



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:53 PM UTC

PDB ID : 2V51 / pdb_00002v51
Title : Structure of MAL-RPEL1 complexed to actin
Authors : Mouilleron, S.; Guettler, S.; Langer, C.A.; Treisman, R.; McDonald, N.Q.
Deposited on : 2008-10-01
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

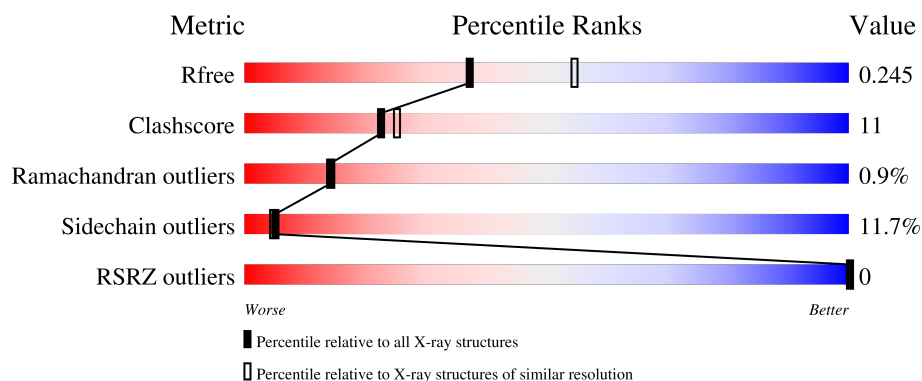
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	B	377	 72% 18% • 7%
1	D	377	 66% 23% 5% • 7%
2	E	32	 50% 25% 12% 12%
2	F	32	 56% 25% 6% 12%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6235 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.

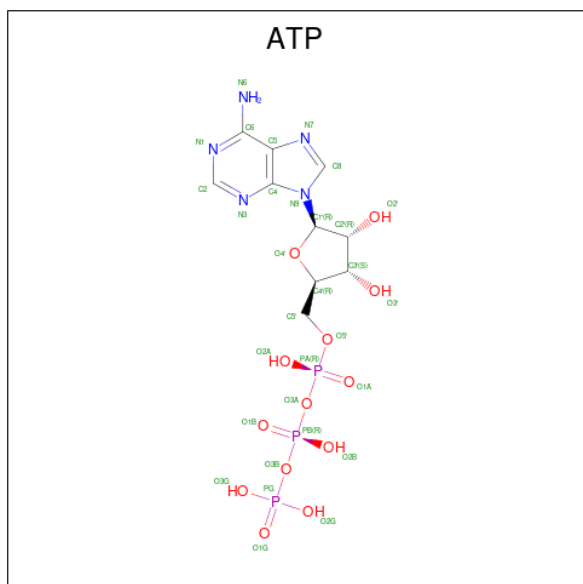
- Molecule 1 is a protein called ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	351	Total	C	N	O	S	0	0	0
			2728	1732	453	525	18			
1	D	352	Total	C	N	O	S	0	0	0
			2734	1735	454	527	18			

- Molecule 2 is a protein called MKL/MYOCARDIN-LIKE PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	28	Total	C	N	O	S	0	0	0
			206	127	41	37	1			
2	F	28	Total	C	N	O	S	0	0	0
			210	129	42	38	1			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

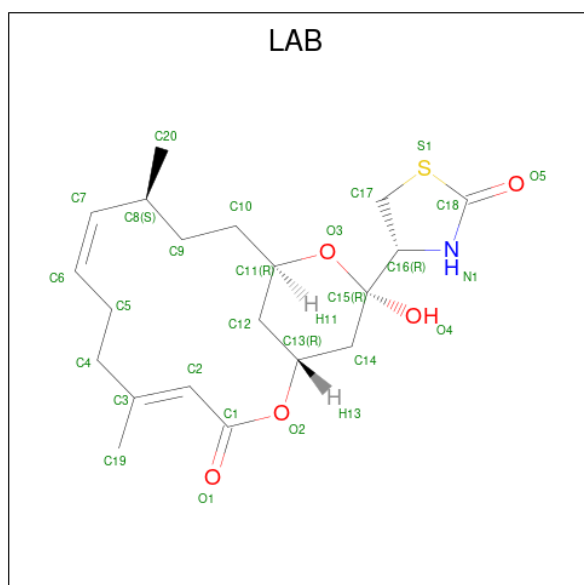


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

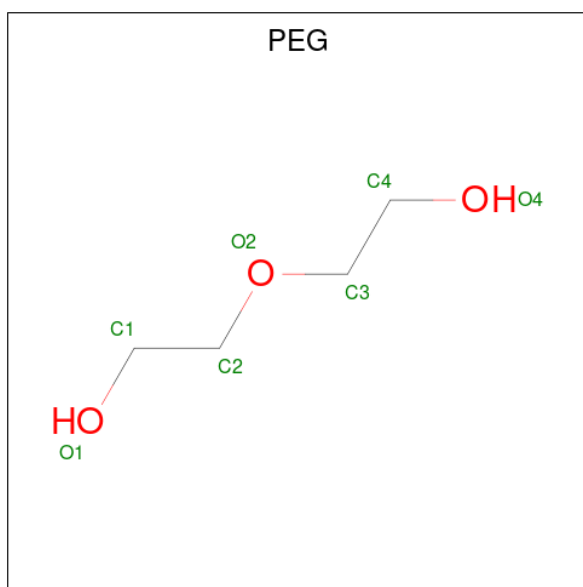
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is LATRUNCULIN B (CCD ID: LAB) (formula: C₂₀H₂₉NO₅S).



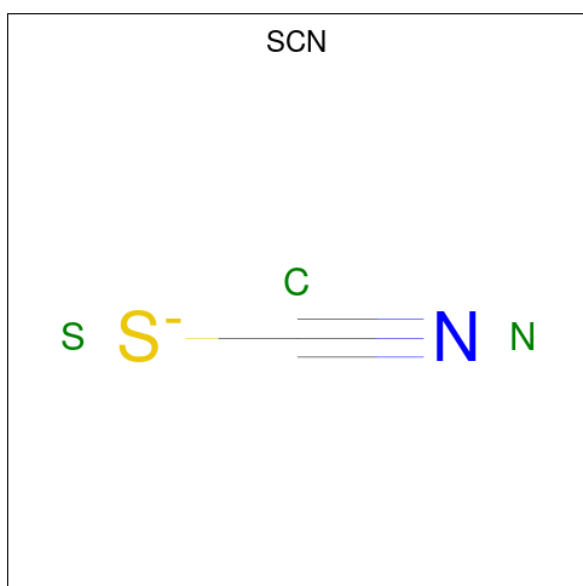
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			27	20	1	5	1		
5	D	1	Total	C	N	O	S	0	0
			27	20	1	5	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	S	0	0
			3	1	1	1		
7	B	1	Total	C	N	S	0	0
			3	1	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	S	0	0
			3	1	1	1		
7	D	1	Total	C	N	S	0	0
			3	1	1	1		

