



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:28 AM UTC

PDB ID : 2ZDG / pdb_00002zdg
Title : Crystal structure of D-Alanine:D-Alanine Ligase with ADP from *Thermus thermophilus* HB8
Authors : Kitamura, Y.; Yokoyama, S.; Kuramitsu, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-11-22
Resolution : 2.20 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

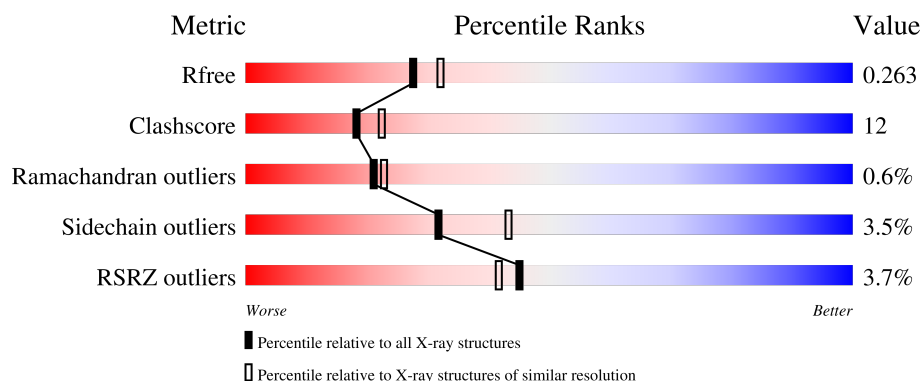
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	319	2% 72% 22% • 5%
1	B	319	3% 74% 18% • 5%
1	C	319	3% 72% 25% •
1	D	319	5% 69% 23% • 5%

2 Entry composition [i](#)

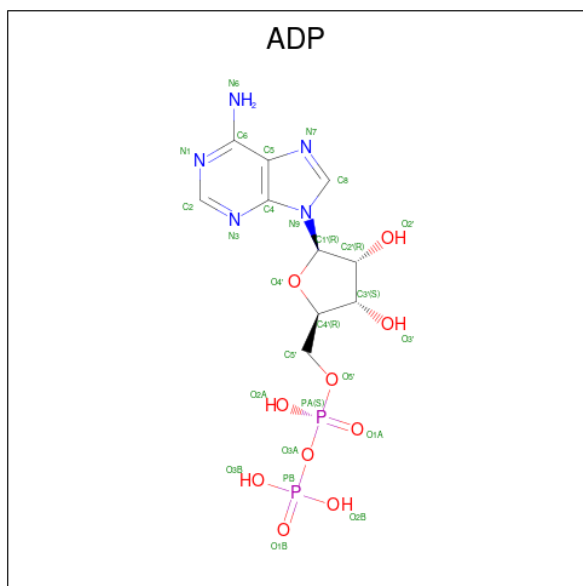
There are 4 unique types of molecules in this entry. The entry contains 9859 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-alanine–D-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2306	1496	385	420	5			
1	B	303	Total	C	N	O	S	0	0	0
			2317	1504	386	422	5			
1	C	319	Total	C	N	O	S	0	0	0
			2449	1591	406	447	5			
1	D	304	Total	C	N	O	S	0	0	0
			2325	1510	387	423	5			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

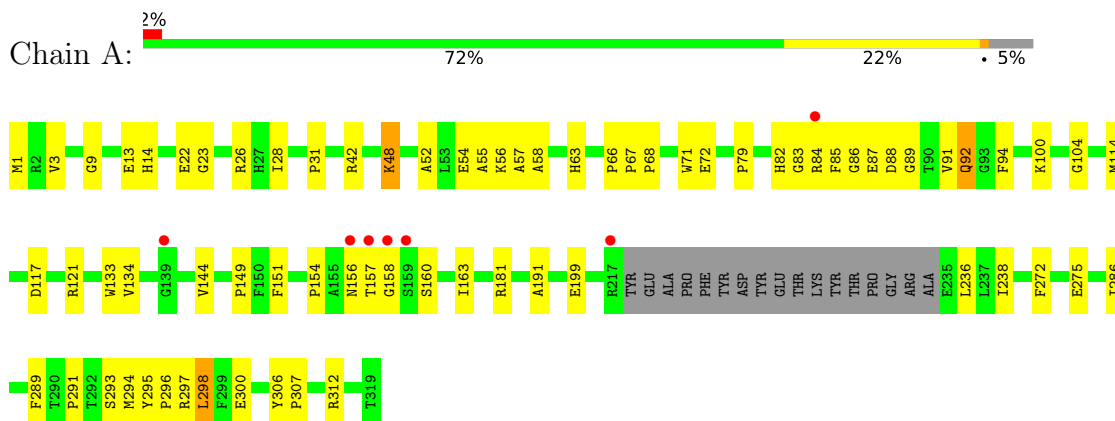
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total	O	0	0
			95	95		
4	B	58	Total	O	0	0
			58	58		
4	C	123	Total	O	0	0
			123	123		
4	D	76	Total	O	0	0
			76	76		

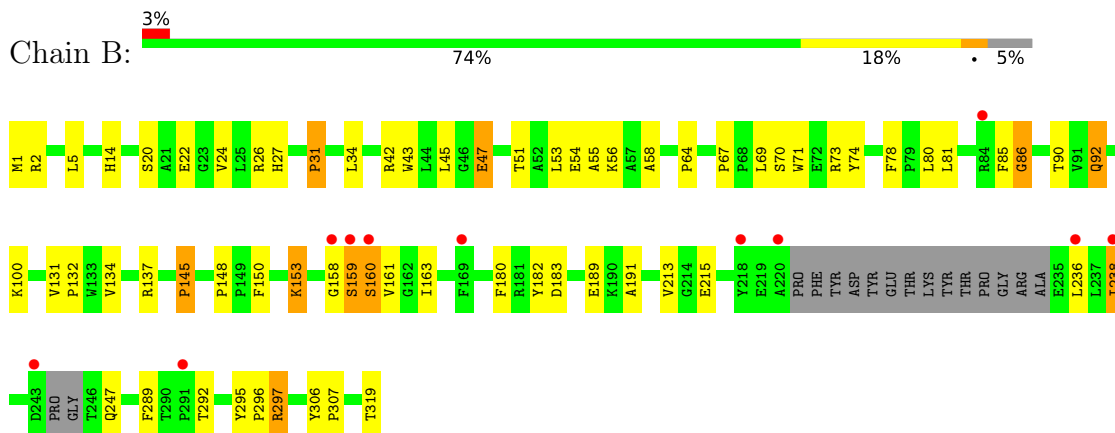
3 Residue-property plots [i](#)

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.

