



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:36 PM UTC

PDB ID : 6K1R / pdb_00006k1r
Title : Crystal structure of Ketopantoate reductase from *Pseudomonas aeruginosa* in complex with NAD⁺ and ketopantoate
Authors : Khanppnavar, B.; Choudhury, A.; Datta, S.
Deposited on : 2019-05-12
Resolution : 2.55 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

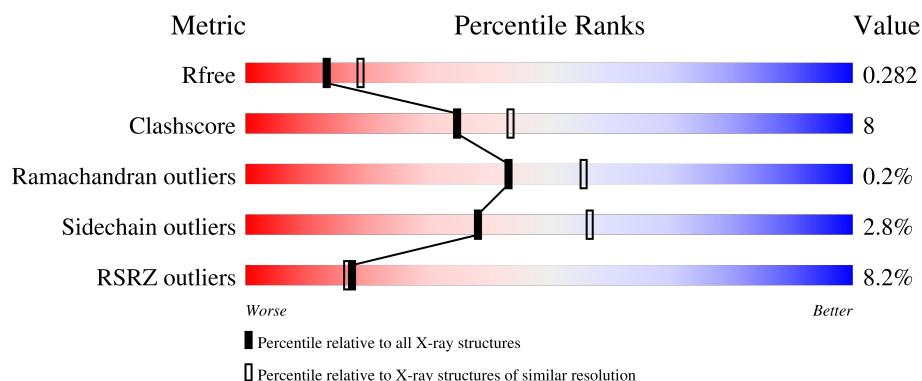
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	323	 2% 79% 15% • 6%
1	B	323	 7% 80% 14% • 6%
1	C	323	 14% 73% 21% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7473 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 Probable 2-dehydropantoate 2-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	1	0
			2354	1462	459	425	8			
1	B	305	Total	C	N	O	S	0	1	0
			2354	1462	459	425	8			
1	C	305	Total	C	N	O	S	0	1	0
			2353	1461	457	427	8			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q9HW09
A	-18	GLY	-	expression tag	UNP Q9HW09
A	-17	SER	-	expression tag	UNP Q9HW09
A	-16	SER	-	expression tag	UNP Q9HW09
A	-15	HIS	-	expression tag	UNP Q9HW09
A	-14	HIS	-	expression tag	UNP Q9HW09
A	-13	HIS	-	expression tag	UNP Q9HW09
A	-12	HIS	-	expression tag	UNP Q9HW09
A	-11	HIS	-	expression tag	UNP Q9HW09
A	-10	HIS	-	expression tag	UNP Q9HW09
A	-9	SER	-	expression tag	UNP Q9HW09
A	-8	SER	-	expression tag	UNP Q9HW09
A	-7	GLY	-	expression tag	UNP Q9HW09
A	-6	LEU	-	expression tag	UNP Q9HW09
A	-5	VAL	-	expression tag	UNP Q9HW09
A	-4	PRO	-	expression tag	UNP Q9HW09
A	-3	ARG	-	expression tag	UNP Q9HW09
A	-2	GLY	-	expression tag	UNP Q9HW09
A	-1	SER	-	expression tag	UNP Q9HW09
A	0	HIS	-	expression tag	UNP Q9HW09
B	-19	MET	-	initiating methionine	UNP Q9HW09
B	-18	GLY	-	expression tag	UNP Q9HW09
B	-17	SER	-	expression tag	UNP Q9HW09

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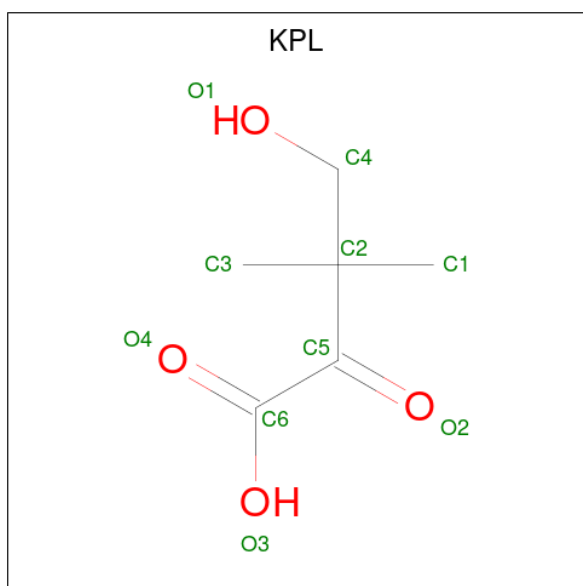
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP Q9HW09
B	-15	HIS	-	expression tag	UNP Q9HW09
B	-14	HIS	-	expression tag	UNP Q9HW09
B	-13	HIS	-	expression tag	UNP Q9HW09
B	-12	HIS	-	expression tag	UNP Q9HW09
B	-11	HIS	-	expression tag	UNP Q9HW09
B	-10	HIS	-	expression tag	UNP Q9HW09
B	-9	SER	-	expression tag	UNP Q9HW09
B	-8	SER	-	expression tag	UNP Q9HW09
B	-7	GLY	-	expression tag	UNP Q9HW09
B	-6	LEU	-	expression tag	UNP Q9HW09
B	-5	VAL	-	expression tag	UNP Q9HW09
B	-4	PRO	-	expression tag	UNP Q9HW09
B	-3	ARG	-	expression tag	UNP Q9HW09
B	-2	GLY	-	expression tag	UNP Q9HW09
B	-1	SER	-	expression tag	UNP Q9HW09
B	0	HIS	-	expression tag	UNP Q9HW09
C	-19	MET	-	initiating methionine	UNP Q9HW09
C	-18	GLY	-	expression tag	UNP Q9HW09
C	-17	SER	-	expression tag	UNP Q9HW09
C	-16	SER	-	expression tag	UNP Q9HW09
C	-15	HIS	-	expression tag	UNP Q9HW09
C	-14	HIS	-	expression tag	UNP Q9HW09
C	-13	HIS	-	expression tag	UNP Q9HW09
C	-12	HIS	-	expression tag	UNP Q9HW09
C	-11	HIS	-	expression tag	UNP Q9HW09
C	-10	HIS	-	expression tag	UNP Q9HW09
C	-9	SER	-	expression tag	UNP Q9HW09
C	-8	SER	-	expression tag	UNP Q9HW09
C	-7	GLY	-	expression tag	UNP Q9HW09
C	-6	LEU	-	expression tag	UNP Q9HW09
C	-5	VAL	-	expression tag	UNP Q9HW09
C	-4	PRO	-	expression tag	UNP Q9HW09
C	-3	ARG	-	expression tag	UNP Q9HW09
C	-2	GLY	-	expression tag	UNP Q9HW09
C	-1	SER	-	expression tag	UNP Q9HW09
C	0	HIS	-	expression tag	UNP Q9HW09

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is KETOPANTOATE (CCD ID: KPL) (formula: $C_6H_{10}O_4$) (labeled as "Ligand of Interest" by depositor).



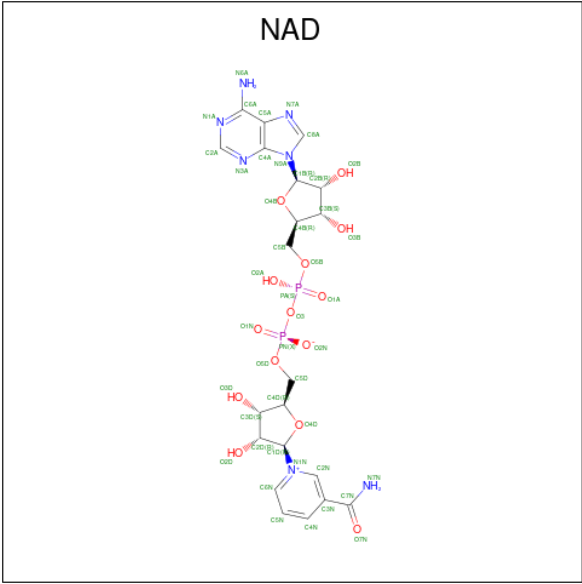
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

