



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:49 am BST

PDB ID : 3CRL
Title : Crystal structure of the PDHK2-L2 complex.
Authors : Popov, K.M.; Luo, M.; Green, T.J.; Grigorian, A.; Klyuyeva, A.; Tuganova, A.
Deposited on : 2008-04-07
Resolution : 2.61 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

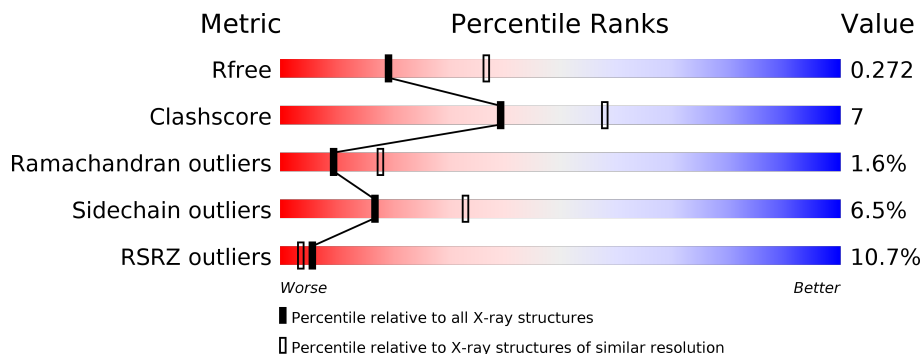
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 on 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	407	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">6% 69% 22% • 6%</p>
1	B	407	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">5% 74% 18% • 6%</p>
2	C	87	<div style="display: flex; align-items: center;"> <div style="width: 34%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">34% 83% 16% •</p>
2	D	87	<div style="display: flex; align-items: center;"> <div style="width: 30%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">30% 91% 9%</p>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7667 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 Pyruvate dehydrogenase [lipoamide] kinase isozyme 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	Total 3040	C 1943	N 504	O 575	S 18	0	0	0
1	B	383	Total 3059	C 1956	N 506	O 579	S 18	0	0	0

- Molecule 2 is a protein called Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	87	Total 680	C 436	N 105	O 133	S 6	0	0	0
2	D	87	Total 680	C 436	N 105	O 133	S 6	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

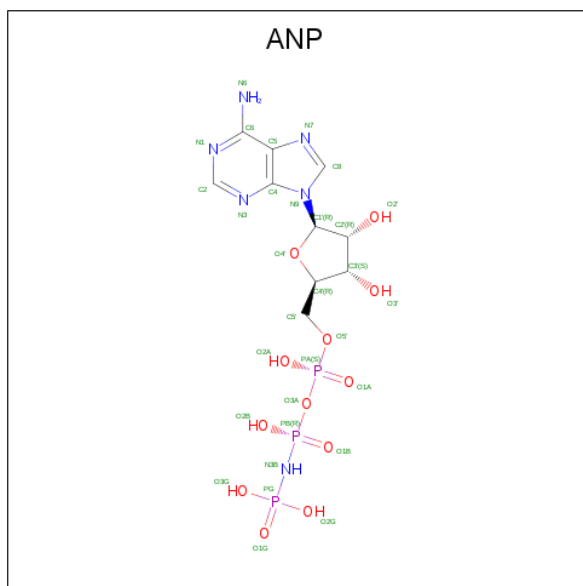
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter

code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

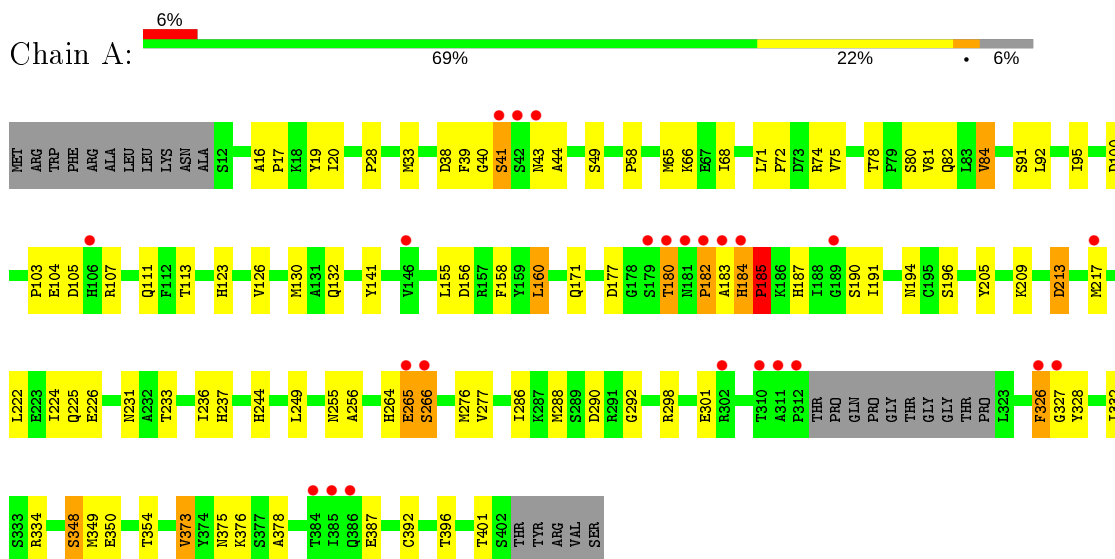
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	70	Total	O	0	0
			70	70		
6	B	59	Total	O	0	0
			59	59		
6	C	8	Total	O	0	0
			8	8		
6	D	5	Total	O	0	0
			5	5		

