Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 04:58 pm BST

PDB ID	:	2WOJ
Title	:	ADP-AlF4 complex of S. cerevisiae GET3
Authors	:	Mateja, A.; Szlachcic, A.; Downing, M.E.; Dobosz, M.; Mariappan, M.; Hegde, R.S.; Keenan, R.J.
Deposited on	:	2009-07-26
Resolution	:	1.99 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:

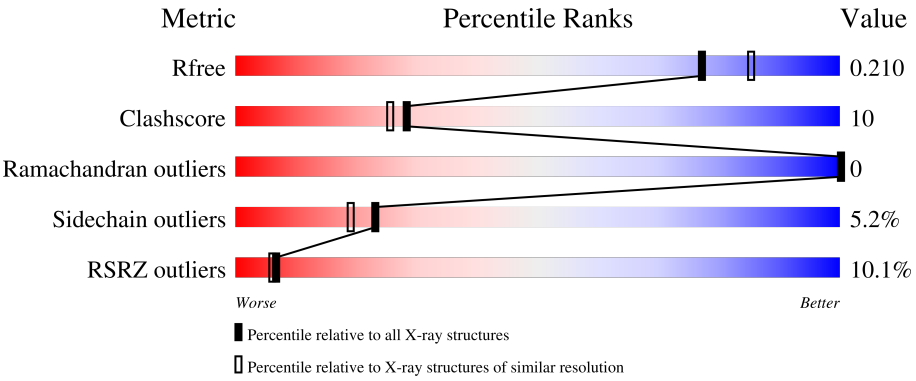
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	354	9% 66% 18% • 15%
1	B	354	7% 70% 13% • 15%
1	C	354	8% 66% 12% • 20%
1	D	354	10% 66% 17% • 14%

2 Entry composition

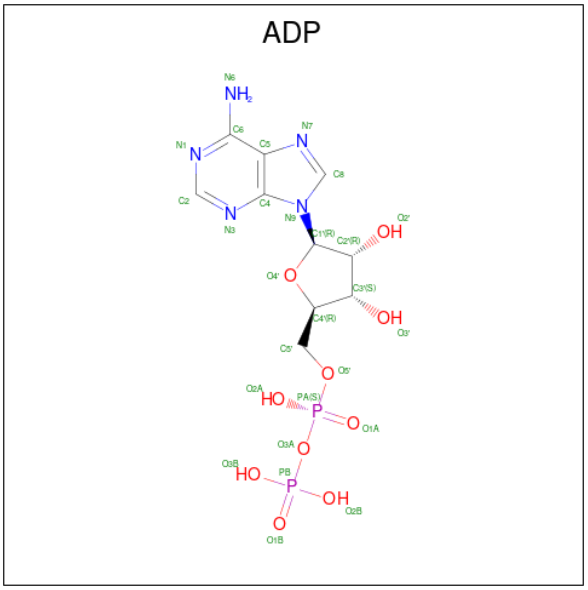
There are 6 unique types of molecules in this entry. The entry contains 10014 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATPASE GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2369	1502	391	459	17			
1	B	301	Total	C	N	O	S	0	0	0
			2372	1506	393	456	17			
1	C	284	Total	C	N	O	S	0	0	0
			2242	1425	371	430	16			
1	D	304	Total	C	N	O	S	0	0	0
			2385	1512	397	459	17			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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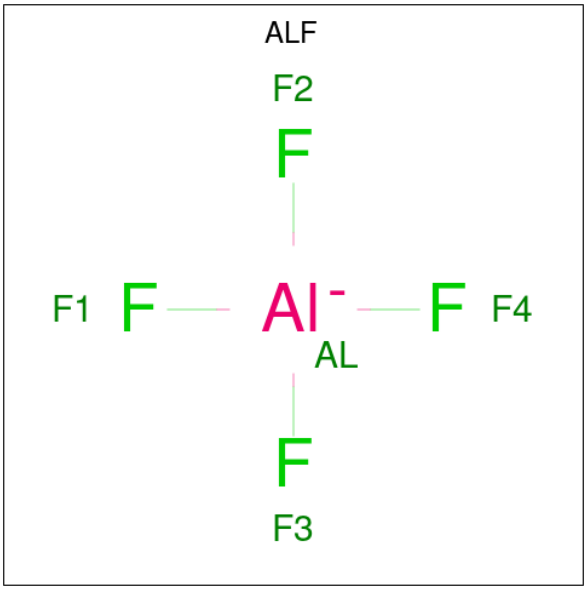
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 27 10 5 10 2	0	0
2	D	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Al F 5 1 4	0	0
3	B	1	Total Al F 5 1 4	0	0
3	C	1	Total Al F 5 1 4	0	0
3	D	1	Total Al F 5 1 4	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	C	1	Total Zn 1 1	0	0

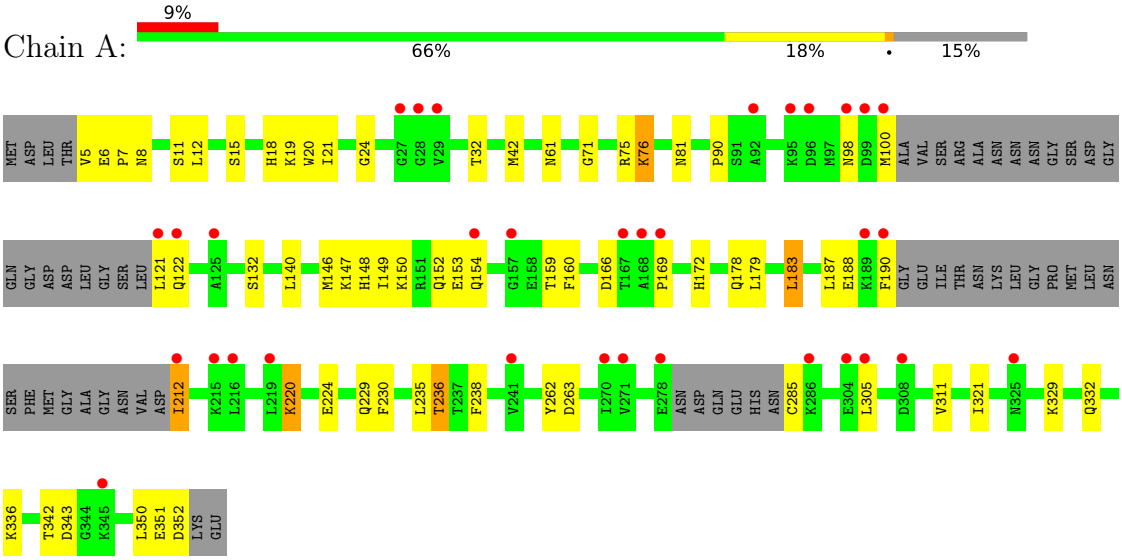
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	134	Total O 134 134	0	0
6	B	154	Total O 154 154	0	0
6	C	118	Total O 118 118	0	0
6	D	106	Total O 106 106	0	0

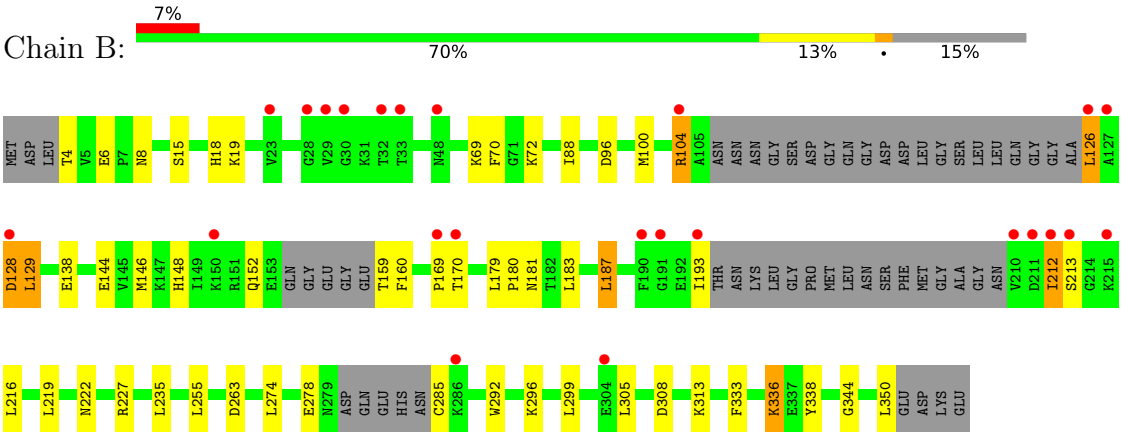
3 Residue-property plots (i)

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.