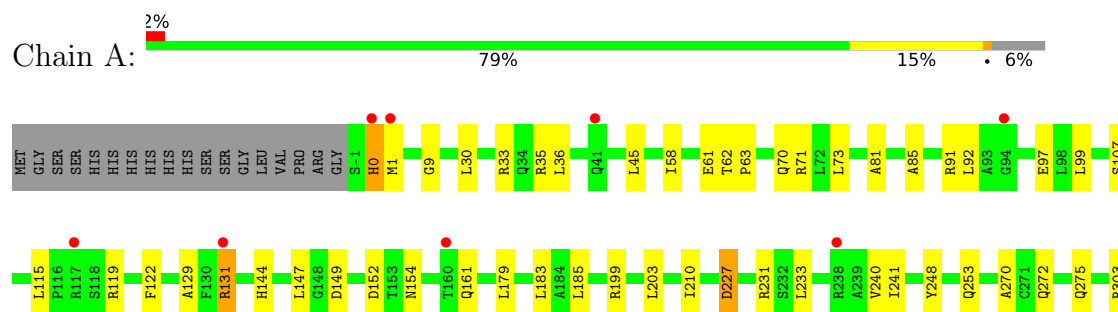
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	104	Total	O	0	0
			104	104		
5	B	101	Total	O	0	0
			101	101		
5	C	77	Total	O	0	0
			77	77		

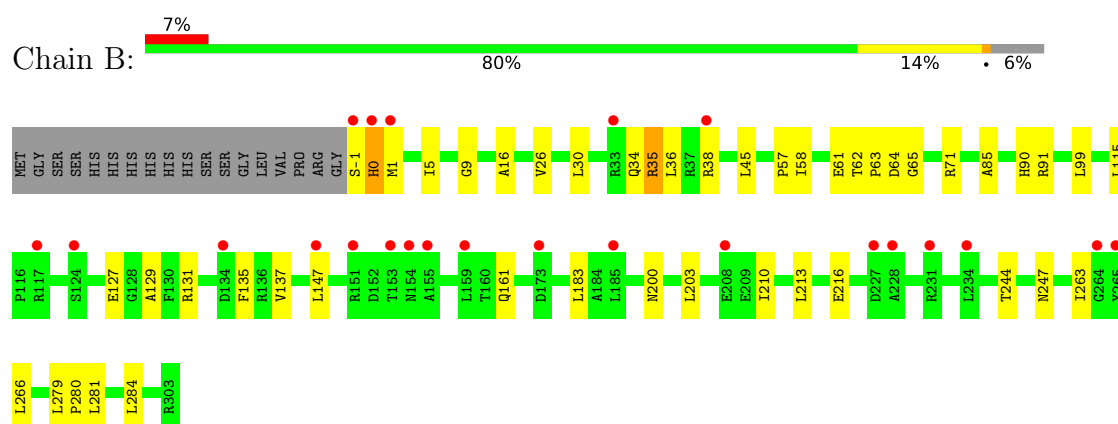
3 Residue-property plots [i](#)

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.

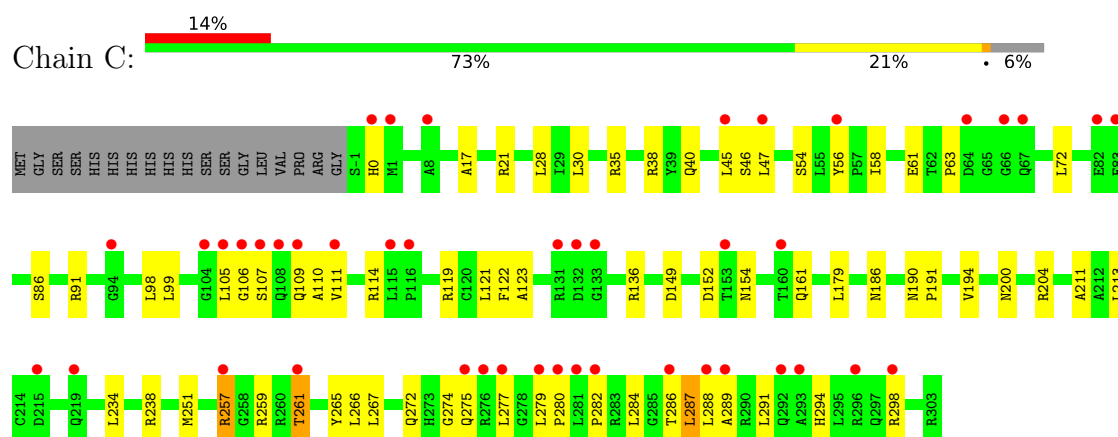
- Molecule 1: Probable 2-dehydropantoate 2-reductase



- Molecule 1: Probable 2-dehydropantoate 2-reductase



- Molecule 1: Probable 2-dehydropantoate 2-reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	130.00Å 130.00Å 155.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.98 – 2.55 22.98 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.0 (22.98-2.55) 97.6 (22.98-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.57Å)	Xtriage
Refinement program	PHENIX (1.12_2829: 000)	Depositor
R, R_{free}	0.244 , 0.269 0.252 , 0.282	Depositor DCC
R_{free} test set	1644 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7473	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 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAD, KPL

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	0.11	0/2401	0.31	0/3256
1	B	0.11	0/2401	0.34	0/3256
1	C	0.12	0/2399	0.32	0/3253
All	All	0.11	0/7201	0.32	0/9765

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2354	0	2347	34	0
1	B	2354	0	2347	30	0
1	C	2353	0	2346	44	0
2	A	12	0	16	1	0
3	A	10	0	9	0	0
3	B	10	0	9	0	0
3	C	10	0	9	4	0
4	A	44	0	24	3	0
4	B	44	0	24	4	0
5	A	104	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	101	0	0	1	0
5	C	77	0	0	2	0
All	All	7473	0	7131	108	0