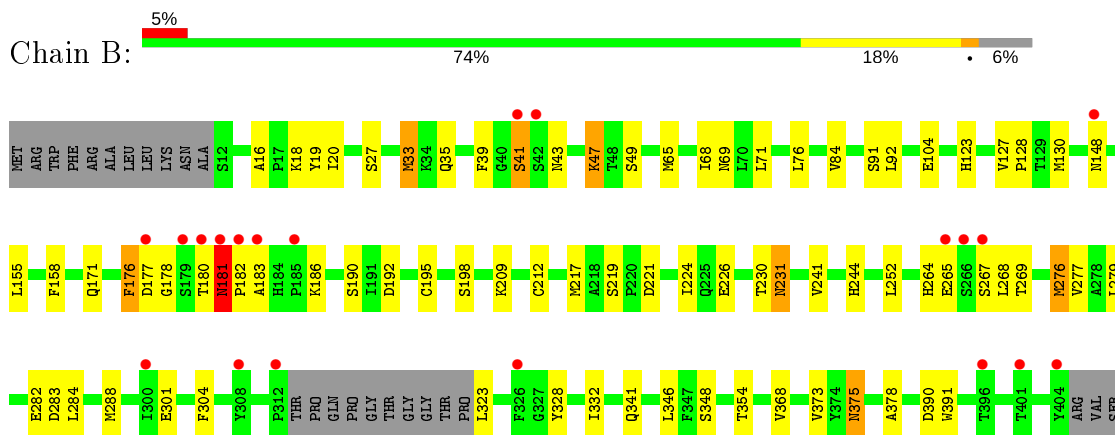
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

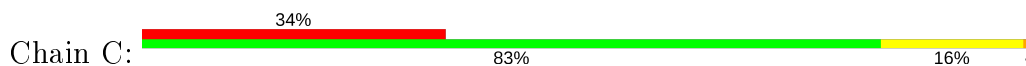
- Molecule 1: Pyruvate dehydrogenase [lipoamide] kinase isozyme 2, mitochondrial

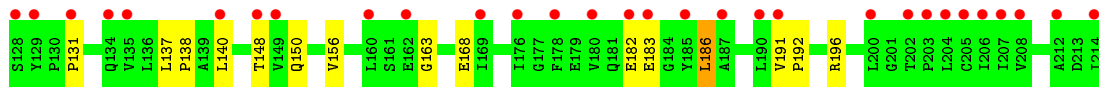


- Molecule 1: Pyruvate dehydrogenase [lipoamide] kinase isozyme 2, mitochondrial

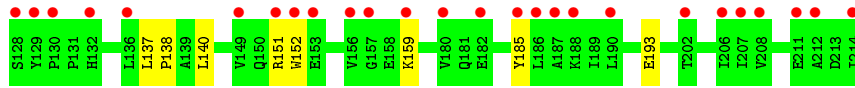
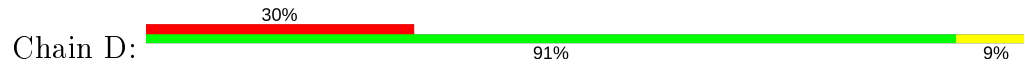


- Molecule 2: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial





- Molecule 2: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.41Å 121.63Å 71.45Å 90.00° 97.29° 90.00°	Depositor
Resolution (Å)	50.00 – 2.61 46.15 – 2.61	Depositor EDS
% Data completeness (in resolution range)	89.7 (50.00-2.61) 89.6 (46.15-2.61)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.221 , 0.274 0.221 , 0.272	Depositor DCC
R_{free} test set	1641 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtrriage
Anisotropy	0.325	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.318 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7667	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: MG, ANP, K, LA2

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	0.40	0/3115	0.54	0/4227
1	B	0.38	0/3135	0.53	0/4255
2	C	0.30	0/671	0.51	0/911
2	D	0.33	0/671	0.51	0/911
All	All	0.38	0/7592	0.53	0/10304

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	THR	Peptide
1	A	185	PRO	Peptide
1	B	176	PHE	Peptide

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	3040	0	2991	57	0
1	B	3059	0	3007	51	0
2	C	680	0	695	6	0
2	D	680	0	695	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	31	0	13	1	0
5	B	31	0	13	1	0
6	A	70	0	0	2	0
6	B	59	0	0	4	0
6	C	8	0	0	0	0
6	D	5	0	0	0	0
All	All	7667	0	7414	111	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 7.