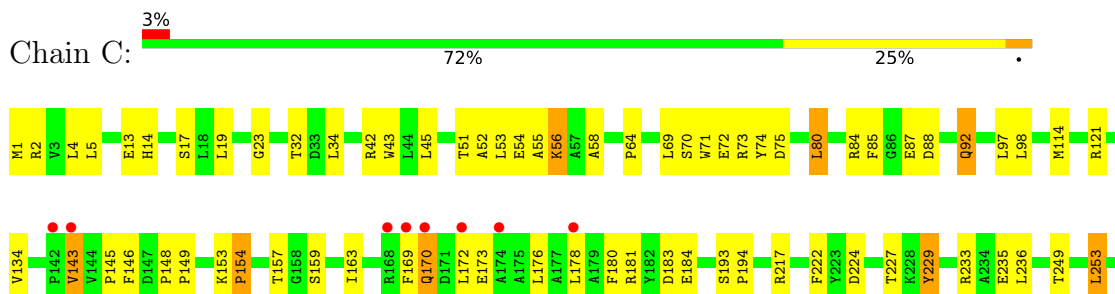
- Molecule 1: D-alanine–D-alanine ligase

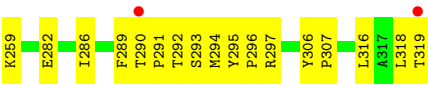


- Molecule 1: D-alanine–D-alanine ligase

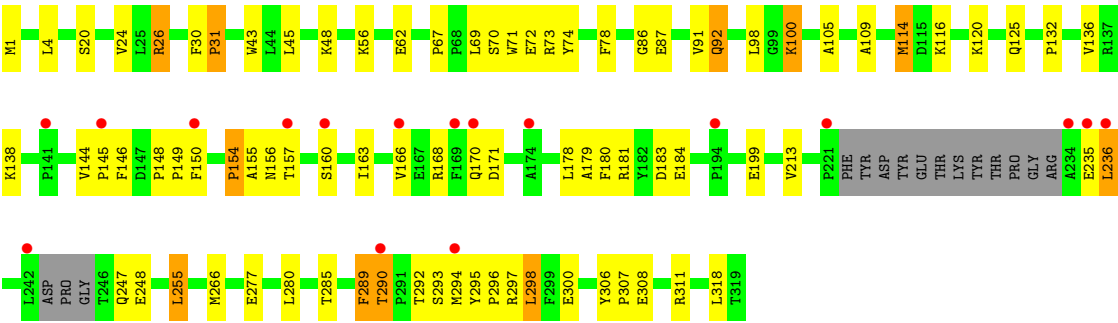


- Molecule 1: D-alanine–D-alanine ligase





● Molecule 1: D-alanine–D-alanine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.10Å 101.07Å 197.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 2.20 49.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.40-2.20) 93.5 (49.40-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.22 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.262 0.214 , 0.263	Depositor DCC
R_{free} test set	6868 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.777	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9859	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: ADP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/2363	0.95	12/3220 (0.4%)
1	B	0.39	0/2373	0.90	2/3232 (0.1%)
1	C	0.43	0/2514	0.92	6/3429 (0.2%)
1	D	0.40	0/2382	0.91	3/3245 (0.1%)
All	All	0.41	0/9632	0.92	23/13126 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	PRO	CA-C-N	6.96	124.67	119.66
1	A	66	PRO	C-N-CA	6.96	124.67	119.66
1	D	300	GLU	N-CA-C	-6.91	103.68	111.14
1	A	144	VAL	CA-C-N	6.63	126.33	119.56
1	A	144	VAL	C-N-CA	6.63	126.33	119.56
1	A	300	GLU	N-CA-C	-6.62	104.06	111.28
1	A	104	GLY	N-CA-C	6.35	121.06	112.17
1	A	67	PRO	N-CA-C	6.27	117.29	110.58
1	A	156	ASN	N-CA-C	6.20	117.88	110.44
1	A	154	PRO	N-CA-C	-6.17	101.57	111.38
1	A	151	PHE	N-CA-C	-5.92	98.62	108.34
1	C	88	ASP	N-CA-C	5.86	120.05	113.02
1	C	318	LEU	N-CA-C	-5.76	106.23	113.20
1	C	43	TRP	N-CA-C	5.67	118.91	110.52
1	C	229	TYR	N-CA-C	5.47	119.94	112.88
1	D	31	PRO	N-CA-C	-5.36	102.78	111.03
1	D	154	PRO	N-CA-C	-5.34	102.75	111.68
1	C	154	PRO	N-CA-C	-5.25	102.95	111.19
1	B	153	LYS	N-CA-C	5.20	116.66	108.23
1	A	272	PHE	N-CA-C	-5.20	101.69	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	VAL	N-CA-C	5.10	115.93	108.53
1	B	31	PRO	N-CA-C	-5.06	103.24	111.03
1	C	32	THR	N-CA-C	5.02	117.24	108.76

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	A	2306	0	2341	45	0
1	B	2317	0	2346	60	0
1	C	2449	0	2466	57	0
1	D	2325	0	2358	71	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	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	95	0	0	1	0
4	B	58	0	0	2	0
4	C	123	0	0	3	0
4	D	76	0	0	2	0
All	All	9859	0	9559	230	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 12.

