



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:30 AM UTC

PDB ID : 6JX2 / pdb_00006jx2
Title : Crystal structure of Ketol-acid reductoisomerase from *Corynebacterium glutamicum*
Authors : Lee, D.; Hong, J.; Kim, K.-J.
Deposited on : 2019-04-22
Resolution : 2.60 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

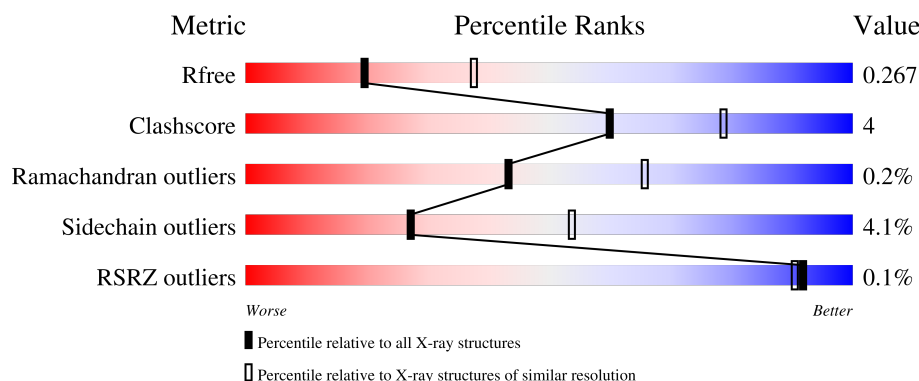
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 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	344	 83% 10% • 6%
1	B	344	 87% 7% • 5%
1	C	344	 79% 13% • 6%
1	D	344	 82% 11% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9995 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 Ketol-acid reductoisomerase (NADP(+)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2441	1535	408	489	9			
1	B	327	Total	C	N	O	S	0	0	0
			2462	1551	411	491	9			
1	C	324	Total	C	N	O	S	0	0	0
			2432	1530	407	487	8			
1	D	322	Total	C	N	O	S	0	0	0
			2419	1521	405	485	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	HIS	-	expression tag	UNP Q57179
A	340	HIS	-	expression tag	UNP Q57179
A	341	HIS	-	expression tag	UNP Q57179
A	342	HIS	-	expression tag	UNP Q57179
A	343	HIS	-	expression tag	UNP Q57179
A	344	HIS	-	expression tag	UNP Q57179
B	339	HIS	-	expression tag	UNP Q57179
B	340	HIS	-	expression tag	UNP Q57179
B	341	HIS	-	expression tag	UNP Q57179
B	342	HIS	-	expression tag	UNP Q57179
B	343	HIS	-	expression tag	UNP Q57179
B	344	HIS	-	expression tag	UNP Q57179
C	339	HIS	-	expression tag	UNP Q57179
C	340	HIS	-	expression tag	UNP Q57179
C	341	HIS	-	expression tag	UNP Q57179
C	342	HIS	-	expression tag	UNP Q57179
C	343	HIS	-	expression tag	UNP Q57179
C	344	HIS	-	expression tag	UNP Q57179
D	339	HIS	-	expression tag	UNP Q57179
D	340	HIS	-	expression tag	UNP Q57179
D	341	HIS	-	expression tag	UNP Q57179

Continued on next page...

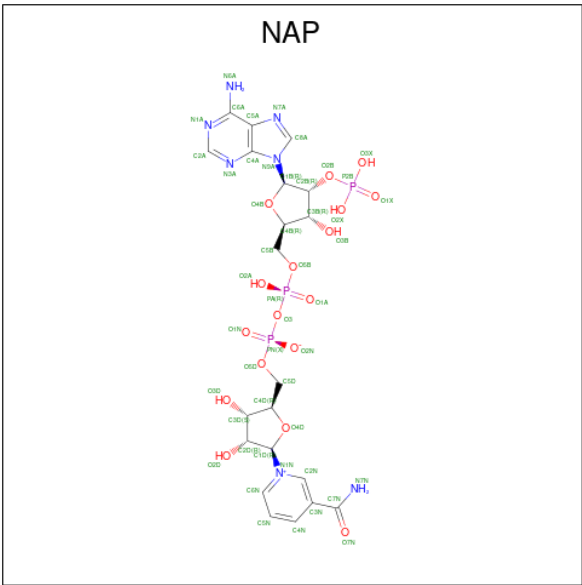
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	342	HIS	-	expression tag	UNP Q57179
D	343	HIS	-	expression tag	UNP Q57179
D	344	HIS	-	expression tag	UNP Q57179