All (111) 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:212:CYS:HA	1:B:323:LEU:HD11	1.54	0.90
1:B:264:HIS:HB3	1:B:267:SER:HB3	1.52	0.89
1:A:392:CYS:SG	1:B:373:VAL:CG2	2.69	0.81
1:B:171:GLN:HE22	1:B:190:SER:H	1.26	0.80
1:A:196:SER:HA	1:A:237:HIS:HD2	1.47	0.80
1:B:264:HIS:HB3	1:B:267:SER:CB	2.12	0.79
1:A:264:HIS:O	1:A:266:SER:N	2.15	0.79
1:A:28:PRO:HD2	1:A:373:VAL:HG12	1.66	0.77
1:A:132:GLN:HG3	6:A:3049:HOH:O	1.87	0.74
5:B:1001:ANP:H5'2	5:B:1001:ANP:H8	1.69	0.74
1:A:107:ARG:O	1:A:111:GLN:HG2	1.91	0.70
1:A:71:LEU:HD13	1:A:75:VAL:HB	1.73	0.70
1:A:392:CYS:SG	1:B:373:VAL:HG22	2.31	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:TRP:HD1	2:D:193:GLU:HG2	1.58	0.68
1:A:209:LYS:O	1:A:213:ASP:HB2	1.94	0.68
1:A:75:VAL:O	1:A:78:THR:HG22	1.94	0.68
1:B:252:LEU:HB3	1:B:288:MET:HE2	1.76	0.67
1:A:196:SER:HA	1:A:237:HIS:CD2	2.32	0.61
1:A:348:SER:HB3	1:A:354:THR:OG1	2.01	0.61
1:A:184:HIS:HB2	1:A:185:PRO:HA	1.83	0.61
1:B:91:SER:OG	1:B:123:HIS:HE1	1.86	0.58
1:B:176:PHE:O	1:B:178:GLY:N	2.32	0.57
1:B:68:ILE:O	1:B:71:LEU:HG	2.05	0.57
1:A:401:THR:HG21	1:B:35:GLN:HA	1.85	0.56
1:B:33:MET:CE	1:B:241:VAL:HG23	2.35	0.56
1:A:72:PRO:HB3	1:A:74:ARG:HH21	1.70	0.56
1:A:376:LYS:HG2	2:C:163:GLY:HA2	1.88	0.55
1:A:171:GLN:NE2	1:A:190:SER:H	2.04	0.55
1:A:28:PRO:HD2	1:A:373:VAL:CG1	2.35	0.55
1:A:68:ILE:O	1:A:71:LEU:HG	2.07	0.55
1:B:267:SER:HB2	6:B:3082:HOH:O	2.06	0.55
1:A:255:ASN:HB3	5:A:1000:ANP:N7	2.22	0.55
1:B:269:THR:HA	6:B:3097:HOH:O	2.06	0.55
1:B:171:GLN:NE2	1:B:190:SER:H	2.00	0.54
1:B:130:MET:CE	1:B:155:LEU:HD21	2.37	0.54
1:A:91:SER:OG	1:A:123:HIS:HE1	1.90	0.54
1:A:91:SER:OG	1:A:123:HIS:CE1	2.62	0.53
1:B:127:VAL:HB	1:B:128:PRO:HD3	1.89	0.53
1:B:33:MET:HE1	1:B:241:VAL:HG23	1.91	0.52
1:B:348:SER:HB3	1:B:354:THR:OG1	2.08	0.52
1:B:226:GLU:HG2	1:B:277:VAL:HB	1.91	0.52
1:B:192:ASP:HB3	1:B:195:CYS:HB2	1.92	0.52
1:A:205:TYR:CE1	1:A:222:LEU:HB2	2.45	0.52
1:B:91:SER:OG	1:B:123:HIS:CE1	2.63	0.51
1:B:190:SER:HA	6:B:3079:HOH:O	2.10	0.51
1:A:184:HIS:CB	1:A:185:PRO:HA	2.39	0.51
1:A:298:ARG:HD3	1:B:282:GLU:OE1	2.11	0.50
1:B:304:PHE:CZ	1:B:346:LEU:HD12	2.46	0.50
1:A:38:ASP:O	1:A:41:SER:HB3	2.12	0.50
1:B:252:LEU:O	1:B:288:MET:HE1	2.12	0.50
1:A:401:THR:HG21	1:B:35:GLN:O	2.11	0.50
2:C:150:GLN:HB3	2:C:168:GLU:HB2	1.94	0.49
1:B:16:ALA:HA	1:B:19:TYR:CD1	2.47	0.49
1:A:123:HIS:O	1:A:126:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ASN:H	1:B:182:PRO:CD	2.25	0.48
1:A:182:PRO:O	1:A:183:ALA:HB3	2.14	0.48
1:B:39:PHE:CZ	1:B:49:SER:HB2	2.49	0.48
1:B:375:ASN:HD22	1:B:378:ALA:H	1.62	0.48
1:A:80:SER:O	1:A:84:VAL:HG12	2.15	0.47
1:B:65:MET:HA	1:B:68:ILE:HD12	1.97	0.47
1:A:33:MET:HG3	1:A:191:ILE:HD13	1.96	0.47
1:A:58:PRO:HD3	1:A:95:ILE:HG21	1.97	0.46
1:A:16:ALA:HA	1:A:19:TYR:CD1	2.51	0.46
1:B:130:MET:HG3	1:B:158:PHE:CE2	2.51	0.46
1:A:171:GLN:HE22	1:A:190:SER:H	1.63	0.46
2:D:159:LYS:HG2	2:D:185:TYR:CE2	2.50	0.46
1:A:130:MET:HE2	1:A:155:LEU:HD21	1.98	0.46
1:A:213:ASP:O	1:A:217:MET:HA	2.16	0.46
1:A:180:THR:O	1:A:182:PRO:HD3	2.16	0.45
1:A:328:TYR:HB3	1:A:332:ILE:HD12	1.99	0.45
1:A:249:LEU:HD21	1:A:286:ILE:HG21	1.99	0.45
1:A:40:GLY:HA2	1:A:44:ALA:HB2	1.96	0.45
1:B:375:ASN:ND2	1:B:378:ALA:H	2.15	0.45
1:A:256:ALA:HB2	1:A:288:MET:CE	2.48	0.44
1:B:39:PHE:HZ	1:B:49:SER:HB2	1.81	0.44
1:A:130:MET:HG3	1:A:158:PHE:CE2	2.52	0.44
1:B:328:TYR:HB3	1:B:332:ILE:HD12	1.99	0.44
2:C:148:THR:HG23	2:C:196:ARG:HA	1.99	0.44
1:B:209:LYS:HG3	1:B:219:SER:OG	2.18	0.44
1:A:74:ARG:HG2	1:A:141:TYR:CZ	2.53	0.43
1:A:156:ASP:O	1:A:160:LEU:HB2	2.18	0.43
1:B:279:LEU:HD13	1:B:284:LEU:HD12	2.00	0.43
1:A:226:GLU:HB3	1:A:236:ILE:HD12	2.01	0.43
1:B:130:MET:HE2	1:B:155:LEU:HD21	2.00	0.43
1:B:16:ALA:O	1:B:20:ILE:HG12	2.18	0.43
1:B:39:PHE:C	1:B:41:SER:H	2.22	0.43
1:A:16:ALA:N	1:A:17:PRO:CD	2.81	0.43
1:A:39:PHE:CZ	1:A:49:SER:HB2	2.54	0.43
1:B:41:SER:HA	6:B:3098:HOH:O	2.19	0.43
1:B:390:ASP:HB3	1:B:391:TRP:CD1	2.54	0.42
1:A:236:ILE:HD13	1:A:277:VAL:HG12	2.01	0.42
1:A:39:PHE:C	1:A:41:SER:H	2.22	0.42
1:B:264:HIS:HB3	1:B:267:SER:HB2	1.96	0.42
1:B:181:ASN:H	1:B:182:PRO:HD3	1.84	0.42
1:A:350:GLU:HB3	1:B:283:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:156:VAL:HA	2:C:186:LEU:HD12	2.01	0.42
2:C:137:LEU:HA	2:C:138:PRO:HD3	1.94	0.42
1:A:276:MET:HG3	6:A:3061:HOH:O	2.20	0.42
1:A:75:VAL:HG12	1:A:81:VAL:HG21	2.01	0.41
1:A:224:ILE:HG22	1:A:225:GLN:N	2.35	0.41
1:B:231:ASN:HD22	1:B:231:ASN:C	2.23	0.41
1:A:375:ASN:H	1:A:378:ALA:HB3	1.86	0.41
2:C:191:VAL:HA	2:C:192:PRO:HD3	1.89	0.41
1:B:130:MET:HE2	1:B:155:LEU:CD2	2.51	0.41
1:A:20:ILE:HD11	1:A:65:MET:CE	2.51	0.41
1:A:290:ASP:OD1	1:A:292:GLY:N	2.48	0.41
1:B:47:LYS:HE3	1:B:104:GLU:HG3	2.03	0.41
1:B:341:GLN:HG2	1:B:368:VAL:O	2.20	0.40
1:A:103:PRO:C	1:A:105:ASP:H	2.25	0.40
2:D:137:LEU:HA	2:D:138:PRO:HD3	1.87	0.40
1:B:276:MET:HE2	1:B:277:VAL:N	2.36	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	377/407 (93%)	347 (92%)	22 (6%)	8 (2%)	7	12
1	B	379/407 (93%)	342 (90%)	31 (8%)	6 (2%)	9	18
2	C	84/87 (97%)	78 (93%)	5 (6%)	1 (1%)	13	25
2	D	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
All	All	924/988 (94%)	844 (91%)	65 (7%)	15 (2%)	9	18

