



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:27 PM UTC

PDB ID : 9QKP / pdb_00009qkp
Title : Structure of the cyanobacteria specific PRK from Chroococcidiopsis (Hyella disjuncta) PCC 6712 (P41212 crystal form)
Authors : Tufail, F.; Yang, L.; Murray, J.W.
Deposited on : 2025-03-20
Resolution : 2.43 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

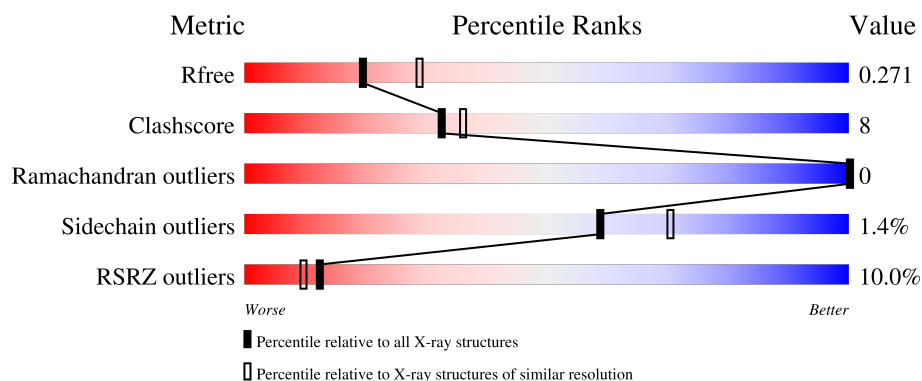
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	311	<div> <div>6%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	B	311	<div> <div>5%</div> <div>80%</div> <div>19%</div> <div>..</div> </div>
1	C	311	<div> <div>12%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	D	311	<div> <div>16%</div> <div>80%</div> <div>15%</div> <div>.</div> </div>

2 Entry composition [i](#)

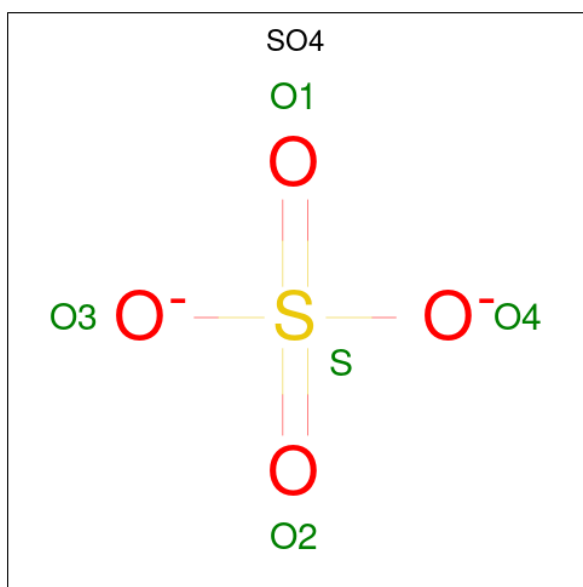
There are 6 unique types of molecules in this entry. The entry contains 9713 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cyanobacteria specific phosphoribulokinase from Chroococcidiopsis PCC 6712.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2416	1525	423	459	9			
1	B	309	Total	C	N	O	S	0	0	0
			2441	1538	427	467	9			
1	C	306	Total	C	N	O	S	0	0	0
			2387	1509	415	454	9			
1	D	299	Total	C	N	O	S	0	0	0
			2235	1409	382	435	9			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

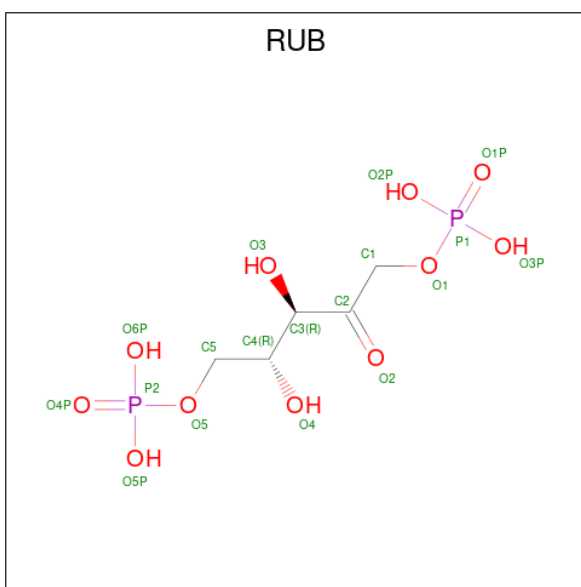
Continued on next page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0

- # ADP

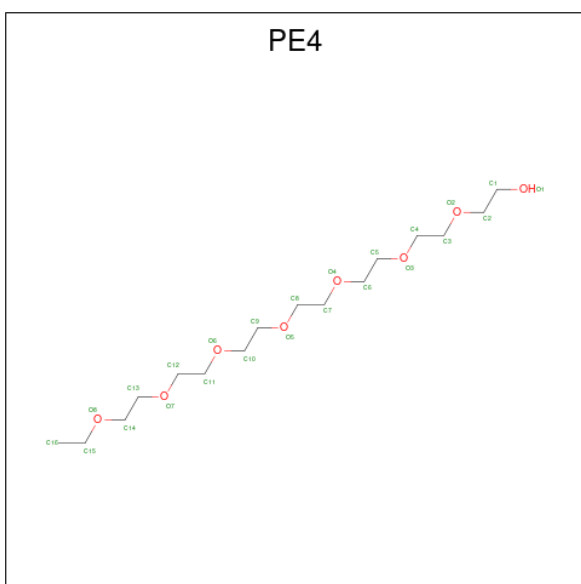
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0

- WORLDWIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 18	C 5	O 11	P 2	0	0
4	B	1	Total 18	C 5	O 11	P 2	0	0
4	C	1	Total 18	C 5	O 11	P 2	0	0
4	D	1	Total 18	C 5	O 11	P 2	0	0

- Molecule 5 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			19	13	6		

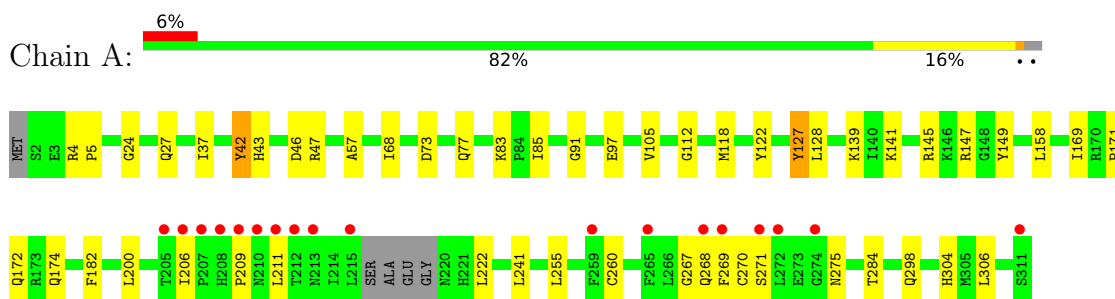
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	7	Total	O	0	0
			7	7		

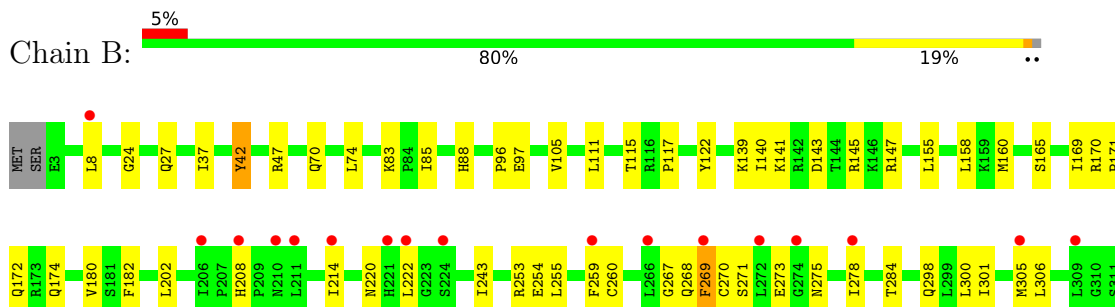
3 Residue-property plots [i](#)

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.

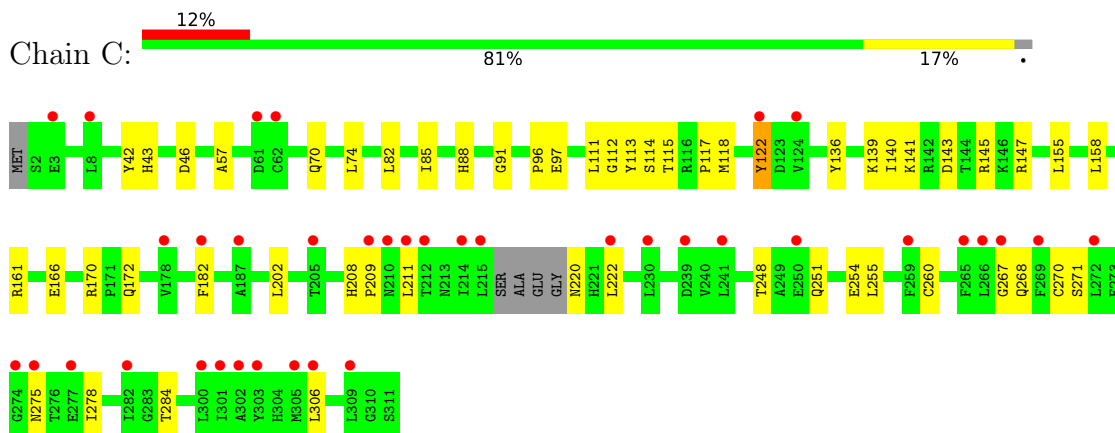
- Molecule 1: cyanobacteria specific phosphoribulokinase from *Chroococcidiopsis* PCC 6712



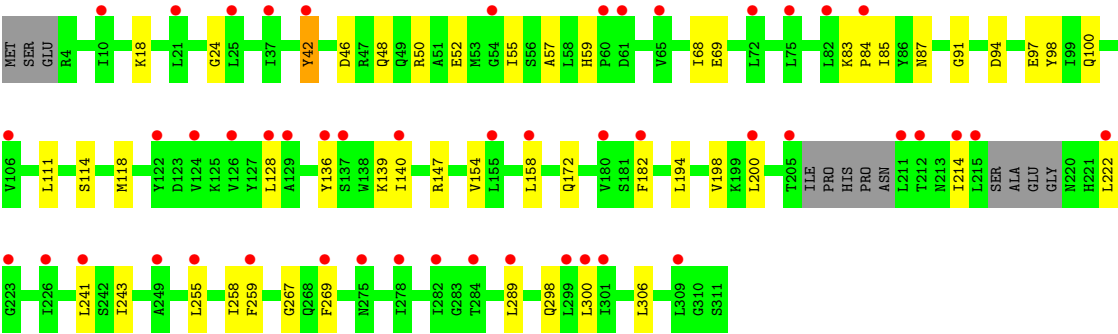
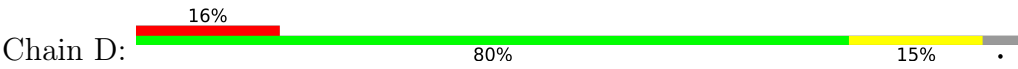
- Molecule 1: cyanobacteria specific phosphoribulokinase from *Chroococcidiopsis* PCC 6712



