



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:59 AM UTC

PDB ID : 1ZBU / pdb_00001zbu
Title : crystal structure of full-length 3'-exonuclease
Authors : Cheng, Y.; Patel, D.J.
Deposited on : 2005-04-08
Resolution : 3.00 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

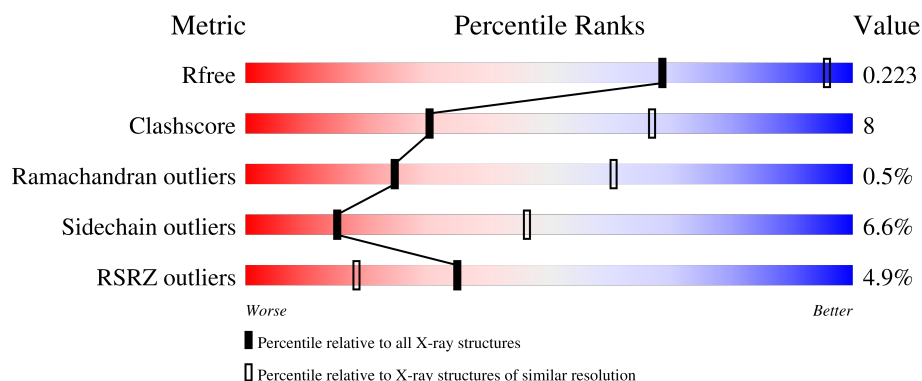
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	349	% 52% 13% 36%
1	B	349	7% 67% 17% • 13%
1	C	349	% 52% 11% • 36%
1	D	349	4% 52% 11% • 36%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8084 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 3'-5' exonuclease ERI1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	Se	0	0	0
			1827	1168	304	341	6	8			
1	B	304	Total	C	N	O	S	Se	0	0	0
			2467	1571	416	462	8	10			
1	C	225	Total	C	N	O	S	Se	0	0	0
			1827	1168	304	341	6	8			
1	D	225	Total	C	N	O	S	Se	0	0	0
			1826	1168	304	340	6	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	modified residue	UNP Q8IV48
A	79	MSE	MET	modified residue	UNP Q8IV48
A	116	MSE	MET	modified residue	UNP Q8IV48
A	213	LEU	TRP	conflict	UNP Q8IV48
A	214	MSE	MET	modified residue	UNP Q8IV48
A	235	MSE	MET	modified residue	UNP Q8IV48
A	280	MSE	MET	modified residue	UNP Q8IV48
A	286	MSE	MET	modified residue	UNP Q8IV48
A	309	MSE	MET	modified residue	UNP Q8IV48
A	322	MSE	MET	modified residue	UNP Q8IV48
A	328	MSE	MET	modified residue	UNP Q8IV48
A	344	MSE	MET	modified residue	UNP Q8IV48
B	1	MSE	-	modified residue	UNP Q8IV48
B	79	MSE	MET	modified residue	UNP Q8IV48
B	116	MSE	MET	modified residue	UNP Q8IV48
B	213	LEU	TRP	conflict	UNP Q8IV48
B	214	MSE	MET	modified residue	UNP Q8IV48
B	235	MSE	MET	modified residue	UNP Q8IV48
B	280	MSE	MET	modified residue	UNP Q8IV48
B	286	MSE	MET	modified residue	UNP Q8IV48
B	309	MSE	MET	modified residue	UNP Q8IV48

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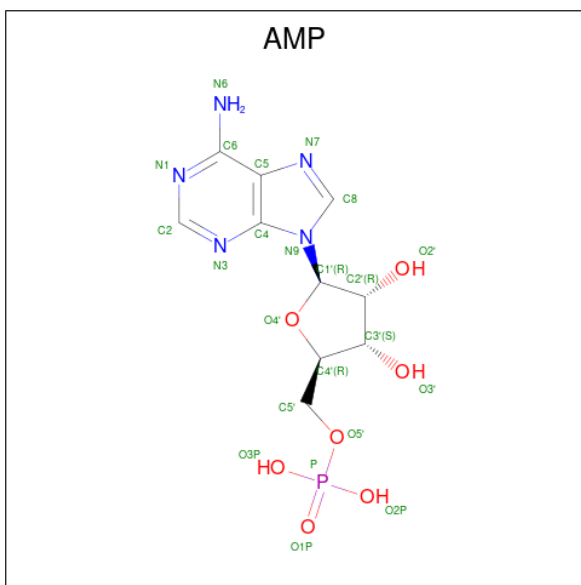
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Chain	Residue	Modelled	Actual	Comment	Reference
B	322	MSE	MET	modified residue	UNP Q8IV48
B	328	MSE	MET	modified residue	UNP Q8IV48
B	344	MSE	MET	modified residue	UNP Q8IV48
C	1	MSE	-	modified residue	UNP Q8IV48
C	79	MSE	MET	modified residue	UNP Q8IV48
C	116	MSE	MET	modified residue	UNP Q8IV48
C	213	LEU	TRP	conflict	UNP Q8IV48
C	214	MSE	MET	modified residue	UNP Q8IV48
C	235	MSE	MET	modified residue	UNP Q8IV48
C	280	MSE	MET	modified residue	UNP Q8IV48
C	286	MSE	MET	modified residue	UNP Q8IV48
C	309	MSE	MET	modified residue	UNP Q8IV48
C	322	MSE	MET	modified residue	UNP Q8IV48
C	328	MSE	MET	modified residue	UNP Q8IV48
C	344	MSE	MET	modified residue	UNP Q8IV48
D	1	MSE	-	modified residue	UNP Q8IV48
D	79	MSE	MET	modified residue	UNP Q8IV48
D	116	MSE	MET	modified residue	UNP Q8IV48
D	213	LEU	TRP	conflict	UNP Q8IV48
D	214	MSE	MET	modified residue	UNP Q8IV48
D	235	MSE	MET	modified residue	UNP Q8IV48
D	280	MSE	MET	modified residue	UNP Q8IV48
D	286	MSE	MET	modified residue	UNP Q8IV48
D	309	MSE	MET	modified residue	UNP Q8IV48
D	322	MSE	MET	modified residue	UNP Q8IV48
D	328	MSE	MET	modified residue	UNP Q8IV48
D	344	MSE	MET	modified residue	UNP Q8IV48

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

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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