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	184	HIS
1	A	185	PRO
1	A	265	GLU
1	A	266	SER
1	A	326	PHE
1	B	41	SER
1	B	268	LEU
1	A	182	PRO
1	B	183	ALA
1	A	327	GLY
1	B	181	ASN
1	B	180	THR
1	B	186	LYS
2	C	131	PRO

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	342/363 (94%)	317 (93%)	25 (7%)	14	27
1	B	344/363 (95%)	321 (93%)	23 (7%)	16	31
2	C	74/74 (100%)	70 (95%)	4 (5%)	22	42
2	D	74/74 (100%)	72 (97%)	2 (3%)	44	69
All	All	834/874 (95%)	780 (94%)	54 (6%)	17	33

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	66	LYS
1	A	82	GLN
1	A	84	VAL
1	A	92	LEU
1	A	100	ASP
1	A	104	GLU

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Mol	Chain	Res	Type
1	A	113	THR
1	A	160	LEU
1	A	177	ASP
1	A	187	HIS
1	A	194	ASN
1	A	213	ASP
1	A	231	ASN
1	A	233	THR
1	A	244	HIS
1	A	265	GLU
1	A	301	GLU
1	A	326	PHE
1	A	334	ARG
1	A	348	SER
1	A	349	MET
1	A	373	VAL
1	A	387	GLU
1	A	396	THR
1	B	18	LYS
1	B	27	SER
1	B	33	MET
1	B	43	ASN
1	B	47	LYS
1	B	69	ASN
1	B	76	LEU
1	B	84	VAL
1	B	92	LEU
1	B	148	ASN
1	B	177	ASP
1	B	181	ASN
1	B	198	SER
1	B	217	MET
1	B	221	ASP
1	B	224	ILE
1	B	230	THR
1	B	231	ASN
1	B	244	HIS
1	B	265	GLU
1	B	276	MET
1	B	301	GLU
1	B	375	ASN
2	C	140	LEU