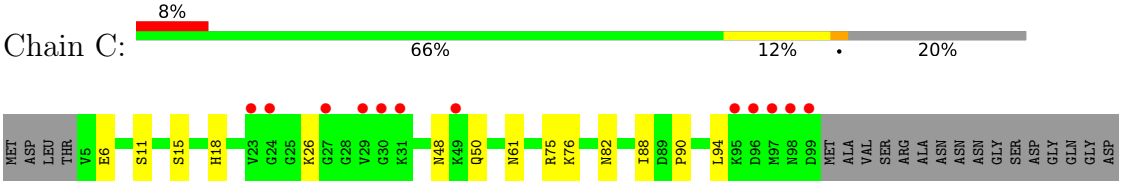
• Molecule 1: ATPASE GET3

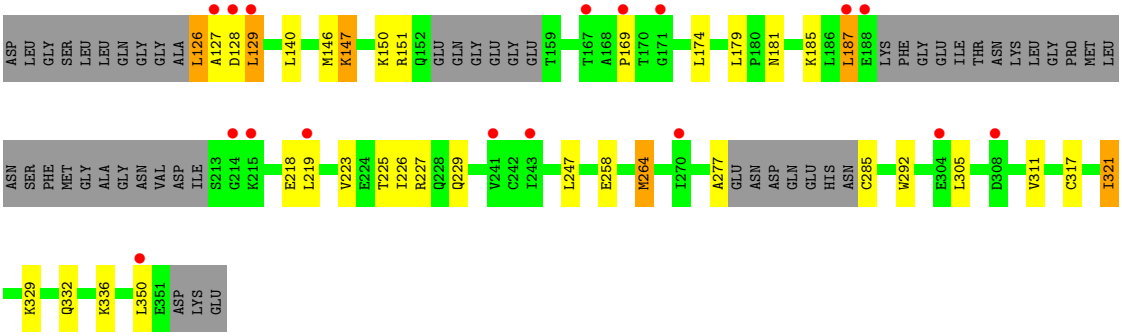


• Molecule 1: ATPASE GET3

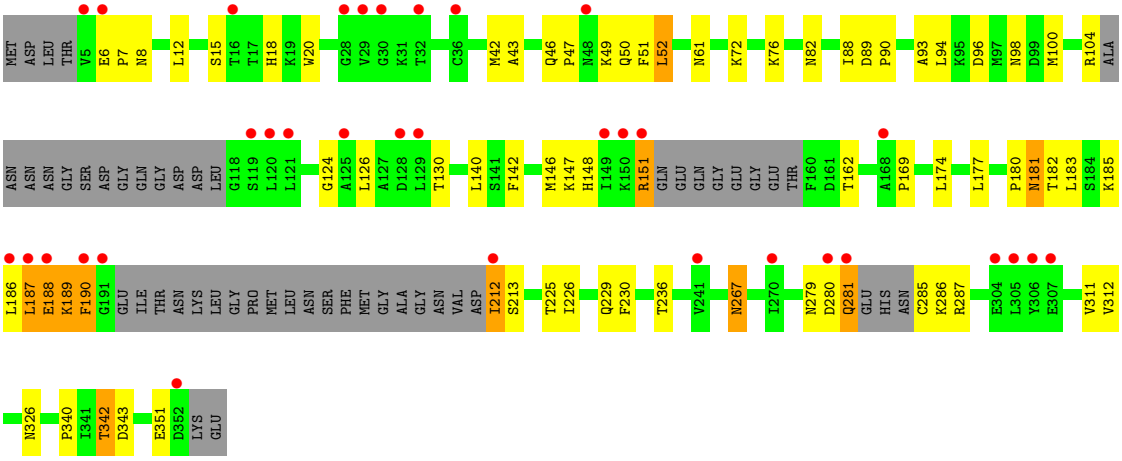


• Molecule 1: ATPASE GET3





• Molecule 1: ATPASE GET3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.61Å 82.63Å 167.28Å 90.00° 98.28° 90.00°	Depositor
Resolution (Å)	37.44 – 1.99 37.44 – 1.99	Depositor EDS
% Data completeness (in resolution range)	95.8 (37.44-1.99) 95.8 (37.44-1.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.176 , 0.213 0.174 , 0.210	Depositor DCC
R_{free} test set	4715 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 70.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10014	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: ALF, MG, ZN, ADP

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	0.53	0/2407	0.61	0/3243
1	B	0.54	0/2409	0.61	0/3247
1	C	0.53	0/2278	0.61	0/3071
1	D	0.49	0/2422	0.60	0/3262
All	All	0.52	0/9516	0.61	0/12823

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

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	2369	0	2361	50	0
1	B	2372	0	2377	46	0
1	C	2242	0	2246	43	0
1	D	2385	0	2385	55	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	134	0	0	7	0
6	B	154	0	0	4	0
6	C	118	0	0	5	0
6	D	106	0	0	2	0
All	All	10014	0	9417	185	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 10.