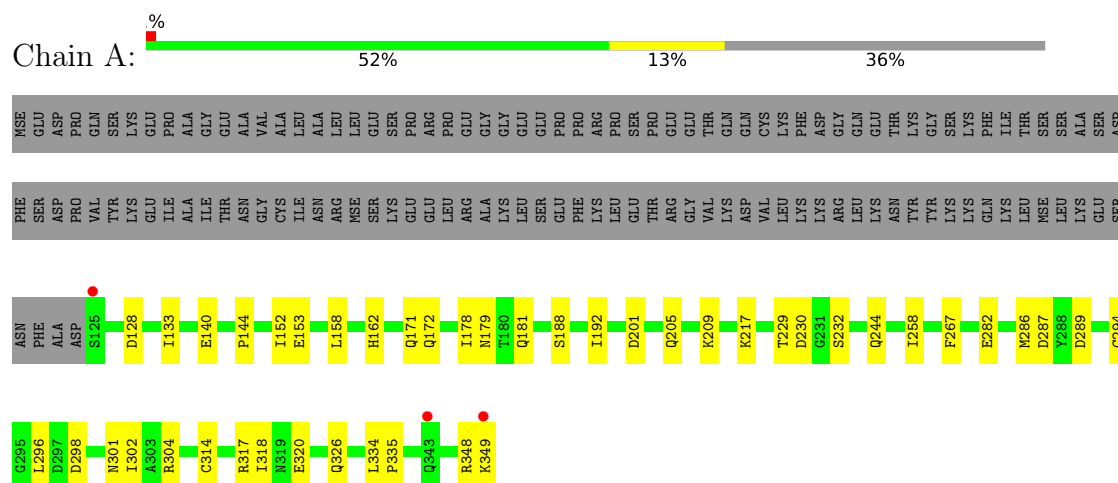
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	1	0
			13	13		
4	B	13	Total	O	5	0
			13	13		
4	C	6	Total	O	2	0
			6	6		
4	D	5	Total	O	2	0
			5	5		

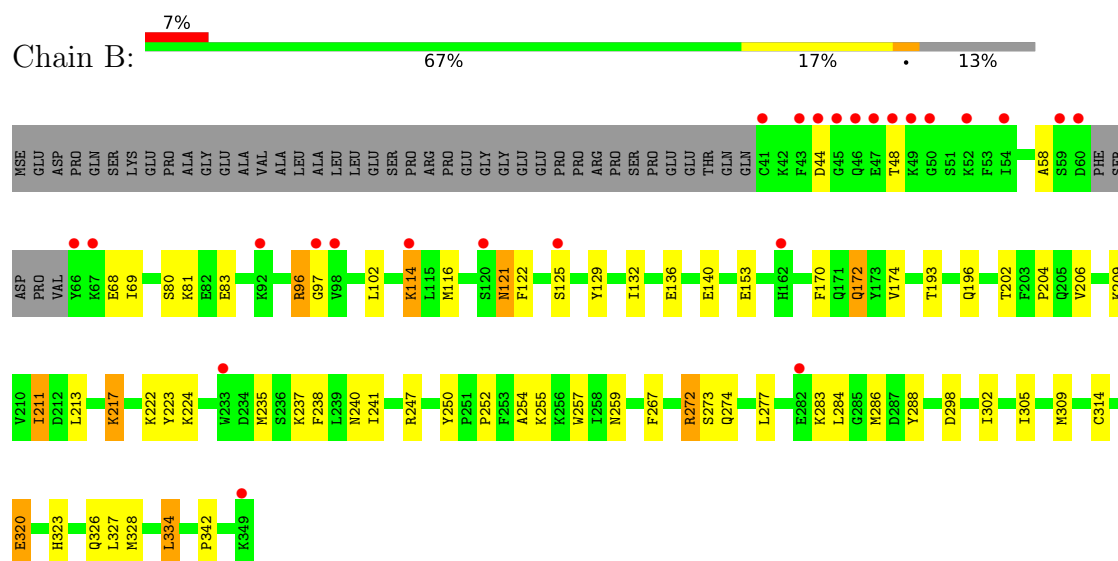
3 Residue-property plots

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.

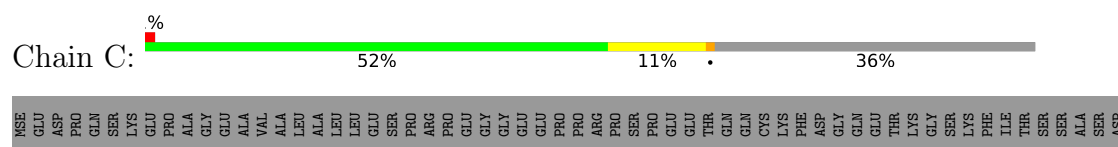
• Molecule 1: 3'-5' exonuclease ERI1

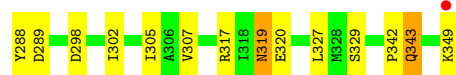


• Molecule 1: 3'-5' exonuclease ERI1

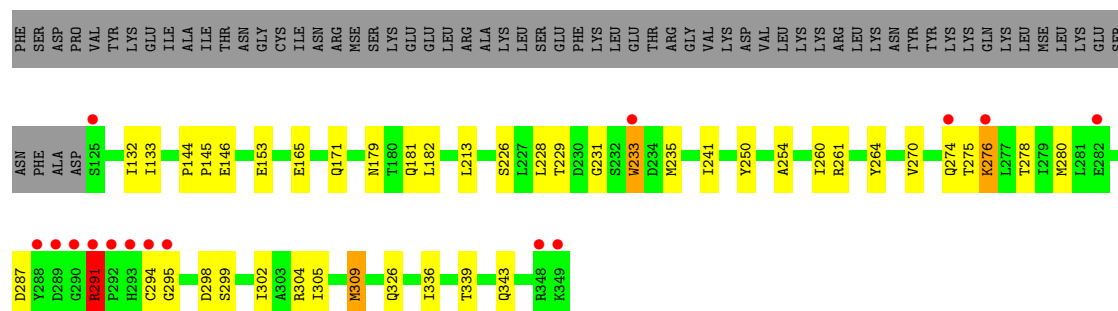


• Molecule 1: 3'-5' exonuclease ERI1





Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.84Å 215.84Å 114.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 3.00 19.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.96-3.00) 97.3 (19.96-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.199 , 0.225 0.200 , 0.223	Depositor DCC
R_{free} test set	6227 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8084	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, MG

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	0.65	0/1861	0.83	0/2501
1	B	0.61	0/2505	0.90	2/3348 (0.1%)
1	C	0.58	0/1861	0.87	2/2501 (0.1%)
1	D	0.59	0/1860	0.81	0/2499
All	All	0.61	0/8087	0.86	4/10849 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	LEU	CA-CB-CG	5.63	135.99	116.30
1	C	144	PRO	CA-C-N	5.61	125.07	119.24
1	C	144	PRO	C-N-CA	5.61	125.07	119.24
1	B	238	PHE	N-CA-C	5.04	116.46	110.97