All (230) 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:297:ARG:HH11	1:B:297:ARG:HB3	1.19	1.01
1:A:84:ARG:HH22	1:A:157:THR:HG23	1.33	0.90
1:D:290:THR:HG23	1:D:292:THR:H	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLN:H	1:B:92:GLN:NE2	1.73	0.87
1:C:178:LEU:HD22	1:C:181:ARG:HH21	1.41	0.85
1:B:153:LYS:HB3	1:B:163:ILE:HG12	1.57	0.84
1:D:178:LEU:O	1:D:181:ARG:HB2	1.81	0.81
1:B:297:ARG:HB3	1:B:297:ARG:NH1	1.94	0.81
1:C:114:MET:HE3	1:C:114:MET:HA	1.62	0.80
1:B:295:TYR:HB3	1:B:296:PRO:HD3	1.64	0.79
1:D:213:VAL:H	1:D:247:GLN:HE21	1.29	0.79
1:A:22:GLU:O	1:A:26:ARG:HG2	1.82	0.77
1:D:295:TYR:HB3	1:D:296:PRO:HD3	1.68	0.76
1:D:166:VAL:HG13	1:D:171:ASP:HB2	1.66	0.76
1:D:26:ARG:CB	1:D:26:ARG:HH11	2.00	0.75
1:C:290:THR:HG22	1:C:293:SER:OG	1.87	0.74
1:D:26:ARG:HH11	1:D:26:ARG:HB2	1.52	0.74
1:D:71:TRP:CD2	1:D:98:LEU:HD21	2.22	0.74
1:B:5:LEU:HD11	1:B:80:LEU:HD12	1.72	0.72
1:C:295:TYR:HB3	1:C:296:PRO:HD3	1.71	0.72
1:C:178:LEU:HD22	1:C:181:ARG:NH2	2.06	0.70
1:D:294:MET:HG3	1:D:298:LEU:HD22	1.73	0.70
1:B:134:VAL:HG11	1:B:145:PRO:HD2	1.73	0.70
1:A:84:ARG:NH2	1:A:157:THR:HG23	2.06	0.70
1:C:306:TYR:HB3	1:C:307:PRO:HD3	1.75	0.69
1:B:14:HIS:HE1	1:B:58:ALA:H	1.41	0.68
1:A:295:TYR:HB3	1:A:296:PRO:HD3	1.75	0.68
1:A:160:SER:HA	1:A:163:ILE:HD12	1.74	0.68
1:A:117:ASP:O	1:A:121:ARG:HG3	1.93	0.68
1:D:236:LEU:HD22	1:D:297:ARG:CZ	2.24	0.68
1:A:92:GLN:NE2	1:A:92:GLN:H	1.92	0.67
1:B:238:ILE:N	1:B:238:ILE:HD12	2.09	0.67
1:B:24:VAL:HG21	1:B:80:LEU:HD11	1.74	0.67
1:B:47:GLU:CD	1:B:47:GLU:H	2.01	0.67
1:B:51:THR:O	1:B:54:GLU:HB2	1.94	0.67
1:A:14:HIS:HE1	1:A:58:ALA:H	1.42	0.66
1:B:92:GLN:H	1:B:92:GLN:HE21	1.41	0.66
1:D:92:GLN:H	1:D:92:GLN:NE2	1.94	0.65
1:D:248:GLU:CD	1:D:248:GLU:H	2.06	0.63
1:C:56:LYS:HE3	1:C:56:LYS:HA	1.81	0.63
1:B:70:SER:O	1:B:73:ARG:HG2	1.99	0.62
1:B:306:TYR:HB3	1:B:307:PRO:HD3	1.81	0.62
1:B:150:PHE:HB2	1:B:189:GLU:O	1.99	0.62
1:A:181:ARG:HD3	1:D:277:GLU:OE2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:GLU:OE1	1:D:294:MET:HG2	2.00	0.62
1:D:213:VAL:CG2	1:D:247:GLN:HG3	2.29	0.61
1:D:71:TRP:HB3	1:D:100:LYS:HD2	1.81	0.61
1:D:236:LEU:HD12	1:D:236:LEU:N	2.16	0.61
1:D:114:MET:HE3	1:D:114:MET:HA	1.82	0.60
1:B:20:SER:HB2	1:B:289:PHE:H	1.65	0.60
1:C:236:LEU:HD12	1:C:294:MET:HE2	1.82	0.60
1:B:292:THR:O	1:B:297:ARG:HD2	2.01	0.59
1:B:14:HIS:CE1	1:B:58:ALA:H	2.20	0.59
1:C:319:THR:HG23	4:C:707:HOH:O	2.01	0.59
1:D:306:TYR:HB3	1:D:307:PRO:HD3	1.84	0.59
1:D:145:PRO:HG2	1:D:146:PHE:HD1	1.67	0.58
1:B:297:ARG:HH11	1:B:297:ARG:CB	2.05	0.58
1:C:290:THR:HG23	1:C:292:THR:H	1.69	0.58
1:A:294:MET:HG3	1:A:298:LEU:HD22	1.84	0.58
1:C:154:PRO:HG2	1:C:157:THR:HB	1.84	0.58
1:C:71:TRP:CD2	1:C:98:LEU:HD21	2.39	0.58
1:D:213:VAL:HG23	1:D:247:GLN:HG3	1.84	0.58
1:C:14:HIS:HE1	1:C:58:ALA:H	1.51	0.57
1:D:294:MET:SD	1:D:298:LEU:HD13	2.45	0.57
1:D:4:LEU:HD23	1:D:74:TYR:CZ	2.40	0.56
1:B:1:MET:O	1:B:31:PRO:HD2	2.06	0.56
1:C:14:HIS:CE1	1:C:58:ALA:H	2.23	0.56
1:C:92:GLN:H	1:C:92:GLN:NE2	2.03	0.56
1:C:169:PHE:O	1:C:172:LEU:HD22	2.06	0.56
1:D:154:PRO:HB2	1:D:157:THR:HG23	1.87	0.56
1:A:42:ARG:HH11	1:A:42:ARG:HG3	1.71	0.56
1:B:42:ARG:HH11	1:B:42:ARG:HG2	1.70	0.55
1:D:154:PRO:HG2	1:D:157:THR:HG21	1.88	0.55
1:D:168:ARG:HB2	1:D:170:GLN:HG2	1.88	0.55
1:D:156:ASN:O	1:D:157:THR:HG23	2.07	0.55
1:D:213:VAL:H	1:D:247:GLN:NE2	2.02	0.54
1:B:71:TRP:C	1:B:100:LYS:HZ3	2.14	0.54
1:C:145:PRO:HG2	1:C:146:PHE:CD1	2.43	0.54
1:C:236:LEU:HD23	1:C:297:ARG:NH1	2.22	0.54
1:D:160:SER:HA	1:D:163:ILE:HD12	1.89	0.54
1:B:134:VAL:HG11	1:B:145:PRO:CD	2.36	0.53
1:B:215:GLU:C	1:B:236:LEU:HD12	2.34	0.53
1:A:72:GLU:N	1:A:72:GLU:OE1	2.41	0.53
1:D:150:PHE:HB2	1:D:166:VAL:HB	1.91	0.53
1:C:143:VAL:HG13	4:C:705:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ARG:NH1	4:A:434:HOH:O	2.41	0.52
1:A:306:TYR:HB3	1:A:307:PRO:HD3	1.92	0.52
1:B:20:SER:CB	1:B:289:PHE:H	2.23	0.52
1:B:150:PHE:HA	1:B:191:ALA:HB2	1.92	0.52
1:B:26:ARG:HG3	1:B:26:ARG:HH11	1.75	0.51
1:B:69:LEU:HD23	1:B:70:SER:N	2.25	0.51
1:D:45:LEU:CD2	1:D:69:LEU:HD12	2.40	0.51
1:D:235:GLU:C	1:D:236:LEU:HD12	2.36	0.51
1:C:172:LEU:HD23	1:C:173:GLU:N	2.24	0.51
1:D:1:MET:O	1:D:31:PRO:HD2	2.10	0.51
1:C:34:LEU:HD22	1:C:53:LEU:HD22	1.92	0.51
1:D:48:LYS:HD2	1:D:62:GLU:OE1	2.11	0.51
1:B:42:ARG:NH1	1:B:64:PRO:HB3	2.26	0.50
1:A:52:ALA:HB1	1:A:58:ALA:HB2	1.92	0.50
1:D:155:ALA:HB3	1:D:183:ASP:OD1	2.11	0.50
1:C:1:MET:HA	1:C:75:ASP:OD2	2.12	0.50
1:B:55:ALA:O	1:B:56:LYS:HB2	2.10	0.50
1:B:137:ARG:NH2	4:B:447:HOH:O	2.43	0.50
1:B:213:VAL:HG23	1:B:247:GLN:HG3	1.94	0.50
1:C:23:GLY:HA3	1:C:291:PRO:HD3	1.94	0.50
1:C:42:ARG:NH1	1:C:64:PRO:HB3	2.27	0.50
1:A:236:LEU:HD12	1:A:236:LEU:N	2.27	0.49
1:D:92:GLN:H	1:D:92:GLN:HE21	1.60	0.49
1:A:9:GLY:O	1:A:14:HIS:HD2	1.95	0.49
1:C:73:ARG:HG2	1:C:73:ARG:HH21	1.76	0.49
1:B:22:GLU:HB2	1:B:53:LEU:HD21	1.95	0.49
1:B:161:VAL:HG22	1:B:182:TYR:CZ	2.48	0.49
1:A:92:GLN:H	1:A:92:GLN:HE21	1.59	0.49
1:B:2:ARG:NE	1:B:73:ARG:HH11	2.10	0.49
1:D:116:LYS:O	1:D:120:LYS:HG3	2.12	0.49
1:A:88:ASP:HB3	1:A:114:MET:HE2	1.95	0.48
1:D:290:THR:HG23	1:D:292:THR:N	2.15	0.48
1:B:26:ARG:HD2	1:B:27:HIS:CE1	2.48	0.48
1:C:97:LEU:HD11	1:D:91:VAL:HA	1.95	0.48
1:A:84:ARG:HH21	1:A:157:THR:HA	1.79	0.48
1:D:168:ARG:CB	1:D:170:GLN:HG2	2.44	0.48
1:A:48:LYS:HE3	1:A:48:LYS:HA	1.96	0.48