All (185) 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:A:98:ASN:HD21	1:A:122:GLN:HG2	1.20	1.00
1:B:159:THR:HG22	1:B:160:PHE:H	1.25	0.99
1:C:285:CYS:HB2	1:D:285:CYS:HB2	1.49	0.94
1:D:326:ASN:HD21	1:D:351:GLU:H	1.12	0.92
1:A:98:ASN:ND2	1:A:122:GLN:HG2	1.85	0.92
1:D:126:LEU:O	1:D:130:THR:HG22	1.76	0.86
1:A:98:ASN:HD21	1:A:122:GLN:CG	1.94	0.80
1:B:336:LYS:O	1:B:336:LYS:HD3	1.81	0.79
1:A:342:THR:HG22	1:A:343:ASP:OD1	1.82	0.79
1:C:151:ARG:O	1:C:151:ARG:HG2	1.83	0.78
1:A:229:GLN:O	1:A:236:THR:HG23	1.84	0.78
1:B:159:THR:HG22	1:B:160:PHE:N	2.00	0.76
1:C:15:SER:OG	1:C:18:HIS:HD2	1.68	0.75
1:D:15:SER:OG	1:D:18:HIS:HD2	1.71	0.74
1:C:50:GLN:NE2	1:C:76:LYS:HE2	2.03	0.73
1:D:94:LEU:HD13	1:D:130:THR:HG23	1.72	0.72
1:A:169:PRO:HG2	1:B:169:PRO:HG2	1.72	0.72
1:B:159:THR:CG2	1:B:160:PHE:H	2.01	0.71
1:D:90:PRO:HA	1:D:140:LEU:CD1	2.21	0.71
1:C:126:LEU:HD12	1:C:128:ASP:H	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLU:O	1:A:352:ASP:HB2	1.93	0.69
1:C:129:LEU:HD22	1:D:186:LEU:HG	1.75	0.69
1:A:230:PHE:HA	1:A:236:THR:HG21	1.75	0.67
1:B:15:SER:OG	1:B:18:HIS:HD2	1.77	0.67
1:B:72:LYS:HE3	1:B:96:ASP:OD1	1.94	0.67
1:C:169:PRO:HG2	1:D:169:PRO:HG2	1.77	0.67
1:B:148:HIS:ND1	1:B:159:THR:HG23	2.09	0.67
1:D:189:LYS:N	1:D:189:LYS:HD3	2.11	0.66
1:D:147:LYS:O	1:D:151:ARG:HD3	1.99	0.63
1:A:178:GLN:NE2	1:A:262:TYR:OH	2.32	0.63
1:A:76:LYS:HE3	1:A:81:ASN:O	1.99	0.63
1:D:280:ASP:O	1:D:281:GLN:HG3	1.99	0.62
1:B:6:GLU:HG3	1:B:8:ASN:ND2	2.15	0.62
1:B:333:PHE:CE2	1:B:336:LYS:HE3	2.35	0.62
1:C:181:ASN:ND2	1:C:227:ARG:HE	1.99	0.61
1:A:183:LEU:O	1:A:187:LEU:HB2	2.00	0.61
1:D:230:PHE:HA	1:D:236:THR:HG21	1.83	0.60
1:A:159:THR:HG22	6:A:2060:HOH:O	2.01	0.60
1:A:212:ILE:HD12	1:A:212:ILE:O	2.01	0.60
1:C:285:CYS:CB	1:D:285:CYS:HB2	2.28	0.60
1:D:142:PHE:HE1	1:D:180:PRO:HG3	1.66	0.59
1:D:280:ASP:C	1:D:281:GLN:HG3	2.22	0.59
1:C:146:MET:HG2	1:C:226:ILE:HD11	1.84	0.59
1:A:15:SER:OG	1:A:18:HIS:HD2	1.83	0.59
1:A:336:LYS:O	1:A:336:LYS:HG3	2.02	0.59
1:B:212:ILE:HD13	1:B:213:SER:N	2.18	0.59
1:A:321:ILE:HG12	1:A:350:LEU:CD2	2.34	0.58
1:C:219:LEU:O	1:C:223:VAL:HG13	2.04	0.57
1:B:128:ASP:OD1	1:B:128:ASP:N	2.37	0.57
1:D:146:MET:HG2	1:D:226:ILE:HD11	1.87	0.57
1:B:6:GLU:CG	1:B:8:ASN:ND2	2.68	0.57
1:D:20:TRP:HD1	1:D:236:THR:HG22	1.70	0.57
1:D:90:PRO:HA	1:D:140:LEU:HD12	1.87	0.56
1:D:49:LYS:O	1:D:82:ASN:OD1	2.23	0.56
1:A:20:TRP:HB2	1:A:236:THR:HB	1.88	0.56
1:B:6:GLU:CG	1:B:8:ASN:HD21	2.19	0.55
1:C:126:LEU:CD1	1:C:128:ASP:H	2.19	0.55
1:A:20:TRP:HD1	1:A:236:THR:HG22	1.72	0.55
1:C:50:GLN:HE22	1:C:76:LYS:HE2	1.69	0.55
1:A:179:LEU:O	1:A:183:LEU:HB2	2.07	0.54
1:C:147:LYS:O	1:C:151:ARG:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:HA	1:B:129:LEU:HD21	1.90	0.54
1:B:181:ASN:ND2	1:B:227:ARG:HE	2.06	0.54
1:A:6:GLU:HG3	1:A:8:ASN:ND2	2.23	0.54
1:C:48:ASN:HB2	6:C:2018:HOH:O	2.07	0.54
1:D:72:LYS:HD3	1:D:89:ASP:H	1.72	0.54
1:B:69:LYS:HE3	1:B:70:PHE:O	2.08	0.53
1:D:187:LEU:O	1:D:190:PHE:HB3	2.07	0.53
1:C:329:LYS:O	1:C:332:GLN:HG2	2.09	0.53
1:D:212:ILE:HD12	1:D:212:ILE:O	2.07	0.53
1:C:151:ARG:O	1:C:151:ARG:CG	2.56	0.53
1:C:317:CYS:SG	1:C:350:LEU:HD12	2.49	0.53
1:D:188:GLU:HB3	1:D:189:LYS:HD3	1.90	0.53
1:A:90:PRO:HA	1:A:140:LEU:CD1	2.38	0.53
1:B:126:LEU:HA	1:B:129:LEU:CD2	2.40	0.52
1:A:71:GLY:HA3	1:A:75:ARG:HH12	1.75	0.52
1:B:126:LEU:HD23	1:B:129:LEU:HD11	1.90	0.52
1:C:50:GLN:HE22	1:C:82:ASN:HA	1.75	0.52
1:D:326:ASN:ND2	1:D:351:GLU:H	1.95	0.51
1:A:220:LYS:HD2	6:A:2078:HOH:O	2.10	0.51
1:C:321:ILE:HD13	1:C:350:LEU:HD13	1.91	0.51
1:D:146:MET:HG2	1:D:226:ILE:CD1	2.40	0.51
1:D:12:LEU:HG	1:D:42:MET:CE	2.41	0.51
1:D:20:TRP:O	1:D:236:THR:HA	2.10	0.51
1:C:126:LEU:HD13	1:C:127:ALA:N	2.24	0.51
1:A:172:HIS:HD2	6:A:2068:HOH:O	1.94	0.51
1:A:172:HIS:HE1	1:B:138:GLU:OE2	1.95	0.50
1:C:50:GLN:NE2	1:C:82:ASN:HA	2.26	0.50
1:D:52:LEU:HD12	1:D:148:HIS:CE1	2.47	0.50
1:A:61:ASN:ND2	6:A:2029:HOH:O	2.43	0.49
1:A:285:CYS:HB3	1:B:285:CYS:HB2	1.93	0.49
1:C:129:LEU:HD23	1:D:182:THR:HG23	1.94	0.49
1:B:179:LEU:CD1	1:B:183:LEU:HD13	2.42	0.49
1:D:20:TRP:CD1	1:D:236:THR:HG22	2.47	0.49
1:C:187:LEU:HD21	1:C:219:LEU:HD23	1.93	0.49
1:D:72:LYS:HE3	1:D:93:ALA:HB2	1.94	0.49
1:D:43:ALA:O	1:D:82:ASN:ND2	2.45	0.49
1:D:51:PHE:CD1	1:D:162:THR:HB	2.49	0.48
1:B:6:GLU:HG2	1:B:8:ASN:HD21	1.78	0.48
1:A:149:ILE:O	1:A:153:GLU:HG2	2.13	0.48
1:B:144:GLU:O	1:B:148:HIS:HD2	1.96	0.48
1:A:229:GLN:O	1:A:236:THR:CG2	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LYS:HD3	1:B:235:LEU:HD22	1.96	0.47
1:A:190:PHE:C	1:A:190:PHE:CD2	2.88	0.47
1:B:179:LEU:HD12	1:B:183:LEU:HD13	1.97	0.47
1:B:274:LEU:HD12	1:B:313:LYS:HB3	1.96	0.47
1:C:181:ASN:ND2	1:C:227:ARG:NE	2.62	0.47
1:A:224:GLU:HG2	6:A:2078:HOH:O	2.14	0.47
1:C:6:GLU:HB3	6:C:2003:HOH:O	2.14	0.46
1:C:181:ASN:HD22	1:C:227:ARG:NE	2.14	0.46
1:A:24:GLY:HA3	1:A:238:PHE:CZ	2.50	0.46
1:A:98:ASN:ND2	6:A:2047:HOH:O	2.48	0.46
1:D:189:LYS:N	1:D:189:LYS:CD	2.78	0.46
1:D:50:GLN:NE2	1:D:76:LYS:HE2	2.31	0.46
1:C:90:PRO:HA	1:C:140:LEU:CD1	2.45	0.46
1:C:26:LYS:HE3	1:C:247:LEU:HB3	1.96	0.45
1:A:148:HIS:O	1:A:152:GLN:HG3	2.17	0.45
1:A:147:LYS:HE3	1:A:147:LYS:HB2	1.45	0.45
1:B:313:LYS:HE3	6:B:2134:HOH:O	2.17	0.45
1:B:19:LYS:NZ	1:B:152:GLN:NE2	2.64	0.45
1:B:299:LEU:HD22	1:B:313:LYS:HE2	1.98	0.44
1:C:146:MET:HG2	1:C:226:ILE:CD1	2.48	0.44
1:A:6:GLU:HA	1:A:7:PRO:HD3	1.82	0.44
1:A:329:LYS:O	1:A:332:GLN:HG2	2.18	0.44
1:D:285:CYS:N	6:D:2081:HOH:O	2.51	0.44
1:A:5:VAL:HG23	1:A:5:VAL:O	2.17	0.44
1:A:19:LYS:HG3	1:A:235:LEU:HD22	1.98	0.44
1:C:88:ILE:HG13	6:C:2050:HOH:O	2.17	0.44
1:B:187:LEU:HD13	1:B:187:LEU:N	2.33	0.44
1:B:278:GLU:CD	1:B:292:TRP:HE1	2.21	0.44
1:B:4:THR:N	6:B:2002:HOH:O	2.51	0.44
1:D:15:SER:OG	1:D:18:HIS:CD2	2.60	0.43
1:D:142:PHE:CE1	1:D:180:PRO:HG3	2.49	0.43
1:B:181:ASN:HD22	1:B:227:ARG:HE	1.66	0.43
1:B:187:LEU:N	1:B:187:LEU:CD1	2.80	0.43
1:C:174:LEU:HD22	1:C:258:GLU:HG2	1.99	0.43
1:B:179:LEU:N	1:B:180:PRO:CD	2.82	0.43
1:C:61:ASN:ND2	6:C:2034:HOH:O	2.51	0.43
1:A:32:THR:OG1	1:A:166:ASP:OD2	2.37	0.43
1:A:121:LEU:N	1:A:122:GLN:OE1	2.52	0.43
1:D:177:LEU:HD23	1:D:177:LEU:HA	1.88	0.43
1:C:277:ALA:HB3	1:C:292:TRP:CD1	2.54	0.43
1:A:159:THR:HG23	1:A:160:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PHE:HA	1:A:236:THR:CG2	2.45	0.43
1:D:181:ASN:OD1	1:D:181:ASN:C	2.57	0.43
1:C:264:MET:HE2	1:C:264:MET:HB2	1.87	0.42
1:C:336:LYS:HG3	1:C:336:LYS:O	2.20	0.42
6:C:2020:HOH:O	1:D:287:ARG:HG2	2.20	0.42
1:D:229:GLN:O	1:D:236:THR:HG23	2.19	0.42
1:B:19:LYS:CE	1:B:152:GLN:NE2	2.83	0.42
1:A:21:ILE:HD13	1:A:42:MET:CE	2.50	0.42
1:D:188:GLU:C	1:D:189:LYS:HD3	2.39	0.42
1:B:126:LEU:N	1:B:128:ASP:OD1	2.53	0.42
1:A:321:ILE:HG12	1:A:350:LEU:HD23	2.01	0.42
1:C:15:SER:OG	1:C:18:HIS:CD2	2.59	0.42
1:D:61:ASN:ND2	6:D:2029:HOH:O	2.51	0.42
1:D:183:LEU:O	1:D:187:LEU:HB2	2.20	0.42
1:A:12:LEU:HG	1:A:42:MET:HE1	2.01	0.42
1:A:212:ILE:N	6:A:2072:HOH:O	2.53	0.42
1:B:170:THR:HG23	1:B:255:LEU:HD13	2.01	0.42
1:C:181:ASN:O	1:C:185:LYS:HG3	2.20	0.41
1:B:146:MET:HG2	1:B:222:ASN:OD1	2.19	0.41
1:C:150:LYS:CE	1:C:218:GLU:OE1	2.68	0.41
1:A:220:LYS:HA	1:A:220:LYS:HD3	1.84	0.41
1:C:126:LEU:HD12	1:C:128:ASP:N	2.28	0.41
1:C:129:LEU:HD21	1:D:185:LYS:HB2	2.02	0.41
1:D:98:ASN:HD21	1:D:124:GLY:HA2	1.86	0.41
1:D:8:ASN:HA	1:D:312:VAL:HG22	2.03	0.41
1:B:296:LYS:HD2	1:B:296:LYS:HA	1.79	0.41
1:C:90:PRO:O	1:C:94:LEU:HG	2.20	0.41
1:D:72:LYS:HE2	1:D:88:ILE:HG13	2.02	0.41
1:D:96:ASP:O	1:D:100:MET:HG3	2.21	0.41
1:A:188:GLU:O	1:A:190:PHE:N	2.54	0.41
1:D:6:GLU:HA	1:D:7:PRO:HD3	1.90	0.41
1:B:338:TYR:OH	1:B:344:GLY:HA2	2.21	0.40
1:D:279:ASN:CG	1:D:340:PRO:HB2	2.41	0.40
1:D:342:THR:HG22	1:D:343:ASP:OD1	2.21	0.40
1:B:100:MET:O	1:B:104:ARG:HB2	2.21	0.40
1:C:225:THR:O	1:C:229:GLN:HG3	2.22	0.40
1:B:193:ILE:HG22	6:B:2087:HOH:O	2.21	0.40
1:B:219:LEU:HB2	6:B:2053:HOH:O	2.22	0.40
1:D:46:GLN:N	1:D:47:PRO:HD3	2.37	0.40
1:D:267:ASN:HD22	1:D:267:ASN:C	2.25	0.40
1:A:90:PRO:HA	1:A:140:LEU:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:THR:CG2	1:B:160:PHE:N	2.70	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	293/354 (83%)	285 (97%)	8 (3%)	0	100	100
1	B	291/354 (82%)	288 (99%)	3 (1%)	0	100	100
1	C	274/354 (77%)	268 (98%)	6 (2%)	0	100	100
1	D	294/354 (83%)	288 (98%)	6 (2%)	0	100	100
All	All	1152/1416 (81%)	1129 (98%)	23 (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	267/309 (86%)	253 (95%)	14 (5%)	23	19
1	B	269/309 (87%)	256 (95%)	13 (5%)	25	22
1	C	255/309 (82%)	244 (96%)	11 (4%)	29	26
1	D	269/309 (87%)	252 (94%)	17 (6%)	18	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1060/1236 (86%)	1005 (95%)	55 (5%)	23 19