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	1827	0	1827	22	0
1	B	2467	0	2496	45	0
1	C	1827	0	1827	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1826	0	1827	37	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	23	0	12	0	0
3	B	23	0	12	0	0
3	C	23	0	12	0	0
3	D	23	0	12	0	0
4	A	13	0	0	0	1
4	B	13	0	0	0	1
4	C	6	0	0	0	0
4	D	5	0	0	0	0
All	All	8084	0	8025	135	1

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 (135) 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:247:ARG:HG2	1:C:247:ARG:HH11	1.09	1.11
1:B:58:ALA:HA	1:B:116:MSE:HE3	1.33	1.04
1:D:305:ILE:HG22	1:D:309:MSE:CE	1.89	1.01
1:B:235:MSE:CE	1:B:254:ALA:HB1	1.92	0.98
1:D:235:MSE:CE	1:D:254:ALA:HB1	1.94	0.98
1:C:259:ASN:H	1:C:319:ASN:HD21	1.01	0.93
1:C:215:LYS:HZ1	1:C:343:GLN:HE22	1.14	0.91
1:C:343:GLN:HE21	1:C:343:GLN:HA	1.35	0.90
1:C:215:LYS:NZ	1:C:343:GLN:HE22	1.69	0.88
1:D:233:TRP:H	1:D:233:TRP:HD1	1.22	0.87
1:D:233:TRP:H	1:D:233:TRP:CD1	1.88	0.87
1:C:247:ARG:HG2	1:C:247:ARG:NH1	1.89	0.85
1:C:343:GLN:HA	1:C:343:GLN:NE2	1.91	0.85
1:D:235:MSE:HE1	1:D:254:ALA:HB1	1.60	0.80
1:B:170:PHE:HZ	1:B:172:GLN:HE21	1.29	0.80
1:C:247:ARG:HH11	1:C:247:ARG:CG	1.93	0.79
1:A:289:ASP:H	1:A:301:ASN:HD21	1.32	0.78
1:D:305:ILE:HG22	1:D:309:MSE:HE2	1.68	0.76
1:B:272:ARG:HH11	1:B:272:ARG:HG3	1.49	0.76
1:C:193:THR:H	1:C:196:GLN:HE21	1.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:MSE:HE1	1:B:254:ALA:HB1	1.69	0.74
1:D:233:TRP:CD1	1:D:233:TRP:N	2.55	0.74
1:D:291:ARG:NH1	1:D:294:CYS:HB3	2.04	0.73
1:B:272:ARG:HH11	1:B:272:ARG:CG	2.08	0.66
1:C:259:ASN:H	1:C:319:ASN:ND2	1.84	0.65
1:B:298:ASP:O	1:B:302:ILE:HG12	1.98	0.64
1:A:287:ASP:OD2	1:C:273:SER:HB2	1.98	0.63
1:B:193:THR:H	1:B:196:GLN:HE21	1.46	0.63
1:C:284:LEU:HB2	1:C:286:MSE:HE2	1.79	0.62
1:D:233:TRP:HD1	1:D:233:TRP:N	1.94	0.61
1:D:291:ARG:HH12	1:D:294:CYS:H	1.47	0.61
1:A:128:ASP:OD2	1:A:162:HIS:HE1	1.84	0.59
1:A:334:LEU:HB2	1:A:335:PRO:HD2	1.84	0.59
1:B:235:MSE:HE2	1:B:254:ALA:HB1	1.82	0.58
1:B:68:GLU:HB3	1:B:116:MSE:HE2	1.84	0.58
1:D:276:LYS:O	1:D:280:MSE:HG3	2.02	0.58
1:B:247:ARG:HH11	1:B:247:ARG:HG2	1.69	0.57
1:B:237:LYS:O	1:B:241:ILE:HG12	2.05	0.57
1:B:193:THR:H	1:B:196:GLN:NE2	2.03	0.57
1:C:286:MSE:HE1	1:C:305:ILE:HG12	1.86	0.57
1:D:305:ILE:CG2	1:D:309:MSE:HE2	2.34	0.57
1:D:153:GLU:OE2	1:D:295:GLY:HA3	2.05	0.57
1:B:58:ALA:CA	1:B:116:MSE:HE3	2.22	0.56
1:C:298:ASP:O	1:C:302:ILE:HG12	2.05	0.56
1:C:281:LEU:HD23	1:C:286:MSE:HE3	1.88	0.56
1:B:96:ARG:O	1:B:102:LEU:HD11	2.06	0.55
1:B:240:ASN:HD22	1:B:240:ASN:C	2.14	0.55
1:D:291:ARG:NH2	1:D:294:CYS:HB2	2.21	0.55
1:A:153:GLU:OE1	1:A:171:GLN:NE2	2.32	0.55
1:B:58:ALA:HB3	1:B:114:LYS:HB3	1.89	0.54
1:C:215:LYS:HZ1	1:C:343:GLN:NE2	1.93	0.54
1:D:291:ARG:NH1	1:D:291:ARG:O	2.40	0.54
1:B:267:PHE:CE1	1:B:314:CYS:HB2	2.43	0.54
1:B:170:PHE:HZ	1:B:172:GLN:NE2	2.02	0.54
1:B:284:LEU:HB2	1:B:286:MSE:HE3	1.89	0.53
1:D:291:ARG:NH1	1:D:294:CYS:CB	2.72	0.53
1:C:232:SER:HB3	1:C:320:GLU:OE1	2.09	0.52
1:C:228:LEU:HD21	1:C:260:ILE:HB	1.92	0.52
1:C:284:LEU:HD12	1:C:286:MSE:HE2	1.91	0.52
1:D:261:ARG:HH12	1:D:276:LYS:HG3	1.74	0.52
1:D:305:ILE:CG2	1:D:309:MSE:CE	2.76	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:ILE:HG22	1:D:309:MSE:HE1	1.88	0.52