1:D:4:LEU:HB2	1:D:74:TYR:CG	2.49	0.48
1:D:290:THR:HG22	1:D:293:SER:OG	2.14	0.48
1:C:70:SER:HB3	1:C:72:GLU:OE1	2.15	0.47
1:C:84:ARG:O	1:C:85:PHE:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:LEU:HD22	1:D:69:LEU:HD12	1.95	0.47
1:A:84:ARG:HH22	1:A:157:THR:CG2	2.15	0.47
1:A:149:PRO:HG2	1:A:191:ALA:HB3	1.97	0.47
1:D:266:MET:SD	1:D:289:PHE:HE1	2.37	0.46
1:C:193:SER:HA	1:C:194:PRO:C	2.38	0.46
1:D:144:VAL:HG21	1:D:150:PHE:CZ	2.50	0.46
1:D:248:GLU:CD	1:D:248:GLU:N	2.72	0.46
1:D:179:ALA:C	1:D:181:ARG:H	2.22	0.46
1:D:236:LEU:N	1:D:236:LEU:CD1	2.78	0.46
1:D:71:TRP:CE3	1:D:98:LEU:HD21	2.49	0.46
1:C:4:LEU:HB2	1:C:74:TYR:CD1	2.50	0.46
1:A:89:GLY:HA2	1:A:92:GLN:NE2	2.31	0.46
1:B:92:GLN:NE2	1:B:92:GLN:N	2.54	0.46
1:C:13:GLU:HA	4:C:666:HOH:O	2.15	0.46
1:C:92:GLN:H	1:C:92:GLN:HE21	1.63	0.46
1:C:180:PHE:HA	1:C:183:ASP:O	2.16	0.46
1:D:1:MET:HG2	1:D:30:PHE:CD1	2.50	0.46
1:A:55:ALA:O	1:A:56:LYS:HB2	2.15	0.46
1:A:79:PRO:O	1:A:286:ILE:HD13	2.15	0.46
1:D:78:PHE:C	1:D:78:PHE:CD2	2.94	0.45
1:C:121:ARG:HG2	1:D:125:GLN:OE1	2.16	0.45
1:C:217:ARG:NH1	1:C:235:GLU:HG2	2.32	0.45
1:B:85:PHE:HA	1:B:90:THR:OG1	2.16	0.45
1:D:70:SER:HB3	1:D:72:GLU:OE1	2.17	0.45
1:A:23:GLY:HA3	1:A:291:PRO:HD3	1.98	0.45
1:B:54:GLU:HB2	4:B:438:HOH:O	2.15	0.45
1:C:172:LEU:O	1:C:176:LEU:HG	2.17	0.45
1:A:83:GLY:C	1:A:114:MET:HE1	2.42	0.45
1:C:183:ASP:OD1	1:C:184:GLU:N	2.50	0.45
1:B:148:PRO:HG3	1:B:150:PHE:CE2	2.52	0.44
1:C:170:GLN:O	1:C:170:GLN:NE2	2.50	0.44
1:B:20:SER:O	1:B:24:VAL:HG23	2.16	0.44
1:C:148:PRO:HB2	1:C:149:PRO:HA	1.99	0.44
1:B:34:LEU:HD22	1:B:53:LEU:HD12	1.99	0.44
1:A:87:GLU:HG2	1:A:286:ILE:HB	1.99	0.44
1:A:121:ARG:HG2	1:A:133:TRP:HZ2	1.83	0.44
1:B:43:TRP:CE3	1:B:67:PRO:HG3	2.52	0.44
1:B:53:LEU:O	1:B:53:LEU:HD23	2.18	0.44
1:B:159:SER:O	1:B:160:SER:C	2.61	0.44
1:A:157:THR:HG22	1:A:158:GLY:N	2.32	0.44
1:B:131:VAL:O	1:B:132:PRO:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:O	1:A:31:PRO:HD2	2.18	0.44
1:C:227:THR:HA	1:C:233:ARG:HG2	1.99	0.44
1:A:199:GLU:OE1	1:A:294:MET:HG2	2.18	0.43
1:D:4:LEU:HD13	1:D:4:LEU:C	2.44	0.43
1:B:2:ARG:HE	1:B:73:ARG:HH11	1.66	0.43
1:D:148:PRO:HA	1:D:149:PRO:C	2.43	0.43
1:C:52:ALA:HB1	1:C:58:ALA:HB2	2.01	0.43
1:C:222:PHE:O	1:C:224:ASP:N	2.52	0.43
1:C:249:THR:HG22	1:C:253:LEU:HD22	2.01	0.43
1:D:78:PHE:C	1:D:78:PHE:HD2	2.26	0.43
1:A:54:GLU:OE1	1:A:54:GLU:HA	2.18	0.43
1:B:131:VAL:HG12	1:B:189:GLU:HB2	2.01	0.43
1:A:71:TRP:O	1:A:100:LYS:HE2	2.19	0.43
1:C:159:SER:HB3	1:C:229:TYR:HE1	1.84	0.43
1:D:136:VAL:HG12	1:D:180:PHE:HZ	1.83	0.42
1:A:48:LYS:HE3	1:A:48:LYS:CA	2.47	0.42
1:C:5:LEU:HD11	1:C:80:LEU:HD12	2.01	0.42
1:A:238:ILE:HD12	1:A:238:ILE:N	2.35	0.42
1:A:63:HIS:CD2	1:A:68:PRO:HG3	2.55	0.42
1:A:82:HIS:CD2	1:A:286:ILE:HG22	2.55	0.42
1:C:172:LEU:HD23	1:C:173:GLU:H	1.84	0.42
1:D:266:MET:SD	1:D:289:PHE:CE1	3.13	0.42
1:D:308:GLU:OE2	1:D:311:ARG:NH2	2.49	0.42
1:C:316:LEU:C	1:C:319:THR:H	2.27	0.42
1:D:132:PRO:HA	4:D:620:HOH:O	2.20	0.42
1:B:74:TYR:O	1:B:100:LYS:HE2	2.20	0.42
1:A:84:ARG:O	1:A:85:PHE:HB2	2.19	0.42
1:D:105:ALA:HB1	1:D:109:ALA:HB3	2.02	0.42
1:B:160:SER:HB2	1:B:163:ILE:HD12	2.01	0.41
1:C:319:THR:OXT	1:C:319:THR:HG22	2.20	0.41
1:D:280:LEU:HD23	1:D:280:LEU:C	2.45	0.41
1:B:158:GLY:O	1:B:160:SER:N	2.53	0.41
1:C:51:THR:O	1:C:54:GLU:HG2	2.20	0.41
1:D:20:SER:O	1:D:24:VAL:HG23	2.20	0.41
1:A:28:ILE:O	1:A:28:ILE:HG23	2.20	0.41
1:A:293:SER:O	1:A:297:ARG:HG3	2.21	0.41
1:B:2:ARG:HE	1:B:73:ARG:NH1	2.18	0.41
1:C:55:ALA:O	1:C:56:LYS:HB2	2.21	0.41
1:C:71:TRP:CG	1:C:98:LEU:HD21	2.54	0.41
1:D:56:LYS:HD3	1:D:56:LYS:HA	1.89	0.41
1:A:298:LEU:HD12	1:A:298:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:MET:HA	1:C:114:MET:CE	2.44	0.41
1:D:43:TRP:CE3	1:D:67:PRO:HG3	2.55	0.41
1:B:137:ARG:HH11	1:B:137:ARG:HG3	1.86	0.41
1:B:319:THR:O	1:B:319:THR:HG22	2.21	0.41
1:B:73:ARG:HG3	1:B:74:TYR:CE2	2.55	0.41
1:C:45:LEU:HD22	1:C:69:LEU:HD21	2.02	0.41
1:D:183:ASP:OD2	1:D:184:GLU:N	2.54	0.41
1:B:81:LEU:HB2	1:B:86:GLY:HA2	2.03	0.41
1:B:78:PHE:C	1:B:78:PHE:CD1	2.99	0.40
1:C:153:LYS:HB3	1:C:163:ILE:HG12	2.03	0.40
1:D:116:LYS:HE2	4:D:674:HOH:O	2.21	0.40
1:D:255:LEU:HD12	1:D:255:LEU:HA	1.95	0.40
1:A:26:ARG:HD3	1:A:26:ARG:N	2.37	0.40
1:C:87:GLU:HG2	1:C:286:ILE:HB	2.03	0.40
1:B:159:SER:O	1:B:161:VAL:N	2.53	0.40
1:C:17:SER:OG	1:C:80:LEU:O	2.36	0.40
1:D:87:GLU:HB2	1:D:285:THR:OG1	2.21	0.40
1:A:91:VAL:O	1:A:94:PHE:HB3	2.22	0.40
1:B:180:PHE:HA	1:B:183:ASP:O	2.22	0.40
1:C:236:LEU:HD23	1:C:297:ARG:HH12	1.87	0.40
1:D:1:MET:HE1	1:D:318:LEU:HD11	2.03	0.40
1:D:138:LYS:HB2	1:D:180:PHE:CD1	2.57	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	298/319 (93%)	285 (96%)	11 (4%)	2 (1%)	18	19
1	B	297/319 (93%)	285 (96%)	8 (3%)	4 (1%)	9	8
1	C	317/319 (99%)	299 (94%)	18 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	298/319 (93%)	282 (95%)	15 (5%)	1 (0%)	36	42
All	All	1210/1276 (95%)	1151 (95%)	52 (4%)	7 (1%)	21	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	SER
1	B	160	SER
1	A	86	GLY
1	A	57	ALA
1	B	145	PRO
1	D	86	GLY
1	B	86	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/256 (94%)	235 (97%)	7 (3%)	37	51
1	B	242/256 (94%)	237 (98%)	5 (2%)	47	63
1	C	255/256 (100%)	243 (95%)	12 (5%)	23	31
1	D	243/256 (95%)	233 (96%)	10 (4%)	27	37
All	All	982/1024 (96%)	948 (96%)	34 (4%)	32	43