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	76	LYS
1	A	100	MET
1	A	132	SER
1	A	146	MET
1	A	150	LYS
1	A	154	GLN
1	A	183	LEU
1	A	212	ILE
1	A	220	LYS
1	A	236	THR
1	A	263	ASP
1	A	305	LEU
1	A	311	VAL
1	B	88	ILE
1	B	104	ARG
1	B	126	LEU
1	B	128	ASP
1	B	129	LEU
1	B	187	LEU
1	B	212	ILE
1	B	216	LEU
1	B	263	ASP
1	B	305	LEU
1	B	308	ASP
1	B	336	LYS
1	B	350	LEU
1	C	11	SER
1	C	75	ARG
1	C	126	LEU
1	C	129	LEU
1	C	147	LYS
1	C	179	LEU
1	C	187	LEU
1	C	264	MET
1	C	305	LEU
1	C	311	VAL

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Mol	Chain	Res	Type
1	C	321	ILE
1	D	52	LEU
1	D	104	ARG
1	D	151	ARG
1	D	174	LEU
1	D	181	ASN
1	D	187	LEU
1	D	188	GLU
1	D	189	LYS
1	D	190	PHE
1	D	212	ILE
1	D	213	SER
1	D	225	THR
1	D	267	ASN
1	D	281	GLN
1	D	286	LYS
1	D	311	VAL
1	D	342	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	41	GLN
1	A	50	GLN
1	A	61	ASN
1	A	98	ASN
1	A	152	GLN
1	A	154	GLN
1	A	172	HIS
1	A	178	GLN
1	A	217	ASN
1	A	222	ASN
1	A	289	GLN
1	A	301	GLN
1	A	325	ASN
1	A	326	ASN
1	B	18	HIS
1	B	41	GLN
1	B	61	ASN
1	B	181	ASN
1	B	217	ASN

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Mol	Chain	Res	Type
1	B	301	GLN
1	B	325	ASN
1	B	326	ASN
1	C	18	HIS
1	C	50	GLN
1	C	61	ASN
1	C	152	GLN
1	C	181	ASN
1	C	217	ASN
1	C	222	ASN
1	C	228	GLN
1	C	301	GLN
1	C	326	ASN
1	D	18	HIS
1	D	41	GLN
1	D	61	ASN
1	D	81	ASN
1	D	98	ASN
1	D	148	HIS
1	D	217	ASN
1	D	222	ASN
1	D	267	ASN
1	D	325	ASN
1	D	326	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	ALF	D	402	2,4,6	0,4,4	-	-	-		
2	ADP	C	401	4,3	24,29,29	1.36	4 (16%)	29,45,45	1.50	6 (20%)
3	ALF	B	402	2,4,6	0,4,4	-	-	-		
3	ALF	A	402	2,4,6	0,4,4	-	-	-		
2	ADP	B	401	4,3	24,29,29	1.04	1 (4%)	29,45,45	1.62	6 (20%)
2	ADP	A	401	4,3	24,29,29	1.37	2 (8%)	29,45,45	1.50	5 (17%)
3	ALF	C	402	2,4,6	0,4,4	-	-	-		
2	ADP	D	401	4,3	24,29,29	1.47	4 (16%)	29,45,45	1.49	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	401	4,3	-	0/12/32/32	0/3/3/3
2	ADP	D	401	4,3	-	0/12/32/32	0/3/3/3
2	ADP	C	401	4,3	-	0/12/32/32	0/3/3/3
2	ADP	A	401	4,3	-	0/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ADP	O4'-C1'	4.30	1.47	1.41
2	D	401	ADP	O4'-C1'	3.41	1.45	1.41
2	D	401	ADP	PB-O3B	-2.66	1.44	1.54
2	A	401	ADP	PB-O3B	-2.59	1.44	1.54
2	C	401	ADP	PB-O1B	2.57	1.58	1.50
2	C	401	ADP	PB-O3B	-2.56	1.45	1.54
2	C	401	ADP	O4'-C1'	2.40	1.44	1.41
2	B	401	ADP	PB-O3B	-2.31	1.45	1.54
2	D	401	ADP	C4-N3	2.24	1.38	1.35
2	D	401	ADP	PB-O1B	2.14	1.57	1.50
2	C	401	ADP	C2'-C1'	2.06	1.56	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	ADP	C1'-N9-C4	-4.08	119.47	126.64
2	C	401	ADP	C1'-N9-C4	-3.92	119.75	126.64
2	B	401	ADP	C1'-N9-C4	-3.78	120.00	126.64
2	D	401	ADP	C1'-N9-C4	-3.71	120.13	126.64
2	B	401	ADP	O2B-PB-O1B	-3.08	98.61	110.68
2	B	401	ADP	PA-O3A-PB	3.02	143.18	132.83
2	B	401	ADP	O3B-PB-O3A	3.01	114.71	104.64
2	D	401	ADP	O3B-PB-O2B	2.93	118.82	107.64
2	B	401	ADP	O3B-PB-O2B	2.69	117.93	107.64
2	A	401	ADP	C4-C5-N7	2.65	112.16	109.40
2	C	401	ADP	O3B-PB-O3A	2.64	113.48	104.64
2	A	401	ADP	PA-O3A-PB	2.59	141.71	132.83
2	D	401	ADP	O2B-PB-O3A	-2.56	96.03	104.64
2	C	401	ADP	O3B-PB-O1B	2.55	120.66	110.68
2	A	401	ADP	O3B-PB-O1B	2.39	120.06	110.68
2	C	401	ADP	PA-O3A-PB	2.34	140.86	132.83
2	A	401	ADP	O3B-PB-O2B	2.33	116.53	107.64
2	C	401	ADP	C4-C5-N7	2.30	111.80	109.40
2	D	401	ADP	O3B-PB-O3A	2.27	112.26	104.64
2	D	401	ADP	PA-O3A-PB	2.23	140.48	132.83
2	B	401	ADP	O3B-PB-O1B	2.19	119.24	110.68
2	C	401	ADP	O2B-PB-O1B	-2.06	102.64	110.68