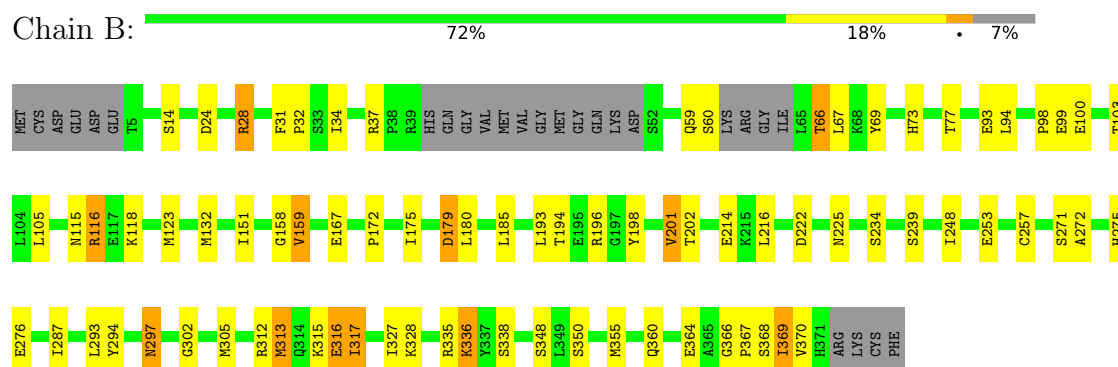
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	103	Total	O	0	0
			103	103		
8	D	97	Total	O	0	0
			97	97		
8	E	6	Total	O	0	0
			6	6		
8	F	7	Total	O	0	0
			7	7		

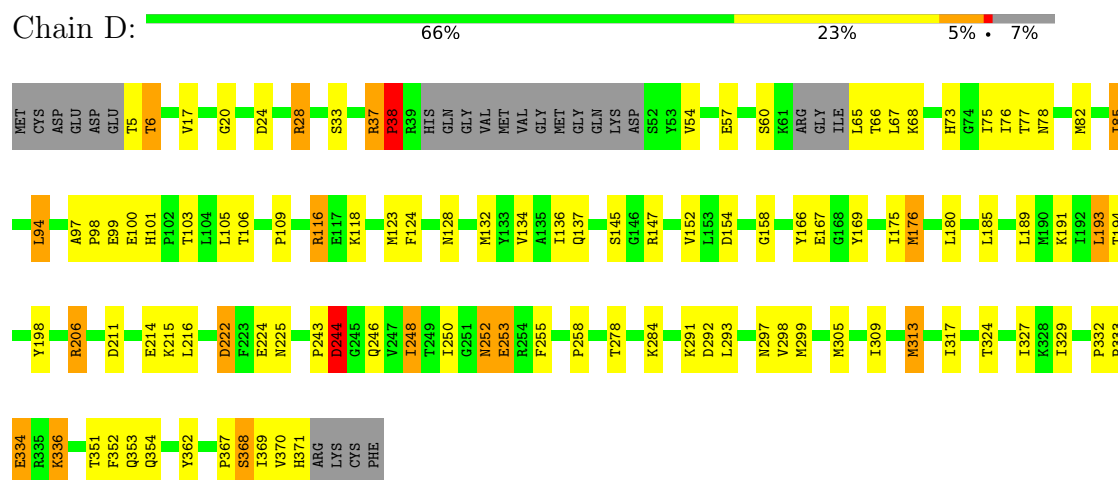
3 Residue-property plots [i](#)

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: ACTIN, ALPHA SKELETAL MUSCLE



• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



• Molecule 2: MKL/MYOCARDIN-LIKE PROTEIN 1



• Molecule 2: MKL/MYOCARDIN-LIKE PROTEIN 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.09Å 59.07Å 166.20Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	86.4 (20.00-2.35) 86.2 (20.00-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.183 , 0.248 0.182 , 0.245	Depositor DCC
R_{free} test set	1890 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 24.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.469 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6235	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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: SCN, ATP, PEG, LAB, CA

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	B	1.15	0/2787	1.20	8/3783 (0.2%)
1	D	1.08	2/2793 (0.1%)	1.20	9/3791 (0.2%)
2	E	1.05	1/207 (0.5%)	1.35	0/279
2	F	1.02	0/211	1.36	1/284 (0.4%)
All	All	1.11	3/5998 (0.1%)	1.21	18/8137 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	332	PRO	CA-C	6.86	1.55	1.51
2	E	94	PRO	CA-C	5.36	1.55	1.52
1	D	75	ILE	CA-CB	5.05	1.60	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	72	ASN	N-CA-C	-8.22	102.29	111.82
1	B	159	VAL	CB-CA-C	-7.82	96.40	110.48
1	B	271	SER	N-CA-C	7.54	120.05	110.24
1	B	69	TYR	CA-C-N	6.56	126.19	119.56
1	B	69	TYR	C-N-CA	6.56	126.19	119.56
1	D	362	TYR	N-CA-C	6.13	118.75	111.33
1	D	336	LYS	N-CA-C	-5.98	105.84	113.01
1	D	244	ASP	N-CA-C	5.93	123.42	110.80
1	D	222	ASP	CB-CA-C	5.83	119.14	110.62
1	D	327	ILE	CB-CA-C	-5.72	102.31	110.83
1	B	275	HIS	N-CA-C	-5.66	105.19	111.36
1	B	118	LYS	N-CA-C	-5.56	105.14	111.14
1	B	316	GLU	CA-C-N	-5.26	112.01	120.64
1	B	316	GLU	C-N-CA	-5.26	112.01	120.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	332	PRO	CA-C-N	-5.24	114.27	119.56
1	D	332	PRO	C-N-CA	-5.24	114.27	119.56
1	D	101	HIS	CA-C-N	-5.18	114.42	119.76
1	D	101	HIS	C-N-CA	-5.18	114.42	119.76

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	B	2728	0	2677	37	0
1	D	2734	0	2682	74	0
2	E	206	0	199	11	0
2	F	210	0	205	6	0
3	B	31	0	12	2	0
3	D	31	0	12	2	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	27	0	29	0	0
5	D	27	0	29	0	0
6	B	7	0	10	0	0
6	D	7	0	10	0	0
7	B	6	0	0	0	0
7	D	6	0	0	0	0
8	B	103	0	0	0	0
8	D	97	0	0	1	0
8	E	6	0	0	0	0
8	F	7	0	0	1	0
All	All	6235	0	5865	125	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 11.