- Molecule 1: cyanobacteria specific phosphoribulokinase from *Chroococcidiopsis* PCC 6712



- Molecule 1: cyanobacteria specific phosphoribulokinase from *Chroococcidiopsis* PCC 6712



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.75Å 92.75Å 407.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.59 – 2.43 65.59 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.8 (65.59-2.43) 99.8 (65.59-2.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.233 , 0.268 0.241 , 0.271	Depositor DCC
R_{free} test set	2025 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 86.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9713	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: RUB, ADP, PE4, SO4

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	0.25	0/2466	0.52	0/3348
1	B	0.26	0/2492	0.53	0/3384
1	C	0.19	0/2436	0.43	0/3310
1	D	0.15	0/2280	0.38	0/3111
All	All	0.22	0/9674	0.47	0/13153

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2416	0	2387	33	0
1	B	2441	0	2410	47	0
1	C	2387	0	2346	36	0
1	D	2235	0	2079	32	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	27	0	12	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	2	0
3	C	27	0	12	1	0
3	D	27	0	12	2	0
4	A	18	0	8	2	0
4	B	18	0	8	4	0
4	C	18	0	8	4	0
4	D	18	0	8	2	0
5	B	19	0	22	4	0
6	A	8	0	0	0	0
6	B	7	0	0	0	0
All	All	9713	0	9324	150	0

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

All (150) 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:147:ARG:HH12	4:B:404:RUB:H11	1.36	0.88
1:D:147:ARG:HH12	4:D:1003:RUB:H11	1.41	0.84
1:D:50:ARG:HH11	1:D:57:ALA:HB2	1.45	0.78
1:A:27:GLN:HB3	1:A:275:ASN:HD21	1.52	0.75
1:A:141:LYS:HZ3	1:A:284:THR:HA	1.53	0.74
3:A:1002:ADP:H8	3:A:1002:ADP:H5'1	1.52	0.74
1:C:147:ARG:HH12	4:C:1003:RUB:H11	1.53	0.73
1:D:85:ILE:HD11	1:D:97:GLU:HB2	1.72	0.72
1:C:141:LYS:HZ3	1:C:284:THR:HA	1.55	0.72
1:A:147:ARG:HH12	4:A:1003:RUB:H11	1.54	0.71
3:D:1002:ADP:H5'1	3:D:1002:ADP:H8	1.56	0.70
1:B:220:ASN:HA	1:B:254:GLU:OE2	1.92	0.70
1:B:74:LEU:HD13	1:C:70:GLN:NE2	2.08	0.69
1:B:85:ILE:HD11	1:B:97:GLU:HB2	1.76	0.68
3:B:403:ADP:H5'1	3:B:403:ADP:H8	1.56	0.68
1:C:220:ASN:HA	1:C:254:GLU:OE2	1.94	0.68
1:B:147:ARG:NH1	4:B:404:RUB:H11	2.08	0.68
1:B:47:ARG:HH11	5:B:401:PE4:H82	1.59	0.67
1:A:141:LYS:NZ	1:A:284:THR:HA	2.09	0.67
3:C:1002:ADP:H5'1	3:C:1002:ADP:H8	1.59	0.67
1:D:50:ARG:NH1	1:D:57:ALA:HB2	2.10	0.67
1:B:27:GLN:HB3	1:B:275:ASN:HD21	1.60	0.66
1:B:47:ARG:NH1	5:B:401:PE4:H82	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LYS:NZ	1:B:145:ARG:HE	1.94	0.65
1:D:139:LYS:HD3	1:D:158:LEU:HD21	1.79	0.64
1:C:85:ILE:HD11	1:C:97:GLU:HB2	1.79	0.63
1:D:87:ASN:HB2	1:D:94:ASP:OD2	2.00	0.62
1:B:141:LYS:HZ2	1:B:145:ARG:HE	1.46	0.62
1:C:222:LEU:HD21	1:C:255:LEU:HD13	1.82	0.61
1:C:141:LYS:NZ	1:C:284:THR:HA	2.17	0.59
1:B:260:CYS:HB2	1:B:270:CYS:HB2	1.84	0.59
1:C:147:ARG:NH1	4:C:1003:RUB:H11	2.19	0.58
1:D:222:LEU:HD21	1:D:255:LEU:HD13	1.84	0.58
1:A:147:ARG:NH1	4:A:1003:RUB:H11	2.19	0.58
1:C:202:LEU:HB3	1:C:208:HIS:CE1	2.39	0.57
1:D:267:GLY:HA3	1:D:306:LEU:HD13	1.85	0.57
1:B:141:LYS:NZ	1:B:284:THR:HA	2.18	0.57
1:D:194:LEU:HD11	1:D:289:LEU:HD13	1.85	0.57
1:C:46:ASP:HB2	1:C:91:GLY:O	2.05	0.57
1:C:139:LYS:HD3	1:C:158:LEU:HD21	1.87	0.56
1:B:47:ARG:HD3	5:B:401:PE4:H61	1.86	0.56
1:B:111:LEU:HA	1:B:172:GLN:HE22	1.72	0.55
1:D:136:TYR:CD1	1:D:158:LEU:HD13	2.42	0.55
1:A:127:TYR:HD1	1:A:128:LEU:N	2.05	0.55
1:C:113:TYR:HE1	1:C:122:TYR:CE2	2.25	0.54
1:D:46:ASP:HB2	1:D:91:GLY:O	2.07	0.54
1:A:127:TYR:HD1	1:A:127:TYR:C	2.16	0.54
1:C:141:LYS:HZ2	1:C:145:ARG:HH11	1.55	0.54
1:D:147:ARG:NH1	4:D:1003:RUB:H11	2.18	0.53
1:B:139:LYS:HD3	1:B:158:LEU:HD21	1.90	0.52
1:C:140:ILE:HD11	1:C:155:LEU:HD21	1.92	0.52
1:A:24:GLY:HA3	1:A:298:GLN:CD	2.34	0.52
1:A:127:TYR:C	1:A:127:TYR:CD1	2.88	0.52
1:D:69:GLU:HG2	1:D:118:MET:HG3	1.92	0.51
1:A:46:ASP:HB2	1:A:91:GLY:O	2.11	0.51
1:B:8:LEU:HD13	1:B:305:MET:SD	2.51	0.50
1:B:27:GLN:HB3	1:B:275:ASN:ND2	2.26	0.50
1:B:37:ILE:HD12	1:B:105:VAL:HG13	1.94	0.50
1:D:214:ILE:HD13	1:D:259:PHE:HE1	1.76	0.50
1:A:139:LYS:HD3	1:A:158:LEU:HD21	1.94	0.50
1:B:70:GLN:NE2	1:C:74:LEU:HD13	2.26	0.50
1:B:169:ILE:O	1:B:172:GLN:HG3	2.12	0.50
1:A:267:GLY:HA3	1:A:306:LEU:HD13	1.93	0.50
1:B:141:LYS:HZ3	1:B:284:THR:HA	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HD11	1:A:304:HIS:CE1	2.46	0.49
1:B:74:LEU:HD13	1:C:70:GLN:HE21	1.76	0.49
1:B:24:GLY:HA3	1:B:298:GLN:CD	2.37	0.49
1:C:111:LEU:HA	1:C:172:GLN:HE22	1.77	0.49
1:D:241:LEU:HD13	1:D:300:LEU:HD13	1.93	0.49
1:C:260:CYS:HB2	1:C:270:CYS:HB2	1.95	0.49
1:D:140:ILE:HA	1:D:154:VAL:HG11	1.94	0.49
1:B:202:LEU:HB3	1:B:208:HIS:CE1	2.47	0.48
1:D:214:ILE:HG23	1:D:258:ILE:HG21	1.95	0.48
1:A:222:LEU:HD21	1:A:255:LEU:HD13	1.95	0.48
1:B:42:TYR:OH	1:B:83:LYS:HG3	2.14	0.48
1:A:43:HIS:CE1	1:A:57:ALA:HB1	2.49	0.48
1:D:182:PHE:HE2	3:D:1002:ADP:HN62	1.61	0.48
1:A:200:LEU:HB2	1:A:241:LEU:HB2	1.96	0.48
1:C:202:LEU:HB3	1:C:208:HIS:HE1	1.79	0.47
1:C:209:PRO:O	1:C:211:LEU:HG	2.14	0.47
1:A:171:PRO:O	1:A:174:GLN:HG2	2.14	0.47
1:D:243:ILE:HD11	1:D:300:LEU:HD12	1.96	0.47
1:C:275:ASN:O	1:C:278:ILE:HG22	2.14	0.47
1:A:85:ILE:HD11	1:A:97:GLU:HB2	1.97	0.47
1:D:24:GLY:HA3	1:D:298:GLN:CD	2.39	0.47
3:A:1002:ADP:H5'1	3:A:1002:ADP:C8	2.43	0.47
1:B:171:PRO:O	1:B:174:GLN:HG2	2.14	0.46
1:C:115:THR:HB	1:C:117:PRO:HD2	1.98	0.46
1:A:4:ARG:HD2	1:A:5:PRO:O	2.15	0.46
1:A:141:LYS:HZ2	1:A:145:ARG:HH11	1.63	0.46
1:D:42:TYR:CD2	1:D:68:ILE:HG12	2.51	0.46
1:B:88:HIS:HE1	4:B:404:RUB:O4	1.97	0.46
1:B:222:LEU:HD21	1:B:255:LEU:HD13	1.98	0.46
1:B:268:GLN:HB2	1:B:271:SER:HB3	1.97	0.45
1:D:24:GLY:HA3	1:D:298:GLN:OE1	2.15	0.45
1:B:267:GLY:HA3	1:B:306:LEU:HD13	1.97	0.45
1:A:268:GLN:HB2	1:A:271:SER:HB3	1.99	0.45
1:A:112:GLY:HA2	1:A:118:MET:HE1	1.99	0.45
1:B:180:VAL:HG21	1:B:301:ILE:HD11	1.98	0.45
1:B:275:ASN:O	1:B:278:ILE:HG22	2.16	0.45
1:B:140:ILE:HD11	1:B:155:LEU:HD21	1.98	0.45
1:C:88:HIS:HE1	4:C:1003:RUB:O4	2.00	0.45
1:C:112:GLY:HA2	1:C:118:MET:HE1	1.99	0.45
1:D:42:TYR:CE1	1:D:83:LYS:HG3	2.52	0.45
1:A:209:PRO:O	1:A:211:LEU:HG	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:HA	1:A:172:GLN:HE21	1.82	0.44
1:D:55:ILE:HD11	1:D:59:HIS:CG	2.52	0.44
1:C:43:HIS:CE1	1:C:57:ALA:HB1	2.52	0.44
1:C:141:LYS:NZ	1:C:145:ARG:HH11	2.15	0.44
1:C:268:GLN:HB2	1:C:271:SER:HB3	2.00	0.44
1:D:198:VAL:HG12	1:D:200:LEU:HD12	2.00	0.44
1:C:143:ASP:OD1	1:C:147:ARG:HD2	2.18	0.44
1:D:98:TYR:HE2	1:D:100:GLN:HE21	1.66	0.44
1:D:198:VAL:HB	1:D:243:ILE:HB	2.00	0.43
1:B:115:THR:HB	1:B:117:PRO:HD2	1.99	0.43
1:B:143:ASP:OD1	1:B:147:ARG:HD2	2.18	0.43
1:C:166:GLU:HA	1:C:170:ARG:HH11	1.83	0.43
1:A:42:TYR:OH	1:A:83:LYS:HG3	2.19	0.42
1:D:111:LEU:HB3	1:D:114:SER:OG	2.19	0.42
1:B:96:PRO:HD3	1:C:96:PRO:HD3	2.00	0.42
1:A:68:ILE:HG21	1:A:118:MET:HE3	2.00	0.42
1:B:243:ILE:HD11	1:B:300:LEU:HD12	2.01	0.42
1:D:18:LYS:HA	1:D:128:LEU:HD11	2.02	0.42
1:A:37:ILE:HD12	1:A:105:VAL:HG13	2.02	0.42
1:A:68:ILE:CG2	1:A:118:MET:HE3	2.50	0.42
1:B:42:TYR:N	1:B:42:TYR:CD1	2.87	0.42
1:A:47:ARG:CZ	1:A:149:TYR:HE1	2.33	0.42
1:A:260:CYS:HB2	1:A:270:CYS:HB2	2.02	0.42
3:B:403:ADP:H5'1	3:B:403:ADP:C8	2.48	0.42
1:D:111:LEU:HA	1:D:172:GLN:HE22	1.84	0.42
1:B:160:MET:HA	1:B:160:MET:HE2	2.02	0.41
1:B:269:PHE:CD1	1:B:269:PHE:N	2.88	0.41
1:B:47:ARG:CD	5:B:401:PE4:H61	2.50	0.41
1:B:147:ARG:HH12	4:B:404:RUB:C1	2.18	0.41
1:B:269:PHE:N	1:B:269:PHE:HD1	2.18	0.41
1:C:161:ARG:HH22	4:C:1003:RUB:H52	1.86	0.41
1:D:48:GLN:O	1:D:52:GLU:HG3	2.20	0.41
1:A:73:ASP:O	1:A:77:GLN:HG3	2.20	0.41
1:B:253:ARG:HH12	1:B:273:GLU:HG2	1.84	0.41
1:B:214:ILE:HD13	1:B:259:PHE:HE1	1.86	0.41
1:A:112:GLY:O	1:A:118:MET:HE2	2.21	0.41
1:B:259:PHE:HB3	1:B:269:PHE:CD2	2.56	0.41
1:C:248:THR:OG1	1:C:251:GLN:HG3	2.20	0.41
1:C:267:GLY:HA3	1:C:306:LEU:HD13	2.02	0.41
1:C:82:LEU:HD12	1:C:82:LEU:HA	1.83	0.40
1:C:111:LEU:HB3	1:C:114:SER:OG	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:TYR:CD1	1:D:84:PRO:HG2	2.57	0.40
1:C:136:TYR:CD1	1:C:158:LEU:HD13	2.56	0.40
1:B:165:SER:O	1:B:170:ARG:HG3	2.21	0.40
1:A:27:GLN:HB3	1:A:275:ASN:ND2	2.29	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	302/311 (97%)	298 (99%)	4 (1%)	0	100	100
1	B	307/311 (99%)	302 (98%)	5 (2%)	0	100	100
1	C	302/311 (97%)	297 (98%)	5 (2%)	0	100	100
1	D	293/311 (94%)	287 (98%)	6 (2%)	0	100	100
All	All	1204/1244 (97%)	1184 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	263/273 (96%)	258 (98%)	5 (2%)	50	63
1	B	266/273 (97%)	262 (98%)	4 (2%)	57	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	257/273 (94%)	254 (99%)	3 (1%)	63	74
1	D	226/273 (83%)	224 (99%)	2 (1%)	70	80
All	All	1012/1092 (93%)	998 (99%)	14 (1%)	59	70