There are no chirality outliers.

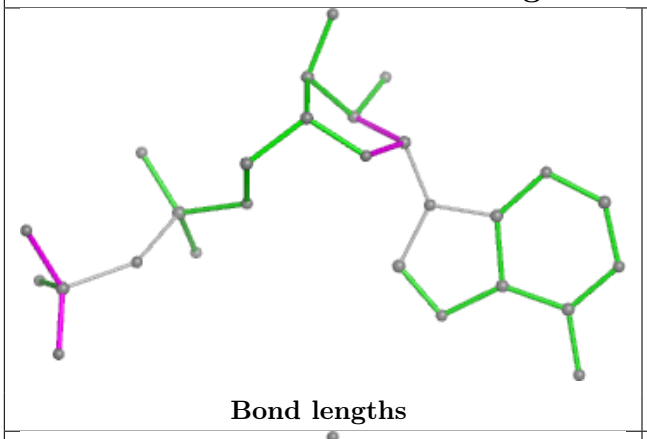
There are no torsion outliers.

There are no ring outliers.

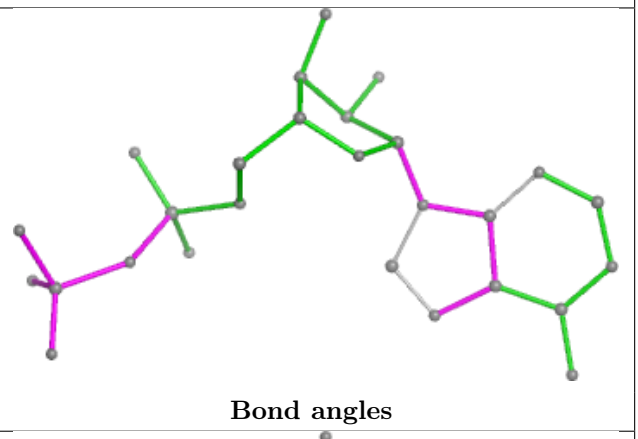
No monomer is involved in short contacts.

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 then 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.