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	48	LYS
1	A	92	GLN
1	A	134	VAL
1	A	275	GLU
1	A	289	PHE
1	A	298	LEU

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Mol	Chain	Res	Type
1	B	45	LEU
1	B	47	GLU
1	B	92	GLN
1	B	238	ILE
1	B	297	ARG
1	C	2	ARG
1	C	19	LEU
1	C	56	LYS
1	C	80	LEU
1	C	92	GLN
1	C	134	VAL
1	C	143	VAL
1	C	170	GLN
1	C	253	LEU
1	C	259	LYS
1	C	282	GLU
1	C	289	PHE
1	D	26	ARG
1	D	73	ARG
1	D	92	GLN
1	D	100	LYS
1	D	114	MET
1	D	236	LEU
1	D	255	LEU
1	D	289	PHE
1	D	290	THR
1	D	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	63	HIS
1	A	82	HIS
1	A	92	GLN
1	A	247	GLN
1	B	14	HIS
1	B	92	GLN
1	B	125	GLN
1	B	156	ASN
1	C	14	HIS
1	C	27	HIS

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Mol	Chain	Res	Type
1	C	92	GLN
1	C	170	GLN
1	C	284	ASN
1	D	92	GLN
1	D	247	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	C	403	3	28,29,29	1.29	3 (10%)	43,45,45	1.93	10 (23%)
2	ADP	D	404	3	28,29,29	1.27	3 (10%)	43,45,45	1.83	9 (20%)
2	ADP	B	402	-	28,29,29	1.21	4 (14%)	43,45,45	1.83	9 (20%)
2	ADP	A	401	-	28,29,29	1.25	4 (14%)	43,45,45	1.85	8 (18%)

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	C	403	3	-	2/16/32/32	0/3/3/3
2	ADP	D	404	3	-	6/16/32/32	0/3/3/3
2	ADP	B	402	-	-	0/16/32/32	0/3/3/3
2	ADP	A	401	-	-	0/16/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	403	ADP	PA-O3A	4.20	1.64	1.59
2	A	401	ADP	PA-O3A	3.74	1.63	1.59
2	D	404	ADP	PA-O3A	3.68	1.63	1.59
2	B	402	ADP	PA-O3A	3.55	1.63	1.59
2	C	403	ADP	O4'-C1'	2.46	1.47	1.42
2	D	404	ADP	O4'-C1'	2.28	1.47	1.42
2	A	401	ADP	O4'-C1'	2.18	1.47	1.42
2	B	402	ADP	PB-O2B	2.17	1.62	1.54
2	B	402	ADP	C5-C4	2.17	1.43	1.39
2	A	401	ADP	PB-O2B	2.13	1.62	1.54
2	A	401	ADP	C5-N7	-2.11	1.35	1.39
2	B	402	ADP	C5-N7	-2.09	1.35	1.39
2	C	403	ADP	C5-N7	-2.07	1.35	1.39
2	D	404	ADP	C5-C4	2.02	1.42	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	403	ADP	C5-C4-N3	-5.56	119.06	126.72
2	D	404	ADP	C5-C4-N3	-5.54	119.09	126.72
2	B	402	ADP	C5-C4-N3	-5.04	119.77	126.72
2	A	401	ADP	C5-C4-N3	-5.03	119.79	126.72
2	C	403	ADP	N3-C2-N1	-4.90	121.17	128.58
2	A	401	ADP	N3-C2-N1	-4.84	121.26	128.58
2	C	403	ADP	N3-C4-N9	4.73	135.21	127.17
2	D	404	ADP	N3-C4-N9	4.70	135.16	127.17
2	B	402	ADP	N3-C2-N1	-4.66	121.53	128.58
2	D	404	ADP	N3-C2-N1	-4.58	121.66	128.58
2	A	401	ADP	N3-C4-N9	4.49	134.80	127.17
2	B	402	ADP	N3-C4-N9	4.22	134.35	127.17
2	C	403	ADP	C2-N3-C4	4.00	121.59	111.83
2	D	404	ADP	C5-N7-C8	3.84	109.48	103.45
2	D	404	ADP	C2-N3-C4	3.83	121.19	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	403	ADP	C5-N7-C8	3.82	109.45	103.45
2	A	401	ADP	C5-N7-C8	3.78	109.39	103.45
2	B	402	ADP	C5-N7-C8	3.71	109.28	103.45
2	B	402	ADP	C2-N3-C4	3.70	120.87	111.83
2	A	401	ADP	C2-N3-C4	3.69	120.84	111.83
2	A	401	ADP	C4-C5-N7	-2.89	107.28	110.58
2	B	402	ADP	C4-C5-N7	-2.85	107.33	110.58
2	D	404	ADP	C4-C5-N7	-2.84	107.33	110.58
2	C	403	ADP	C4-C5-N7	-2.79	107.39	110.58
2	C	403	ADP	O2A-PA-O3A	2.55	114.17	107.27
2	B	402	ADP	N9-C8-N7	-2.52	110.37	113.94
2	A	401	ADP	PA-O5'-C5'	-2.46	107.26	121.35
2	B	402	ADP	PA-O5'-C5'	-2.45	107.31	121.35
2	A	401	ADP	N9-C8-N7	-2.43	110.50	113.94
2	B	402	ADP	O2B-PB-O3A	2.35	112.52	104.64
2	C	403	ADP	O2B-PB-O3A	2.33	112.44	104.64
2	D	404	ADP	PA-O5'-C5'	-2.23	108.57	121.35
2	D	404	ADP	N9-C8-N7	-2.20	110.81	113.94
2	C	403	ADP	N9-C8-N7	-2.19	110.83	113.94
2	D	404	ADP	O2B-PB-O3A	2.18	111.94	104.64
2	C	403	ADP	PA-O5'-C5'	-2.12	109.17	121.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