All (125) 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:116:ARG:HH11	1:B:116:ARG:CB	1.52	1.20
1:B:116:ARG:HB3	1:B:116:ARG:NH1	1.61	1.13
1:B:116:ARG:HH11	1:B:116:ARG:HB3	0.84	1.00
1:D:176:MET:HE3	1:D:176:MET:HA	1.46	0.95
2:E:93:MET:HE3	2:E:94:PRO:HD2	1.52	0.91
1:D:313:MET:HE2	1:D:317:ILE:CD1	2.09	0.83
1:D:116:ARG:CG	1:D:116:ARG:HH11	1.97	0.78
1:D:37:ARG:HG3	1:D:38:PRO:HD2	1.66	0.77
1:D:5:THR:HG22	1:D:6:THR:H	1.50	0.77
1:D:206:ARG:HG2	1:D:206:ARG:HH11	1.49	0.76
1:B:196:ARG:HD2	1:B:253:GLU:OE1	1.87	0.75
1:D:176:MET:HA	1:D:176:MET:CE	2.19	0.72
1:B:116:ARG:HH11	1:B:116:ARG:CG	2.03	0.71
1:D:313:MET:HE2	1:D:317:ILE:HD12	1.73	0.70
1:D:116:ARG:HH11	1:D:116:ARG:HG3	1.56	0.69
1:B:116:ARG:CB	1:B:116:ARG:NH1	2.38	0.69
2:E:93:MET:CE	2:E:94:PRO:HD2	2.24	0.67
1:B:367:PRO:O	1:B:370:VAL:HG12	1.95	0.67
2:F:92:ILE:O	8:F:2007:HOH:O	2.14	0.66
1:D:17:VAL:HG23	1:D:33:SER:HB3	1.79	0.64
1:D:244:ASP:HB2	1:D:246:GLN:H	1.63	0.63
1:D:116:ARG:HH11	1:D:116:ARG:CB	2.10	0.63
1:D:333:PRO:HD2	1:D:334:GLU:OE2	1.98	0.63
1:D:313:MET:CE	1:D:317:ILE:CD1	2.76	0.63
1:B:214:GLU:HG2	3:B:1372:ATP:C5	2.34	0.62
1:D:252:ASN:HD22	1:D:253:GLU:N	1.96	0.62
1:D:5:THR:HG22	1:D:6:THR:N	2.13	0.62
1:D:5:THR:CG2	1:D:6:THR:H	2.13	0.60
1:D:313:MET:HE2	1:D:317:ILE:HD11	1.84	0.60
1:B:34:ILE:HD12	1:B:67:LEU:HD13	1.84	0.59
1:D:37:ARG:HG3	1:D:38:PRO:CD	2.31	0.59
1:D:206:ARG:HG2	1:D:206:ARG:NH1	2.18	0.59
2:E:83:THR:HG22	2:E:85:GLU:H	1.66	0.59
1:B:172:PRO:HA	1:B:175:ILE:HD12	1.85	0.58
1:B:116:ARG:NH1	1:B:116:ARG:CG	2.64	0.58
1:D:116:ARG:HH11	1:D:116:ARG:HB2	1.68	0.58
1:D:368:SER:O	1:D:369:ILE:C	2.48	0.57
2:E:83:THR:HB	2:E:86:GLU:HG3	1.87	0.56
1:D:244:ASP:CB	1:D:246:GLN:H	2.18	0.56
2:E:88:VAL:CG1	2:F:89:SER:HB3	2.35	0.56
1:D:98:PRO:C	1:D:100:GLU:H	2.14	0.56
2:E:95:PRO:O	2:E:96:LEU:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:MET:CE	1:B:317:ILE:HG23	2.36	0.55
1:D:76:ILE:HD13	1:D:82:MET:HG2	1.88	0.55
1:D:206:ARG:HH11	1:D:206:ARG:CG	2.20	0.55
1:D:24:ASP:OD2	1:D:28:ARG:NH1	2.40	0.54
1:D:214:GLU:HG2	3:D:1372:ATP:C5	2.42	0.54
2:E:83:THR:HG22	2:E:85:GLU:N	2.22	0.54
1:D:166:TYR:CE1	1:D:167:GLU:HG3	2.43	0.54
1:D:313:MET:CE	1:D:317:ILE:HD11	2.39	0.52
1:D:211:ASP:O	1:D:215:LYS:HG2	2.08	0.52
2:F:93:MET:HE3	2:F:94:PRO:HD2	1.91	0.52
1:B:37:ARG:O	1:B:66:THR:HB	2.10	0.52
1:D:351:THR:HG23	2:E:75:GLN:HE21	1.77	0.50
1:B:32:PRO:HB2	1:B:34:ILE:HG12	1.94	0.49
1:B:302:GLY:HA2	1:B:336:LYS:HG3	1.95	0.49
1:D:222:ASP:OD2	1:D:225:ASN:ND2	2.46	0.48
2:F:83:THR:HB	2:F:86:GLU:H	1.77	0.48
1:D:37:ARG:O	1:D:65:LEU:N	2.46	0.48
1:D:299:MET:HE2	1:D:329:ILE:CG2	2.43	0.48
1:D:37:ARG:O	1:D:38:PRO:C	2.57	0.47
1:D:73:HIS:HD2	1:D:158:GLY:O	1.97	0.47
1:D:291:LYS:HE3	1:D:292:ASP:OD2	2.15	0.47
2:E:93:MET:HE2	2:E:94:PRO:O	2.15	0.47
1:B:99:GLU:H	1:B:99:GLU:CD	2.22	0.46
1:D:255:PHE:O	1:D:258:PRO:HD2	2.14	0.46
2:F:83:THR:HG22	2:F:85:GLU:H	1.81	0.46
1:D:132:MET:HE2	1:D:134:VAL:HG23	1.96	0.46
1:D:352:PHE:O	1:D:354:GLN:N	2.48	0.46
1:B:201:VAL:HG12	1:B:202:THR:HG23	1.97	0.46
1:B:355:MET:HA	1:B:355:MET:HE2	1.97	0.46
1:B:24:ASP:OD2	1:B:28:ARG:NH1	2.49	0.46
1:D:106:THR:HB	1:D:137:GLN:HG3	1.97	0.46
1:B:312:ARG:O	1:B:316:GLU:HG2	2.16	0.46
1:D:169:TYR:CE1	2:E:84:ARG:HG2	2.50	0.45
1:D:299:MET:HE2	1:D:329:ILE:HG21	1.98	0.45
1:B:366:GLY:O	1:B:369:ILE:HG22	2.17	0.45
1:D:145:SER:OG	1:D:147:ARG:HD2	2.16	0.45
1:D:194:THR:HA	1:D:198:TYR:O	2.17	0.45
2:E:84:ARG:HE	2:E:84:ARG:HB3	1.34	0.45
1:B:239:SER:HA	1:B:248:ILE:O	2.17	0.45
1:B:105:LEU:HD11	1:B:123:MET:HG3	1.99	0.45
1:D:116:ARG:CG	1:D:116:ARG:NH1	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:93:MET:HE2	2:F:94:PRO:O	2.17	0.45
1:D:152:VAL:HG22	1:D:298:VAL:HB	2.00	0.44
1:D:198:TYR:CZ	1:D:248:ILE:HB	2.52	0.44
1:D:250:ILE:HB	1:D:253:GLU:HG2	2.00	0.44
1:D:189:LEU:HG	1:D:193:LEU:HD22	1.99	0.44
1:D:97:ALA:O	1:D:100:GLU:HB2	2.18	0.43
1:B:317:ILE:HD11	1:B:327:ILE:HG23	2.01	0.43
1:D:98:PRO:C	1:D:100:GLU:N	2.75	0.43
1:D:103:THR:O	1:D:132:MET:HA	2.17	0.43
1:D:278:THR:HG21	1:D:317:ILE:HD11	2.01	0.43
1:D:154:ASP:OD2	1:D:154:ASP:C	2.61	0.43
1:B:297:ASN:HB2	1:B:328:LYS:O	2.19	0.43
1:D:252:ASN:HD22	1:D:253:GLU:H	1.62	0.43
1:D:367:PRO:O	1:D:370:VAL:HG12	2.19	0.43
1:B:73:HIS:HD2	1:B:158:GLY:O	2.02	0.43
1:D:132:MET:CE	1:D:134:VAL:HG23	2.49	0.42
1:B:201:VAL:HG12	1:B:202:THR:N	2.34	0.42
1:B:305:MET:HB2	3:B:1372:ATP:C6	2.54	0.42
1:D:166:TYR:CD1	1:D:167:GLU:HG3	2.55	0.42
1:D:99:GLU:HA	1:D:128:ASN:O	2.19	0.42
1:D:124:PHE:CZ	1:D:132:MET:HG2	2.55	0.42
1:B:272:ALA:HB1	1:B:276:GLU:HB3	2.02	0.41
1:B:103:THR:O	1:B:132:MET:HA	2.19	0.41
1:D:105:LEU:O	1:D:134:VAL:HA	2.20	0.41
1:D:291:LYS:HE2	1:D:291:LYS:HB3	1.63	0.41
1:D:193:LEU:HD12	1:D:193:LEU:HA	1.94	0.41
1:B:73:HIS:CD2	1:B:179:ASP:OD1	2.73	0.41
1:B:194:THR:HA	1:B:198:TYR:O	2.21	0.41
1:D:116:ARG:HB2	1:D:116:ARG:NH1	2.35	0.41
1:D:305:MET:HB2	3:D:1372:ATP:C6	2.56	0.41
1:D:313:MET:CE	1:D:317:ILE:HG13	2.51	0.41
1:D:20:GLY:HA2	1:D:94:LEU:HD11	2.02	0.40
1:D:136:ILE:O	1:D:137:GLN:C	2.63	0.40
1:B:294:TYR:CD1	1:B:317:ILE:CD1	3.04	0.40
1:B:335:ARG:HA	1:B:338:SER:OG	2.20	0.40
1:D:54:VAL:HG11	1:D:85:ILE:HA	2.02	0.40
1:B:31:PHE:CE2	1:B:93:GLU:HG3	2.56	0.40
1:B:98:PRO:C	1:B:100:GLU:H	2.29	0.40
1:D:105:LEU:HD11	1:D:123:MET:HG3	2.03	0.40
1:D:118:LYS:NZ	8:D:2038:HOH:O	2.51	0.40
1:D:109:PRO:HB3	1:D:175:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ASP:OD2	1:B:225:ASN:ND2	2.55	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	B	345/377 (92%)	327 (95%)	16 (5%)	2 (1%)	21	24
1	D	346/377 (92%)	321 (93%)	21 (6%)	4 (1%)	10	9
2	E	26/32 (81%)	22 (85%)	3 (12%)	1 (4%)	2	1
2	F	26/32 (81%)	26 (100%)	0	0	100	100
All	All	743/818 (91%)	696 (94%)	40 (5%)	7 (1%)	14	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	THR
1	D	38	PRO
1	D	244	ASP
1	D	353	GLN
2	E	96	LEU
1	D	6	THR
1	B	369	ILE