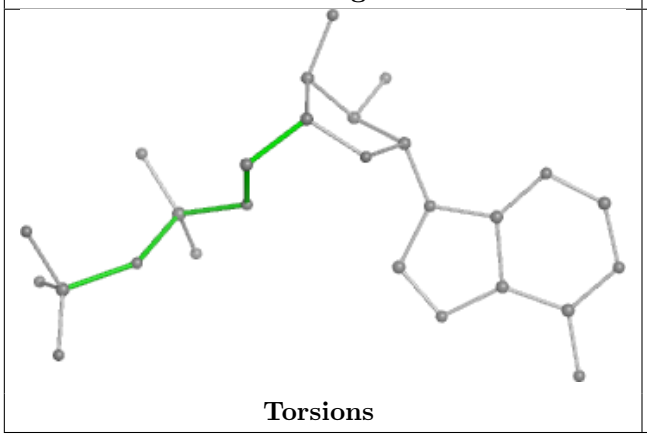
Ligand ADP C 401



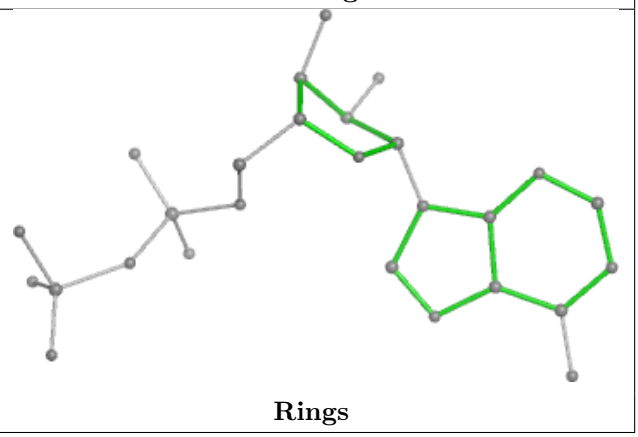
Bond lengths



Bond angles

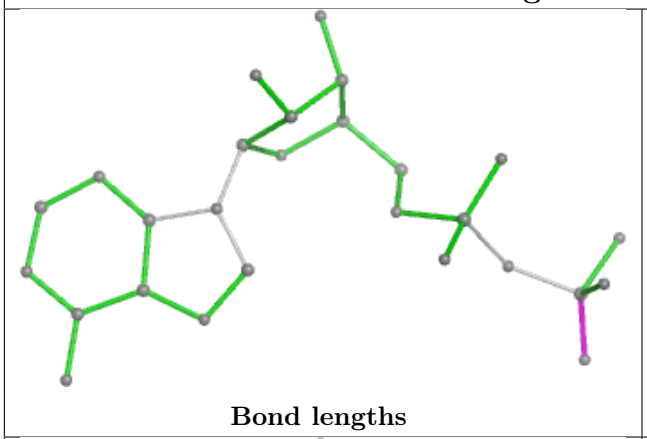


Torsions

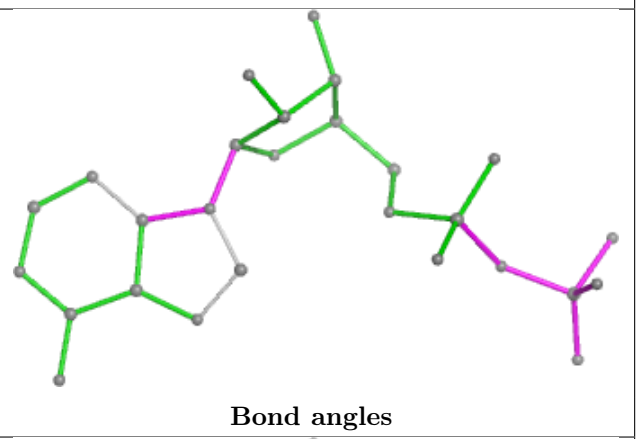


Rings

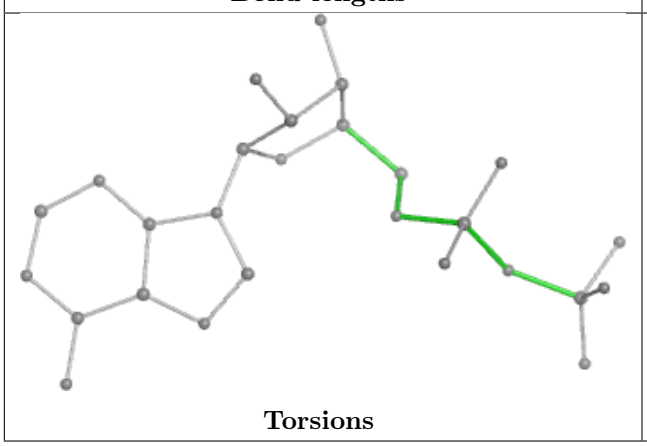
Ligand ADP B 401



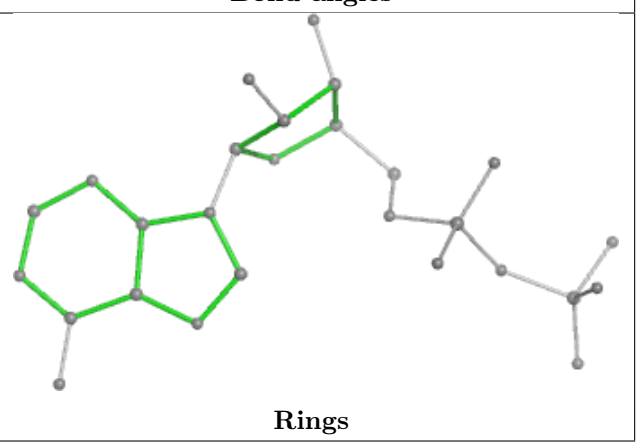
Bond lengths



Bond angles

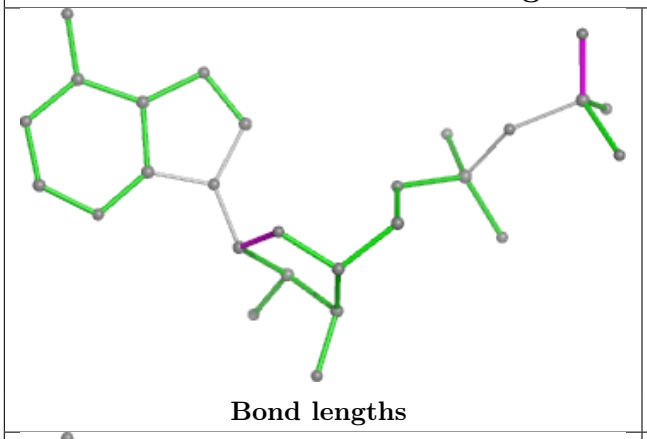


Torsions

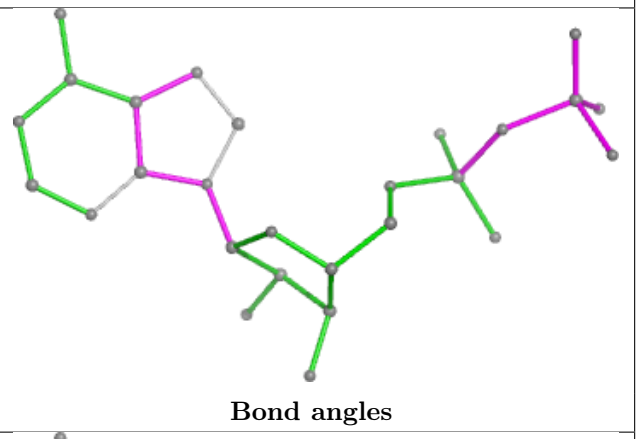


Rings

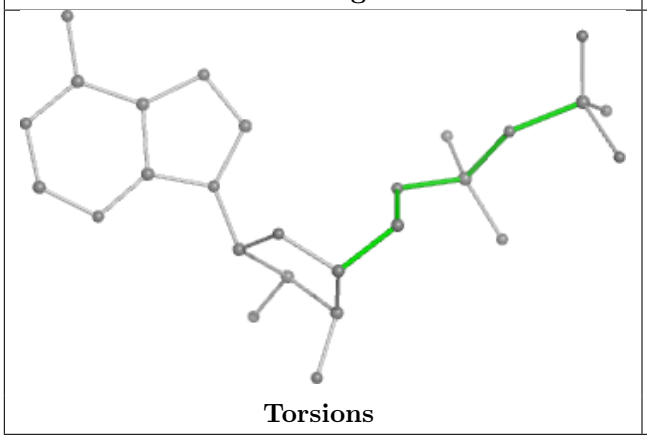
Ligand ADP A 401



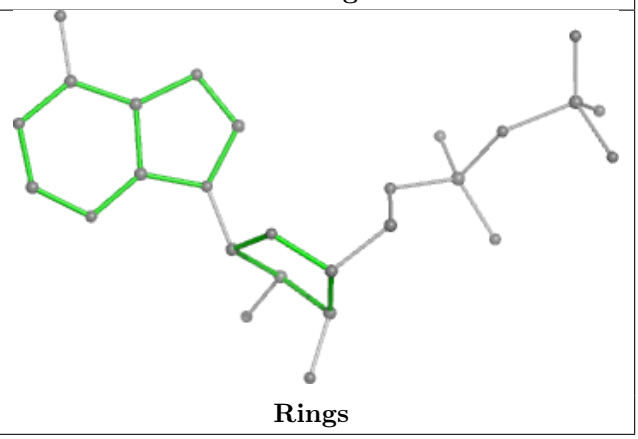
Bond lengths



Bond angles

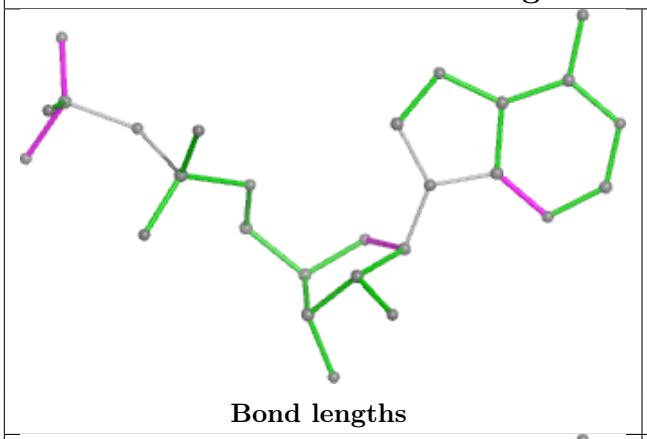


Torsions

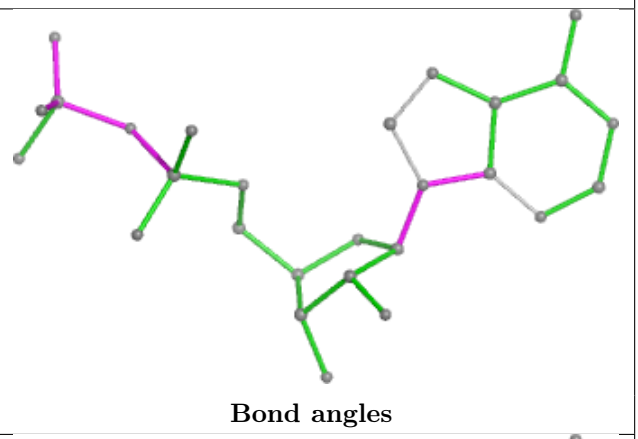


Rings

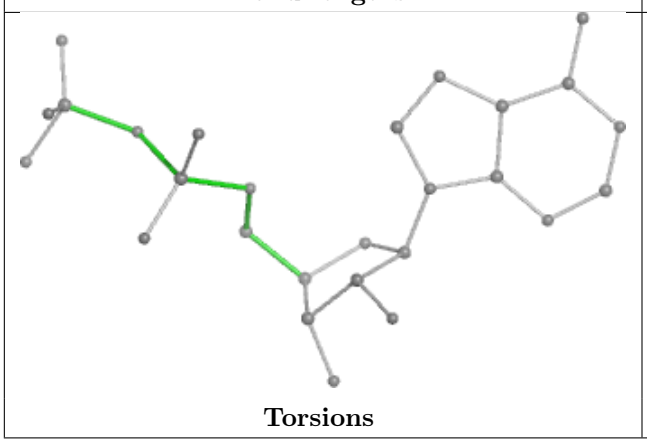
Ligand ADP D 401



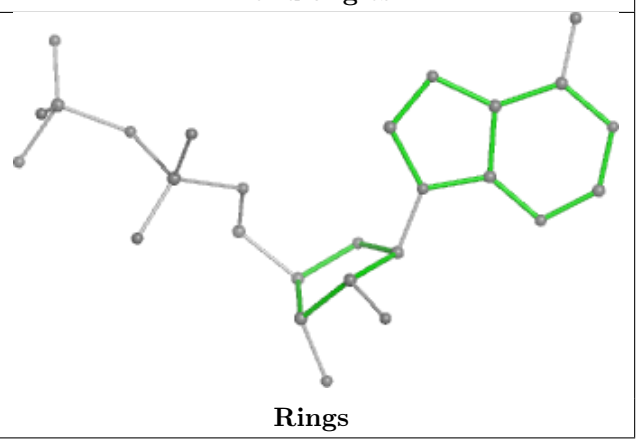
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	301/354 (85%)	0.51	33 (10%) 5 5	22, 43, 81, 100	0
1	B	301/354 (85%)	0.33	24 (7%) 12 11	21, 39, 73, 93	0
1	C	284/354 (80%)	0.51	29 (10%) 6 6	25, 41, 73, 102	0
1	D	304/354 (85%)	0.67	34 (11%) 5 4	30, 50, 78, 105	0
All	All	1190/1416 (84%)	0.50	120 (10%) 7 6	21, 44, 79, 105	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	190	PHE	10.6
1	A	121	LEU	7.3
1	B	210	VAL	6.1
1	D	150	LYS	5.9
1	D	120	LEU	5.5
1	C	214	GLY	5.3
1	B	126	LEU	5.1
1	C	95	LYS	5.1
1	A	100	MET	5.0
1	D	187	LEU	4.6
1	C	97	MET	4.6
1	D	212	ILE	4.5
1	C	98	ASN	4.5
1	A	99	ASP	4.5
1	B	212	ILE	4.5
1	D	16	THR	4.4
1	D	188	GLU	4.3
1	C	96	ASP	4.3
1	D	191	GLY	4.3
1	D	186	LEU	4.2
1	A	125	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	99	ASP	3.9
1	C	241	VAL	3.8
1	A	212	ILE	3.7
1	D	280	ASP	3.7
1	B	215	LYS	3.7
1	D	281	GLN	3.6
1	C	29	VAL	3.5
1	D	32	THR	3.5
1	A	29	VAL	3.5
1	B	190	PHE	3.4
1	B	193	ILE	3.4
1	B	29	VAL	3.3
1	C	304	GLU	3.3
1	D	48	ASN	3.3
1	C	27	GLY	3.2
1	A	98	ASN	3.2
1	D	241	VAL	3.1
1	C	187	LEU	3.1
1	C	127	ALA	3.1
1	C	350	LEU	3.0
1	D	129	LEU	3.0
1	D	5	VAL	3.0
1	A	157	GLY	2.9
1	D	151	ARG	2.9
1	B	30	GLY	2.9
1	A	96	ASP	2.9
1	D	36	CYS	2.9
1	A	241	VAL	2.8
1	A	95	LYS	2.8
1	C	23	VAL	2.8
1	A	345	LYS	2.8
1	C	215	LYS	2.7
1	D	119	SER	2.7
1	A	27	GLY	2.7
1	B	169	PRO	2.7
1	B	128	ASP	2.6
1	D	29	VAL	2.6
1	A	28	GLY	2.6
1	B	28	GLY	2.6