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

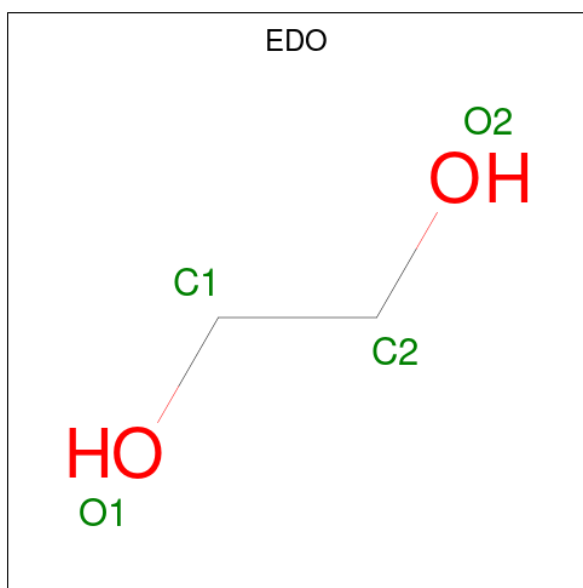
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Mg	0	0
			4	4		
2	B	5	Total	Mg	0	0
			5	5		
2	C	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

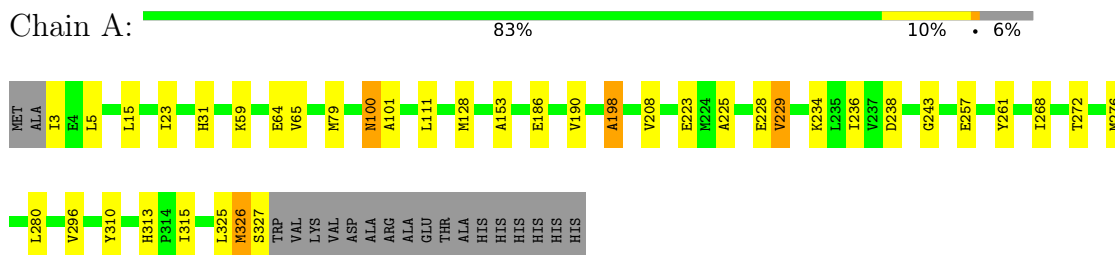
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	45	Total	O	0	0
			45	45		
5	B	31	Total	O	0	0
			31	31		
5	C	9	Total	O	0	0
			9	9		
5	D	13	Total	O	0	0
			13	13		

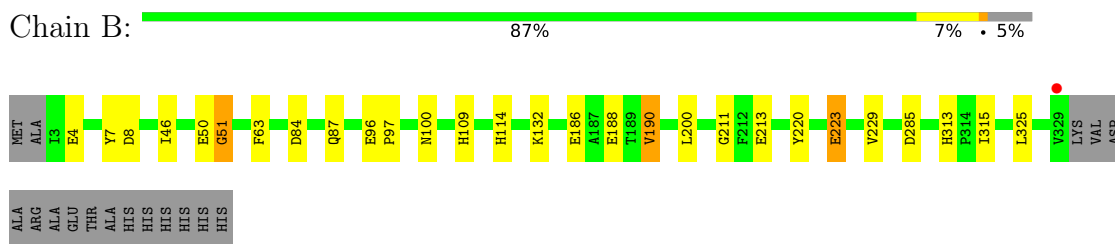
3 Residue-property plots

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.

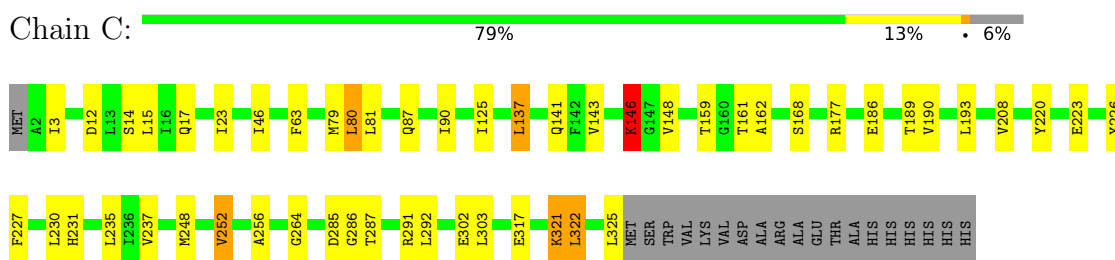
• Molecule 1: Ketol-acid reductoisomerase (NADP(+))



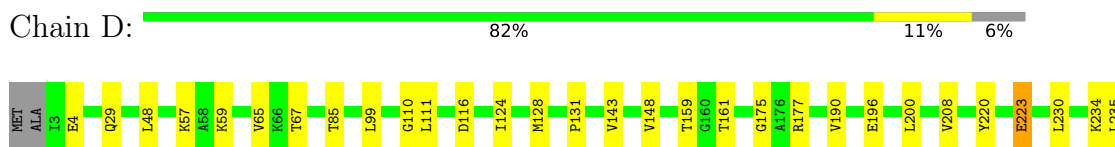
• Molecule 1: Ketol-acid reductoisomerase (NADP(+))