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Mol	Chain	Res	Type
2	C	182	GLU
2	C	183	GLU
2	C	186	LEU
2	D	140	LEU
2	D	151	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	171	GLN
1	A	231	ASN
1	A	234	GLN
1	A	237	HIS
1	B	43	ASN
1	B	111	GLN
1	B	123	HIS
1	B	148	ASN
1	B	171	GLN
1	B	231	ASN
1	B	375	ASN
2	C	134	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](#)

2 non-standard protein/DNA/RNA residues 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
2	LA2	C	173	2	17,19,20	0.34	0	12,21,23	1.80	3 (25%)
2	LA2	D	173	2	17,19,20	0.37	0	12,21,23	1.86	3 (25%)

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	LA2	C	173	2	-	7/18/20/22	-
2	LA2	D	173	2	-	8/18/20/22	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	173	LA2	C7-C8-S8	-5.16	108.36	113.74
2	C	173	LA2	C7-C8-S8	-4.54	109.01	113.74
2	C	173	LA2	CD-CE-NZ	-2.29	105.66	112.21
2	D	173	LA2	CE-NZ-C1	2.26	127.04	122.84
2	D	173	LA2	CD-CE-NZ	-2.23	105.84	112.21
2	C	173	LA2	CE-NZ-C1	2.15	126.82	122.84

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	173	LA2	C4-C5-C6-S6
2	C	173	LA2	C5-C6-C7-C8
2	D	173	LA2	C4-C5-C6-S6
2	D	173	LA2	C4-C5-C6-C7
2	D	173	LA2	C1-C2-C3-C4
2	C	173	LA2	C3-C4-C5-C6
2	D	173	LA2	C2-C3-C4-C5
2	C	173	LA2	C2-C3-C4-C5
2	C	173	LA2	CE-CD-CG-CB
2	C	173	LA2	C4-C5-C6-C7
2	D	173	LA2	CE-CD-CG-CB
2	C	173	LA2	C1-C2-C3-C4
2	D	173	LA2	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	D	173	LA2	O1-C1-C2-C3
2	D	173	LA2	NZ-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	ANP	B	1001	3	29,33,33	1.87	9 (31%)	31,52,52	1.93	8 (25%)
5	ANP	A	1000	3	29,33,33	1.87	8 (27%)	31,52,52	1.58	7 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	B	1001	3	-	6/14/38/38	0/3/3/3
5	ANP	A	1000	3	-	3/14/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1001	ANP	PG-N3B	4.61	1.75	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1000	ANP	PG-N3B	4.60	1.75	1.63
5	A	1000	ANP	PB-N3B	4.36	1.74	1.63
5	B	1001	ANP	PB-N3B	4.29	1.74	1.63
5	B	1001	ANP	PG-O1G	3.42	1.51	1.46
5	A	1000	ANP	PB-O1B	3.40	1.51	1.46
5	A	1000	ANP	PG-O1G	3.22	1.51	1.46
5	B	1001	ANP	PB-O1B	3.16	1.51	1.46
5	B	1001	ANP	C5-C4	2.61	1.47	1.40
5	A	1000	ANP	C5-C4	2.52	1.47	1.40
5	B	1001	ANP	PB-O3A	2.43	1.62	1.59
5	B	1001	ANP	O4'-C1'	2.26	1.44	1.41
5	B	1001	ANP	PB-O2B	-2.09	1.51	1.56
5	A	1000	ANP	PG-O3G	-2.04	1.51	1.56
5	A	1000	ANP	PG-O2G	-2.03	1.51	1.56
5	A	1000	ANP	O4'-C1'	2.03	1.43	1.41
5	B	1001	ANP	PG-O3G	-2.01	1.51	1.56

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	ANP	O1G-PG-N3B	-5.06	104.32	111.77
5	B	1001	ANP	O2B-PB-O1B	4.09	118.50	109.92
5	A	1000	ANP	O2B-PB-O1B	3.83	117.95	109.92
5	B	1001	ANP	O1B-PB-N3B	-3.78	106.21	111.77
5	A	1000	ANP	N3-C2-N1	-3.77	122.78	128.68
5	B	1001	ANP	C3'-C2'-C1'	3.30	105.95	100.98
5	B	1001	ANP	N3-C2-N1	-3.27	123.56	128.68
5	A	1000	ANP	O1G-PG-N3B	-2.84	107.59	111.77
5	B	1001	ANP	C4-C5-N7	-2.67	106.62	109.40
5	A	1000	ANP	PA-O3A-PB	-2.40	124.18	132.62
5	A	1000	ANP	C4-C5-N7	-2.36	106.94	109.40
5	A	1000	ANP	C2-N1-C6	2.31	122.71	118.75
5	B	1001	ANP	O3G-PG-O2G	2.27	113.69	107.64
5	A	1000	ANP	O3G-PG-O2G	2.24	113.60	107.64
5	B	1001	ANP	PA-O3A-PB	-2.15	125.04	132.62

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1001	ANP	PB-N3B-PG-O1G
5	B	1001	ANP	PG-N3B-PB-O1B

