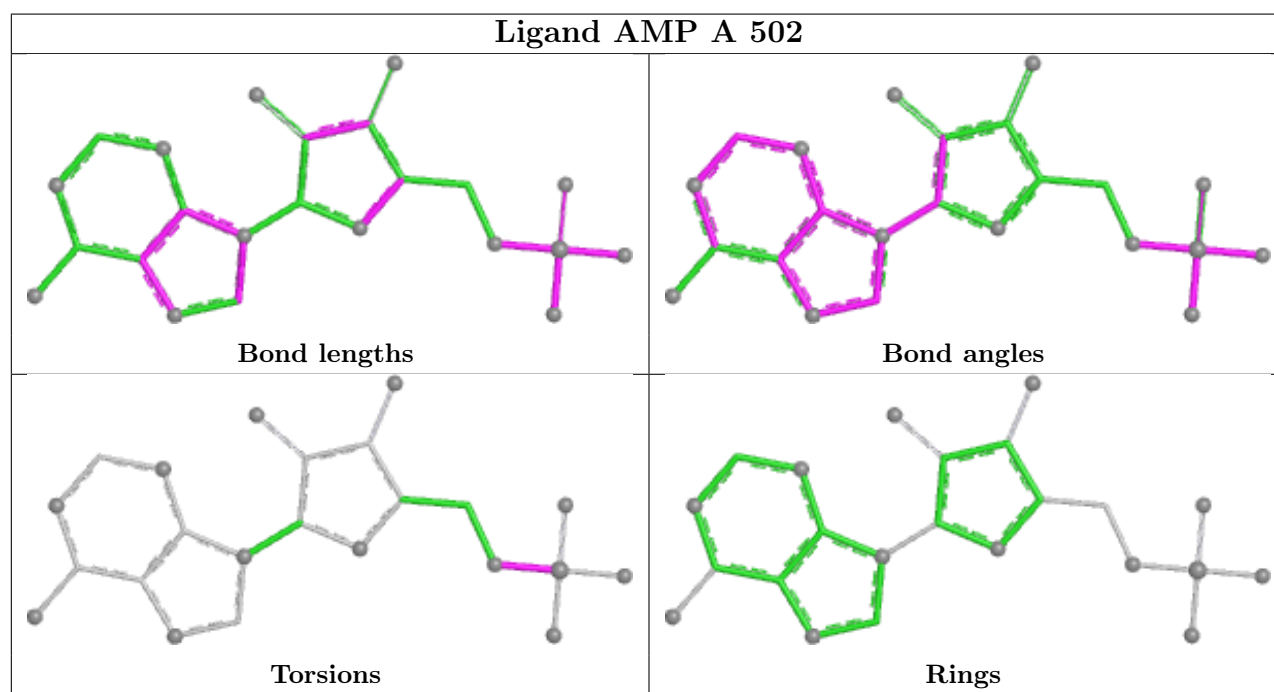
Mol	Chain	Res	Type	Atoms
2	A	501	AMP	C5'-O5'-P-O2P
2	A	501	AMP	C5'-O5'-P-O3P
2	A	502	AMP	C5'-O5'-P-O2P
2	A	502	AMP	C5'-O5'-P-O3P
2	A	503	AMP	C5'-O5'-P-O1P
2	A	503	AMP	C5'-O5'-P-O2P
2	A	503	AMP	C5'-O5'-P-O3P
2	A	501	AMP	O4'-C4'-C5'-O5'
2	A	501	AMP	C3'-C4'-C5'-O5'
2	A	501	AMP	C5'-O5'-P-O1P
2	A	502	AMP	C5'-O5'-P-O1P