1:A:178:ILE:HG22	1:A:179:ASN:N	2.25	0.51
1:D:228:LEU:HD11	1:D:260:ILE:HD12	1.91	0.51
1:B:174:VAL:HG22	1:B:206:VAL:HG21	1.93	0.51
1:D:287:ASP:O	1:D:304:ARG:NH2	2.43	0.51
1:C:281:LEU:HA	1:C:286:MSE:HE3	1.93	0.50
1:B:252:PRO:HA	1:B:255:LYS:HE2	1.93	0.50
1:D:291:ARG:CZ	1:D:294:CYS:HB2	2.42	0.50
1:A:286:MSE:HE1	1:A:304:ARG:HB3	1.93	0.50
1:A:301:ASN:ND2	1:A:304:ARG:NH1	2.59	0.50
1:C:215:LYS:NZ	1:C:343:GLN:NE2	2.50	0.50
1:B:44:ASP:HB3	1:B:122:PHE:CE1	2.47	0.49
1:C:266:ASN:O	1:C:269:LYS:HE3	2.12	0.49
1:D:264:TYR:CD2	1:D:275:THR:HG22	2.47	0.49
1:B:247:ARG:HG2	1:B:247:ARG:NH1	2.26	0.49
1:C:288:TYR:C	1:C:288:TYR:CD2	2.91	0.49
1:D:264:TYR:HD2	1:D:275:THR:HG22	1.78	0.49
1:A:152:ILE:HD12	1:A:192:ILE:HD12	1.94	0.49
1:B:272:ARG:CG	1:B:272:ARG:NH1	2.73	0.49
1:B:121:ASN:ND2	1:B:121:ASN:H	2.10	0.49
1:B:257:TRP:CZ2	1:B:320:GLU:HG2	2.48	0.49
1:B:284:LEU:CB	1:B:286:MSE:HE3	2.43	0.48
1:B:136:GLU:HB2	1:B:153:GLU:HB3	1.95	0.48
1:B:211:ILE:HG23	1:B:342:PRO:HB2	1.94	0.48
1:C:319:ASN:H	1:C:319:ASN:HD22	1.61	0.48
1:A:232:SER:HB3	1:A:320:GLU:OE2	2.14	0.48
1:B:222:LYS:HD3	1:B:223:TYR:CZ	2.48	0.48
1:D:231:GLY:HA3	1:D:233:TRP:HE1	1.79	0.48
1:B:170:PHE:CZ	1:B:172:GLN:HB2	2.48	0.47
1:D:291:ARG:HH12	1:D:294:CYS:HB3	1.77	0.47
1:B:235:MSE:HE3	1:B:250:TYR:OH	2.14	0.47
1:A:287:ASP:OD2	1:C:273:SER:CB	2.63	0.47
1:C:211:ILE:HG22	1:C:215:LYS:HD2	1.96	0.47
1:B:277:LEU:HD13	1:B:302:ILE:HD13	1.96	0.47
1:D:146:GLU:OE2	1:D:146:GLU:HA	2.14	0.47
1:A:301:ASN:HD22	1:A:304:ARG:NH1	2.13	0.45
1:D:299:SER:HA	1:D:302:ILE:HD12	1.98	0.45
1:B:44:ASP:HB3	1:B:122:PHE:HE1	1.81	0.45
1:C:258:ILE:HG12	1:C:317:ARG:C	2.42	0.45
1:A:140:GLU:HB2	1:A:144:PRO:CD	2.46	0.45
1:B:125:SER:HB2	1:B:224:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ARG:NH1	1:C:349:LYS:O	2.51	0.44
1:D:144:PRO:HA	1:D:145:PRO:HD3	1.77	0.44
1:D:291:ARG:CZ	1:D:294:CYS:CB	2.96	0.44
1:A:244:GLN:HA	1:A:348:ARG:HH12	1.83	0.44
1:D:291:ARG:HH22	1:D:294:CYS:N	2.16	0.43
1:A:171:GLN:HB2	1:A:296:LEU:HD22	2.00	0.43
1:A:133:ILE:O	1:A:229:THR:HG22	2.19	0.43
1:C:170:PHE:CD2	1:C:170:PHE:C	2.97	0.43
1:A:267:PHE:CE1	1:A:314:CYS:HB2	2.54	0.43
1:D:132:ILE:HG12	1:D:228:LEU:HD22	2.01	0.43
1:D:305:ILE:HG22	1:D:309:MSE:HE3	1.90	0.43
1:B:259:ASN:C	1:B:259:ASN:OD1	2.62	0.43
1:A:172:GLN:NE2	1:A:209:LYS:HD2	2.34	0.42
1:B:170:PHE:CD2	1:B:170:PHE:C	2.97	0.42
1:B:323:HIS:HB3	1:B:328:MSE:HE1	2.00	0.42
1:D:235:MSE:HE3	1:D:250:TYR:OH	2.19	0.42
1:B:129:TYR:OH	1:B:217:LYS:HE3	2.20	0.42
1:C:193:THR:OG1	1:C:196:GLN:HG3	2.19	0.42
1:C:277:LEU:HD13	1:C:302:ILE:HD13	2.02	0.41
1:A:230:ASP:HB2	1:A:302:ILE:CD1	2.51	0.41
1:C:211:ILE:HD12	1:C:342:PRO:HB2	2.02	0.41
1:D:133:ILE:O	1:D:229:THR:HG22	2.20	0.41
1:B:80:SER:OG	1:B:83:GLU:HG3	2.20	0.41
1:B:305:ILE:O	1:B:309:MSE:HG3	2.20	0.41
1:D:226:SER:HA	1:D:339:THR:OG1	2.20	0.41
1:A:201:ASP:HB3	1:A:205:GLN:HB2	2.02	0.41
1:D:336:ILE:H	1:D:336:ILE:HD12	1.86	0.41
1:A:301:ASN:ND2	1:A:304:ARG:HH11	2.18	0.40
1:C:164:LEU:HG	1:C:307:VAL:HG13	2.03	0.40
1:A:258:ILE:HG12	1:A:317:ARG:C	2.46	0.40
1:B:202:THR:HB	1:B:204:PRO:HD2	2.04	0.40
1:B:172:GLN:HE22	1:B:209:LYS:HD2	1.86	0.40
1:B:288:TYR:OH	1:B:298:ASP:OD1	2.33	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1003:HOH:O	4:B:2007:HOH:O[3_654]	1.39	0.81