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	TYR
1	A	122	TYR
1	A	127	TYR
1	A	182	PHE
1	A	269	PHE
1	B	42	TYR
1	B	122	TYR
1	B	182	PHE
1	B	269	PHE
1	C	42	TYR
1	C	122	TYR
1	C	182	PHE
1	D	42	TYR
1	D	269	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	157	GLN
1	A	167	ASN
1	A	172	GLN
1	A	193	ASN
1	A	275	ASN
1	A	304	HIS
1	B	27	GLN
1	B	70	GLN
1	B	88	HIS
1	B	193	ASN
1	C	43	HIS
1	C	70	GLN
1	C	88	HIS
1	C	172	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	268	GLN
1	D	157	GLN
1	D	172	GLN
1	D	193	ASN
1	D	268	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 ⓘ

13 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	$\# Z > 2$
3	ADP	C	1002	-	28,29,29	1.37	4 (14%)	43,45,45	1.89	9 (20%)
4	RUB	C	1003	-	17,17,17	0.50	0	17,25,25	0.65	0
2	SO4	A	1001	-	4,4,4	0.56	0	6,6,6	0.24	0
2	SO4	B	402	-	4,4,4	0.22	0	6,6,6	0.57	0
4	RUB	B	404	-	17,17,17	0.54	0	17,25,25	0.91	0
4	RUB	A	1003	-	17,17,17	0.49	0	17,25,25	0.69	0
4	RUB	D	1003	-	17,17,17	0.48	0	17,25,25	0.60	0
3	ADP	D	1002	-	28,29,29	1.37	5 (17%)	43,45,45	1.89	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	1001	-	4,4,4	0.67	0	6,6,6	0.08	0
3	ADP	A	1002	-	28,29,29	1.30	5 (17%)	43,45,45	1.79	12 (27%)
3	ADP	B	403	-	28,29,29	1.35	5 (17%)	43,45,45	1.89	12 (27%)
5	PE4	B	401	-	18,18,23	0.35	0	17,17,22	0.43	0
2	SO4	C	1001	-	4,4,4	0.64	0	6,6,6	0.13	0

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	ADP	C	1002	-	-	2/16/32/32	0/3/3/3
4	RUB	B	404	-	-	9/20/20/20	-
4	RUB	A	1003	-	-	9/20/20/20	-
4	RUB	D	1003	-	-	7/20/20/20	-
3	ADP	D	1002	-	-	1/16/32/32	0/3/3/3
3	ADP	A	1002	-	-	1/16/32/32	0/3/3/3
3	ADP	B	403	-	-	2/16/32/32	0/3/3/3
5	PE4	B	401	-	-	5/16/16/21	-
4	RUB	C	1003	-	-	9/20/20/20	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	ADP	C5-C4	4.61	1.47	1.39
3	D	1002	ADP	C5-C4	4.57	1.47	1.39
3	A	1002	ADP	C5-C4	4.44	1.47	1.39
3	B	403	ADP	C5-C4	4.36	1.46	1.39
3	B	403	ADP	C5-N7	-2.67	1.34	1.39
3	C	1002	ADP	C5-C6	2.58	1.48	1.41
3	A	1002	ADP	C5-N7	-2.55	1.34	1.39
3	D	1002	ADP	C5-N7	-2.51	1.34	1.39
3	C	1002	ADP	C5-N7	-2.40	1.34	1.39
3	D	1002	ADP	C5-C6	2.32	1.47	1.41
3	B	403	ADP	C5-C6	2.30	1.47	1.41
3	A	1002	ADP	C4-N9	-2.18	1.33	1.37
3	A	1002	ADP	C8-N7	2.15	1.35	1.31
3	C	1002	ADP	C8-N7	2.11	1.35	1.31
3	B	403	ADP	C4-N9	-2.08	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	ADP	C5-C6	2.08	1.46	1.41
3	B	403	ADP	C8-N7	2.04	1.35	1.31
3	D	1002	ADP	PA-O3A	2.02	1.61	1.59
3	D	1002	ADP	C8-N7	2.00	1.35	1.31

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1002	ADP	C5-C4-N3	-6.10	118.32	126.72
3	C	1002	ADP	C5-C4-N3	-6.06	118.37	126.72
3	B	403	ADP	C5-C4-N3	-5.82	118.70	126.72
3	D	1002	ADP	N3-C4-N9	5.28	136.15	127.17
3	A	1002	ADP	C5-C4-N3	-5.19	119.58	126.72
3	C	1002	ADP	N3-C4-N9	4.90	135.51	127.17
3	B	403	ADP	N3-C4-N9	4.82	135.37	127.17
3	A	1002	ADP	N3-C4-N9	4.35	134.57	127.17
3	C	1002	ADP	C2-N3-C4	3.75	120.99	111.83
3	D	1002	ADP	C2-N3-C4	3.73	120.94	111.83
3	B	403	ADP	C2-N3-C4	3.62	120.67	111.83
3	A	1002	ADP	N3-C2-N1	-3.52	123.26	128.58
3	A	1002	ADP	C2-N3-C4	3.46	120.28	111.83
3	C	1002	ADP	C2'-C1'-N9	-3.32	105.06	113.30
3	D	1002	ADP	N3-C2-N1	-3.20	123.74	128.58
3	B	403	ADP	N3-C2-N1	-3.16	123.80	128.58
3	C	1002	ADP	N3-C2-N1	-3.14	123.83	128.58
3	C	1002	ADP	C4-C5-N7	-3.13	107.00	110.58
3	D	1002	ADP	C2'-C1'-N9	-2.81	106.32	113.30
3	B	403	ADP	C4-C5-N7	-2.70	107.50	110.58
3	B	403	ADP	O3A-PA-O1A	-2.62	102.83	110.70
3	A	1002	ADP	O2A-PA-O3A	2.58	114.25	107.27
3	D	1002	ADP	C4-C5-N7	-2.49	107.74	110.58
3	D	1002	ADP	C4-N9-C8	2.47	108.33	105.74
3	A	1002	ADP	C4-N9-C8	2.41	108.26	105.74
3	B	403	ADP	C4-N9-C8	2.40	108.25	105.74
3	C	1002	ADP	C3'-C2'-C1'	2.38	105.96	101.46
3	B	403	ADP	C3'-C2'-C1'	2.37	105.94	101.46
3	C	1002	ADP	C4-N9-C8	2.36	108.22	105.74
3	A	1002	ADP	C2'-C1'-N9	-2.35	107.47	113.30
3	A	1002	ADP	C4-C5-N7	-2.34	107.91	110.58
3	C	1002	ADP	C5-N7-C8	2.29	107.05	103.45
3	B	403	ADP	O2A-PA-O3A	2.17	113.15	107.27
3	B	403	ADP	C2'-C1'-N9	-2.17	107.92	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1002	ADP	C3'-C2'-C1'	2.16	105.56	101.46
3	A	1002	ADP	C2-N1-C6	2.12	122.22	118.73
3	D	1002	ADP	N6-C6-N1	2.12	123.09	118.38
3	B	403	ADP	O3B-PB-O2B	2.10	115.67	107.80
3	A	1002	ADP	C3'-C2'-C1'	2.04	105.31	101.46
3	A	1002	ADP	O3B-PB-O2B	2.02	115.37	107.80
3	A	1002	ADP	O3A-PA-O1A	-2.01	104.67	110.70
3	B	403	ADP	C5-N7-C8	2.00	106.60	103.45