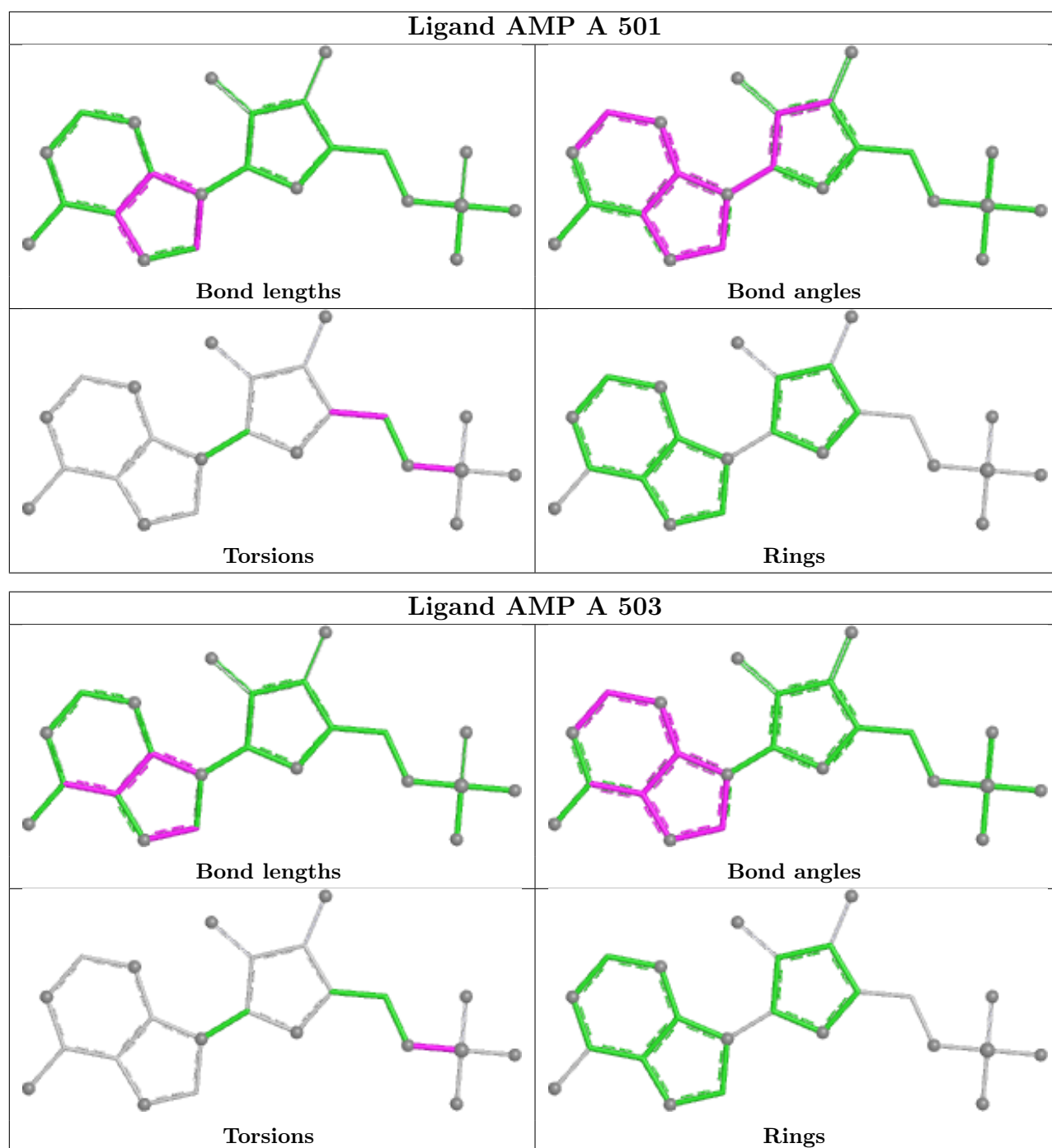
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AMP	1	0
2	A	503	AMP	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	314/393 (79%)	0.35	22 (7%)	22 18	39, 74, 121, 145	0
1	B	292/393 (74%)	0.62	42 (14%)	6 5	25, 76, 144, 160	0
All	All	606/786 (77%)	0.48	64 (10%)	11 9	25, 74, 139, 160	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	VAL	6.0
1	A	222	VAL	5.6
1	B	372	THR	5.3
1	B	236	PRO	5.2
1	B	337	PHE	5.2
1	B	338	GLY	5.1
1	B	287	ASP	4.0
1	A	223	ALA	4.0
1	B	414	ILE	3.9
1	A	304	ASP	3.8
1	A	400	PRO	3.8
1	B	44	SER	3.7
1	B	336	PHE	3.7
1	B	211	VAL	3.6
1	B	206	SER	3.6
1	B	279	TYR	3.4
1	A	220	SER	3.3
1	B	371	LEU	3.2
1	B	258	LYS	3.1
1	B	251	HIS	3.1
1	B	373	PRO	3.1
1	B	235	LEU	3.0
1	B	289	ASP	2.8
1	A	358	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	232	ALA	2.7
1	B	252	VAL	2.7
1	A	297	GLU	2.7
1	B	233	LYS	2.7
1	B	356	SER	2.6
1	A	406	ARG	2.6
1	B	354	HIS	2.6
1	A	128	ASN	2.6
1	B	358	PRO	2.6
1	B	247	GLY	2.5
1	B	272	ALA	2.5
1	B	259	ASN	2.5
1	B	250	LEU	2.5
1	A	416	THR	2.4
1	B	208	ARG	2.4
1	B	406	ARG	2.4
1	A	246	GLU	2.3
1	B	339	PRO	2.3
1	B	407	PHE	2.3
1	B	246	GLU	2.3
1	B	39	SER	2.3
1	A	401	GLU	2.2
1	B	210	THR	2.2
1	B	413	ASN	2.2
1	A	354	HIS	2.2
1	A	402	GLN	2.2
1	B	175	HIS	2.1
1	A	32	LYS	2.1
1	B	344	PRO	2.1
1	A	399	ASN	2.1
1	A	139	PHE	2.1
1	A	298	VAL	2.1
1	A	359	LYS	2.0
1	A	405	LYS	2.0
1	B	209	LEU	2.0
1	B	212	HIS	2.0
1	A	338	GLY	2.0
1	B	232	ALA	2.0
1	B	357	SER	2.0
1	B	248	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