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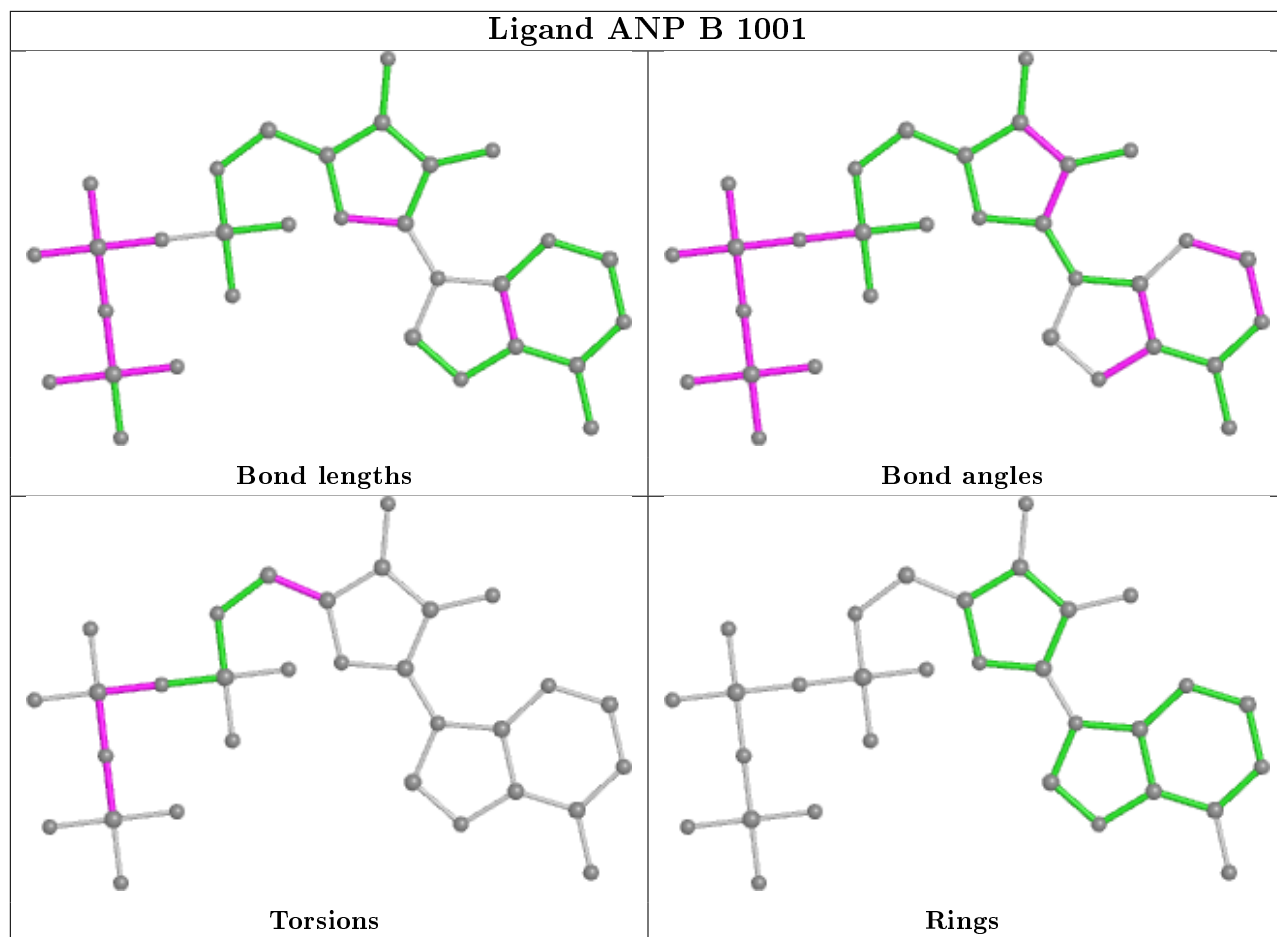
Mol	Chain	Res	Type	Atoms
5	B	1001	ANP	PA-O3A-PB-O1B
5	B	1001	ANP	PA-O3A-PB-O2B
5	B	1001	ANP	C3'-C4'-C5'-O5'
5	A	1000	ANP	PB-N3B-PG-O1G
5	A	1000	ANP	PG-N3B-PB-O1B
5	B	1001	ANP	O4'-C4'-C5'-O5'
5	A	1000	ANP	PA-O3A-PB-O2B