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	RUB	O1-C1-C2-C3
4	A	1003	RUB	O1-C1-C2-O2
4	A	1003	RUB	C2-C3-C4-C5
4	A	1003	RUB	C2-C3-C4-O4
4	A	1003	RUB	O3-C3-C4-O4
4	A	1003	RUB	C5-O5-P2-O4P
4	A	1003	RUB	C5-O5-P2-O5P
4	A	1003	RUB	C5-O5-P2-O6P
4	B	404	RUB	O1-C1-C2-C3
4	B	404	RUB	O1-C1-C2-O2
4	B	404	RUB	C2-C3-C4-C5
4	B	404	RUB	C2-C3-C4-O4
4	B	404	RUB	O3-C3-C4-O4
4	B	404	RUB	C5-O5-P2-O4P
4	B	404	RUB	C5-O5-P2-O5P
4	B	404	RUB	C5-O5-P2-O6P
4	C	1003	RUB	O1-C1-C2-C3
4	C	1003	RUB	O1-C1-C2-O2
4	C	1003	RUB	C2-C3-C4-C5
4	C	1003	RUB	C5-O5-P2-O4P
4	C	1003	RUB	C5-O5-P2-O5P
4	C	1003	RUB	C5-O5-P2-O6P
4	D	1003	RUB	O1-C1-C2-C3
4	D	1003	RUB	O1-C1-C2-O2
4	D	1003	RUB	C2-C3-C4-C5
4	D	1003	RUB	C5-O5-P2-O4P
4	D	1003	RUB	C5-O5-P2-O5P
4	D	1003	RUB	C5-O5-P2-O6P
5	B	401	PE4	O2-C3-C4-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	401	PE4	O6-C11-C12-O7
5	B	401	PE4	C5-C6-O4-C7
4	C	1003	RUB	C2-C3-C4-O4
4	D	1003	RUB	C2-C3-C4-O4
3	C	1002	ADP	O4'-C4'-C5'-O5'
3	D	1002	ADP	O4'-C4'-C5'-O5'
3	A	1002	ADP	O4'-C4'-C5'-O5'
3	B	403	ADP	O4'-C4'-C5'-O5'
5	B	401	PE4	C9-C10-O6-C11
4	C	1003	RUB	O3-C3-C4-O4
4	A	1003	RUB	O3-C3-C4-C5
4	B	404	RUB	O3-C3-C4-C5
4	C	1003	RUB	O3-C3-C4-C5
3	B	403	ADP	PB-O3A-PA-O1A
3	C	1002	ADP	PB-O3A-PA-O1A
5	B	401	PE4	C7-C8-O5-C9

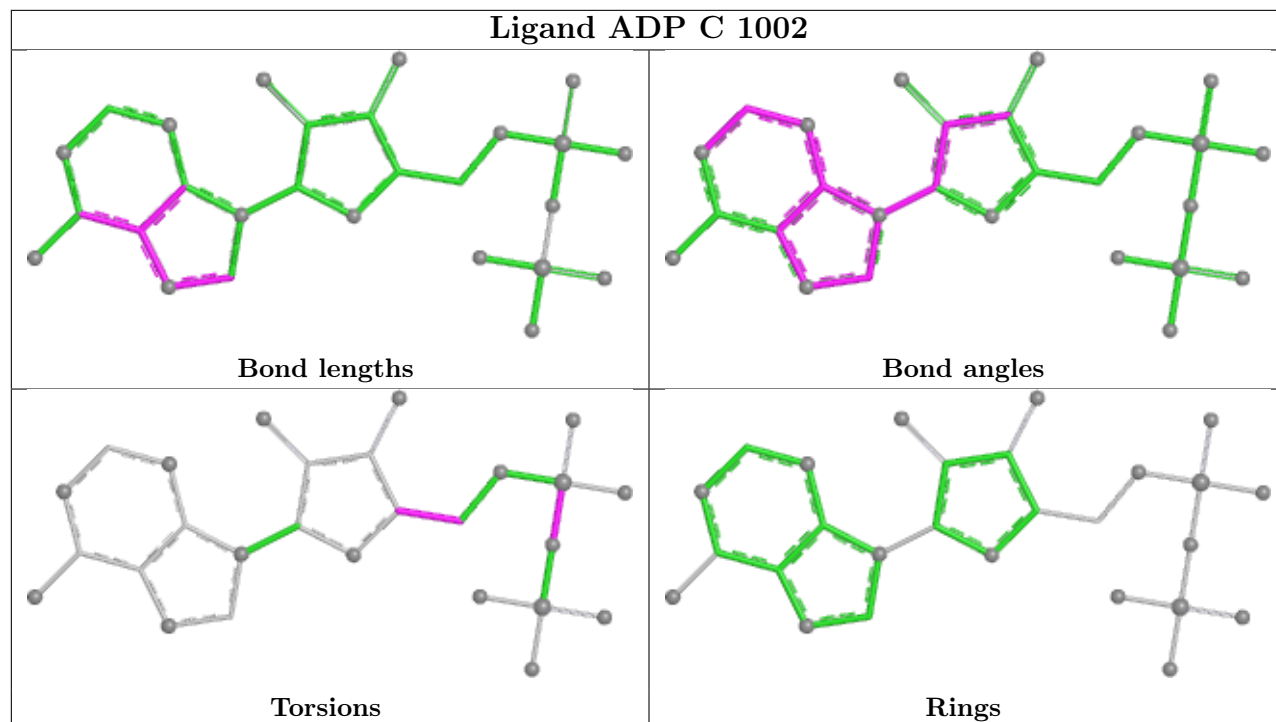
There are no ring outliers.

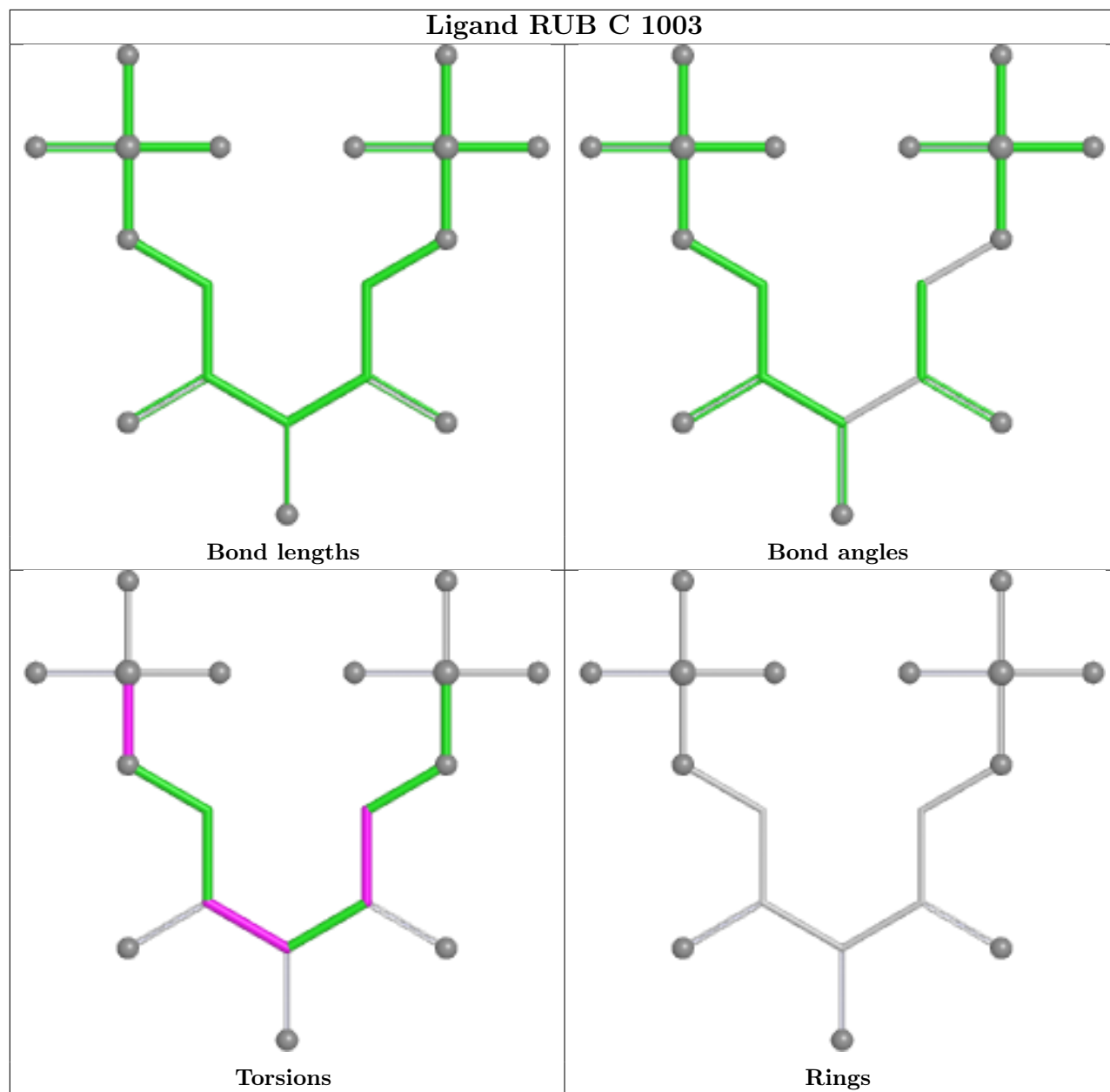
9 monomers are involved in 23 short contacts:

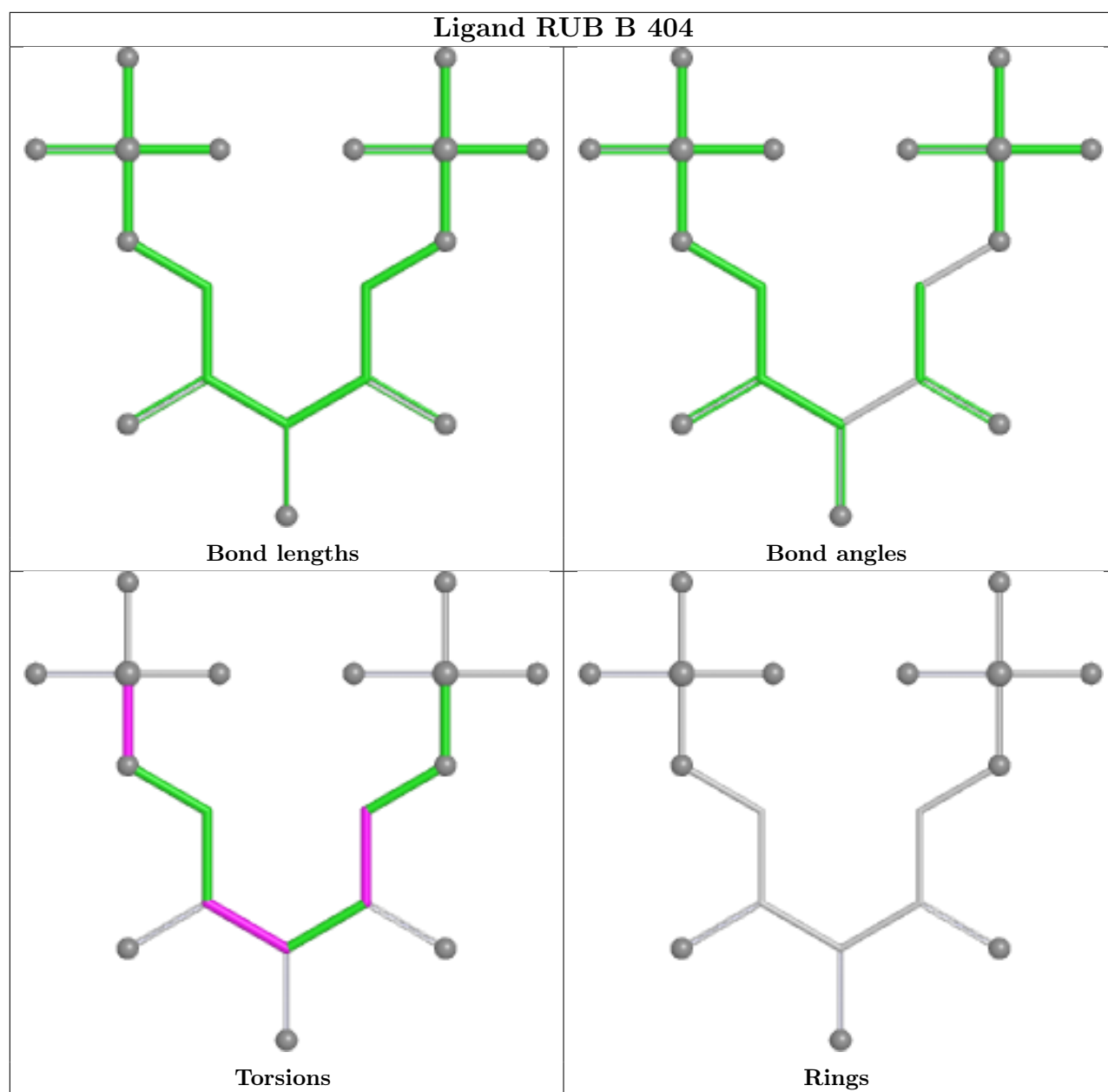
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1002	ADP	1	0
4	C	1003	RUB	4	0
4	B	404	RUB	4	0
4	A	1003	RUB	2	0
4	D	1003	RUB	2	0
3	D	1002	ADP	2	0
3	A	1002	ADP	2	0
3	B	403	ADP	2	0
5	B	401	PE4	4	0

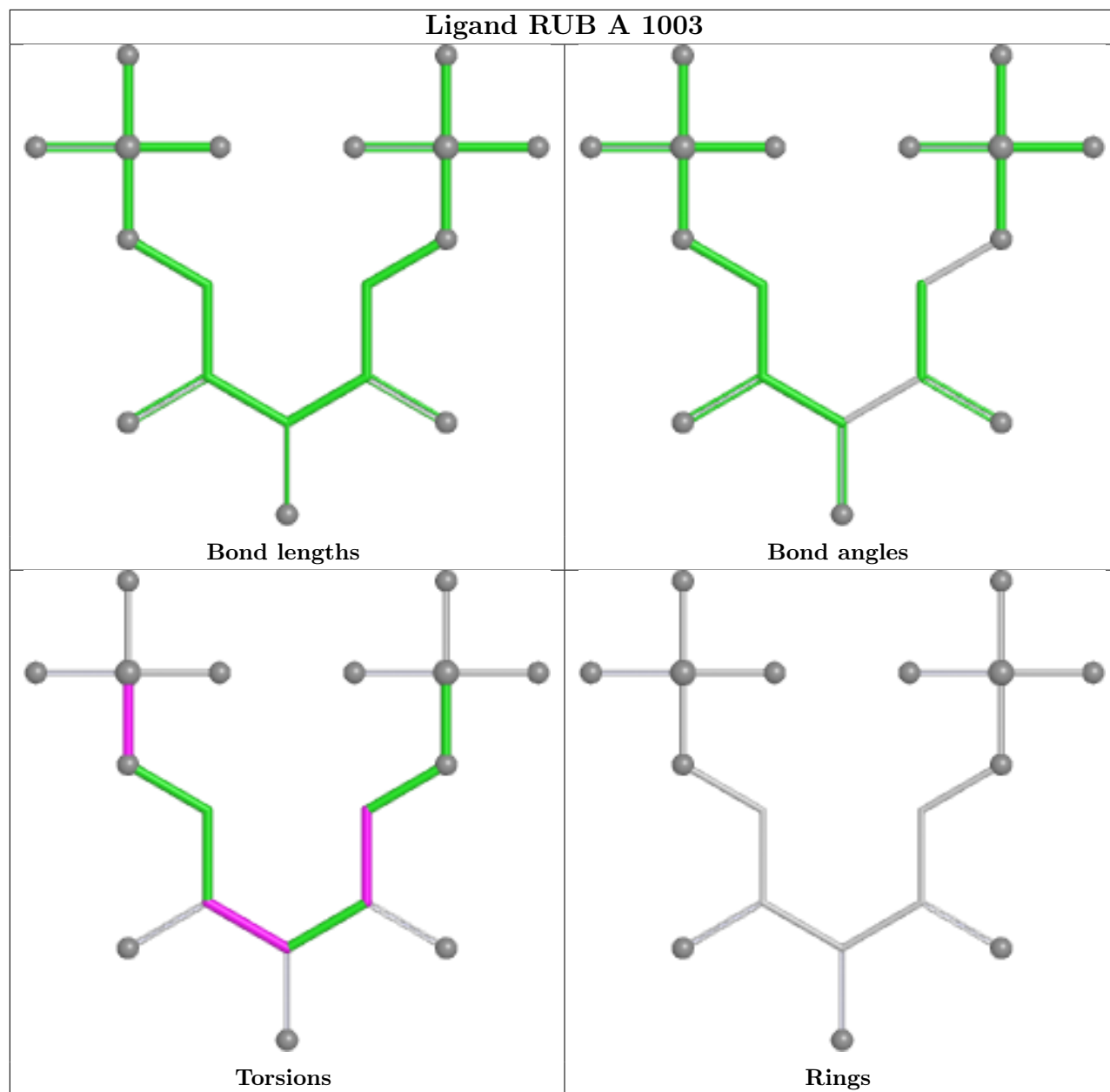
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

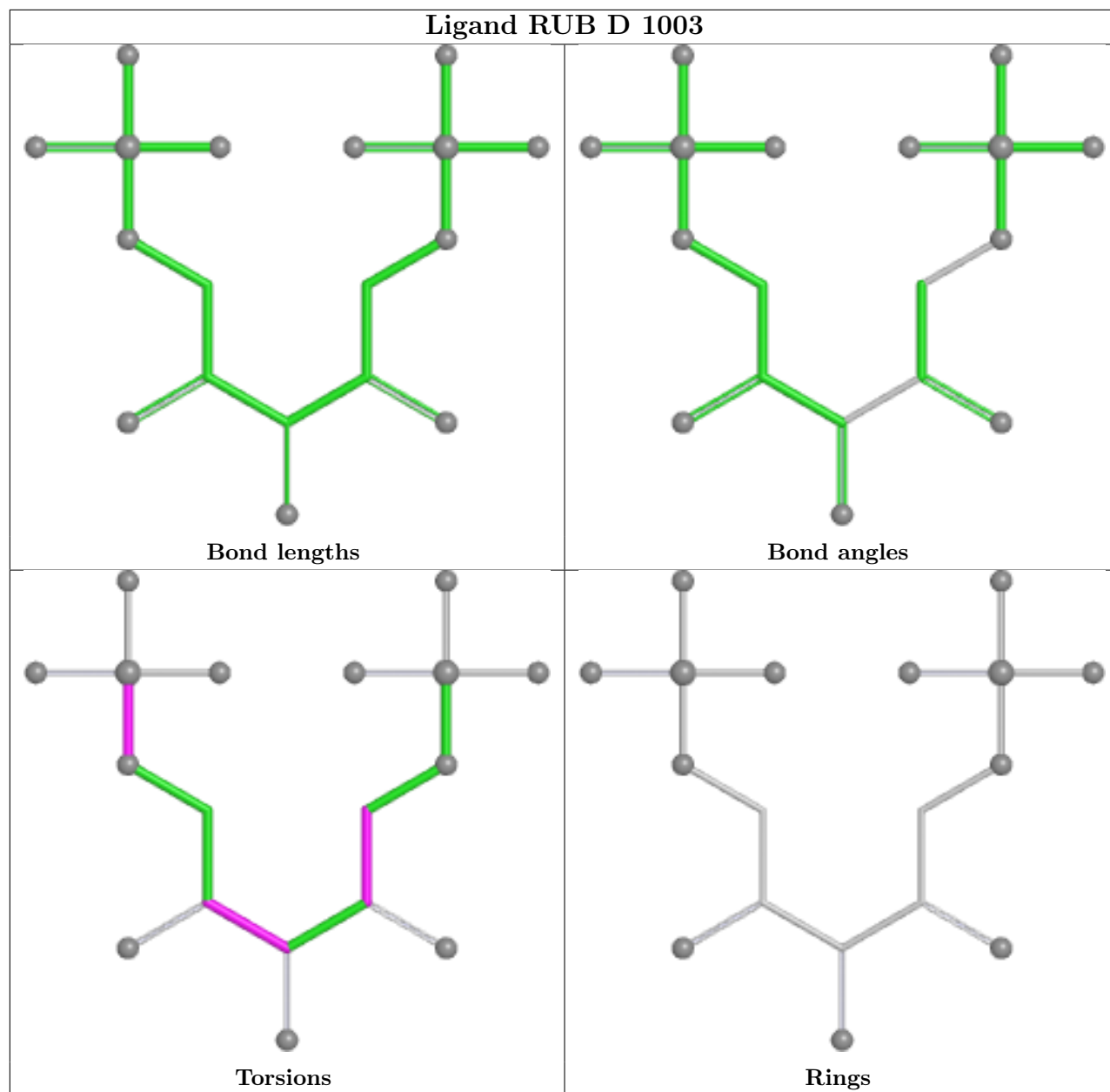
equivalents in the CSD to analyse the geometry.