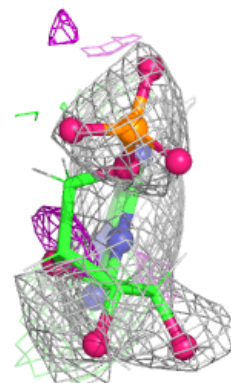
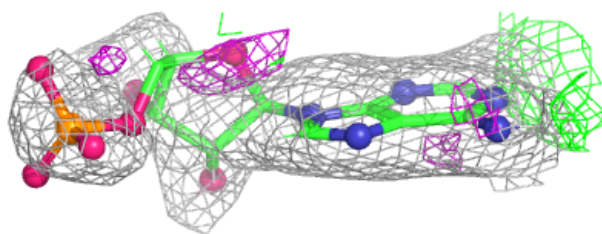
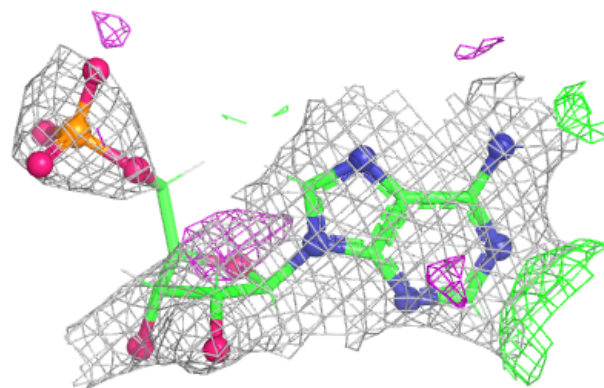
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AMP	A	501	23/23	0.72	0.15	84,142,184,195	0
2	AMP	A	502	23/23	0.91	0.13	66,84,102,109	0
2	AMP	A	503	23/23	0.97	0.07	58,76,92,94	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.