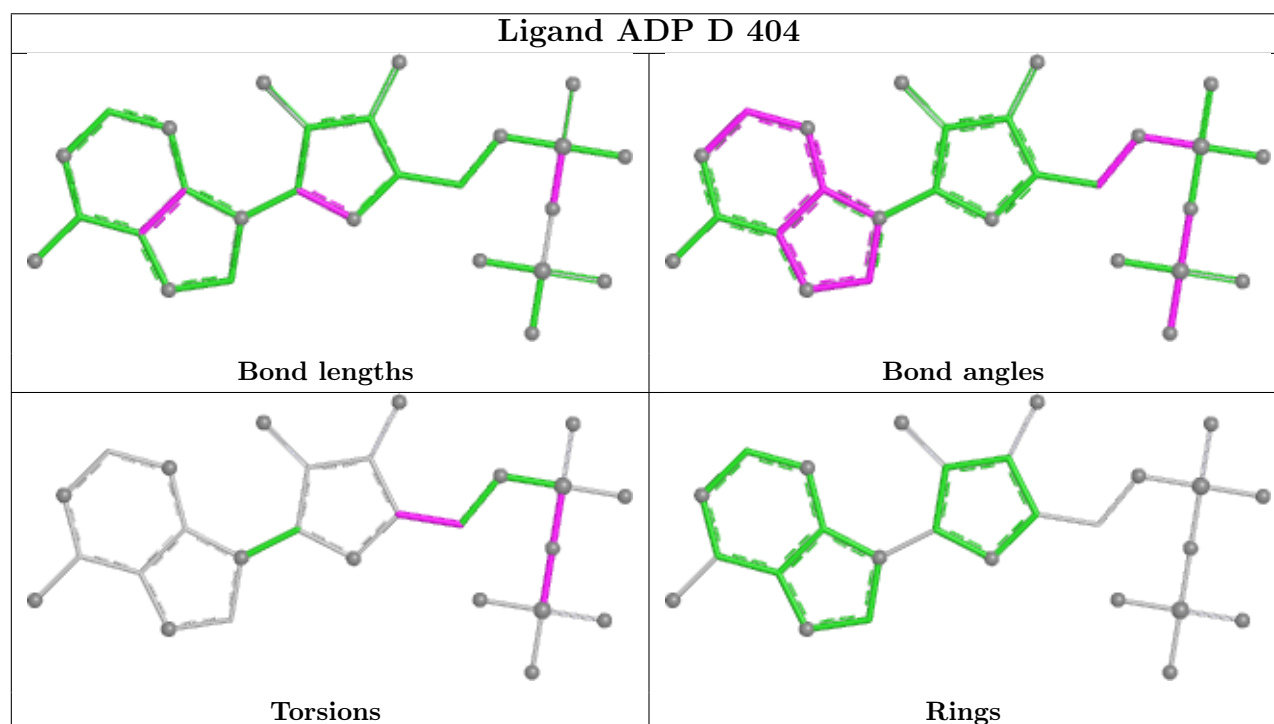
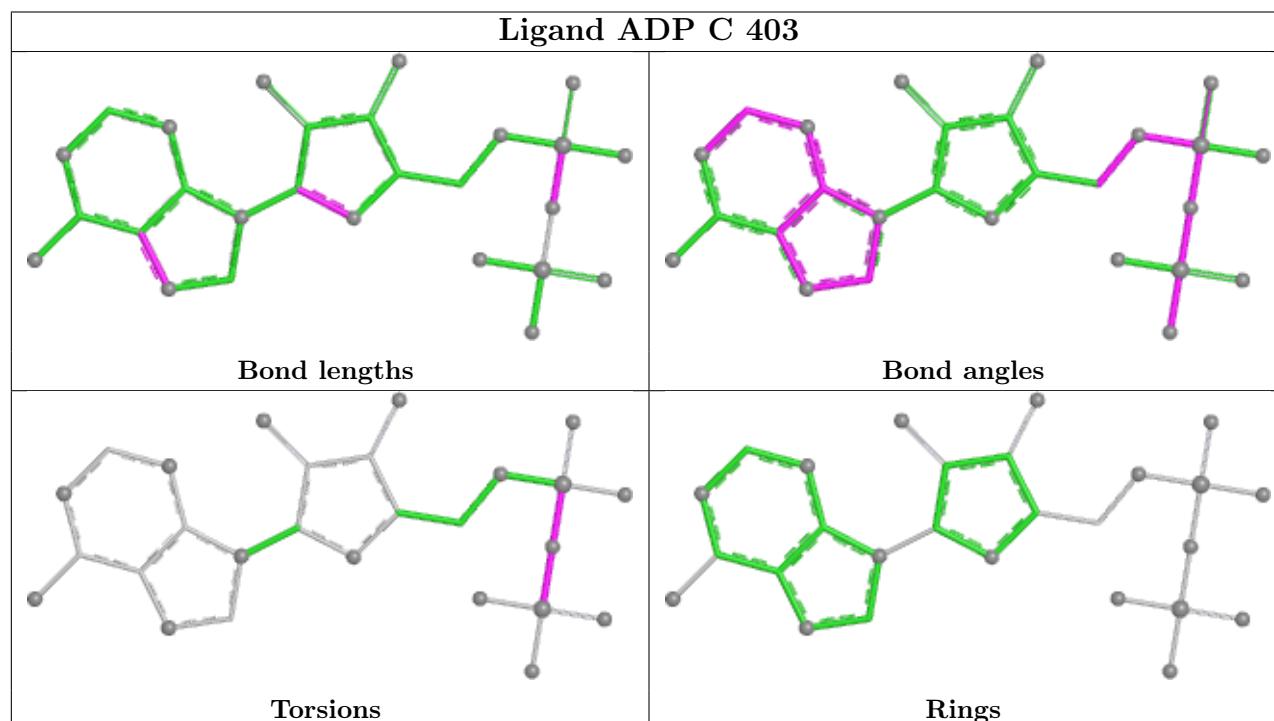
Mol	Chain	Res	Type	Atoms
2	D	404	ADP	PA-O3A-PB-O2B
2	D	404	ADP	PA-O3A-PB-O3B
2	D	404	ADP	O4'-C4'-C5'-O5'
2	D	404	ADP	C3'-C4'-C5'-O5'
2	D	404	ADP	PB-O3A-PA-O5'
2	C	403	ADP	PB-O3A-PA-O2A
2	C	403	ADP	PA-O3A-PB-O1B
2	D	404	ADP	PA-O3A-PB-O1B