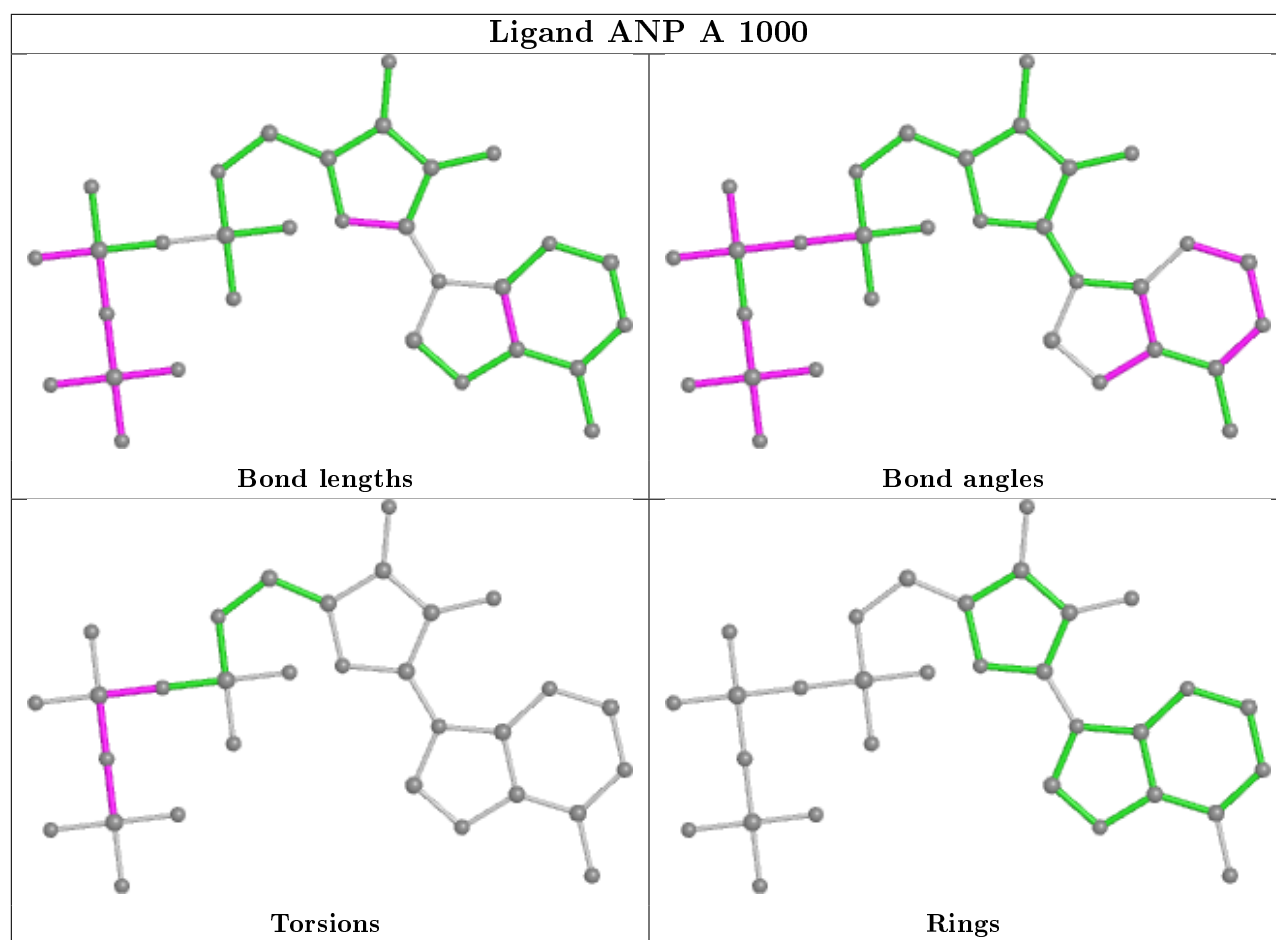
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1001	ANP	1	0
5	A	1000	ANP	1	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	381/407 (93%)	0.49	24 (6%) 20 15	22, 42, 58, 65	0
1	B	383/407 (94%)	0.50	20 (5%) 27 21	20, 42, 63, 73	0
2	C	86/87 (98%)	1.84	30 (34%) 0 0	69, 80, 92, 95	0
2	D	86/87 (98%)	1.53	26 (30%) 0 0	68, 80, 92, 95	0
All	All	936/988 (94%)	0.72	100 (10%) 6 4	20, 45, 84, 95	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	214	ILE	8.3
1	A	385	ILE	7.8
1	B	182	PRO	7.0
1	B	266	SER	7.0
1	A	42	SER	6.8
2	C	206	ILE	6.8
1	A	311	ALA	6.5
2	D	128	SER	6.1
2	D	212	ALA	6.1
1	A	182	PRO	5.8
1	B	404	TYR	5.7
1	A	183	ALA	5.5
2	D	156	VAL	5.3
1	A	312	PRO	5.3
2	D	129	TYR	5.0
2	C	190	LEU	5.0
2	D	130	PRO	4.8
2	D	206	ILE	4.7
2	C	208	VAL	4.6
2	C	187	ALA	4.6
1	B	265	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	43	ASN	4.5
2	C	169	ILE	4.5
2	D	159	LYS	4.1
2	C	149	VAL	4.1
1	B	312	PRO	3.8
2	C	183	GLU	3.8
2	D	186	LEU	3.6
2	D	214	ILE	3.6
2	D	208	VAL	3.6
1	B	179	SER	3.5
1	B	181	ASN	3.5
2	C	160	LEU	3.4
2	C	131	PRO	3.4
2	C	182	GLU	3.4
2	C	200	LEU	3.4
2	C	203	PRO	3.3
2	C	180	VAL	3.3
2	C	135	VAL	3.2
2	C	202	THR	3.2
2	C	178	PHE	3.2
1	A	310	THR	3.1
1	A	180	THR	3.0
1	A	265	GLU	3.0
1	A	326	PHE	2.9
1	B	308	TYR	2.9
1	A	106	HIS	2.9
2	D	136	LEU	2.9
1	A	179	SER	2.9
1	B	185	PRO	2.8
2	D	180	VAL	2.8
2	C	191	VAL	2.8
1	A	266	SER	2.8
1	B	396	THR	2.8
1	B	267	SER	2.8
2	D	132	HIS	2.8
1	A	386	GLN	2.7
2	C	148	THR	2.7
2	D	188	LYS	2.7
1	B	401	THR	2.7
1	A	302	ARG	2.7
2	D	182	GLU	2.6
2	C	134	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	384	THR	2.6
1	B	180	THR	2.5
2	C	212	ALA	2.5
2	C	204	LEU	2.5
1	B	148	ASN	2.5
1	B	183	ALA	2.5
1	B	300	ILE	2.5
2	C	205	CYS	2.5
1	A	327	GLY	2.5
2	D	157	GLY	2.5
1	B	177	ASP	2.5
1	B	42	SER	2.4
2	C	176	ILE	2.4
2	C	162	GLU	2.4
2	D	207	ILE	2.4
1	A	146	VAL	2.4
1	A	217	MET	2.3
2	C	128	SER	2.3
1	A	181	ASN	2.3
2	D	152	TRP	2.3
2	D	202	THR	2.3
2	D	187	ALA	2.3
1	B	326	PHE	2.3
2	D	153	GLU	2.3
1	A	189	GLY	2.2
1	B	41	SER	2.2
2	D	185	TYR	2.2
2	D	151	ARG	2.2
2	D	211	GLU	2.2
1	A	184	HIS	2.1
2	C	129	TYR	2.1
2	D	190	LEU	2.1
1	A	41	SER	2.1
2	C	207	ILE	2.1
2	C	185	TYR	2.1
2	D	149	VAL	2.0
2	C	140	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LA2	C	173	20/21	0.88	0.28	65,66,68,68	0
2	LA2	D	173	20/21	0.91	0.23	65,66,68,68	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