1	B	286	LYS	2.6
1	D	168	ALA	2.6
1	C	167	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	305	LEU	2.5
1	B	127	ALA	2.5
1	A	216	LEU	2.5
1	C	128	ASP	2.5
1	D	352	ASP	2.5
1	D	306	TYR	2.5
1	A	308	ASP	2.5
1	A	215	LYS	2.5
1	B	150	LYS	2.5
1	D	30	GLY	2.5
1	C	129	LEU	2.5
1	A	190	PHE	2.5
1	C	188	GLU	2.5
1	A	278	GLU	2.4
1	A	122	GLN	2.4
1	C	31	LYS	2.4
1	B	48	ASN	2.4
1	D	307	GLU	2.4
1	B	213	SER	2.4
1	B	211	ASP	2.3
1	B	32	THR	2.3
1	A	271	VAL	2.3
1	C	30	GLY	2.3
1	A	286	LYS	2.3
1	C	169	PRO	2.3
1	C	308	ASP	2.3
1	D	270	ILE	2.3
1	A	167	THR	2.3
1	C	219	LEU	2.3
1	A	92	ALA	2.2
1	B	104	ARG	2.2
1	D	28	GLY	2.2
1	A	270	ILE	2.2
1	D	121	LEU	2.2
1	B	23	VAL	2.2
1	C	270	ILE	2.2
1	A	168	ALA	2.2
1	B	170	THR	2.2
1	C	24	GLY	2.1
1	C	171	GLY	2.1
1	D	304	GLU	2.1
1	D	6	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	49	LYS	2.1
1	A	325	ASN	2.1
1	B	33	THR	2.1
1	D	125	ALA	2.1
1	A	154	GLN	2.1
1	C	243	ILE	2.1
1	D	149	ILE	2.1
1	A	219	LEU	2.1
1	D	305	LEU	2.1
1	B	191	GLY	2.1
1	A	189	LYS	2.0
1	B	304	GLU	2.0
1	A	169	PRO	2.0
1	A	304	GLU	2.0
1	D	128	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ALF	A	402	5/5	0.97	0.15	24,29,33,34	0
3	ALF	C	402	5/5	0.97	0.15	28,29,33,41	0
4	MG	A	403	1/1	0.97	0.13	28,28,28,28	0
4	MG	B	403	1/1	0.97	0.17	27,27,27,27	0
4	MG	D	403	1/1	0.97	0.18	35,35,35,35	0
5	ZN	A	1353	1/1	0.97	0.06	43,43,43,43	0
2	ADP	D	401	27/27	0.98	0.15	28,32,37,41	0
3	ALF	D	402	5/5	0.98	0.15	28,30,37,41	0

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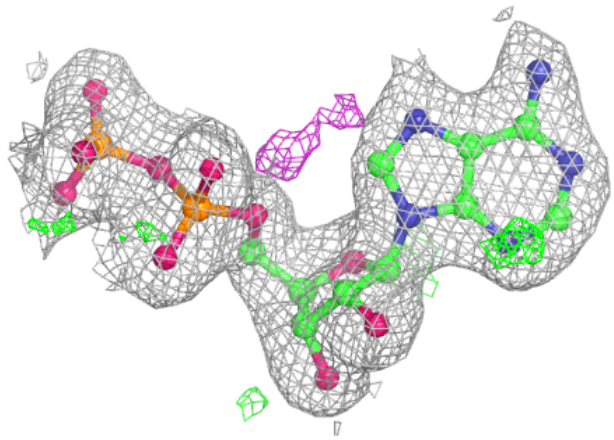
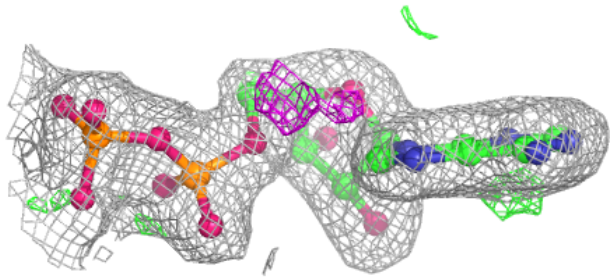
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ALF	B	402	5/5	0.98	0.18	25,27,31,35	0
5	ZN	C	1352	1/1	0.98	0.05	40,40,40,40	0
4	MG	C	403	1/1	0.99	0.16	30,30,30,30	0
2	ADP	B	401	27/27	0.99	0.19	20,26,33,39	0
2	ADP	C	401	27/27	0.99	0.15	24,28,34,34	0
2	ADP	A	401	27/27	0.99	0.15	21,25,33,37	0

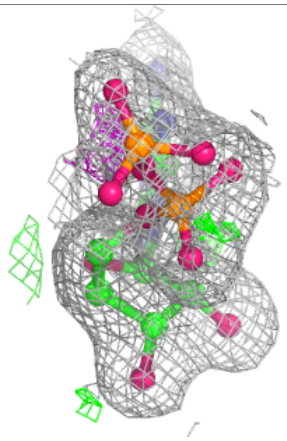
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP D 401:

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

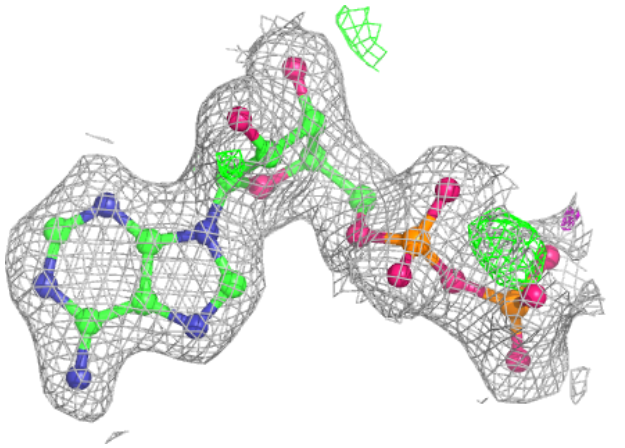


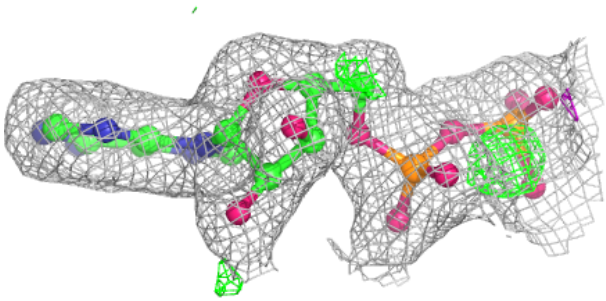


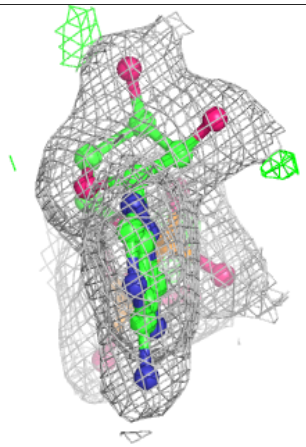


Electron density around ADP B 401:

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

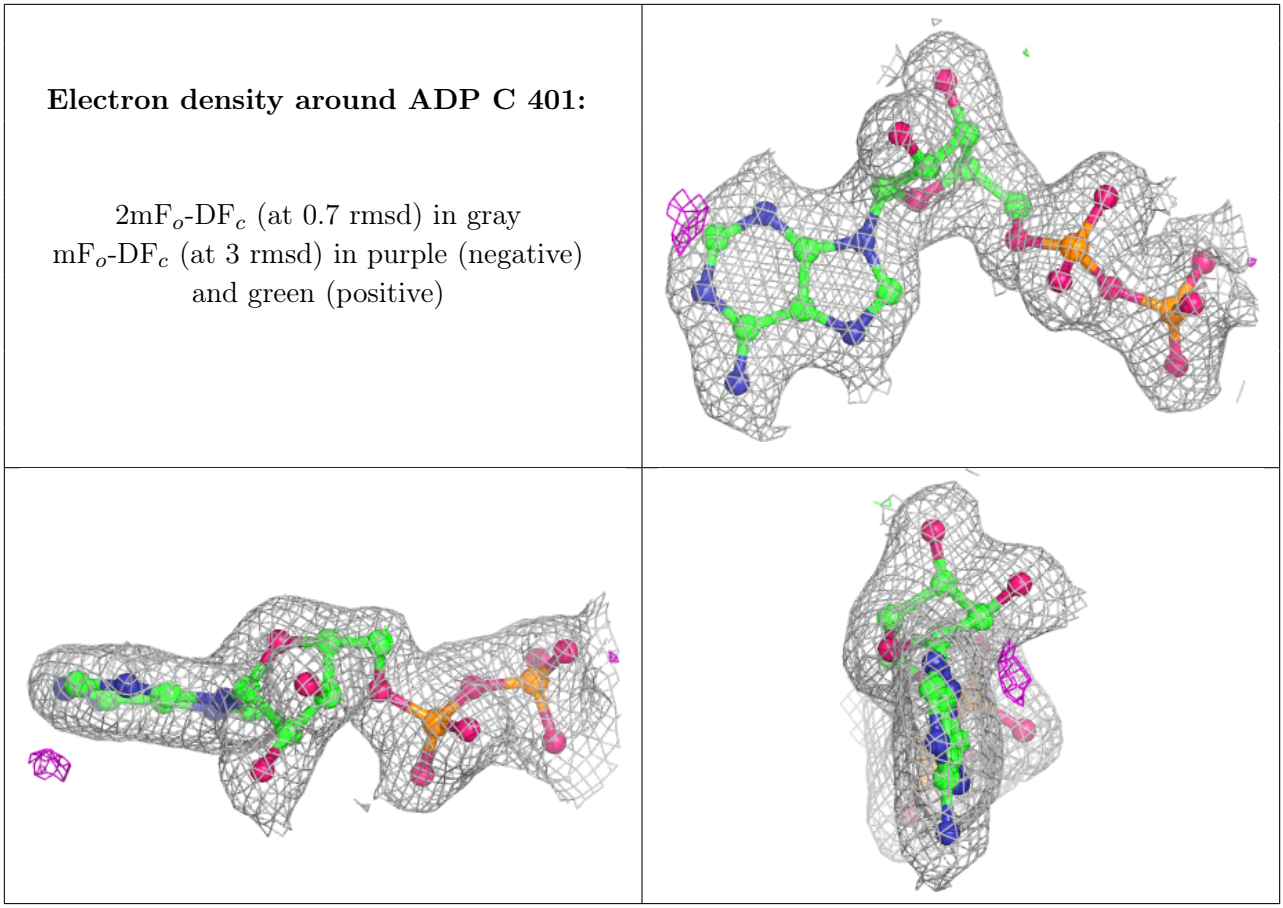






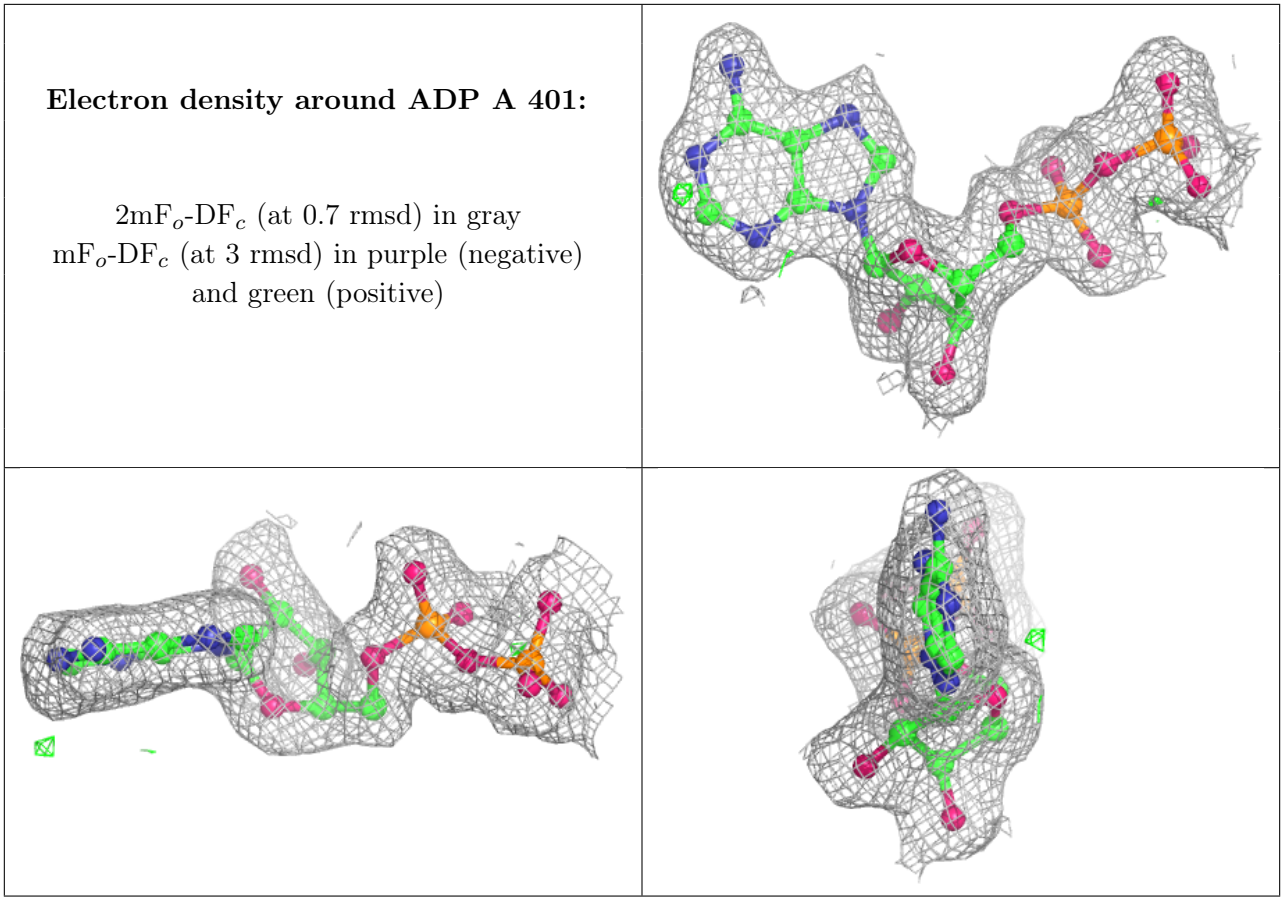
Electron density around ADP C 401:

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



Electron density around ADP A 401:

$2mF_o$-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

There are no such residues in this entry.