• Molecule 1: Ketol-acid reductoisomerase (NADP(+))



• Molecule 1: Ketol-acid reductoisomerase (NADP(+))



I236	V237	T255	A256	E257	Y261	K277	T281	D285	G286	T287	K290	D324	LEU	MET	SER	TRP	VAL	LYS	VAL	ASP	ALA	ARG	ALA	GLU	THR	ALA	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.95Å 90.18Å 157.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.91 – 2.60 78.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (78.91-2.60) 97.9 (78.91-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.94 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.179 , 0.267 0.183 , 0.267	Depositor DCC
R_{free} test set	1865 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9995	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: EDO, MG, NAP

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	0.90	0/2480	1.04	3/3362 (0.1%)
1	B	0.85	0/2503	1.01	2/3395 (0.1%)
1	C	0.83	0/2471	1.01	5/3351 (0.1%)
1	D	0.76	0/2458	1.03	0/3333
All	All	0.84	0/9912	1.02	10/13441 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	148	VAL	CA-C-N	-5.76	114.32	120.03
1	C	148	VAL	C-N-CA	-5.76	114.32	120.03
1	A	326	MET	N-CA-C	5.65	118.78	110.59
1	B	87	GLN	N-CA-C	5.57	118.28	111.82
1	A	243	GLY	N-CA-C	-5.40	100.39	113.18
1	B	51	GLY	N-CA-C	-5.05	101.21	113.18
1	C	146	LYS	CB-CA-C	-5.03	102.82	112.43
1	C	264	GLY	CA-C-N	5.03	124.69	119.56
1	C	264	GLY	C-N-CA	5.03	124.69	119.56
1	A	198	ALA	N-CA-C	5.01	116.74	111.28

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	2441	0	2402	24	0
1	B	2462	0	2421	18	0
1	C	2432	0	2393	38	0
1	D	2419	0	2377	19	0
2	A	4	0	0	0	0
2	B	5	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	31	0	11	0	0
3	C	48	0	25	1	0
3	D	31	0	11	0	0
4	A	8	0	12	0	0
4	B	12	0	18	0	0
5	A	45	0	0	0	0
5	B	31	0	0	2	0
5	C	9	0	0	1	0
5	D	13	0	0	0	0
All	All	9995	0	9670	84	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 4.