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

All (108) 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:C:106:GLY:HA2	1:C:265:TYR:HB3	1.67	0.74
1:B:129:ALA:H	4:B:402:NAD:H72N	1.37	0.73
1:C:251:MET:HG3	1:C:261:THR:HG21	1.71	0.72
1:A:129:ALA:H	4:A:404:NAD:H72N	1.40	0.69
1:B:203:LEU:HB3	1:B:210:ILE:HD11	1.76	0.68
1:C:121:LEU:HD23	1:C:149:ASP:HB2	1.78	0.66
1:C:267:LEU:HD21	1:C:287:LEU:HD13	1.80	0.64
1:C:107:SER:HB2	1:C:110:ALA:HB3	1.80	0.64
1:A:248:TYR:O	1:A:253:GLN:NE2	2.31	0.63
1:B:71:ARG:NH1	1:B:161:GLN:OE1	2.32	0.62
1:C:279:LEU:HD12	1:C:280:PRO:HD2	1.81	0.61
1:A:99:LEU:HD11	1:A:147:LEU:HD22	1.82	0.60
1:A:275:GLN:NE2	5:A:501:HOH:O	2.32	0.59
1:A:33:ARG:HG2	1:A:62:THR:HG21	1.84	0.59
1:C:105:LEU:HD22	1:C:109:GLN:HE22	1.67	0.59
1:B:34:GLN:HG2	1:B:38:ARG:HE	1.69	0.58
1:C:107:SER:O	1:C:111:VAL:N	2.26	0.58
1:A:183:LEU:HD21	1:A:270:ALA:HB2	1.86	0.57
1:C:21:ARG:NH1	5:C:503:HOH:O	2.38	0.57
1:A:1:MET:HE2	1:A:71:ARG:HB2	1.85	0.57
3:C:401:KPL:O2	3:C:401:KPL:O1	2.23	0.56
1:C:267:LEU:HG	1:C:288:LEU:HB2	1.87	0.56
1:A:185:LEU:HD21	1:A:240:VAL:HG21	1.89	0.55
1:A:9:GLY:HA3	4:A:404:NAD:O5B	2.07	0.55
1:C:194:VAL:HG21	1:C:251:MET:HG2	1.88	0.54
1:B:281:LEU:HD13	1:B:284:LEU:HD12	1.89	0.54
1:C:38:ARG:NH1	5:C:504:HOH:O	2.41	0.53
1:A:144:HIS:HB3	2:A:401:GOL:H11	1.91	0.53
1:B:5:ILE:HD12	1:B:26:VAL:HG13	1.89	0.53
1:A:0[B]:HIS:CE1	1:A:71:ARG:HH22	2.28	0.52
1:A:30:LEU:HD12	1:A:36:LEU:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:HD11	1:C:123:ALA:HB2	1.92	0.51
1:B:183:LEU:HG	1:B:266:LEU:HA	1.92	0.51
1:C:30:LEU:O	1:C:63:PRO:HD3	2.10	0.51
1:B:45:LEU:HD12	1:B:58:ILE:HD12	1.93	0.51
1:C:61:GLU:OE1	1:C:91:ARG:NH2	2.42	0.50
1:C:200:ASN:ND2	3:C:401:KPL:H11	2.27	0.50
1:B:45:LEU:HD23	1:B:135:PHE:HB3	1.93	0.50
1:A:152:ASP:OD1	1:A:154:ASN:ND2	2.44	0.50
1:C:186:ASN:HB2	1:C:266:LEU:HD11	1.93	0.50
1:A:199:ARG:NH2	1:B:247:ASN:OD1	2.44	0.50
1:A:30:LEU:O	1:A:63:PRO:HD3	2.12	0.49
1:C:204:ARG:HG2	1:C:238:ARG:HH22	1.76	0.49
1:B:64:ASP:OD1	1:B:65:GLY:N	2.42	0.49
1:A:203:LEU:HD22	1:A:210:ILE:HD11	1.94	0.49
4:B:402:NAD:H8A	5:B:521:HOH:O	2.13	0.48
1:A:0[B]:HIS:CG	1:A:1:MET:N	2.82	0.48
1:A:122:PHE:HB3	1:A:179:LEU:HD11	1.96	0.48
1:B:-1:SER:O	1:B:0[B]:HIS:HB2	2.14	0.48
1:C:122:PHE:HB3	1:C:179:LEU:HD11	1.95	0.48
1:C:274:GLY:O	1:C:279:LEU:N	2.40	0.48
1:C:272:GLN:O	1:C:275:GLN:HG2	2.14	0.47
1:B:131:ARG:HG2	1:B:137:VAL:HG22	1.96	0.47
1:C:119:ARG:NH2	1:C:154:ASN:O	2.44	0.47
1:A:85:ALA:HB1	1:A:115:LEU:HD11	1.97	0.47
1:B:216:GLU:HB3	1:B:281:LEU:HD22	1.95	0.47
1:C:47:LEU:O	1:C:54:SER:N	2.48	0.47
1:C:149:ASP:HB3	1:C:152:ASP:O	2.15	0.46
1:B:5:ILE:HD13	1:B:16:ALA:HB2	1.96	0.46
1:B:61:GLU:OE1	1:B:91:ARG:NH2	2.32	0.46
1:C:72:LEU:HB3	1:C:98:LEU:HG	1.98	0.46
1:C:257:ARG:HB3	1:C:259:ARG:HD3	1.96	0.46
1:A:0[B]:HIS:CE1	1:A:161:GLN:HE22	2.34	0.46
1:C:191:PRO:HB3	1:C:291:LEU:HD22	1.97	0.46
1:B:127:GLU:O	4:B:402:NAD:H4N	2.16	0.45
1:A:1:MET:SD	1:A:71:ARG:NH2	2.89	0.45
1:A:97:GLU:HG2	1:A:119:ARG:HD3	1.98	0.45
1:C:286:THR:HA	1:C:289:ALA:HB3	1.97	0.45
1:A:1:MET:HE3	1:A:70:GLN:HB3	1.99	0.45
1:C:17:ALA:O	1:C:21:ARG:HG3	2.16	0.45
1:A:149:ASP:HB3	1:A:152:ASP:O	2.16	0.45
1:C:294:HIS:O	1:C:298:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:LEU:HD11	1:C:45:LEU:HD11	2.00	0.44
1:C:194:VAL:CG2	1:C:251:MET:HG2	2.47	0.44
1:C:45:LEU:HD12	1:C:58:ILE:HD12	2.00	0.44
1:C:204:ARG:HG2	1:C:238:ARG:HH12	1.82	0.44
1:B:279:LEU:HD12	1:B:280:PRO:HD2	2.01	0.43
1:B:57:PRO:HB3	1:C:40:GLN:HA	1.99	0.43
1:C:110:ALA:O	1:C:114:ARG:N	2.39	0.43
1:B:36:LEU:HD22	1:B:62:THR:HG23	2.00	0.43
1:A:227:ASP:N	1:A:227:ASP:OD1	2.51	0.43
1:B:147:LEU:HD23	1:B:147:LEU:HA	1.71	0.43
1:A:81:ALA:HB3	1:A:107:SER:HB2	2.00	0.42
1:C:200:ASN:HD21	3:C:401:KPL:H11	1.83	0.42
1:B:99:LEU:HD11	1:B:147:LEU:HD21	2.02	0.42
1:A:61:GLU:OE2	1:A:91:ARG:NH2	2.37	0.42
1:A:73:LEU:HD12	1:A:99:LEU:HB3	2.02	0.42
1:C:105:LEU:HD23	1:C:105:LEU:HA	1.88	0.42
1:A:9:GLY:HA2	1:A:131:ARG:NH2	2.34	0.42
1:A:129:ALA:N	4:A:404:NAD:H72N	2.13	0.41
1:A:45:LEU:HD12	1:A:58:ILE:HD12	2.02	0.41
1:C:46:SER:O	1:C:136:ARG:HA	2.20	0.41
1:C:56:TYR:HB3	1:C:58:ILE:HG13	2.03	0.41
1:C:213:LEU:HD22	1:C:284:LEU:HD23	2.03	0.41
1:B:200:ASN:HB2	1:B:244:THR:O	2.21	0.41
1:B:213:LEU:HD22	1:B:284:LEU:HD23	2.01	0.41
1:A:92:LEU:HD11	1:A:115:LEU:HD13	2.03	0.41
1:B:9:GLY:HA3	4:B:402:NAD:O5B	2.20	0.41
1:B:-1:SER:O	1:B:0[B]:HIS:CB	2.70	0.41
1:B:85:ALA:HB1	1:B:115:LEU:HD11	2.03	0.41
1:C:121:LEU:CD2	1:C:149:ASP:HB2	2.49	0.40
1:B:90:HIS:CE1	1:B:91:ARG:HG3	2.56	0.40
1:C:190:ASN:OD1	3:C:401:KPL:H32	2.21	0.40
1:B:35:ARG:HH22	1:B:131:ARG:HH12	1.68	0.40
1:B:30:LEU:O	1:B:63:PRO:HD3	2.21	0.40
1:C:211:ALA:HA	1:C:234:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	304/323 (94%)	291 (96%)	13 (4%)	0	100	100
1	B	304/323 (94%)	292 (96%)	10 (3%)	2 (1%)	18	25
1	C	304/323 (94%)	292 (96%)	11 (4%)	1 (0%)	36	45
All	All	912/969 (94%)	875 (96%)	34 (4%)	3 (0%)	43	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	282	PRO
1	B	0[A]	HIS
1	B	0[B]	HIS

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	236/250 (94%)	226 (96%)	10 (4%)	26	40
1	B	236/250 (94%)	233 (99%)	3 (1%)	61	76
1	C	236/250 (94%)	228 (97%)	8 (3%)	32	48
All	All	708/750 (94%)	687 (97%)	21 (3%)	38	53

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0[A]	HIS
1	A	0[B]	HIS
1	A	35	ARG
1	A	131	ARG
1	A	227	ASP
1	A	231	ARG
1	A	233	LEU
1	A	241	ILE
1	A	272	GLN
1	A	303	ARG
1	B	1	MET
1	B	35	ARG
1	B	263	ILE
1	C	0	HIS
1	C	35	ARG
1	C	86	SER
1	C	161	GLN
1	C	257	ARG
1	C	261	THR
1	C	277	LEU
1	C	287	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	161	GLN
1	A	190	ASN
1	A	196	HIS
1	A	219	GLN
1	A	297	GLN
1	B	205	GLN
1	B	294	HIS
1	C	200	ASN
1	C	294	HIS