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	223/349 (64%)	218 (98%)	5 (2%)	0	100	100
1	B	300/349 (86%)	285 (95%)	13 (4%)	2 (1%)	18	53
1	C	223/349 (64%)	214 (96%)	9 (4%)	0	100	100
1	D	223/349 (64%)	209 (94%)	11 (5%)	3 (1%)	9	38
All	All	969/1396 (69%)	926 (96%)	38 (4%)	5 (0%)	24	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	276	LYS
1	B	97	GLY
1	B	114	LYS
1	D	274	GLN
1	D	291	ARG

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	208/306 (68%)	198 (95%)	10 (5%)	23	57
1	B	279/306 (91%)	260 (93%)	19 (7%)	14	45
1	C	208/306 (68%)	192 (92%)	16 (8%)	12	40
1	D	208/306 (68%)	193 (93%)	15 (7%)	13	43
All	All	903/1224 (74%)	843 (93%)	60 (7%)	15	46

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	LEU
1	A	181	GLN
1	A	188	SER
1	A	217	LYS
1	A	282	GLU
1	A	294	CYS
1	A	298	ASP
1	A	318	ILE
1	A	326	GLN
1	A	349	LYS
1	B	48	THR
1	B	69	ILE
1	B	81	LYS
1	B	96	ARG
1	B	121	ASN
1	B	132	ILE
1	B	140	GLU
1	B	172	GLN
1	B	211	ILE
1	B	213	LEU
1	B	217	LYS
1	B	272	ARG
1	B	273	SER
1	B	274	GLN
1	B	283	LYS
1	B	320	GLU
1	B	326	GLN
1	B	327	LEU
1	B	334	LEU
1	C	130	ILE
1	C	134	ASP
1	C	140	GLU
1	C	151	ILE
1	C	158	LEU
1	C	164	LEU
1	C	172	GLN
1	C	178	ILE
1	C	229	THR
1	C	247	ARG
1	C	273	SER
1	C	289	ASP
1	C	319	ASN

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Mol	Chain	Res	Type
1	C	327	LEU
1	C	329	SER
1	C	343	GLN
1	D	165	GLU
1	D	171	GLN
1	D	179	ASN
1	D	181	GLN
1	D	182	LEU
1	D	213	LEU
1	D	233	TRP
1	D	241	ILE
1	D	270	VAL
1	D	278	THR
1	D	291	ARG
1	D	298	ASP
1	D	309	MSE
1	D	326	GLN
1	D	343	GLN

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

Mol	Chain	Res	Type
1	A	143	ASN
1	A	162	HIS
1	A	172	GLN
1	A	266	ASN
1	A	301	ASN
1	B	121	ASN
1	B	171	GLN
1	B	172	GLN
1	B	181	GLN
1	B	196	GLN
1	B	240	ASN
1	B	343	GLN
1	C	143	ASN
1	C	171	GLN
1	C	172	GLN
1	C	179	ASN
1	C	196	GLN
1	C	266	ASN
1	C	319	ASN
1	C	343	GLN

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Mol	Chain	Res	Type
1	D	293	HIS
1	D	301	ASN

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	AMP	B	2002	2	25,25,25	1.50	4 (16%)	37,38,38	1.89	10 (27%)
3	AMP	A	1002	2	25,25,25	1.53	4 (16%)	37,38,38	1.88	9 (24%)
3	AMP	D	4002	2	25,25,25	1.55	4 (16%)	37,38,38	1.96	11 (29%)
3	AMP	C	3002	2	25,25,25	1.53	4 (16%)	37,38,38	1.94	8 (21%)

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	AMP	B	2002	2	-	3/10/26/26	0/3/3/3
3	AMP	A	1002	2	-	2/10/26/26	0/3/3/3
3	AMP	D	4002	2	-	0/10/26/26	0/3/3/3
3	AMP	C	3002	2	-	0/10/26/26	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4002	AMP	C5-C4	5.31	1.48	1.39
3	A	1002	AMP	C5-C4	5.17	1.48	1.39
3	C	3002	AMP	C5-C4	5.15	1.48	1.39
3	B	2002	AMP	C5-C4	5.13	1.48	1.39
3	D	4002	AMP	C5-C6	3.01	1.49	1.41
3	A	1002	AMP	C5-C6	2.79	1.48	1.41
3	B	2002	AMP	C5-C6	2.77	1.48	1.41
3	C	3002	AMP	C5-C6	2.71	1.48	1.41
3	D	4002	AMP	C8-N7	2.53	1.36	1.31
3	B	2002	AMP	C8-N7	2.40	1.36	1.31
3	C	3002	AMP	C5-N7	-2.37	1.34	1.39
3	A	1002	AMP	C8-N7	2.30	1.36	1.31
3	C	3002	AMP	C8-N7	2.26	1.36	1.31
3	A	1002	AMP	C5-N7	-2.11	1.35	1.39
3	B	2002	AMP	C5-N7	-2.03	1.35	1.39
3	D	4002	AMP	C5-N7	-2.02	1.35	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4002	AMP	C5-C4-N3	-5.82	118.70	126.72
3	C	3002	AMP	C5-C4-N3	-5.71	118.86	126.72
3	B	2002	AMP	C5-C4-N3	-5.45	119.21	126.72
3	A	1002	AMP	C5-C4-N3	-5.07	119.74	126.72
3	C	3002	AMP	N3-C4-N9	4.86	135.44	127.17
3	D	4002	AMP	N3-C4-N9	4.65	135.07	127.17
3	B	2002	AMP	N3-C4-N9	4.60	134.99	127.17
3	A	1002	AMP	N3-C4-N9	4.35	134.56	127.17
3	D	4002	AMP	C2-N3-C4	3.85	121.23	111.83
3	B	2002	AMP	N3-C2-N1	-3.78	122.86	128.58
3	C	3002	AMP	C2-N3-C4	3.72	120.92	111.83
3	C	3002	AMP	N3-C2-N1	-3.72	122.95	128.58
3	B	2002	AMP	C2-N3-C4	3.72	120.91	111.83
3	D	4002	AMP	N3-C2-N1	-3.64	123.07	128.58
3	A	1002	AMP	C2'-C1'-N9	-3.59	104.39	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	AMP	N3-C2-N1	-3.39	123.46	128.58
3	A	1002	AMP	C2-N3-C4	3.37	120.07	111.83
3	D	4002	AMP	C4-C5-N7	-3.31	106.80	110.58
3	B	2002	AMP	C4-C5-N7	-3.05	107.10	110.58
3	C	3002	AMP	C4-C5-N7	-3.01	107.14	110.58
3	A	1002	AMP	C4-C5-N7	-2.87	107.30	110.58
3	A	1002	AMP	C4-N9-C8	2.75	108.63	105.74
3	B	2002	AMP	C4-N9-C8	2.72	108.60	105.74
3	D	4002	AMP	C2'-C1'-N9	-2.58	106.88	113.30
3	C	3002	AMP	C4-N9-C8	2.52	108.39	105.74
3	D	4002	AMP	C5-N7-C8	2.45	107.31	103.45
3	C	3002	AMP	C5-N7-C8	2.38	107.19	103.45
3	B	2002	AMP	C5-N7-C8	2.32	107.10	103.45
3	C	3002	AMP	C2-N1-C6	2.26	122.44	118.73
3	D	4002	AMP	O4'-C1'-N9	2.25	112.41	108.09
3	A	1002	AMP	C5-N7-C8	2.20	106.90	103.45
3	B	2002	AMP	C2-N1-C6	2.19	122.33	118.73
3	D	4002	AMP	C6-C5-N7	2.16	136.25	132.09
3	B	2002	AMP	C6-C5-N7	2.15	136.24	132.09
3	D	4002	AMP	C4-N9-C8	2.10	107.94	105.74
3	A	1002	AMP	C6-C5-N7	2.05	136.03	132.09
3	D	4002	AMP	C2-N1-C6	2.03	122.06	118.73
3	B	2002	AMP	C2'-C1'-N9	-2.02	108.27	113.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