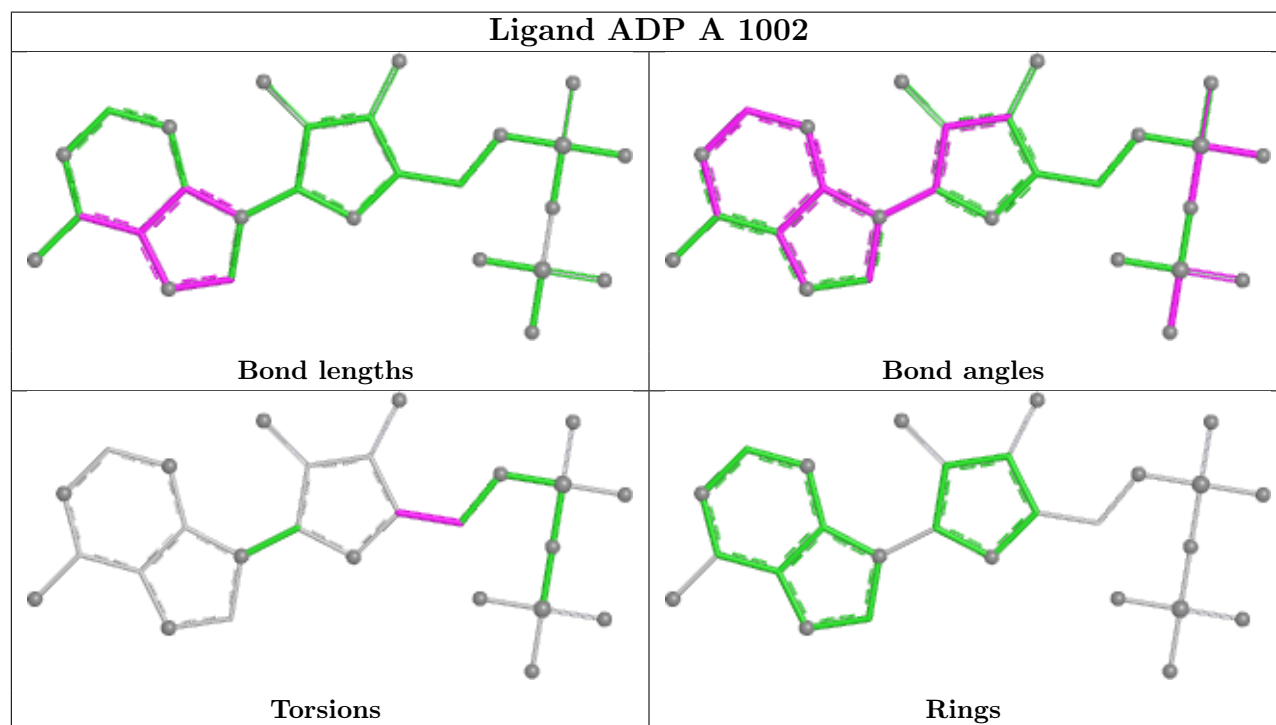
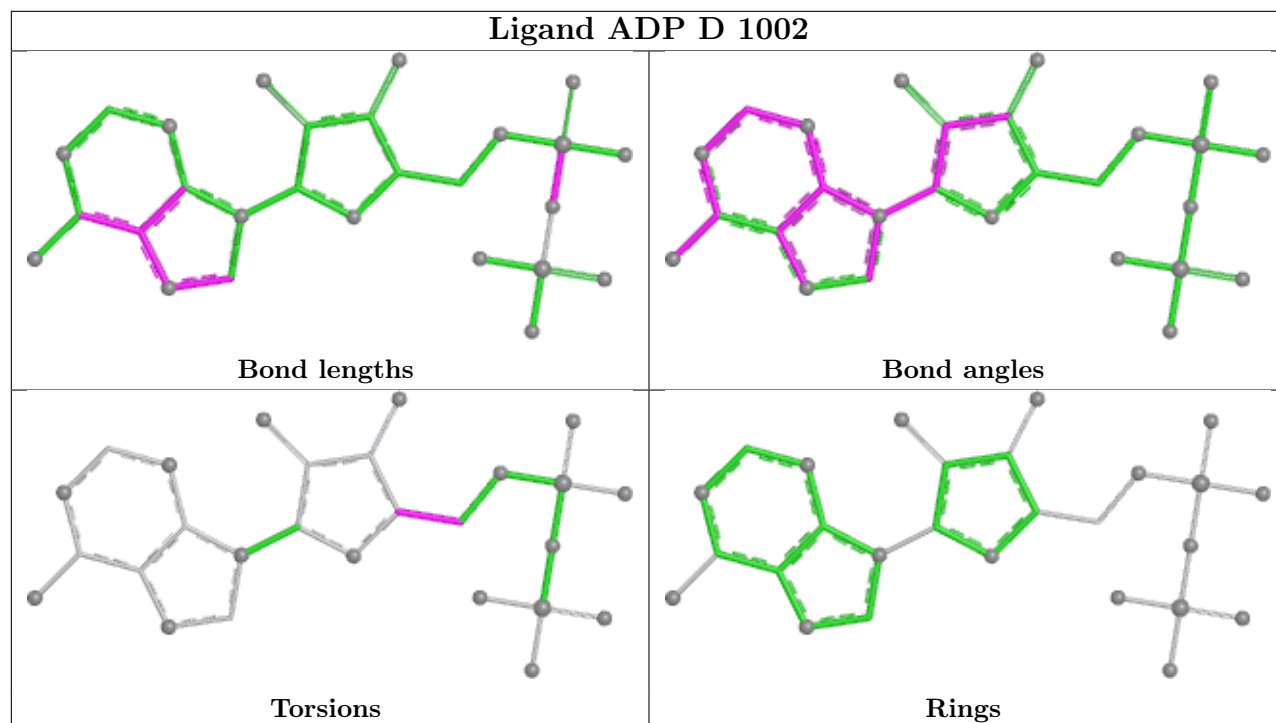