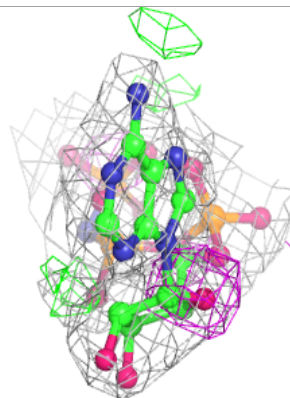
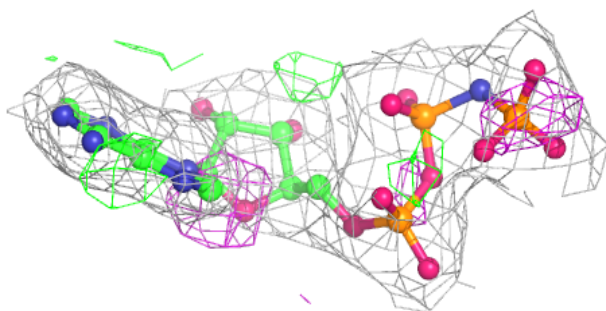
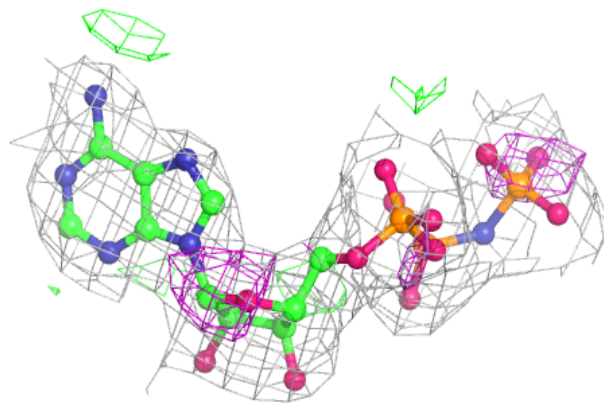
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	B	3001	1/1	0.91	0.27	92,92,92,92	0
3	MG	B	2001	1/1	0.93	0.18	56,56,56,56	0
5	ANP	B	1001	31/31	0.94	0.16	54,58,59,61	0
4	K	A	3002	1/1	0.94	0.11	82,82,82,82	0
3	MG	A	2000	1/1	0.94	0.06	42,42,42,42	0
5	ANP	A	1000	31/31	0.96	0.13	44,51,57,58	0

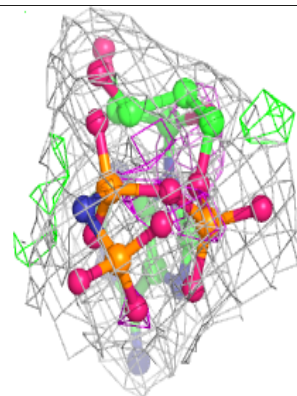
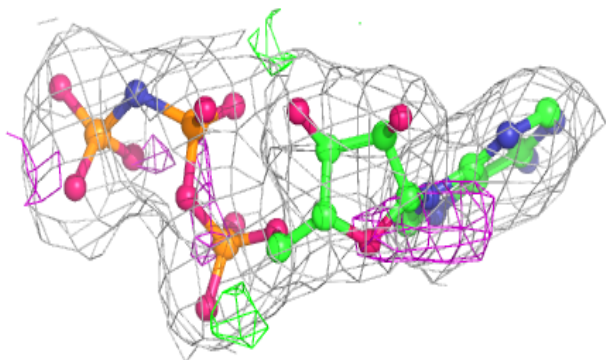
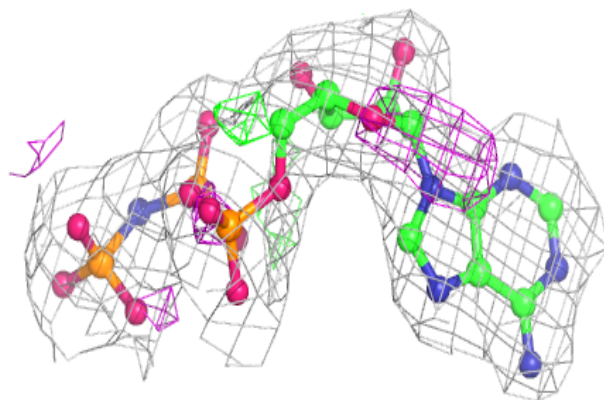
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 1001:

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

**Electron density around ANP A 1000:**

$2mF_o-DF_c$ (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.