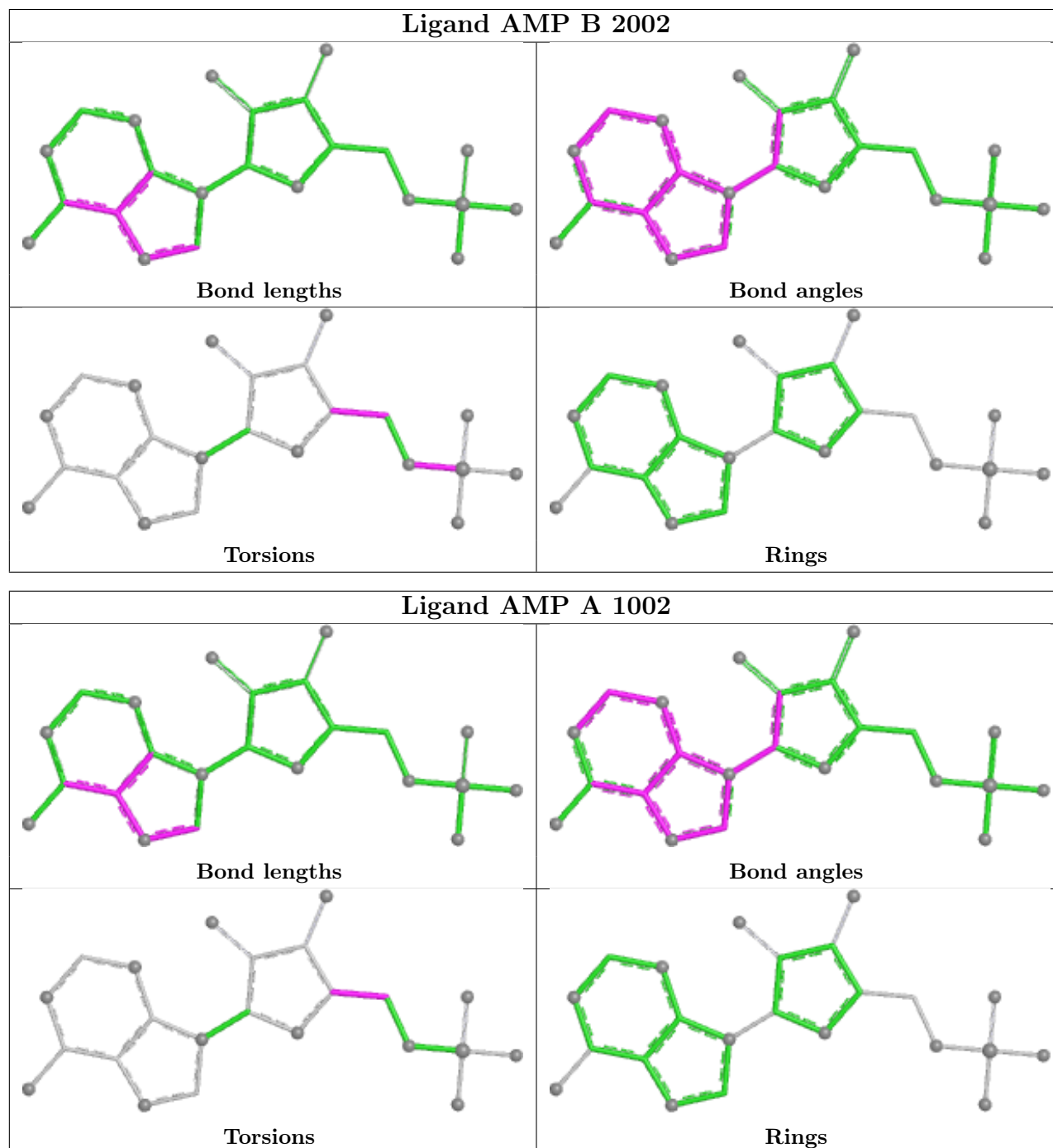
Mol	Chain	Res	Type	Atoms
3	B	2002	AMP	O4'-C4'-C5'-O5'
3	A	1002	AMP	O4'-C4'-C5'-O5'
3	B	2002	AMP	C3'-C4'-C5'-O5'
3	B	2002	AMP	C5'-O5'-P-O1P
3	A	1002	AMP	C3'-C4'-C5'-O5'

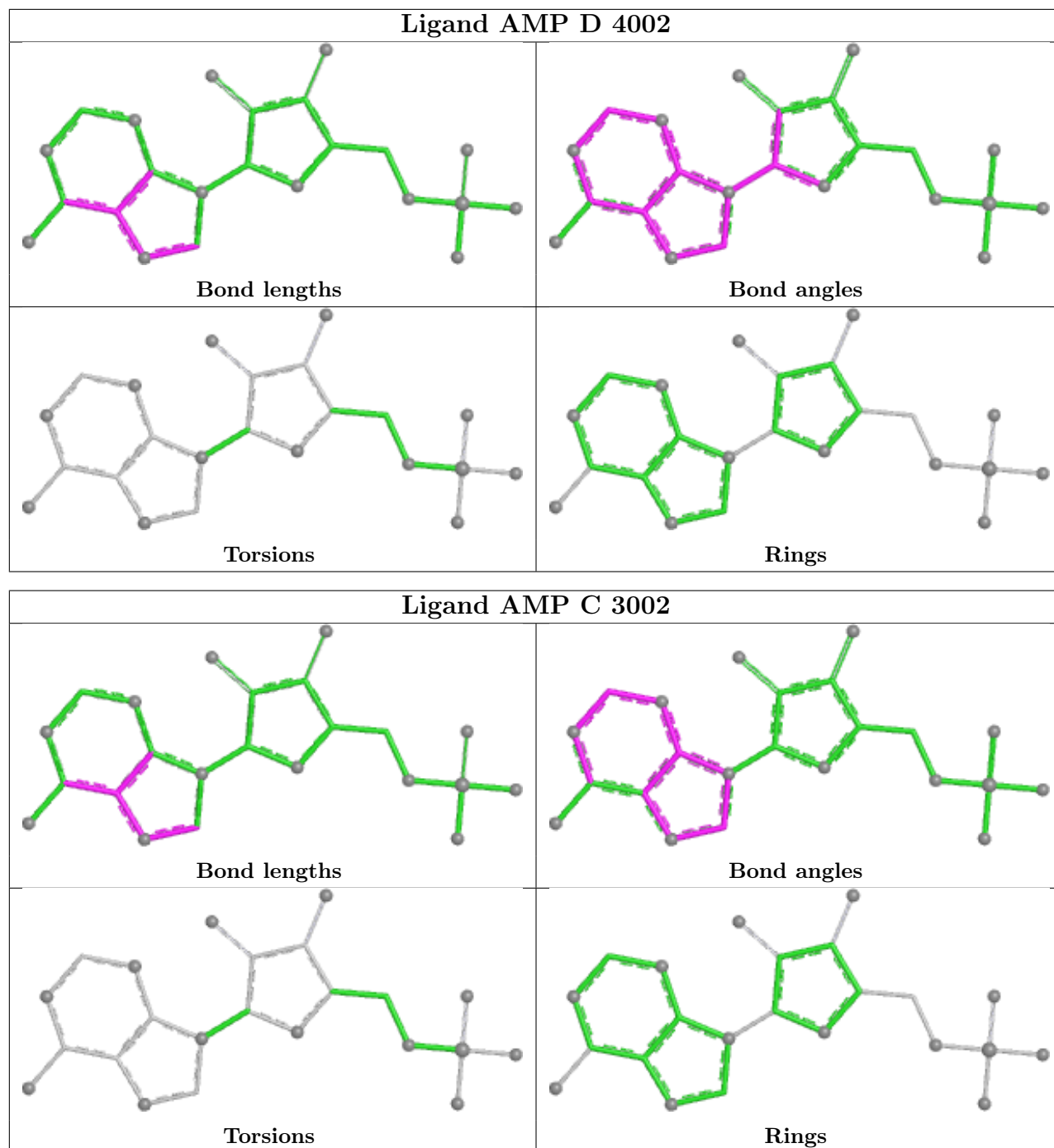
There are no ring outliers.