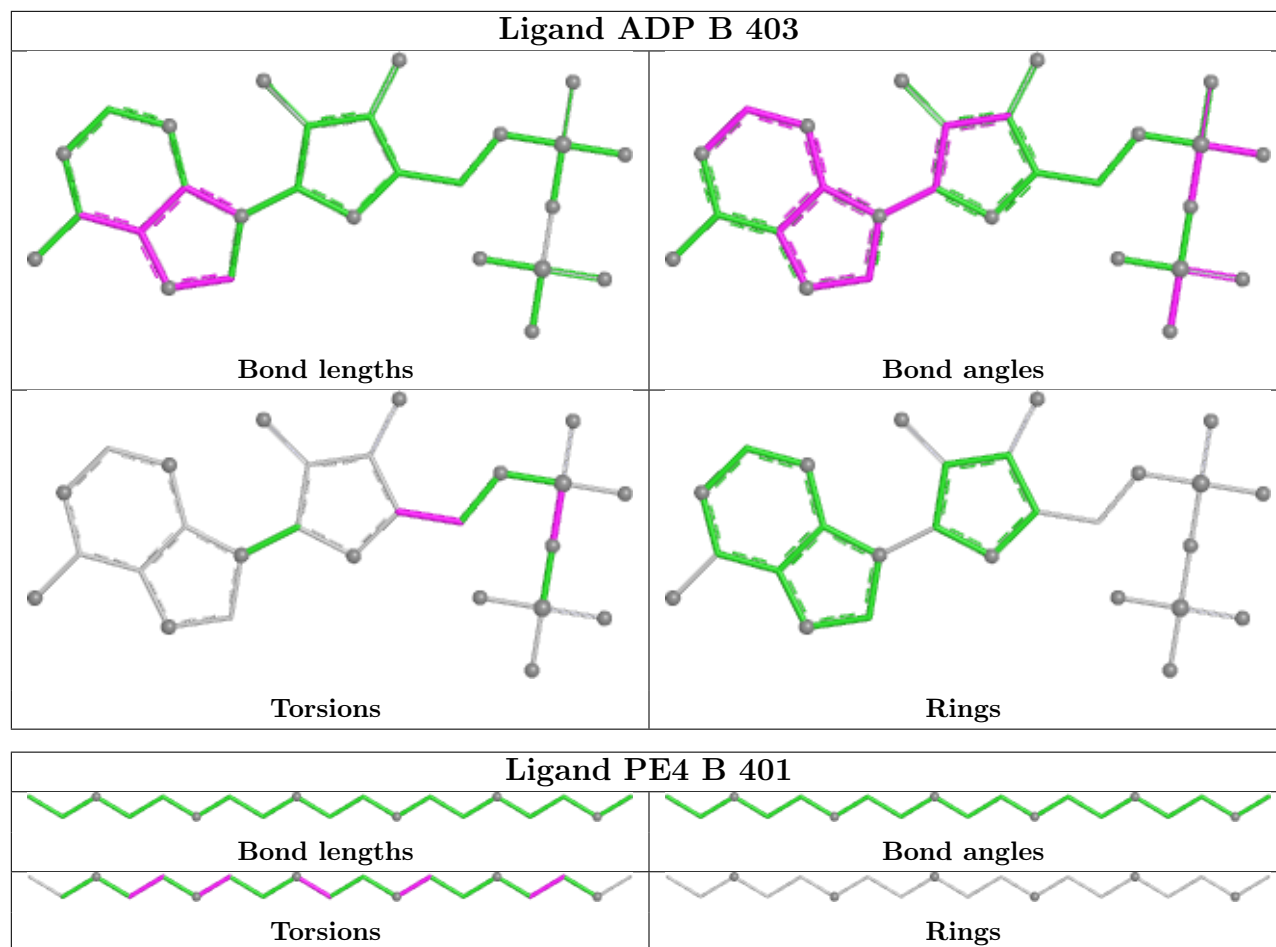












5.7 Other polymers [i](#)

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	306/311 (98%)	0.35	18 (5%)	28 25	54, 79, 149, 229	0
1	B	309/311 (99%)	0.39	17 (5%)	30 28	52, 76, 160, 197	0
1	C	306/311 (98%)	0.93	38 (12%)	8 6	67, 136, 219, 269	0
1	D	299/311 (96%)	1.23	49 (16%)	4 3	188, 234, 294, 355	0
All	All	1220/1244 (98%)	0.72	122 (10%)	12 10	52, 118, 261, 355	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	305	MET	6.1
1	C	301	ILE	4.8
1	D	155	LEU	4.6
1	B	259	PHE	4.2
1	C	215	LEU	4.2
1	C	272	LEU	4.2
1	A	210	ASN	4.0
1	D	72	LEU	4.0
1	B	210	ASN	3.9
1	D	301	ILE	3.7
1	A	259	PHE	3.7
1	C	267	GLY	3.6
1	D	75	LEU	3.5
1	D	10	ILE	3.4
1	C	62	CYS	3.4
1	D	124	VAL	3.4
1	A	215	LEU	3.3
1	B	214	ILE	3.3
1	D	223	GLY	3.2
1	D	241	LEU	3.2
1	D	275	ASN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	214	ILE	3.2
1	A	211	LEU	3.1
1	C	214	ILE	3.1
1	C	275	ASN	3.1
1	A	271	SER	3.0
1	C	209	PRO	3.0
1	C	124	VAL	2.9
1	C	302	ALA	2.9
1	D	284	THR	2.9
1	B	222	LEU	2.9
1	B	224	SER	2.9
1	B	305	MET	2.9
1	C	282	ILE	2.8
1	D	299	LEU	2.8
1	C	205	THR	2.8
1	B	266	LEU	2.8
1	D	278	ILE	2.8
1	A	206	ILE	2.7
1	D	65	VAL	2.7
1	B	272	LEU	2.7
1	C	277	GLU	2.7
1	A	208	HIS	2.7
1	D	140	ILE	2.7
1	A	213	ASN	2.7
1	D	255	LEU	2.7
1	D	82	LEU	2.6
1	C	211	LEU	2.6
1	D	226	ILE	2.6
1	C	8	LEU	2.6
1	C	241	LEU	2.6
1	D	289	LEU	2.6
1	D	300	LEU	2.6
1	D	282	ILE	2.6
1	B	309	LEU	2.6
1	D	200	LEU	2.6
1	A	311	SER	2.6
1	C	303	TYR	2.6
1	B	274	GLY	2.5
1	D	21	LEU	2.5
1	A	212	THR	2.5
1	C	122	TYR	2.5
1	A	207	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	269	PHE	2.5
1	C	230	LEU	2.5
1	D	215	LEU	2.5
1	D	37	ILE	2.5
1	B	8	LEU	2.5
1	D	259	PHE	2.5
1	D	249	ALA	2.5
1	C	300	LEU	2.5
1	C	306	LEU	2.4
1	D	84	PRO	2.4
1	D	128	LEU	2.4
1	C	212	THR	2.4
1	C	182	PHE	2.4
1	A	205	THR	2.3
1	D	205	THR	2.3
1	C	61	ASP	2.3
1	A	272	LEU	2.3
1	D	309	LEU	2.3
1	D	106	VAL	2.3
1	B	208	HIS	2.3
1	D	269	PHE	2.3
1	D	60	PRO	2.3
1	A	274	GLY	2.3
1	B	221	HIS	2.3
1	C	3	GLU	2.3
1	D	180	VAL	2.3
1	C	187	ALA	2.2
1	D	211	LEU	2.2
1	D	126	VAL	2.2
1	C	269	PHE	2.2
1	C	222	LEU	2.2
1	D	222	LEU	2.2
1	D	54	GLY	2.2
1	C	178	VAL	2.1
1	B	211	LEU	2.1
1	C	309	LEU	2.1
1	D	158	LEU	2.1
1	D	136	TYR	2.1
1	D	137	SER	2.1
1	A	265	PHE	2.1
1	C	265	PHE	2.1
1	D	129	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	209	PRO	2.1
1	C	259	PHE	2.1
1	C	274	GLY	2.1
1	B	206	ILE	2.1
1	B	269	PHE	2.0
1	D	182	PHE	2.0
1	C	210	ASN	2.0
1	C	266	LEU	2.0
1	C	250	GLU	2.0
1	D	212	THR	2.0
1	D	61	ASP	2.0
1	A	268	GLN	2.0
1	D	25	LEU	2.0
1	B	278	ILE	2.0
1	C	239	ASP	2.0
1	D	42	TYR	2.0
1	D	122	TYR	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(\AA^2)	Q<0.9
3	ADP	D	1002	27/27	0.71	0.10	219,229,248,250	0
4	RUB	D	1003	18/18	0.81	0.08	228,238,241,246	0
2	SO4	D	1001	5/5	0.85	0.06	218,224,230,240	0
5	PE4	B	401	19/24	0.88	0.16	57,81,101,103	0
4	RUB	C	1003	18/18	0.89	0.12	99,121,140,144	0
2	SO4	C	1001	5/5	0.91	0.09	100,115,140,145	0

Continued on next page...

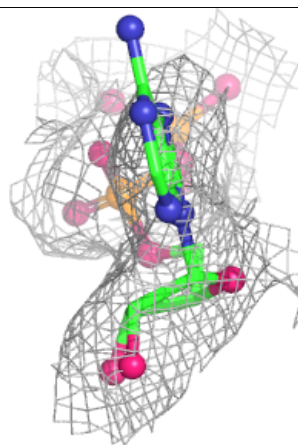
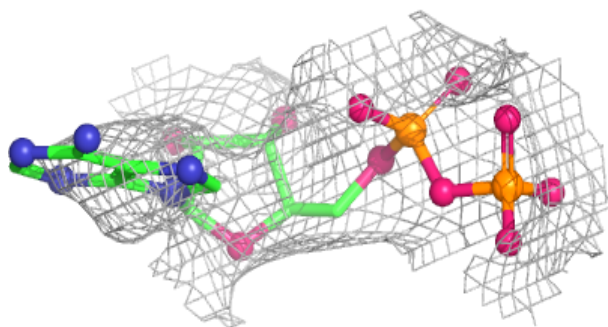
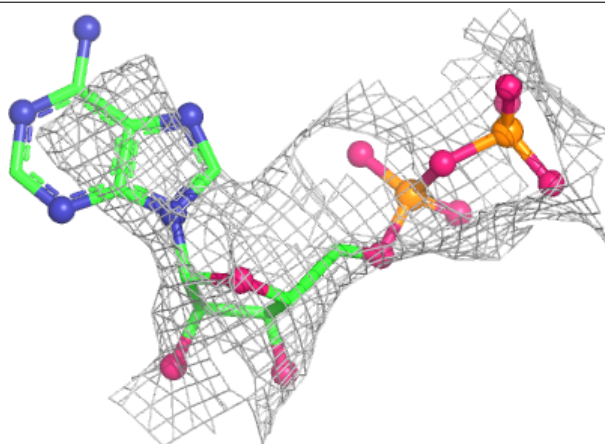
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADP	C	1002	27/27	0.93	0.10	96,129,144,145	0
4	RUB	B	404	18/18	0.94	0.11	55,75,101,103	0
4	RUB	A	1003	18/18	0.94	0.10	56,90,108,108	0
3	ADP	B	403	27/27	0.97	0.07	63,72,80,91	0
2	SO4	A	1001	5/5	0.97	0.08	75,81,91,107	0
2	SO4	B	402	5/5	0.97	0.09	57,65,77,82	0
3	ADP	A	1002	27/27	0.97	0.06	60,73,85,104	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.

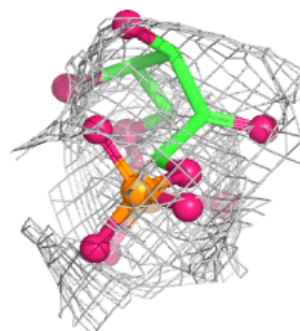
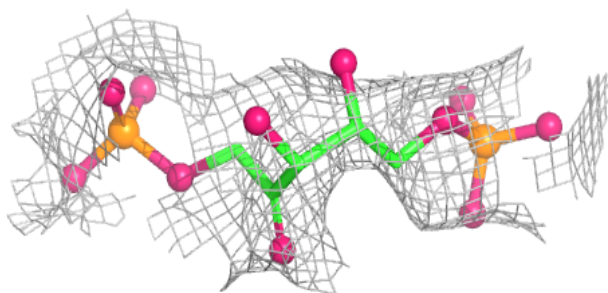
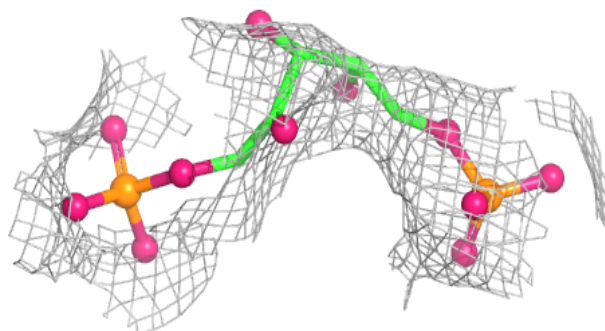
Electron density around ADP D 1002:

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

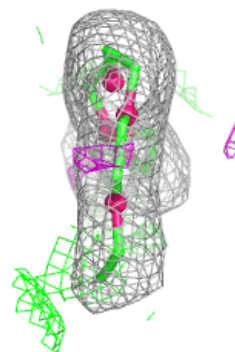
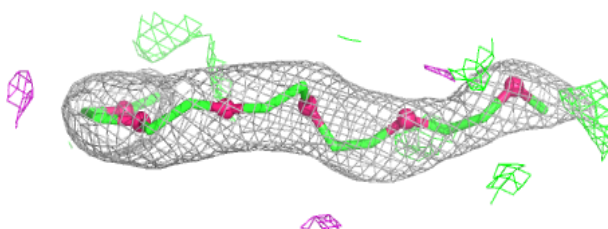
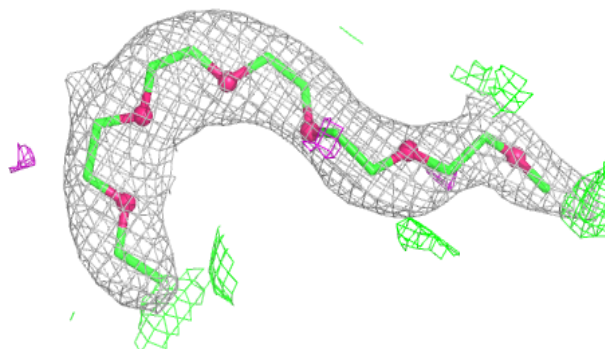


Electron density around RUB D 1003:

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

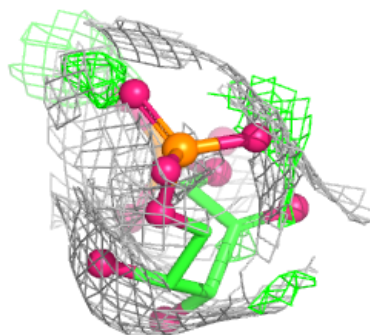
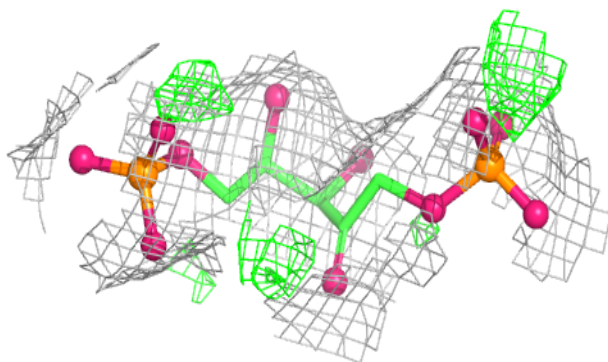
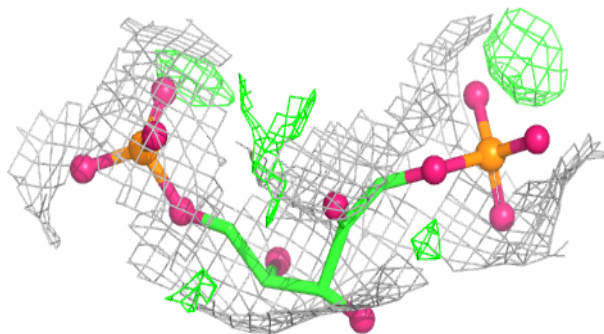
**Electron density around PE4 B 401:**