5.3.3 RNA ⓘ

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](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	KPL	A	403	-	9,9,9	0.99	0	11,13,13	1.71	4 (36%)
3	KPL	B	401	-	9,9,9	1.06	0	11,13,13	1.73	4 (36%)
2	GOL	A	401	-	5,5,5	0.92	0	5,5,5	1.22	1 (20%)
2	GOL	A	402	-	5,5,5	0.82	0	5,5,5	1.21	1 (20%)
4	NAD	B	402	-	46,48,48	3.88	18 (39%)	64,73,73	2.35	15 (23%)
3	KPL	C	401	-	9,9,9	1.02	0	11,13,13	1.83	4 (36%)
4	NAD	A	404	-	46,48,48	3.83	19 (41%)	64,73,73	2.37	16 (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
3	KPL	A	403	-	-	0/13/13/13	-
3	KPL	B	401	-	-	8/13/13/13	-
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-
4	NAD	B	402	-	-	16/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KPL	C	401	-	-	3/13/13/13	-
4	NAD	A	404	-	-	2/30/62/62	0/5/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	NAD	O4D-C1D	16.72	1.62	1.40
4	A	404	NAD	O4D-C1D	16.59	1.62	1.40
4	A	404	NAD	C3B-C4B	-8.63	1.31	1.53
4	B	402	NAD	C3B-C4B	-8.54	1.31	1.53
4	B	402	NAD	O4B-C4B	7.90	1.62	1.45
4	A	404	NAD	O4B-C4B	7.61	1.61	1.45
4	A	404	NAD	C7N-N7N	6.35	1.44	1.33
4	B	402	NAD	O4D-C4D	-6.26	1.31	1.45
4	A	404	NAD	O4D-C4D	-6.25	1.31	1.45
4	B	402	NAD	C7N-N7N	6.11	1.44	1.33
4	B	402	NAD	PN-O3	5.81	1.65	1.59
4	B	402	NAD	PA-O3	5.75	1.65	1.59
4	A	404	NAD	PN-O3	5.55	1.65	1.59
4	A	404	NAD	PA-O3	4.91	1.64	1.59
4	A	404	NAD	O4B-C1B	-4.53	1.31	1.42
4	B	402	NAD	O4B-C1B	-4.52	1.31	1.42
4	B	402	NAD	C6A-N6A	3.68	1.43	1.34
4	A	404	NAD	C6A-N6A	3.60	1.43	1.34
4	B	402	NAD	O2B-C2B	-3.35	1.34	1.43
4	A	404	NAD	O2B-C2B	-3.32	1.34	1.43
4	A	404	NAD	O7N-C7N	-3.10	1.18	1.24
4	B	402	NAD	O7N-C7N	-3.03	1.18	1.24
4	A	404	NAD	C4N-C3N	-2.98	1.34	1.39
4	B	402	NAD	C4N-C3N	-2.92	1.35	1.39
4	A	404	NAD	O3B-C3B	2.92	1.50	1.43
4	B	402	NAD	O2D-C2D	2.90	1.50	1.43
4	B	402	NAD	O3B-C3B	2.88	1.50	1.43
4	A	404	NAD	C8A-N9A	-2.77	1.32	1.37
4	A	404	NAD	O2D-C2D	2.75	1.49	1.43
4	A	404	NAD	O3D-C3D	-2.75	1.36	1.43
4	B	402	NAD	O3D-C3D	-2.72	1.36	1.43
4	B	402	NAD	C8A-N9A	-2.72	1.32	1.37
4	B	402	NAD	C5A-C4A	-2.65	1.34	1.39
4	A	404	NAD	C5A-C4A	-2.60	1.34	1.39
4	B	402	NAD	C5A-N7A	-2.48	1.34	1.39
4	A	404	NAD	C5A-N7A	-2.42	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	NAD	C5N-C4N	-2.13	1.35	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	NAD	C4A-N9A-C1B	-8.75	106.17	126.63
4	B	402	NAD	C4A-N9A-C1B	-8.41	106.95	126.63
4	A	404	NAD	C1B-N9A-C8A	7.68	144.14	127.09
4	B	402	NAD	C1B-N9A-C8A	7.51	143.77	127.09
4	B	402	NAD	C5A-C4A-N3A	-5.72	118.84	126.72
4	A	404	NAD	C5A-C4A-N3A	-5.64	118.96	126.72
4	B	402	NAD	N3A-C2A-N1A	-5.35	120.49	128.58
4	A	404	NAD	N3A-C2A-N1A	-5.35	120.49	128.58
4	A	404	NAD	N3A-C4A-N9A	5.16	135.94	127.17
4	B	402	NAD	N3A-C4A-N9A	5.12	135.88	127.17
4	A	404	NAD	N9A-C8A-N7A	-3.83	108.50	113.94
4	A	404	NAD	C4A-N9A-C8A	3.76	109.69	105.74
4	B	402	NAD	N9A-C8A-N7A	-3.67	108.72	113.94
4	B	402	NAD	C2A-N3A-C4A	3.64	120.72	111.83
4	A	404	NAD	C2A-N3A-C4A	3.63	120.70	111.83
4	B	402	NAD	C2B-C1B-N9A	-3.50	104.60	113.30
4	B	402	NAD	C4A-N9A-C8A	3.37	109.28	105.74
3	B	401	KPL	O3-C6-C5	3.26	121.87	112.88
4	B	402	NAD	O7N-C7N-N7N	-3.16	118.05	122.62
3	C	401	KPL	O3-C6-C5	3.12	121.48	112.88
4	A	404	NAD	C2B-C1B-N9A	-3.08	105.65	113.30
3	A	403	KPL	O3-C6-C5	2.86	120.75	112.88
3	C	401	KPL	O1-C4-C2	-2.74	107.54	112.76
3	A	403	KPL	O3-C6-O4	-2.68	117.52	123.90
4	A	404	NAD	C5D-C4D-C3D	-2.66	105.65	115.21
4	B	402	NAD	O4B-C1B-C2B	-2.63	100.99	106.62
4	B	402	NAD	C3N-C7N-N7N	2.54	120.86	117.74
3	C	401	KPL	O3-C6-O4	-2.45	118.08	123.90
3	B	401	KPL	C4-C2-C5	2.44	114.16	108.97
3	B	401	KPL	O2-C5-C2	-2.43	116.21	121.87
4	A	404	NAD	C5B-C4B-C3B	-2.42	106.48	115.21
4	A	404	NAD	C4D-O4D-C1D	-2.40	107.73	109.92
4	B	402	NAD	C5B-C4B-C3B	-2.37	106.69	115.21
3	B	401	KPL	O3-C6-O4	-2.34	118.32	123.90
3	A	403	KPL	O2-C5-C2	-2.30	116.53	121.87
4	A	404	NAD	O7N-C7N-N7N	-2.30	119.30	122.62
4	B	402	NAD	C6A-C5A-C4A	2.27	120.28	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	NAD	C6A-C5A-C4A	2.20	120.18	117.18
3	A	403	KPL	C3-C2-C5	2.18	113.84	108.73
4	A	404	NAD	C3N-C7N-N7N	2.16	120.41	117.74
3	C	401	KPL	C3-C2-C5	2.14	113.76	108.73
4	A	404	NAD	C5A-N7A-C8A	2.13	106.81	103.45
4	B	402	NAD	C5A-N7A-C8A	2.13	106.80	103.45
2	A	401	GOL	C3-C2-C1	-2.01	104.43	111.80
2	A	402	GOL	C3-C2-C1	-2.01	104.43	111.80

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	KPL	C2-C5-C6-O4
3	B	401	KPL	C2-C5-C6-O3
3	B	401	KPL	C5-C2-C4-O1
3	B	401	KPL	C3-C2-C4-O1
3	B	401	KPL	C1-C2-C4-O1
3	C	401	KPL	C5-C2-C4-O1
3	C	401	KPL	C1-C2-C4-O1
4	B	402	NAD	C5B-O5B-PA-O1A
4	B	402	NAD	C5B-O5B-PA-O3
4	B	402	NAD	PN-O3-PA-O5B
4	B	402	NAD	C5D-O5D-PN-O3
4	B	402	NAD	C5D-O5D-PN-O1N
4	B	402	NAD	C5D-O5D-PN-O2N
4	B	402	NAD	O4D-C1D-N1N-C2N
4	B	402	NAD	O4D-C1D-N1N-C6N
4	B	402	NAD	C2D-C1D-N1N-C2N
4	B	402	NAD	C2D-C1D-N1N-C6N
4	B	402	NAD	O4B-C4B-C5B-O5B
4	B	402	NAD	C3D-C4D-C5D-O5D
4	B	402	NAD	C3B-C4B-C5B-O5B
2	A	401	GOL	C1-C2-C3-O3
4	B	402	NAD	O4D-C4D-C5D-O5D
2	A	401	GOL	O2-C2-C3-O3
4	A	404	NAD	O4B-C4B-C5B-O5B
4	A	404	NAD	C3B-C4B-C5B-O5B
3	B	401	KPL	C1-C2-C5-C6
3	B	401	KPL	C1-C2-C5-O2
3	C	401	KPL	C3-C2-C4-O1
4	B	402	NAD	C5B-O5B-PA-O2A