No monomer is involved in short contacts.

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	217/349 (62%)	-0.41	3 (1%) 73 51	11, 20, 30, 41	0
1	B	294/349 (84%)	0.27	25 (8%) 16 8	10, 20, 37, 57	0
1	C	217/349 (62%)	-0.31	3 (1%) 73 51	10, 20, 31, 37	0
1	D	217/349 (62%)	0.12	15 (6%) 23 12	8, 19, 37, 50	0
All	All	945/1396 (67%)	-0.05	46 (4%) 35 18	8, 20, 34, 57	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	ASP	6.6
1	B	66	TYR	6.5
1	B	48	THR	4.9
1	B	43	PHE	4.8
1	B	52	LYS	4.7
1	D	294	CYS	4.5
1	B	41	CYS	4.5
1	D	233	TRP	4.2
1	D	293	HIS	4.2
1	B	44	ASP	4.1
1	B	46	GLN	4.1
1	D	349	LYS	4.0
1	B	349	LYS	4.0
1	B	47	GLU	3.8
1	D	295	GLY	3.7
1	D	291	ARG	3.6
1	D	289	ASP	3.6
1	D	125	SER	3.4
1	A	349	LYS	3.3
1	A	125	SER	3.2
1	B	114	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	349	LYS	3.1
1	A	343	GLN	3.0
1	B	59	SER	3.0
1	B	92	LYS	2.9
1	B	97	GLY	2.9
1	D	290	GLY	2.9
1	C	125	SER	2.8
1	D	274	GLN	2.7
1	B	45	GLY	2.7
1	B	233	TRP	2.6
1	B	54	ILE	2.6
1	C	272	ARG	2.6
1	B	67	LYS	2.5
1	B	50	GLY	2.5
1	B	282	GLU	2.5
1	D	288	TYR	2.4
1	B	162	HIS	2.4
1	B	49	LYS	2.4
1	B	120	SER	2.3
1	D	282	GLU	2.3
1	B	98	VAL	2.2
1	B	125	SER	2.1
1	D	292	PRO	2.1
1	D	276	LYS	2.0
1	D	348	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

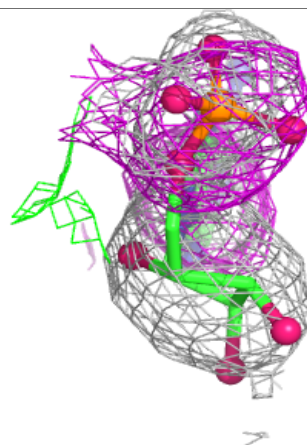
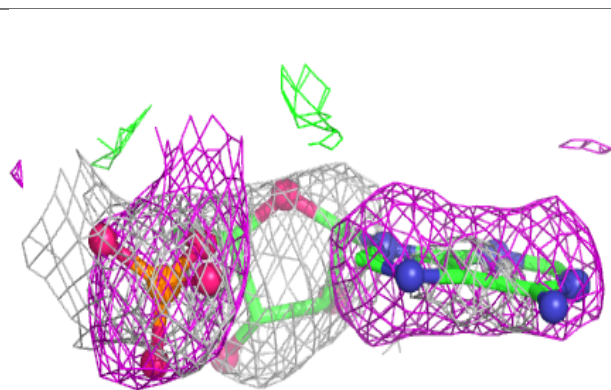
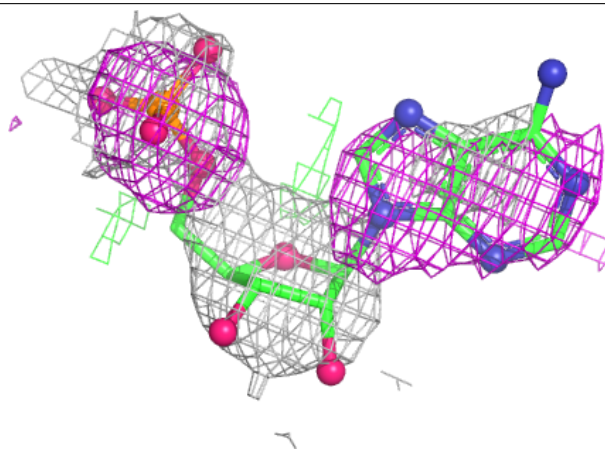
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	B	2000	1/1	0.67	0.16	52,52,52,52	0
3	AMP	D	4002	23/23	0.75	0.23	83,86,90,91	0
2	MG	A	1000	1/1	0.83	0.12	32,32,32,32	0
2	MG	D	4000	1/1	0.85	0.33	60,60,60,60	0
3	AMP	C	3002	23/23	0.86	0.15	49,52,59,59	0
3	AMP	B	2002	23/23	0.86	0.16	57,60,64,65	0
2	MG	C	3000	1/1	0.89	0.14	54,54,54,54	0
2	MG	B	2001	1/1	0.89	0.36	42,42,42,42	0
2	MG	D	4001	1/1	0.89	0.21	59,59,59,59	0
3	AMP	A	1002	23/23	0.90	0.13	29,31,40,41	0
2	MG	C	3001	1/1	0.90	0.43	40,40,40,40	0
2	MG	A	1001	1/1	0.96	0.39	42,42,42,42	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.