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

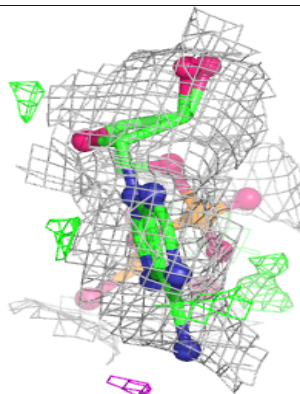
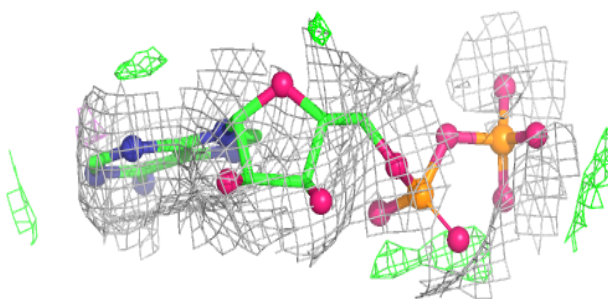
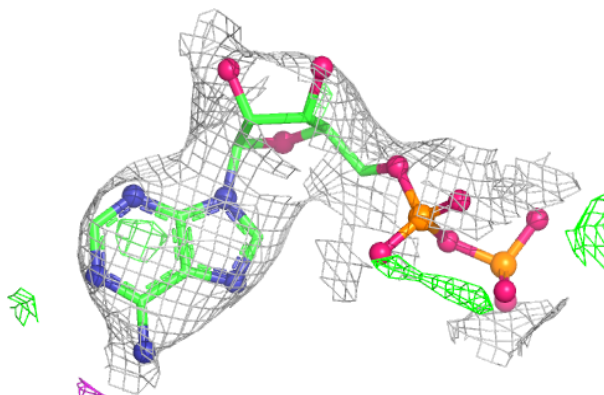


Electron density around RUB C 1003:

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

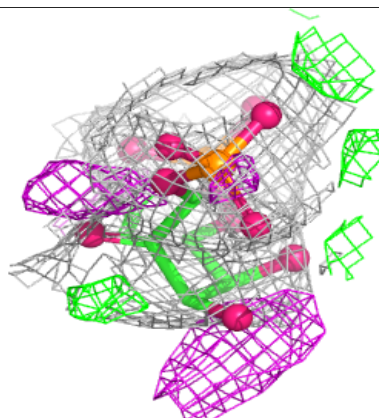
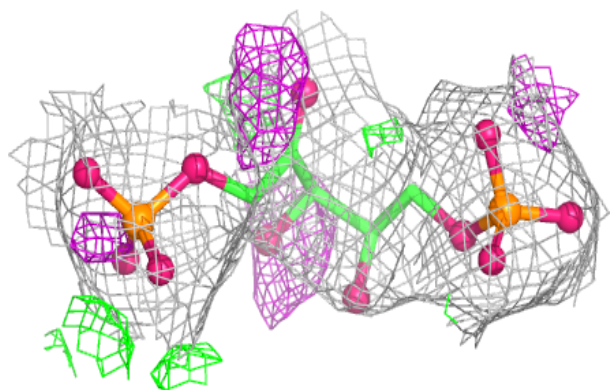
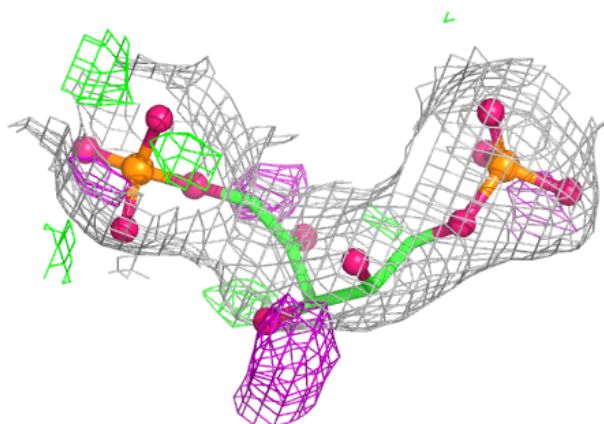
**Electron density around ADP C 1002:**

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

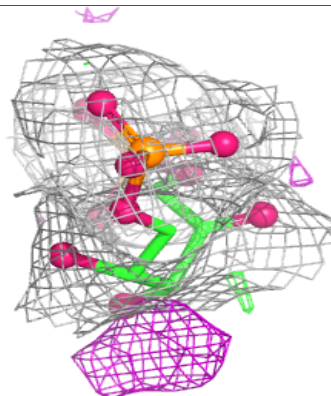
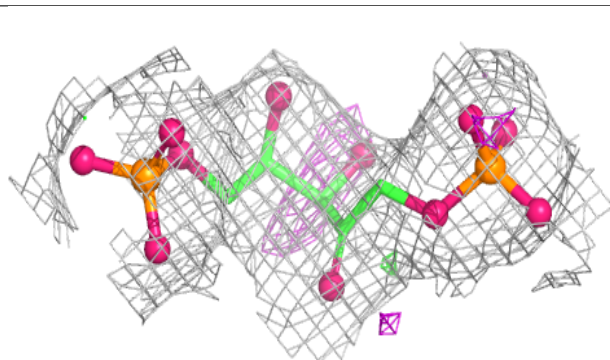
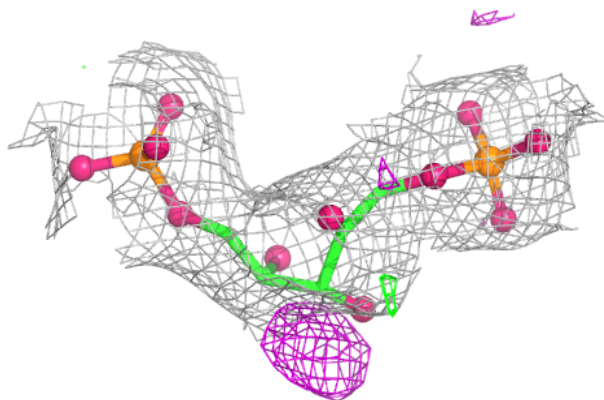


Electron density around RUB B 404:

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

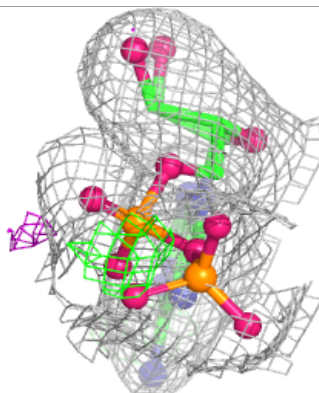
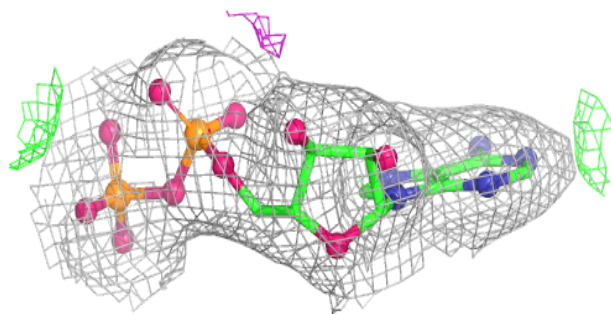
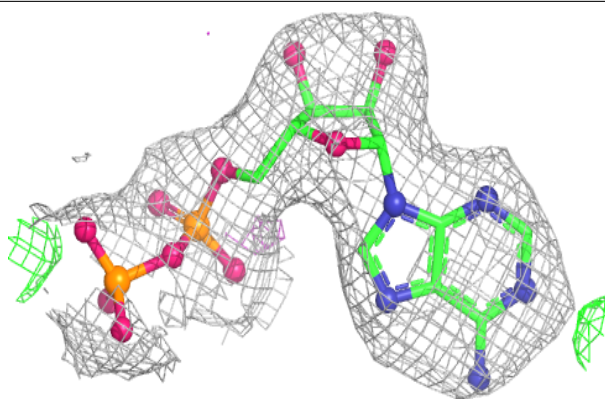
**Electron density around RUB A 1003:**

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

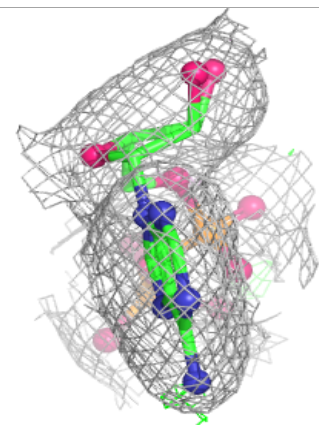
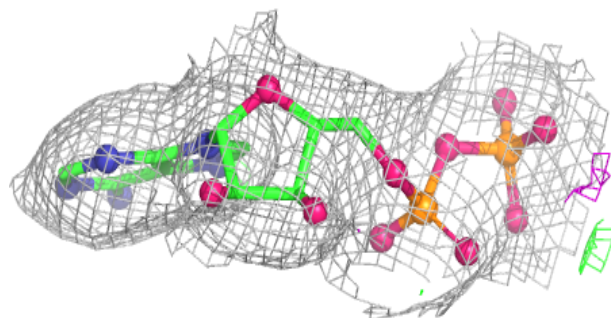
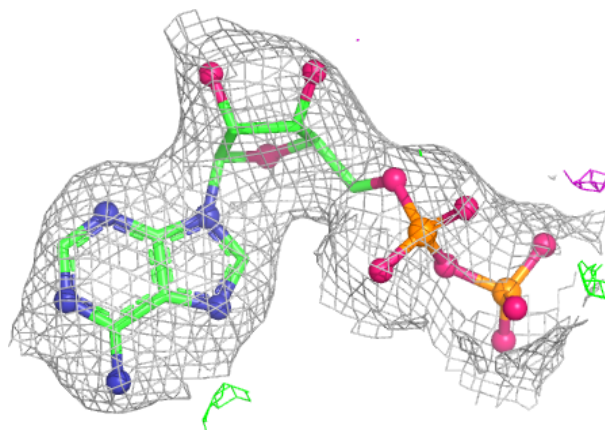


Electron density around ADP B 403:

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

**Electron density around ADP 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.