5.3.2 Protein sidechains [i](#)

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	B	294/320 (92%)	263 (90%)	31 (10%)	6	6
1	D	295/320 (92%)	260 (88%)	35 (12%)	5	4
2	E	20/31 (64%)	16 (80%)	4 (20%)	1	1
2	F	21/31 (68%)	17 (81%)	4 (19%)	1	1
All	All	630/702 (90%)	556 (88%)	74 (12%)	5	5

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	SER
1	B	28	ARG
1	B	59	GLN
1	B	60	SER
1	B	77	THR
1	B	94	LEU
1	B	115	ASN
1	B	116	ARG
1	B	151	ILE
1	B	159	VAL
1	B	167	GLU
1	B	179	ASP
1	B	180	LEU
1	B	185	LEU
1	B	193	LEU
1	B	201	VAL
1	B	216	LEU
1	B	234	SER
1	B	257	CYS
1	B	287	ILE
1	B	293	LEU
1	B	297	ASN
1	B	313	MET
1	B	315	LYS
1	B	317	ILE
1	B	336	LYS
1	B	348	SER
1	B	350	SER
1	B	360	GLN
1	B	364	GLU

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Mol	Chain	Res	Type
1	B	368	SER
1	D	28	ARG
1	D	37	ARG
1	D	38	PRO
1	D	57	GLU
1	D	60	SER
1	D	66	THR
1	D	67	LEU
1	D	68	LYS
1	D	77	THR
1	D	78	ASN
1	D	85	ILE
1	D	94	LEU
1	D	116	ARG
1	D	176	MET
1	D	180	LEU
1	D	185	LEU
1	D	191	LYS
1	D	193	LEU
1	D	206	ARG
1	D	216	LEU
1	D	224	GLU
1	D	243	PRO
1	D	248	ILE
1	D	252	ASN
1	D	253	GLU
1	D	284	LYS
1	D	293	LEU
1	D	297	ASN
1	D	309	ILE
1	D	313	MET
1	D	324	THR
1	D	334	GLU
1	D	336	LYS
1	D	368	SER
1	D	371	HIS
2	E	74	LEU
2	E	84	ARG
2	E	89	SER
2	E	93	MET
2	F	72	ASN
2	F	74	LEU

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Mol	Chain	Res	Type
2	F	90	GLN
2	F	93	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	59	GLN
1	B	73	HIS
1	B	246	GLN
1	B	280	ASN
1	B	360	GLN
1	D	73	HIS
1	D	78	ASN
1	D	92	ASN
1	D	121	GLN
1	D	162	ASN
1	D	246	GLN
1	D	252	ASN
1	D	280	ASN
2	E	75	GLN
2	F	75	GLN