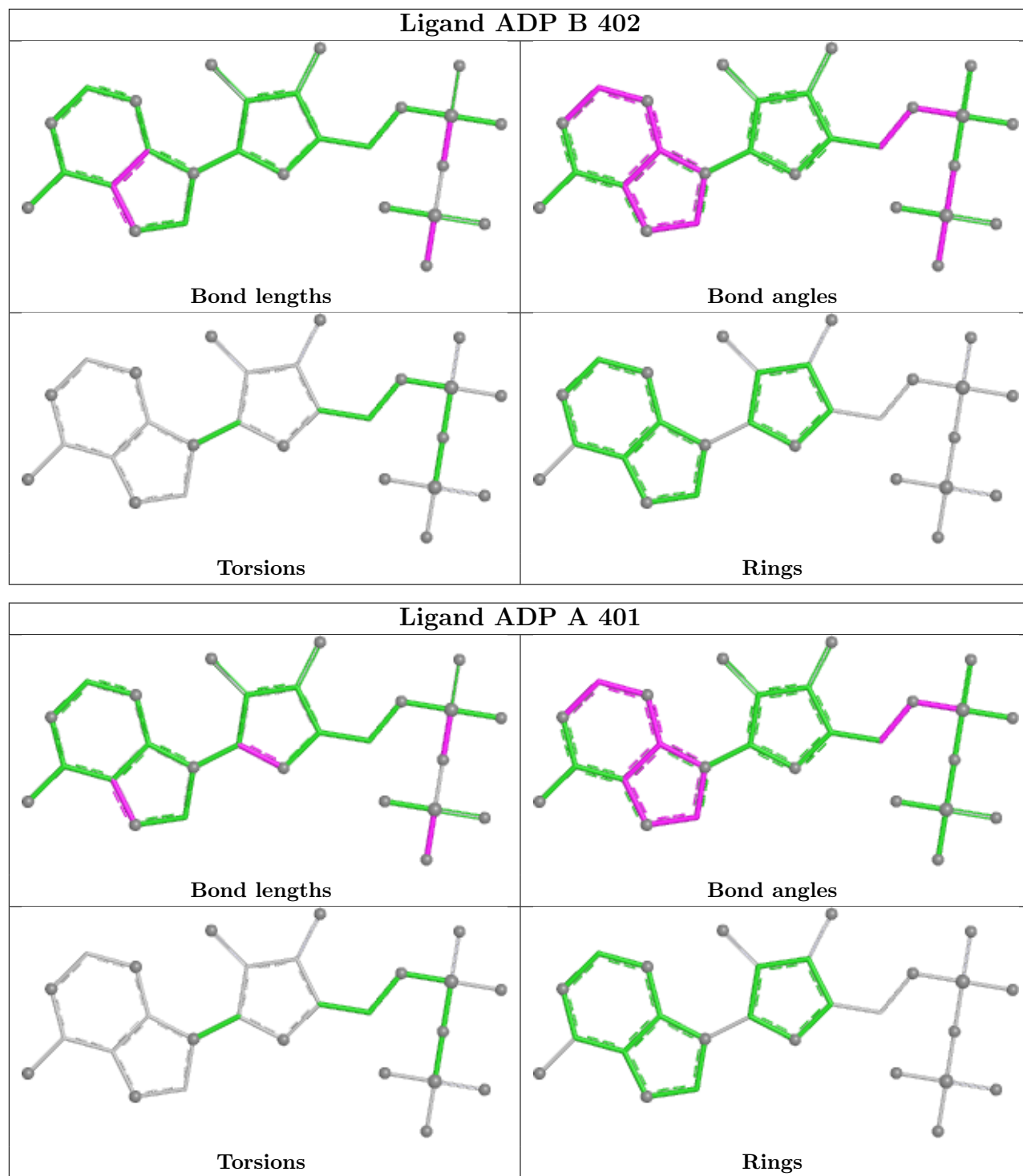
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	302/319 (94%)	-0.00	7 (2%) 61 58	18, 32, 48, 58	0
1	B	303/319 (94%)	0.43	11 (3%) 46 43	24, 39, 59, 69	0
1	C	319/319 (100%)	0.03	10 (3%) 51 48	18, 32, 51, 74	0
1	D	304/319 (95%)	0.37	17 (5%) 30 27	19, 38, 61, 80	0
All	All	1228/1276 (96%)	0.20	45 (3%) 45 42	18, 34, 57, 80	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	172	LEU	5.3
1	B	220	ALA	3.6
1	A	157	THR	3.6
1	B	159	SER	3.5
1	D	169	PHE	3.4
1	B	236	LEU	3.3
1	C	178	LEU	3.1
1	D	234	ALA	3.1
1	C	143	VAL	3.1
1	D	235	GLU	3.0
1	C	169	PHE	3.0
1	D	166	VAL	3.0
1	D	294	MET	2.8
1	C	168	ARG	2.8
1	B	84	ARG	2.8
1	B	218	TYR	2.7
1	C	319	THR	2.7
1	D	160	SER	2.6
1	B	169	PHE	2.6
1	B	158	GLY	2.6
1	B	243	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	242	LEU	2.5
1	B	160	SER	2.5
1	C	170	GLN	2.5
1	D	157	THR	2.4
1	A	217	ARG	2.4
1	C	174	ALA	2.3
1	A	159	SER	2.3
1	D	221	PRO	2.3
1	D	236	LEU	2.3
1	A	156	ASN	2.3
1	A	84	ARG	2.3
1	D	170	GLN	2.2
1	D	174	ALA	2.2
1	C	142	PRO	2.2
1	C	290	THR	2.2
1	D	150	PHE	2.1
1	D	194	PRO	2.1
1	A	139	GLY	2.1
1	A	158	GLY	2.1
1	B	291	PRO	2.1
1	D	141	PRO	2.1
1	D	145	PRO	2.1
1	B	238	ILE	2.0
1	D	290	THR	2.0

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

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

6.3 Carbohydrates [i](#)

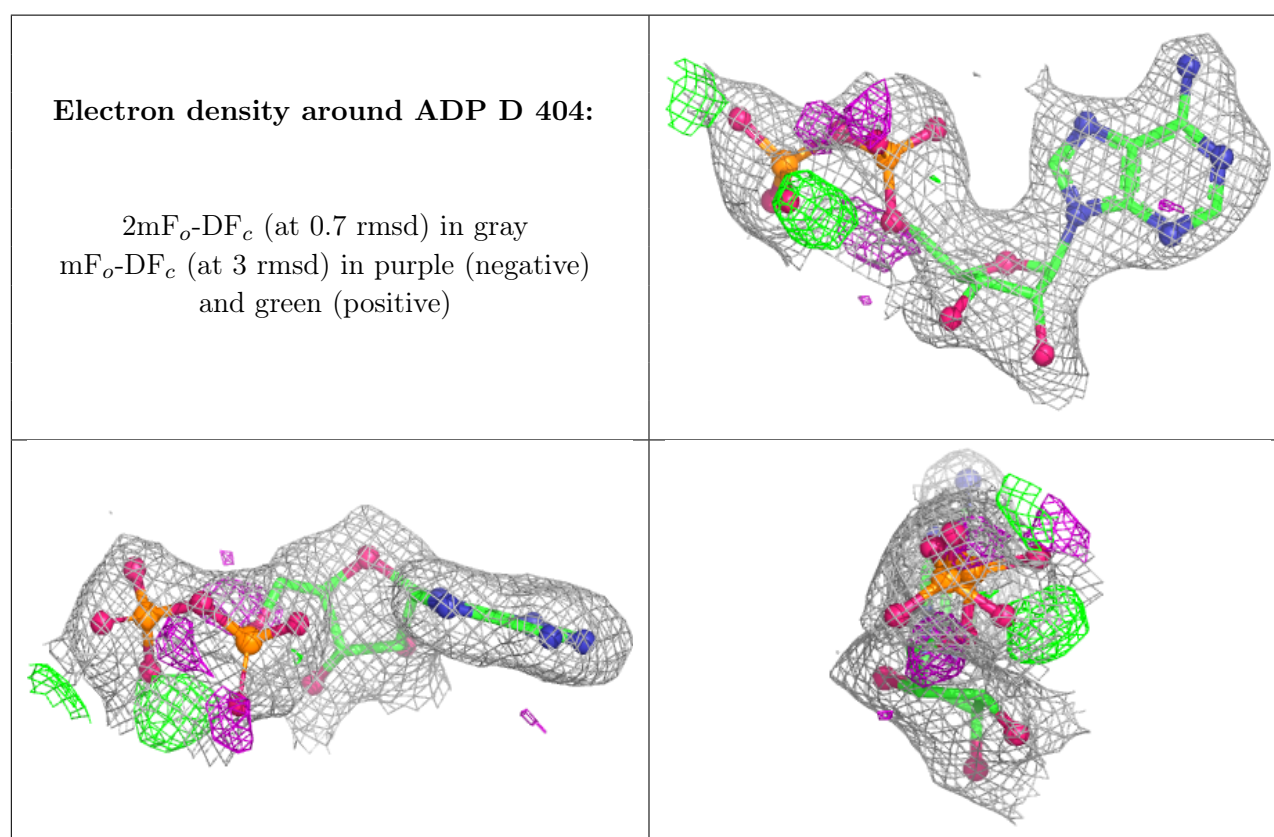
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