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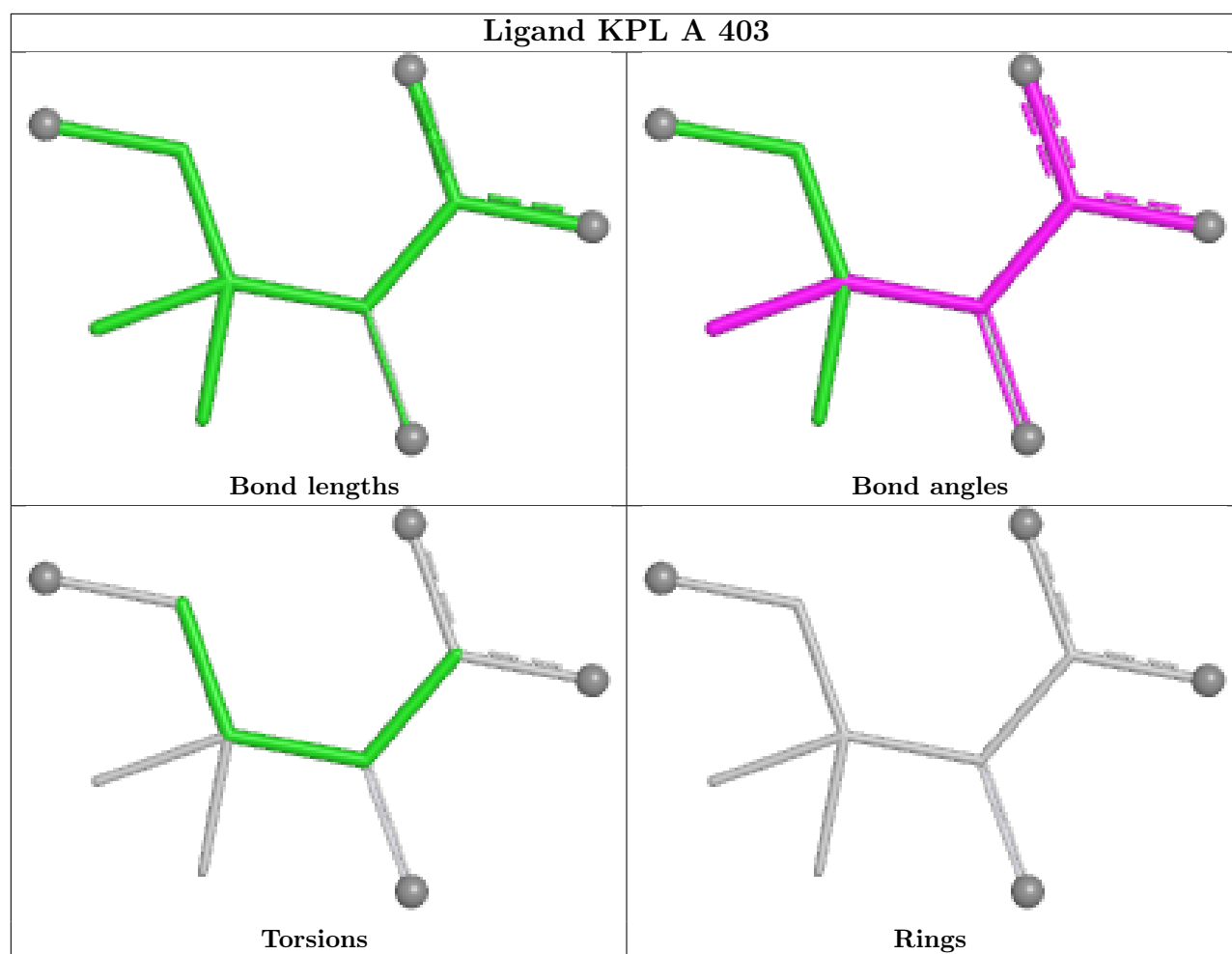
Mol	Chain	Res	Type	Atoms
4	B	402	NAD	PA-O3-PN-O2N
3	B	401	KPL	C4-C2-C5-C6

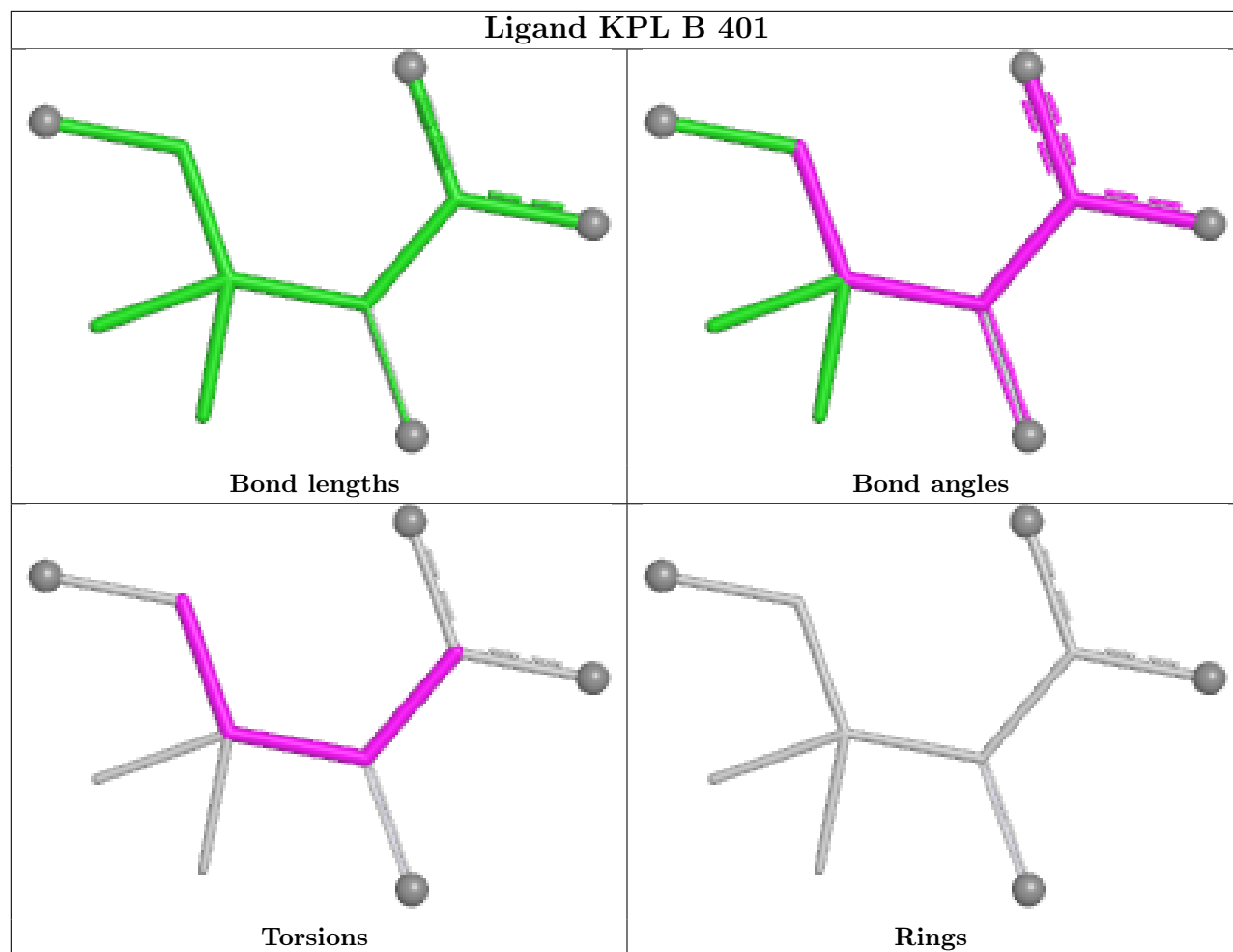
There are no ring outliers.