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, 2 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	LAB	B	1374	-	28,29,29	1.78	4 (14%)	29,41,41	2.38	8 (27%)
7	SCN	D	1375	-	1,2,2	1.76	0	0,1,1	-	-
3	ATP	B	1372	4	32,33,33	1.48	5 (15%)	48,52,52	2.35	16 (33%)
7	SCN	D	1376	-	1,2,2	1.41	0	0,1,1	-	-
5	LAB	D	1374	-	28,29,29	1.70	3 (10%)	29,41,41	2.14	9 (31%)
6	PEG	D	1377	-	6,6,6	0.61	0	5,5,5	0.85	0
7	SCN	B	1376	-	1,2,2	1.96	0	0,1,1	-	-
3	ATP	D	1372	4	32,33,33	1.57	7 (21%)	48,52,52	2.30	19 (39%)
7	SCN	B	1377	-	1,2,2	0.76	0	0,1,1	-	-
6	PEG	B	1375	-	6,6,6	0.69	0	5,5,5	1.24	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LAB	B	1374	-	-	3/21/49/49	0/2/3/3
3	ATP	B	1372	4	-	1/22/38/38	0/3/3/3
5	LAB	D	1374	-	-	3/21/49/49	0/2/3/3
6	PEG	D	1377	-	-	2/4/4/4	-
3	ATP	D	1372	4	-	2/22/38/38	0/3/3/3
6	PEG	B	1375	-	-	3/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1374	LAB	O2-C1	5.15	1.45	1.34
5	D	1374	LAB	O2-C1	5.14	1.45	1.34
5	B	1374	LAB	C18-S1	-5.10	1.67	1.77
5	D	1374	LAB	C18-S1	-5.00	1.67	1.77
3	B	1372	ATP	PB-O3B	4.61	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1372	ATP	C5-C4	4.50	1.47	1.39
3	D	1372	ATP	PA-O3A	3.12	1.62	1.59
3	B	1372	ATP	C5-N7	-3.11	1.33	1.39
3	B	1372	ATP	C8-N9	-2.98	1.32	1.37
3	B	1372	ATP	C5-C4	2.87	1.44	1.39
5	D	1374	LAB	O4-C15	2.84	1.45	1.40
3	D	1372	ATP	C5-C6	2.75	1.48	1.41
5	B	1374	LAB	C14-C15	2.67	1.56	1.52
3	D	1372	ATP	PB-O3B	2.50	1.62	1.59
5	B	1374	LAB	O4-C15	2.47	1.45	1.40
3	D	1372	ATP	C5-N7	-2.41	1.34	1.39
3	D	1372	ATP	C8-N7	2.36	1.36	1.31
3	D	1372	ATP	C8-N9	-2.28	1.33	1.37
3	B	1372	ATP	C5-C6	2.08	1.46	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1374	LAB	C17-S1-C18	6.89	96.03	92.04
3	B	1372	ATP	C5-C4-N3	-6.84	117.30	126.72
3	D	1372	ATP	C5-C4-N3	-6.45	117.83	126.72
5	D	1374	LAB	C17-S1-C18	6.45	95.78	92.04
3	B	1372	ATP	N3-C2-N1	-6.03	119.45	128.58
3	B	1372	ATP	N3-C4-N9	5.88	137.17	127.17
5	B	1374	LAB	O2-C1-C2	5.57	124.12	111.20
3	D	1372	ATP	N3-C2-N1	-5.35	120.49	128.58
3	B	1372	ATP	C2-N3-C4	5.28	124.73	111.83
3	D	1372	ATP	N3-C4-N9	5.14	135.92	127.17
3	D	1372	ATP	C2-N3-C4	4.82	123.61	111.83
5	D	1374	LAB	O2-C1-C2	4.49	121.60	111.20
5	B	1374	LAB	O4-C15-O3	-4.45	101.36	110.00
3	D	1372	ATP	C4-C5-N7	-4.04	105.96	110.58
5	B	1374	LAB	O2-C1-O1	-3.64	117.50	123.34
3	D	1372	ATP	C2-N1-C6	3.53	124.54	118.73
3	B	1372	ATP	O2A-PA-O3A	3.33	116.27	107.27
5	D	1374	LAB	C4-C5-C6	-3.28	105.45	112.57
5	B	1374	LAB	C19-C3-C4	3.23	120.84	115.23
5	B	1374	LAB	O1-C1-C2	-3.22	118.21	126.23
3	D	1372	ATP	C5-N7-C8	3.10	108.31	103.45
3	B	1372	ATP	O3A-PA-O1A	-3.05	101.53	110.70
3	D	1372	ATP	C4-N9-C8	3.02	108.91	105.74
5	D	1374	LAB	O1-C1-C2	-2.97	118.84	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1372	ATP	O3'-C3'-C4'	-2.90	102.75	111.08
3	D	1372	ATP	C2'-C1'-N9	-2.85	106.23	113.30
3	B	1372	ATP	C2-N1-C6	2.79	123.31	118.73
3	B	1372	ATP	O4'-C1'-C2'	-2.78	100.67	106.62
3	D	1372	ATP	O4'-C1'-N9	2.70	113.28	108.09
3	B	1372	ATP	O3B-PB-O1B	2.70	118.83	110.70
3	D	1372	ATP	O2B-PB-O3A	2.69	114.53	107.27
3	D	1372	ATP	O4'-C1'-C2'	-2.68	100.87	106.62
5	B	1374	LAB	O2-C13-C12	-2.66	101.51	107.77
3	B	1372	ATP	O2B-PB-O3A	2.65	114.43	107.27
5	D	1374	LAB	O4-C15-O3	-2.62	104.91	110.00
3	B	1372	ATP	O4'-C1'-N9	2.60	113.09	108.09
3	D	1372	ATP	C6-C5-N7	2.56	137.03	132.09
3	D	1372	ATP	O3'-C3'-C4'	-2.56	103.72	111.08
3	B	1372	ATP	C4-N9-C8	2.49	108.35	105.74
3	B	1372	ATP	C4-C5-N7	-2.48	107.75	110.58
5	B	1374	LAB	C19-C3-C2	-2.44	115.70	122.90
5	D	1374	LAB	O2-C1-O1	-2.38	119.52	123.34
3	D	1372	ATP	N9-C8-N7	-2.38	110.57	113.94
5	D	1374	LAB	C19-C3-C4	2.36	119.32	115.23
6	B	1375	PEG	C3-O2-C2	2.33	123.44	113.26
3	D	1372	ATP	O2A-PA-O3A	2.24	113.33	107.27
3	D	1372	ATP	O3'-C3'-C2'	-2.22	104.69	111.82
5	D	1374	LAB	C9-C10-C11	-2.17	110.10	114.06
5	D	1374	LAB	O2-C13-C14	2.16	113.17	107.64
3	D	1372	ATP	O3G-PG-O2G	2.16	115.90	107.80
3	D	1372	ATP	O2G-PG-O3B	-2.13	97.50	104.64
3	B	1372	ATP	C5-N7-C8	2.11	106.76	103.45
3	B	1372	ATP	N6-C6-N1	2.07	123.00	118.38

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1374	LAB	O3-C15-C16-C17
5	D	1374	LAB	O3-C15-C16-C17
6	D	1377	PEG	O1-C1-C2-O2
6	B	1375	PEG	C4-C3-O2-C2
3	D	1372	ATP	PG-O3B-PB-O1B
6	B	1375	PEG	O2-C3-C4-O4
6	D	1377	PEG	C1-C2-O2-C3
6	B	1375	PEG	O1-C1-C2-O2

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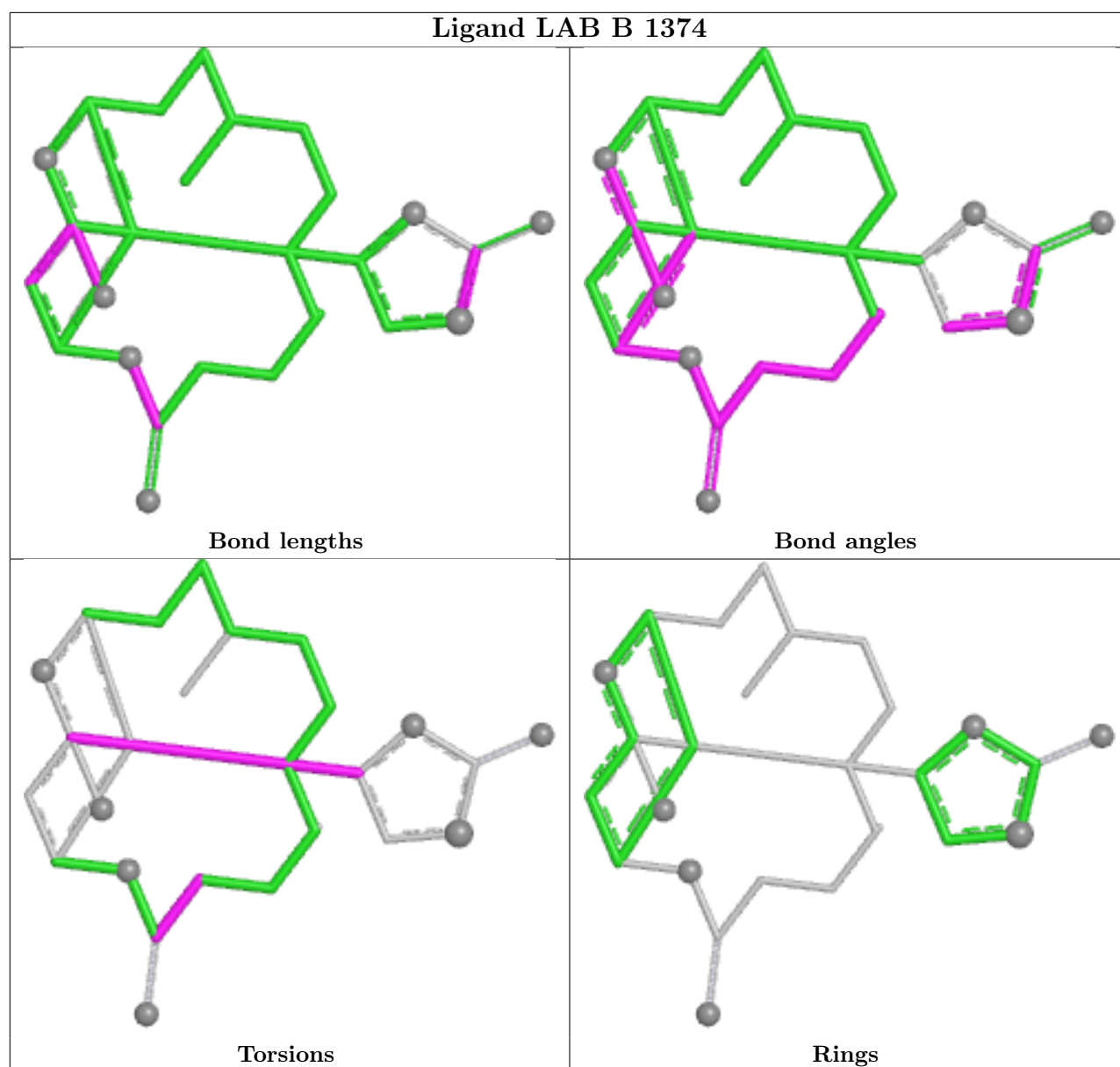
Mol	Chain	Res	Type	Atoms
5	D	1374	LAB	O2-C1-C2-C3
5	B	1374	LAB	O2-C1-C2-C3
5	B	1374	LAB	O1-C1-C2-C3
5	D	1374	LAB	C7-C8-C9-C10
3	B	1372	ATP	PG-O3B-PB-O2B
3	D	1372	ATP	PG-O3B-PB-O2B