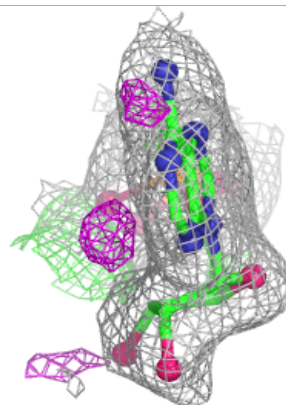
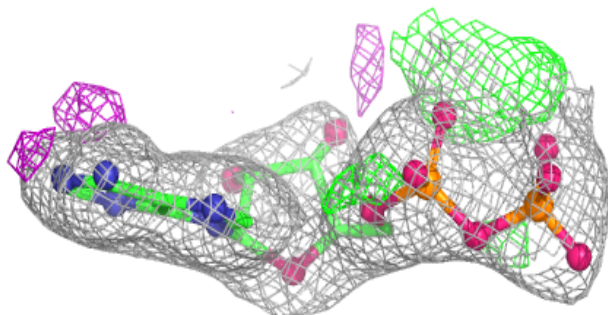
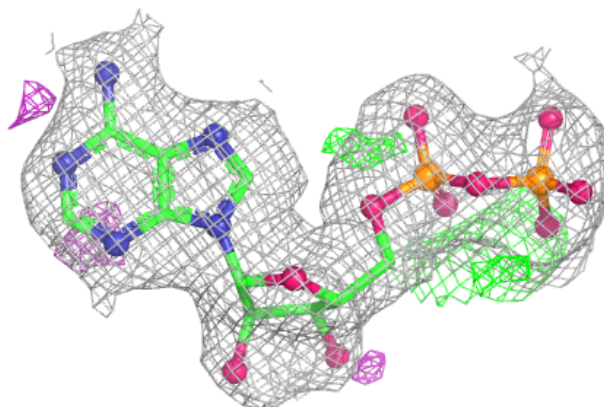
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	D	602	1/1	0.88	0.14	49,49,49,49	0
2	ADP	D	404	27/27	0.90	0.11	40,45,51,52	0
2	ADP	A	401	27/27	0.91	0.09	25,37,47,49	0
2	ADP	B	402	27/27	0.92	0.09	35,39,45,47	0
3	MG	C	601	1/1	0.94	0.08	34,34,34,34	0
2	ADP	C	403	27/27	0.97	0.06	21,24,28,31	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.



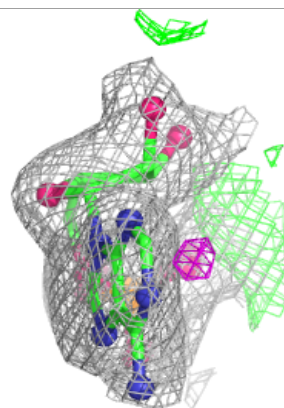
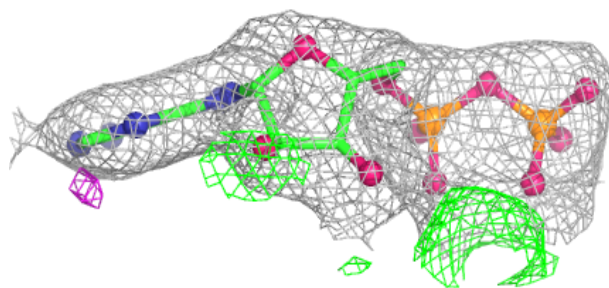
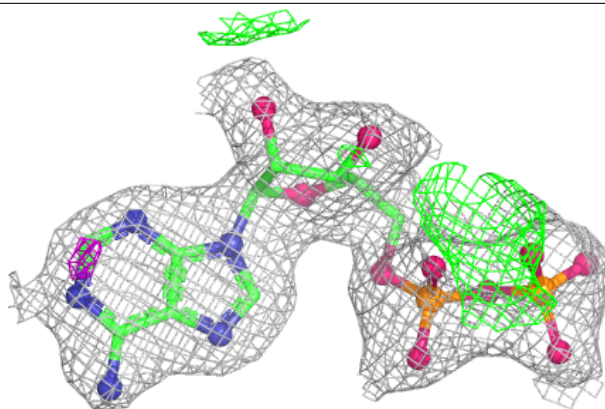
Electron density around ADP A 401:

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

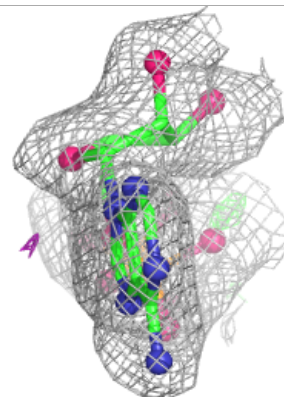
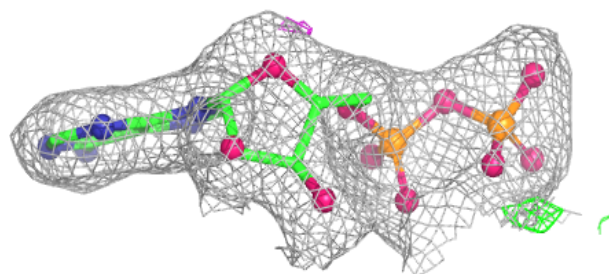
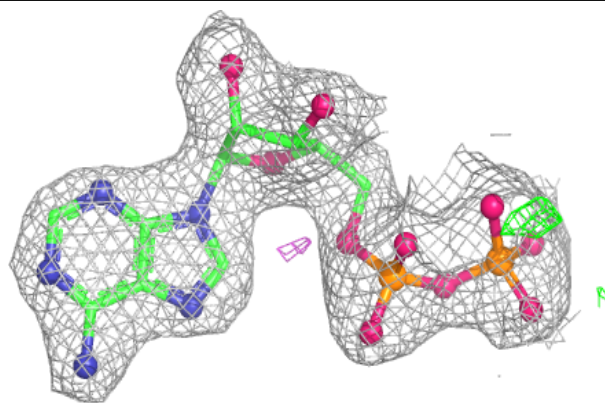


Electron density around ADP B 402:

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

**Electron density around ADP C 403:**

$2mF_o-DF_c$ (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.