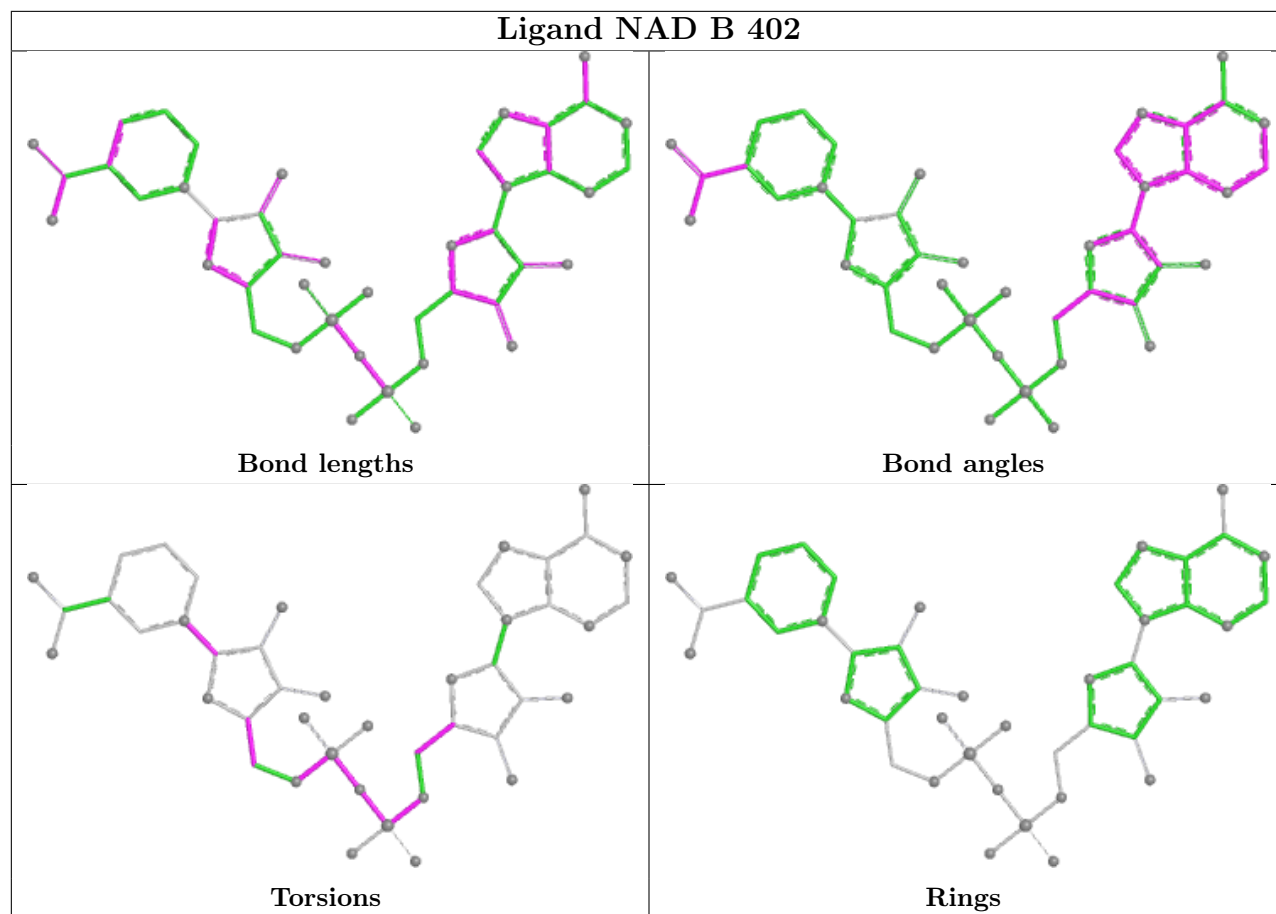
4 monomers are involved in 12 short contacts:

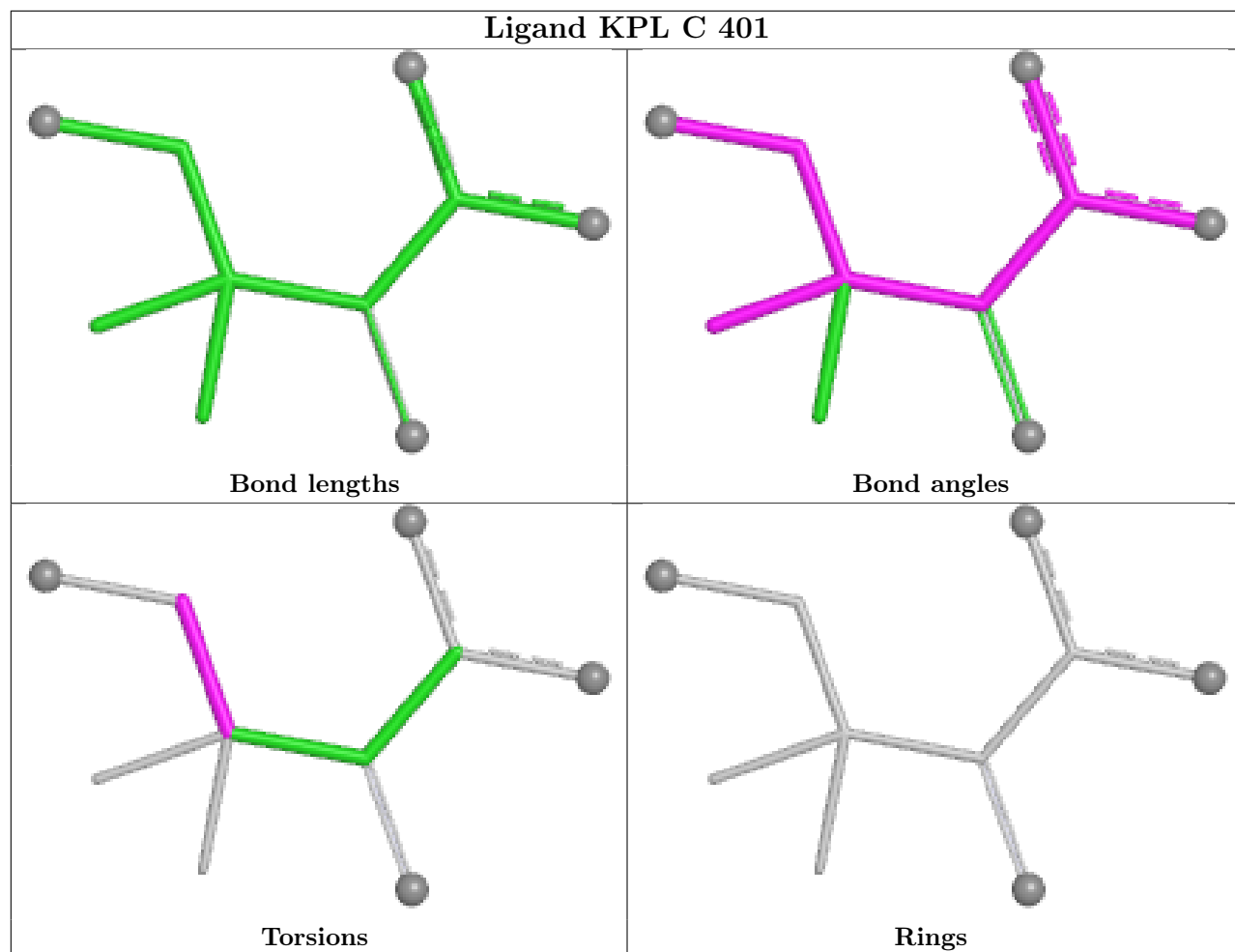
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GOL	1	0
4	B	402	NAD	4	0
3	C	401	KPL	4	0
4	A	404	NAD	3	0