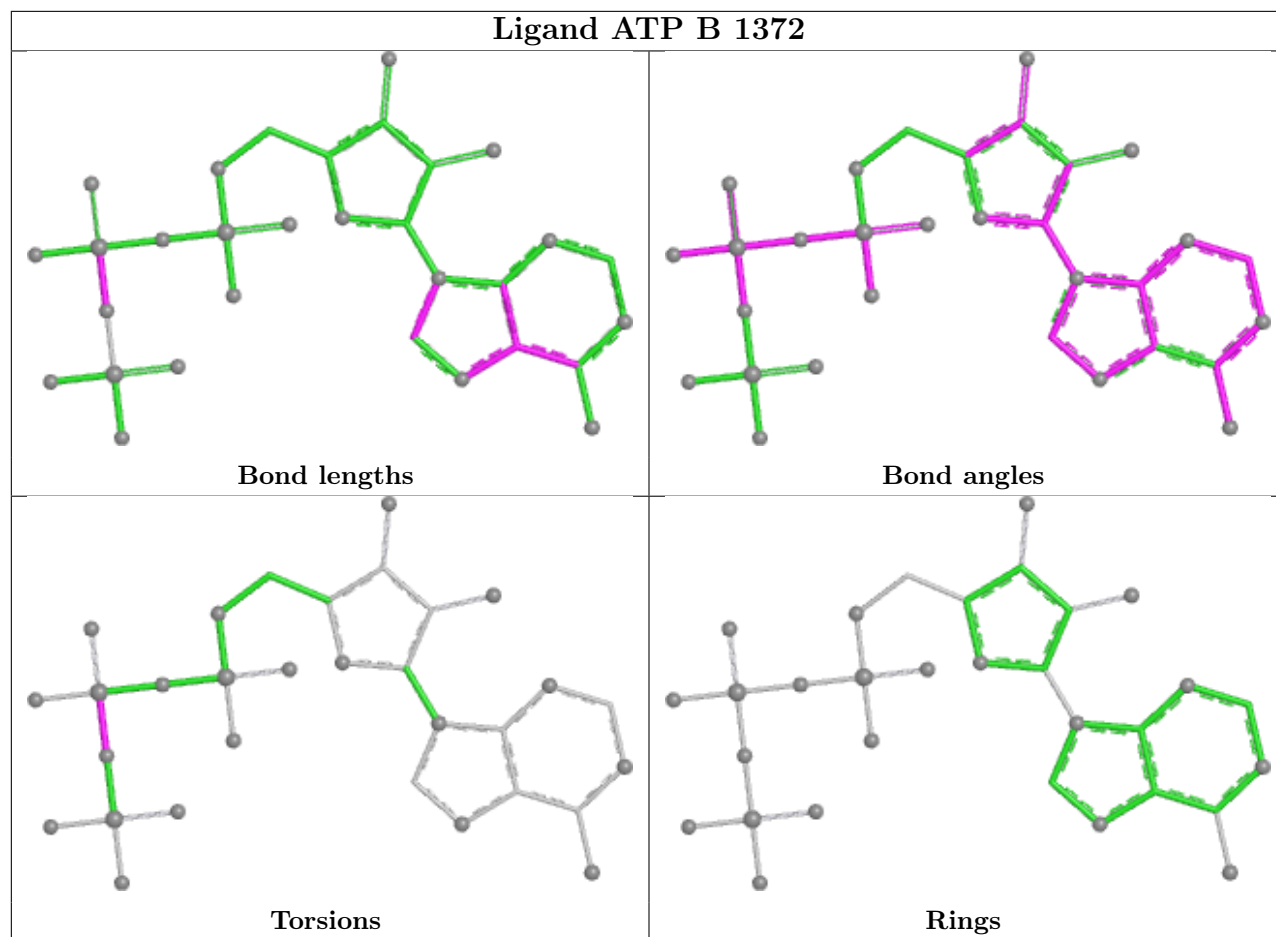
There are no ring outliers.

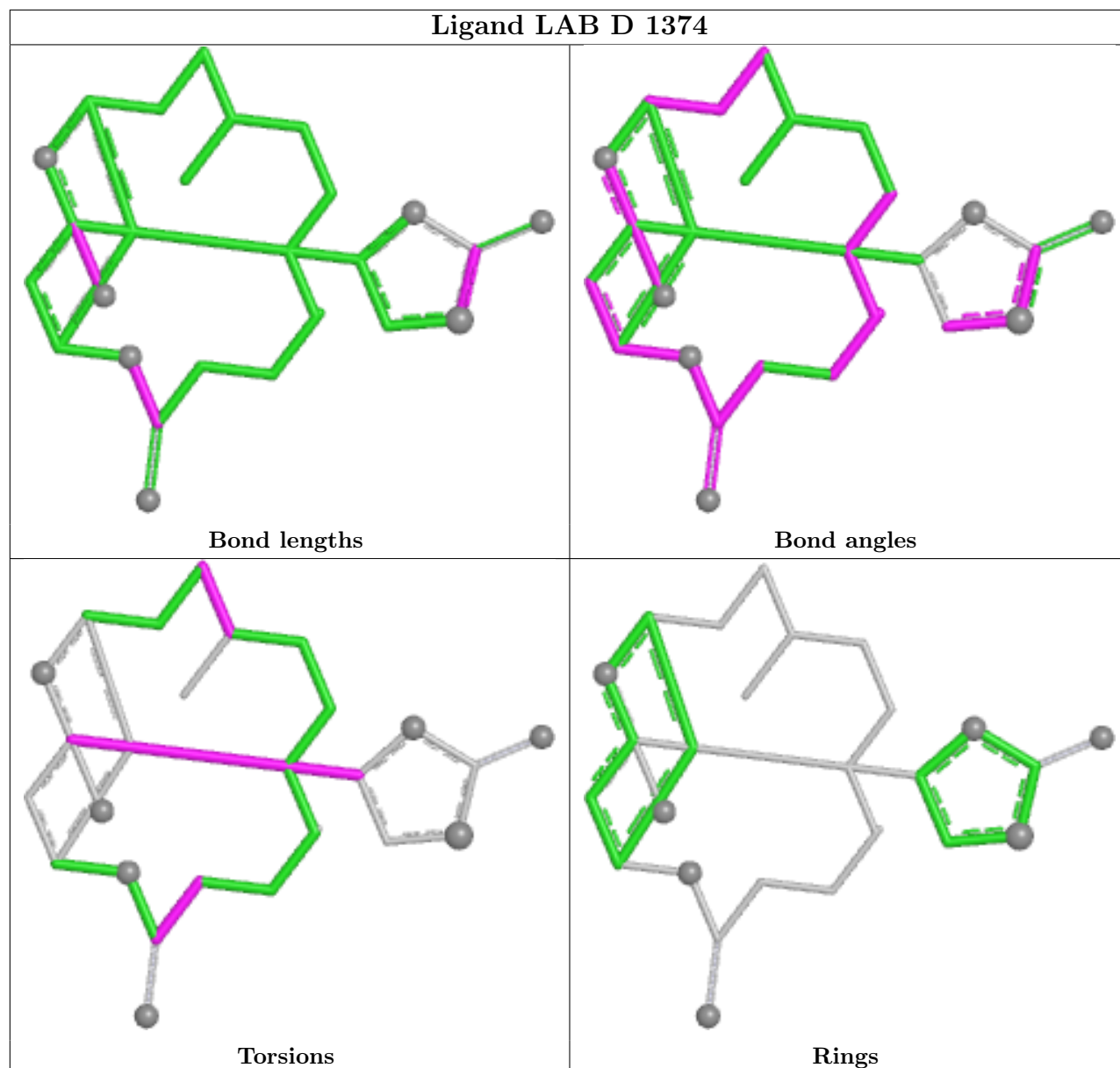
2 monomers are involved in 4 short contacts:

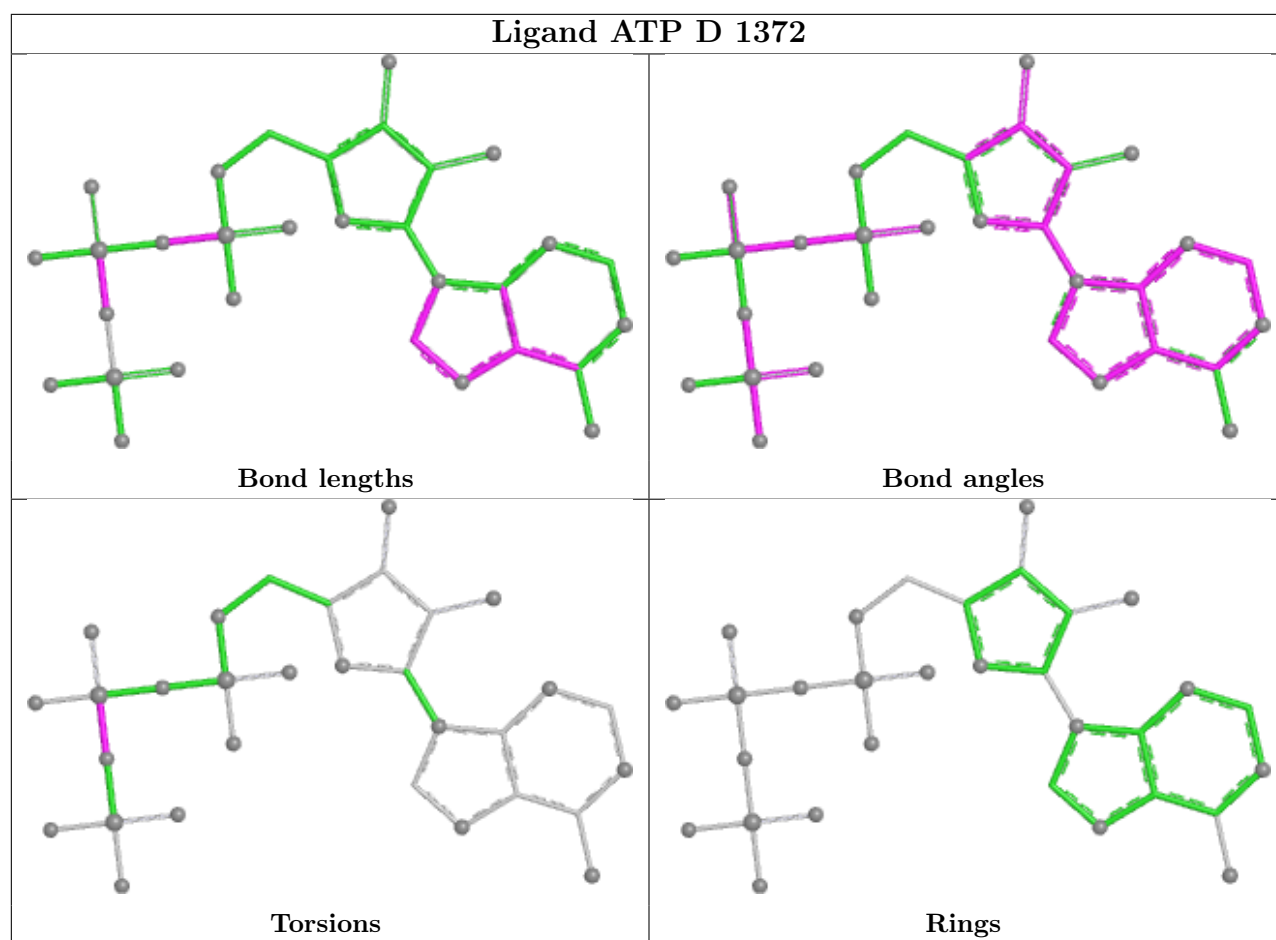
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1372	ATP	2	0
3	D	1372	ATP	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	351/377 (93%)	-1.53	0 100 100	27, 34, 46, 61	0
1	D	352/377 (93%)	-1.50	0 100 100	27, 34, 46, 58	0
2	E	28/32 (87%)	-1.45	0 100 100	31, 37, 41, 42	0
2	F	28/32 (87%)	-1.43	0 100 100	32, 39, 42, 43	0
All	All	759/818 (92%)	-1.51	0 100 100	27, 34, 46, 61	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PEG	B	1375	7/7	0.97	0.06	44,45,54,56	0
6	PEG	D	1377	7/7	0.98	0.06	47,49,52,52	0
7	SCN	D	1376	3/3	0.98	0.06	69,69,69,70	0
7	SCN	B	1376	3/3	0.99	0.03	51,51,51,52	0