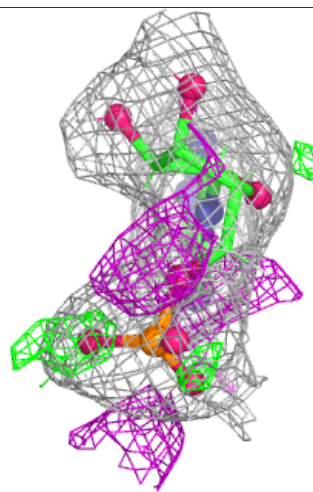
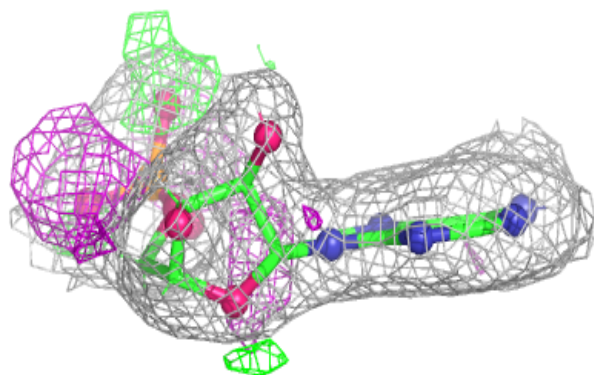
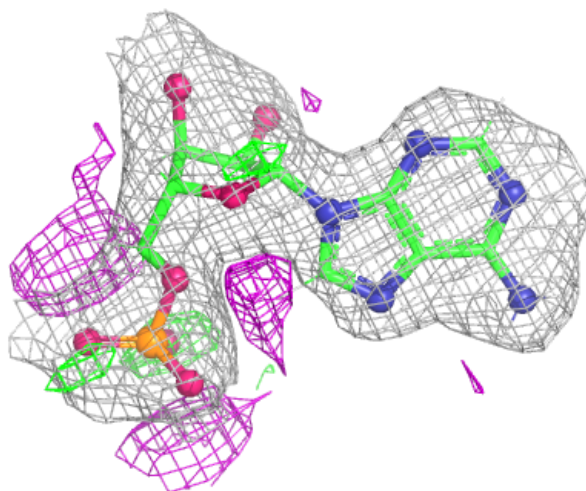
Electron density around AMP A 501:

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



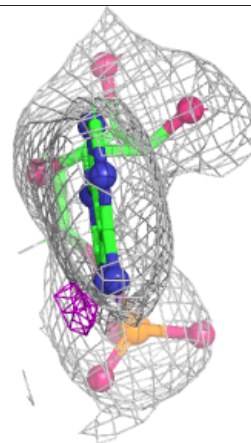
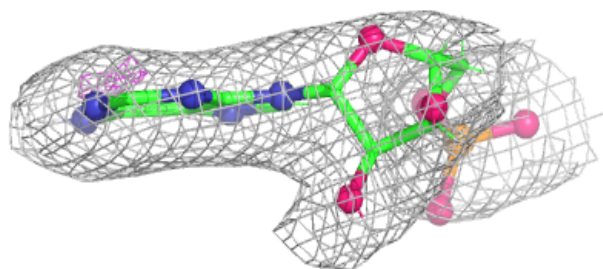
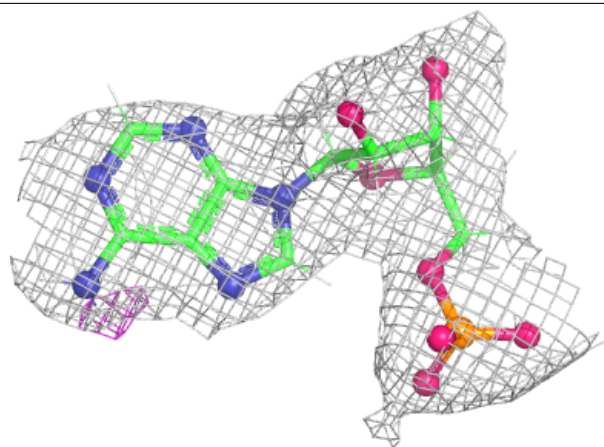
Electron density around AMP A 502:

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



Electron density around AMP A 503:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.