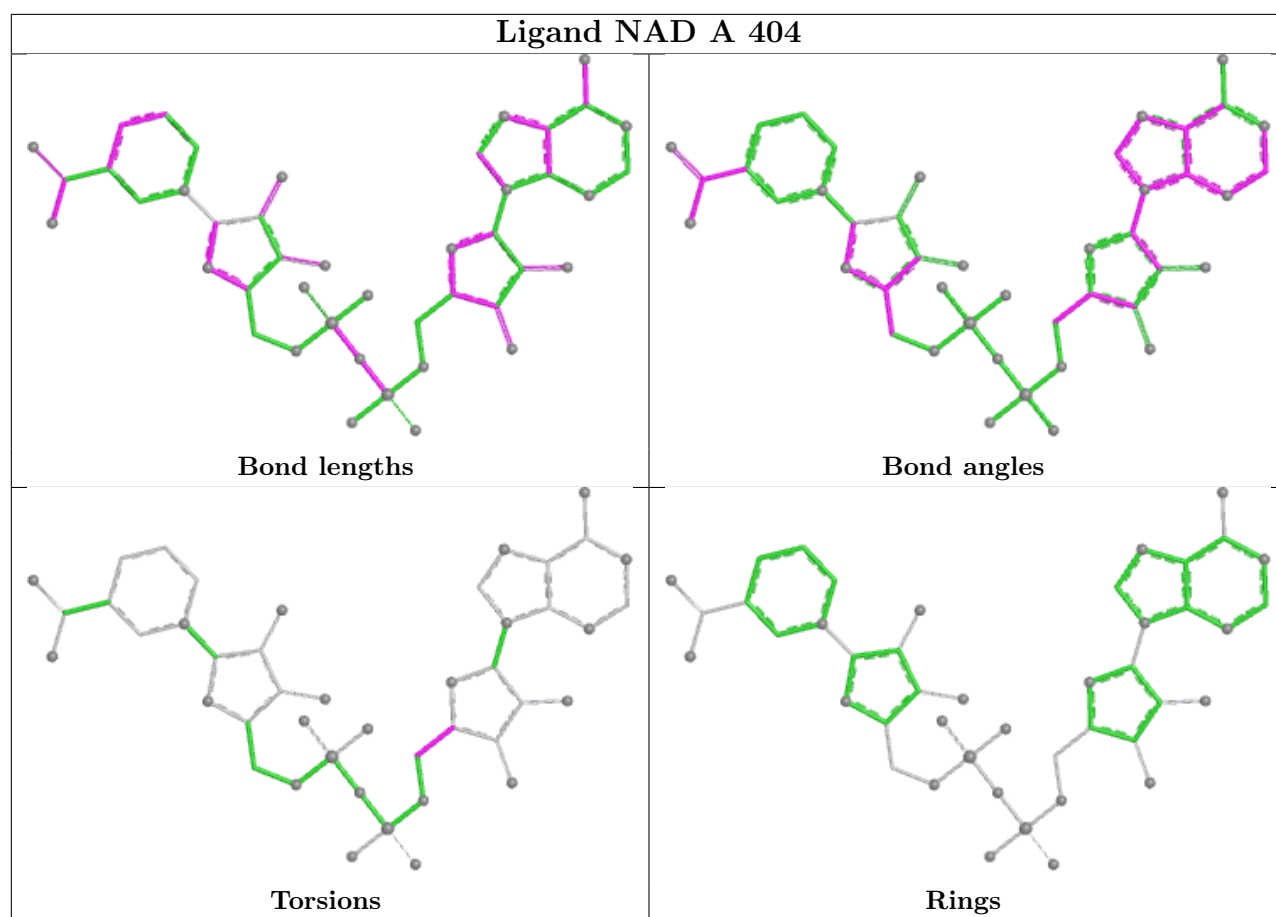
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	305/323 (94%)	0.45	8 (2%) 57 58	30, 42, 60, 80	9 (2%)
1	B	305/323 (94%)	0.62	23 (7%) 20 19	26, 44, 66, 81	10 (3%)
1	C	305/323 (94%)	0.97	44 (14%) 6 5	27, 48, 72, 85	24 (7%)
All	All	915/969 (94%)	0.68	75 (8%) 17 17	26, 45, 66, 85	43 (4%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0[A]	HIS	6.4
1	C	277	LEU	5.0
1	A	0[A]	HIS	4.9
1	C	64	ASP	4.3
1	C	107	SER	4.0
1	C	0	HIS	3.8
1	B	-1	SER	3.6
1	C	289	ALA	3.5
1	C	279	LEU	3.5
1	A	160	THR	3.4
1	C	160	THR	3.2
1	C	286	THR	3.1
1	B	154	ASN	3.1
1	C	104	GLY	3.1
1	C	275	GLN	3.0
1	C	292	GLN	3.0
1	C	66	GLY	3.0
1	B	155	ALA	2.9
1	B	231	ARG	2.9
1	B	1	MET	2.9
1	B	134	ASP	2.9
1	C	257	ARG	2.8
1	C	282	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	264	GLY	2.7
1	B	38	ARG	2.7
1	A	41	GLN	2.6
1	C	133	GLY	2.6
1	B	33	ARG	2.6
1	C	106	GLY	2.6
1	B	234	LEU	2.6
1	A	1	MET	2.5
1	C	1	MET	2.5
1	C	281	LEU	2.5
1	C	109	GLN	2.5
1	C	293	ALA	2.5
1	C	288	LEU	2.5
1	C	131	ARG	2.5
1	B	228	ALA	2.5
1	C	116	PRO	2.4
1	B	153	THR	2.4
1	C	215	ASP	2.4
1	C	67	GLN	2.4
1	C	83	GLU	2.4
1	A	131	ARG	2.3
1	C	108	GLN	2.3
1	C	132	ASP	2.3
1	C	276	ARG	2.3
1	B	147	LEU	2.3
1	C	47	LEU	2.3
1	B	173	ASP	2.3
1	C	82[A]	GLU	2.3
1	C	8	ALA	2.3
1	B	227	ASP	2.3
1	B	151	ARG	2.3
1	C	219	GLN	2.3
1	B	159	LEU	2.3
1	C	111	VAL	2.3
1	A	117	ARG	2.3
1	C	153	THR	2.2
1	C	105	LEU	2.2
1	B	208	GLU	2.2
1	C	298	ARG	2.2
1	C	280	PRO	2.2
1	C	45	LEU	2.1
1	A	94	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	296	ARG	2.1
1	B	265	TYR	2.1
1	C	56	TYR	2.1
1	B	117	ARG	2.1
1	B	185	LEU	2.1
1	C	94	GLY	2.1
1	C	261	THR	2.1
1	A	238	ARG	2.0
1	C	115	LEU	2.0
1	B	124	SER	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](#)

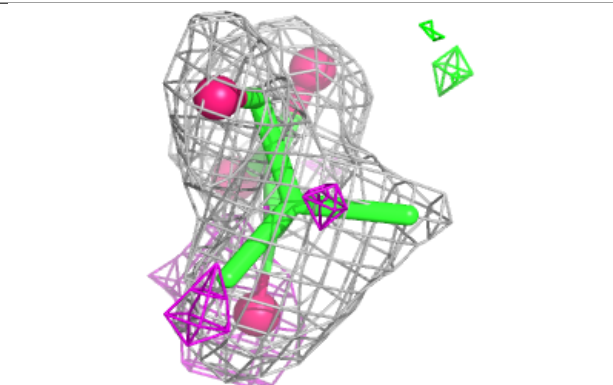
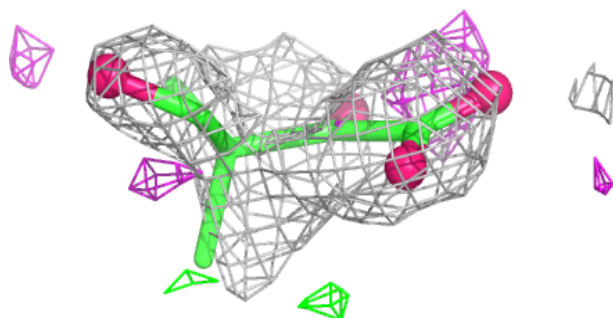
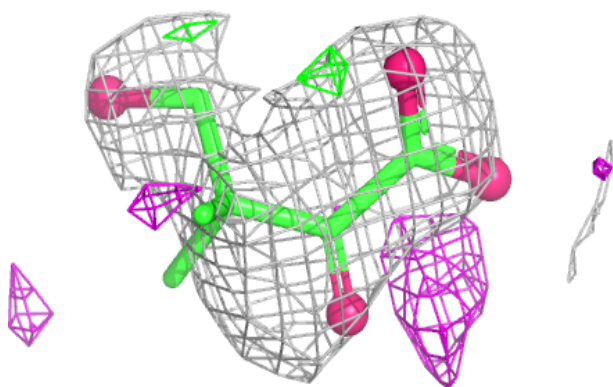
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	KPL	B	401	10/10	0.73	0.28	50,54,59,66	0
3	KPL	C	401	10/10	0.78	0.18	34,42,48,53	10
3	KPL	A	403	10/10	0.81	0.23	48,53,61,64	0
2	GOL	A	401	6/6	0.82	0.14	50,51,57,64	0
2	GOL	A	402	6/6	0.90	0.10	32,36,38,41	0
4	NAD	A	404	44/44	0.90	0.13	27,45,55,61	44
4	NAD	B	402	44/44	0.93	0.09	29,47,61,66	0