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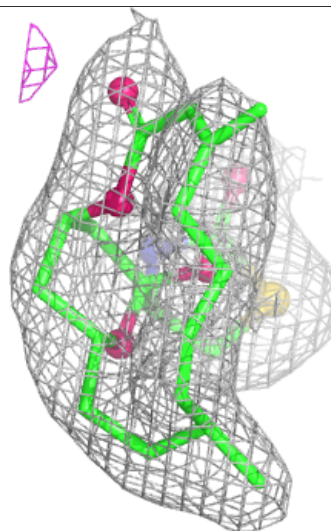
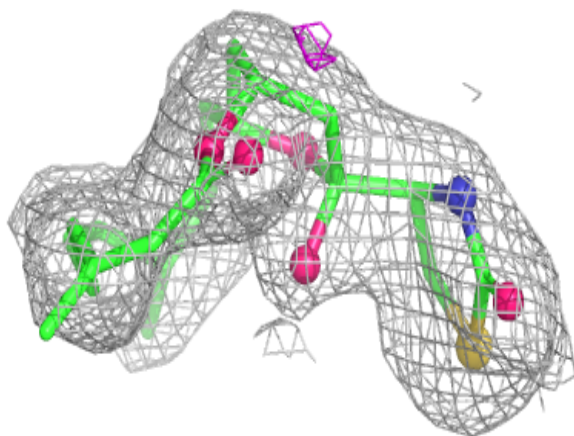
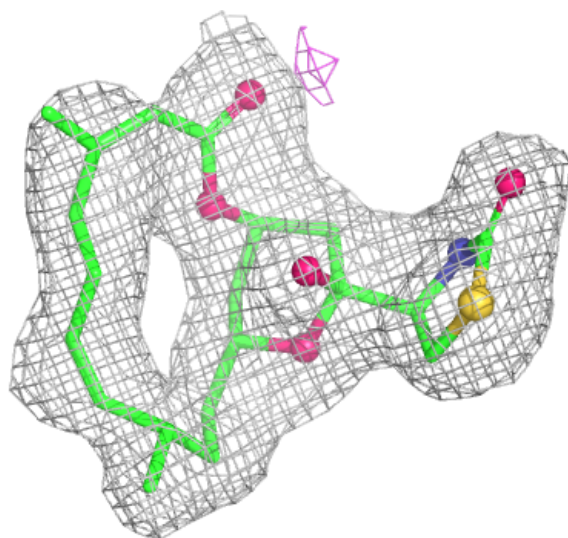
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SCN	B	1377	3/3	0.99	0.04	58,58,59,62	0
7	SCN	D	1375	3/3	0.99	0.05	57,57,57,58	0
5	LAB	D	1374	27/27	0.99	0.03	26,32,38,41	0
4	CA	B	1373	1/1	1.00	0.05	39,39,39,39	0
4	CA	D	1373	1/1	1.00	0.07	41,41,41,41	0
5	LAB	B	1374	27/27	1.00	0.03	27,30,36,37	0
3	ATP	B	1372	31/31	1.00	0.02	29,33,36,37	0
3	ATP	D	1372	31/31	1.00	0.03	29,35,38,40	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.

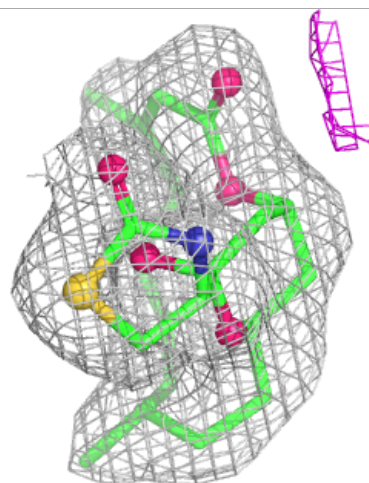
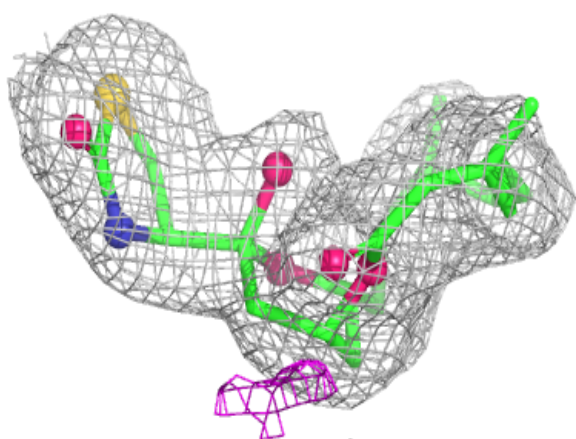
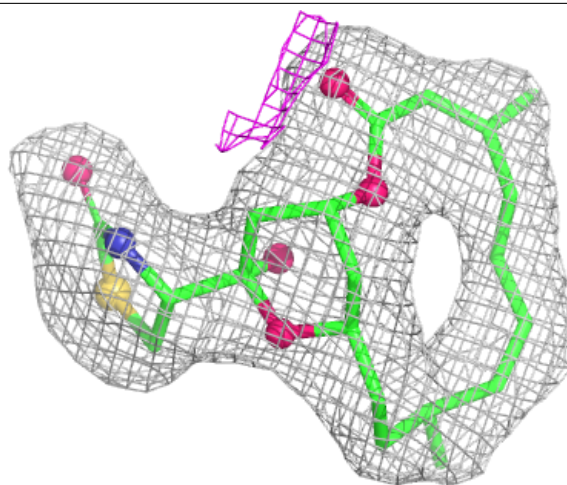
Electron density around LAB D 1374:

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



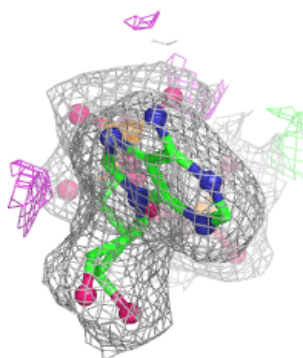
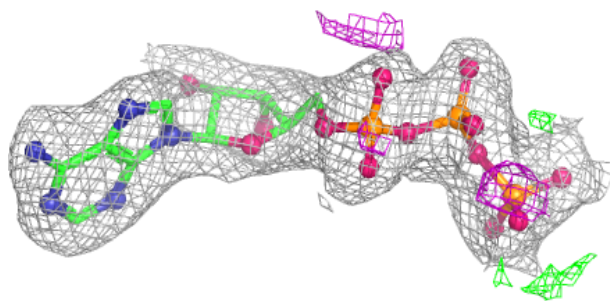
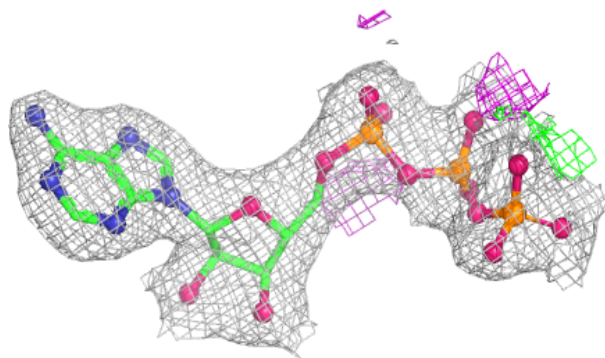
Electron density around LAB B 1374:

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

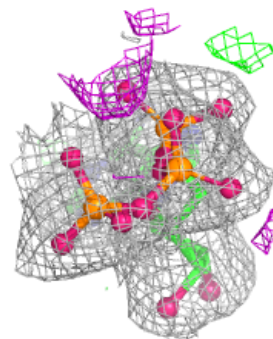
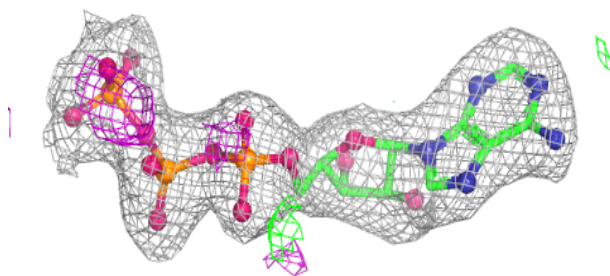
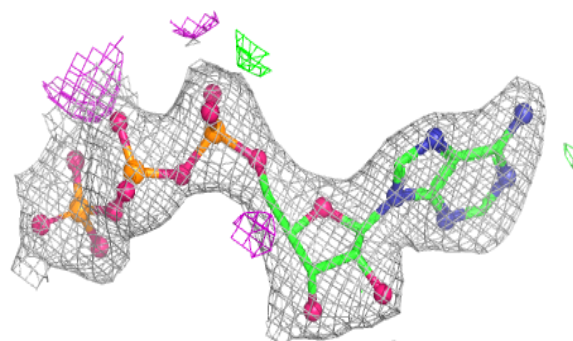


Electron density around ATP B 1372:

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

**Electron density around ATP D 1372:**

$2mF_o-DF_c$ (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.