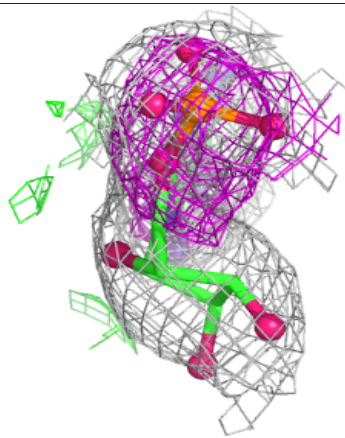
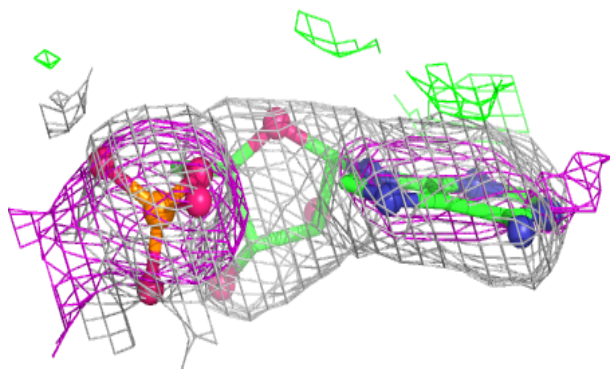
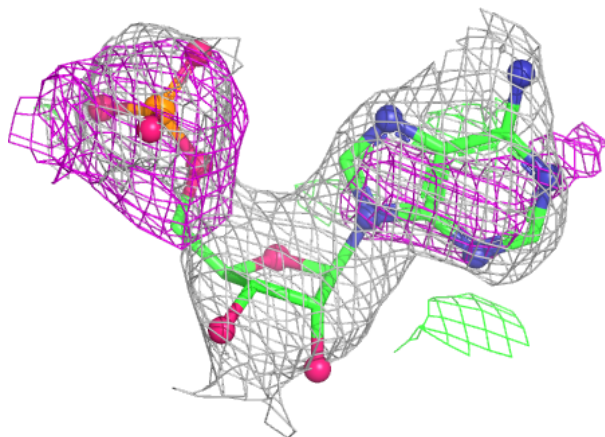
Electron density around AMP D 4002:

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



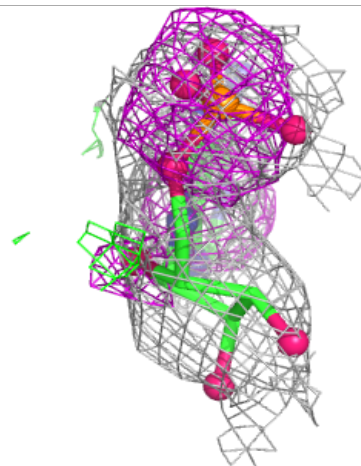
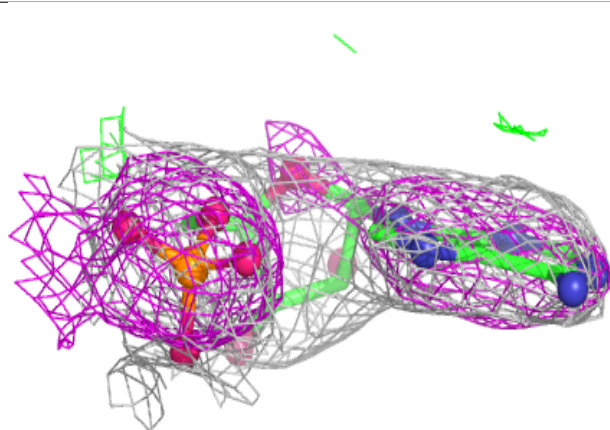
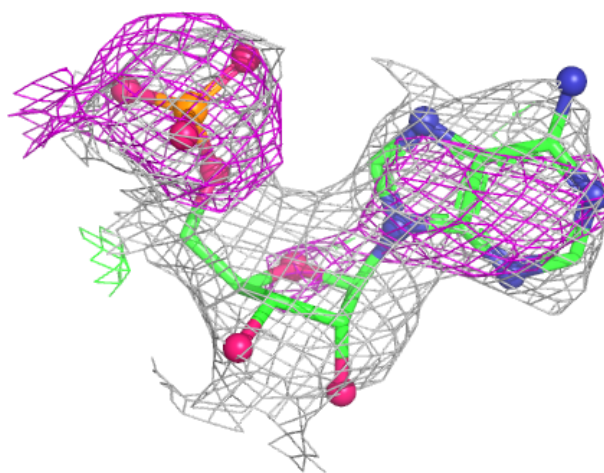
Electron density around AMP C 3002:

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



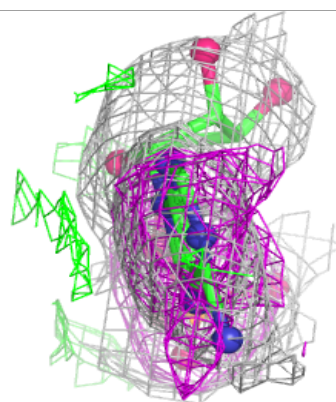
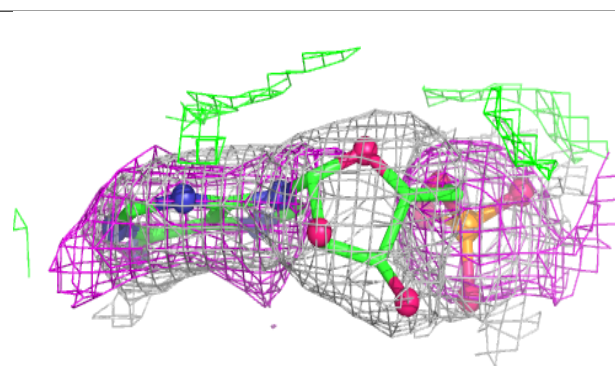
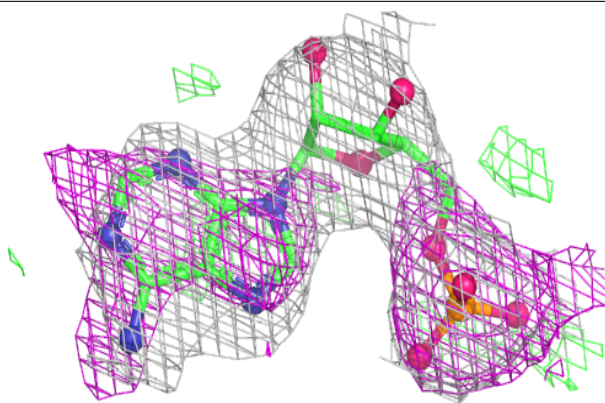
Electron density around AMP B 2002:

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



Electron density around AMP A 1002:

$2mF_o-DF_c$ (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.