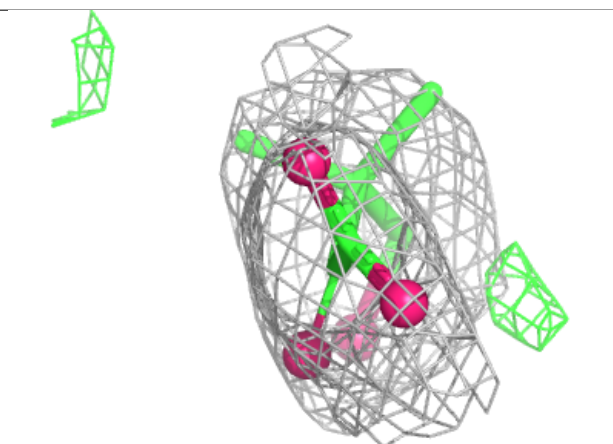
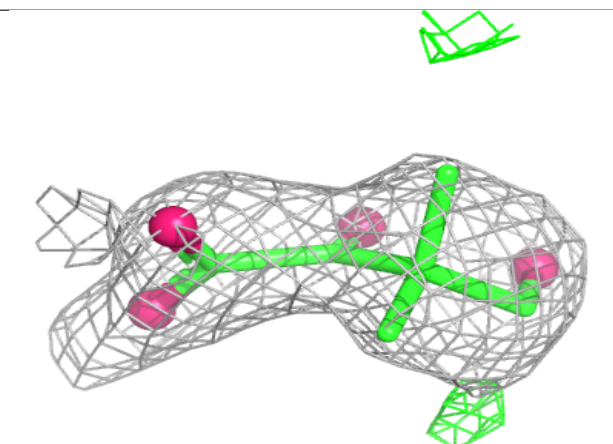
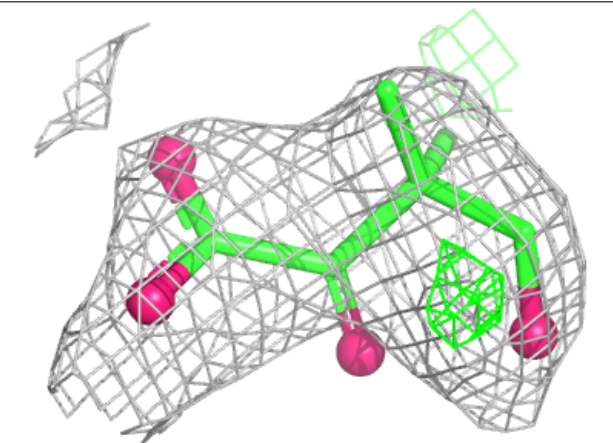
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KPL 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)

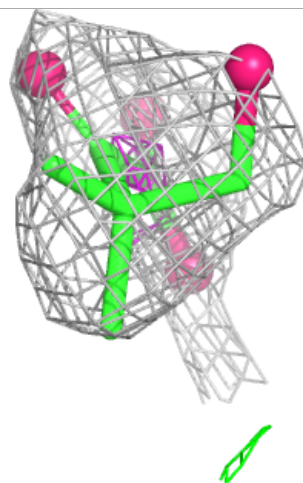
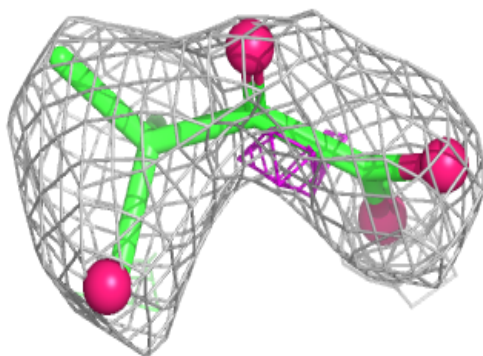
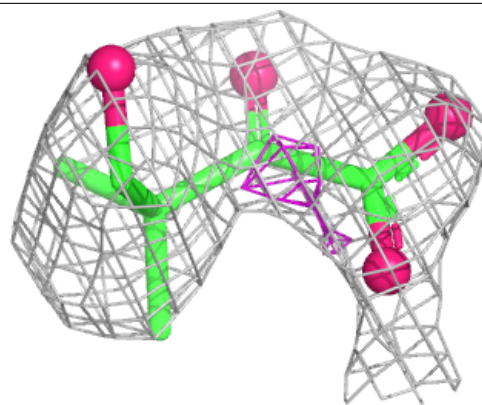
**Electron density around KPL C 401:**

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



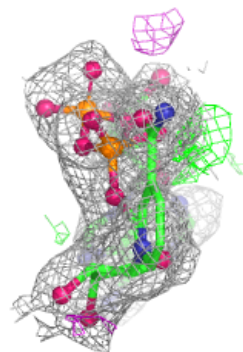
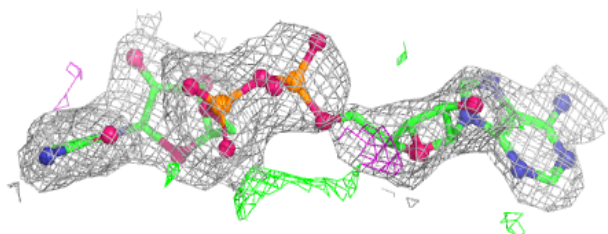
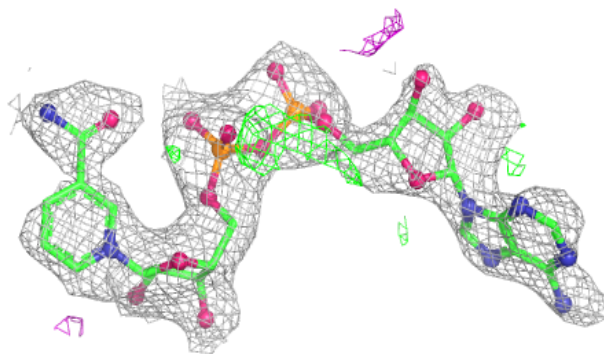
Electron density around KPL A 403:

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

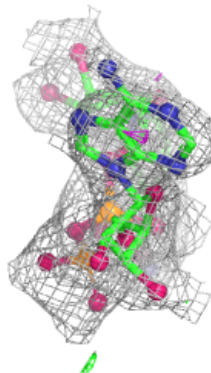
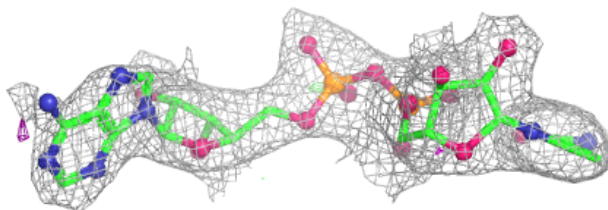
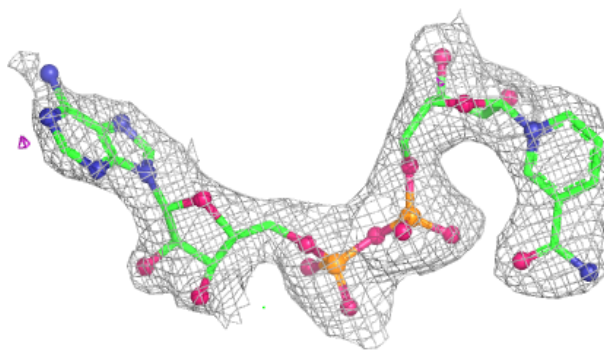


Electron density around NAD A 404:

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

**Electron density around NAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.