All (84) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:VAL:HB	5:B:525:HOH:O	1.63	0.97
1:C:137:LEU:O	1:C:137:LEU:HD12	1.95	0.67
1:A:5:LEU:HD12	1:B:325:LEU:HD13	1.79	0.65
1:C:159:THR:HB	1:C:161:THR:HG22	1.80	0.63
1:A:190:VAL:HG21	1:B:220:TYR:CZ	2.34	0.62
1:C:317:GLU:HG2	1:C:321:LYS:NZ	2.15	0.62
1:C:317:GLU:HG2	1:C:321:LYS:HZ2	1.65	0.60
1:C:285:ASP:OD1	1:C:287:THR:HG23	2.01	0.60
1:C:252:VAL:HG13	1:C:256:ALA:HB3	1.85	0.58
1:C:220:TYR:OH	1:D:190:VAL:HG21	2.04	0.58
1:A:23:ILE:HD13	1:A:79:MET:HB3	1.87	0.56
1:A:276:MET:HE1	1:B:211:GLY:CA	2.37	0.53
1:B:213:GLU:OE2	1:B:313:HIS:HE1	1.92	0.53
1:C:23:ILE:HD13	1:C:79:MET:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:VAL:HG22	1:C:143:VAL:O	2.08	0.53
1:D:48:LEU:HD12	1:D:65:VAL:HG21	1.90	0.53
1:A:276:MET:HE1	1:B:211:GLY:HA2	1.90	0.53
1:C:285:ASP:OD1	1:C:286:GLY:N	2.42	0.53
1:A:268:ILE:HG23	1:A:272:THR:HG21	1.93	0.50
1:C:79:MET:HE3	1:C:81:LEU:HD21	1.93	0.50
1:A:276:MET:CE	1:B:211:GLY:HA2	2.41	0.50
1:A:5:LEU:CD1	1:B:325:LEU:HD13	2.43	0.49
1:C:317:GLU:CG	1:C:321:LYS:HZ2	2.25	0.49
1:D:48:LEU:HD12	1:D:65:VAL:CG2	2.43	0.49
1:D:257:GLU:HG2	1:D:261:TYR:CE2	2.48	0.48
1:A:3:ILE:HG21	1:B:223:GLU:HG3	1.96	0.48
1:A:228:GLU:OE2	1:B:132:LYS:NZ	2.47	0.48
1:C:226:TYR:CZ	1:C:230:LEU:HD22	2.48	0.48
1:C:317:GLU:CG	1:C:321:LYS:NZ	2.77	0.47
1:A:236:ILE:CD1	1:B:200:LEU:HB3	2.44	0.47
1:D:196:GLU:HA	1:D:200:LEU:HB2	1.95	0.47
1:C:186:GLU:O	1:C:190:VAL:HG22	2.14	0.47
1:C:322:LEU:HD22	1:C:322:LEU:HA	1.72	0.47
1:D:159:THR:OG1	1:D:161:THR:HG22	2.15	0.47
1:A:326:MET:HE2	1:A:327:SER:O	2.14	0.47
1:A:280:LEU:HD11	5:B:525:HOH:O	2.15	0.47
1:C:80:LEU:HD22	1:C:87:GLN:HG2	1.96	0.47
1:C:190:VAL:HG21	1:D:220:TYR:OH	2.16	0.46
1:B:186:GLU:O	1:B:190:VAL:HG13	2.15	0.46
1:A:257:GLU:HG2	1:A:261:TYR:CE2	2.49	0.46
1:C:46:ILE:HD13	1:C:63:PHE:HB3	1.97	0.46
1:C:125:ILE:HG23	1:C:162:ALA:HB2	1.99	0.45
1:C:141:GLN:O	1:C:146:LYS:O	2.34	0.45
1:C:189:THR:HG22	1:C:193:LEU:HD12	1.98	0.45
1:C:3:ILE:HG22	1:D:223:GLU:HG3	1.98	0.45
1:C:291:ARG:NH2	1:C:302:GLU:OE2	2.49	0.45
1:A:186:GLU:O	1:A:190:VAL:HG22	2.17	0.45
1:C:226:TYR:CE1	1:C:230:LEU:HD22	2.52	0.45
1:C:14:SER:HA	1:C:17:GLN:HB2	1.98	0.45
1:D:110:GLY:CA	1:D:128:MET:HE2	2.47	0.45
1:D:111:LEU:C	1:D:111:LEU:HD23	2.42	0.45
1:C:231:HIS:HD2	5:C:502:HOH:O	2.00	0.45
1:C:237:VAL:HG21	1:D:237:VAL:HG21	1.98	0.44
1:D:99:LEU:HD13	1:D:124:ILE:HD13	1.99	0.44
1:D:29:GLN:HE22	1:D:131:PRO:HG2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ALA:HB1	1:A:276:MET:HE3	2.00	0.43
1:C:190:VAL:HG21	1:D:220:TYR:CZ	2.53	0.43
1:A:225:ALA:O	1:A:229:VAL:HB	2.18	0.43
1:D:148:VAL:O	1:D:175:GLY:HA2	2.19	0.42
1:A:234:LYS:HE3	1:A:238:ASP:OD2	2.18	0.42
1:B:313:HIS:HD2	1:B:315:ILE:H	1.66	0.42
1:C:12:ASP:O	1:C:168:SER:OG	2.36	0.42
1:C:248:MET:C	1:C:248:MET:SD	3.03	0.42
1:C:230:LEU:HD23	1:C:230:LEU:C	2.44	0.42
1:C:227:PHE:CZ	1:C:322:LEU:HD11	2.55	0.42
1:B:285:ASP:OD1	1:B:285:ASP:C	2.63	0.42
1:C:141:GLN:HG3	1:C:146:LYS:HB3	2.01	0.42
1:A:111:LEU:C	1:A:111:LEU:HD23	2.45	0.41
1:A:128:MET:HE2	1:A:153:ALA:HB3	2.01	0.41
1:C:227:PHE:CE2	1:C:322:LEU:HD11	2.56	0.41
1:B:96:GLU:HB3	1:B:97:PRO:HD3	2.02	0.41
1:B:109:HIS:HD2	1:B:188:GLU:OE2	2.04	0.41
1:C:90:ILE:HD11	3:C:403:NAP:C6A	2.50	0.41
1:D:285:ASP:OD1	1:D:287:THR:HG22	2.20	0.41
1:C:141:GLN:CG	1:C:146:LYS:HB3	2.51	0.41
1:D:230:LEU:C	1:D:230:LEU:HD23	2.46	0.41
1:A:313:HIS:HD2	1:A:315:ILE:H	1.69	0.41
1:B:114:HIS:CD2	1:B:186:GLU:HA	2.56	0.41
1:D:277:LYS:O	1:D:281:THR:HG23	2.20	0.41
1:A:100:ASN:O	1:A:101:ALA:C	2.64	0.40
1:C:292:LEU:HD22	1:D:255:THR:HG23	2.03	0.40
1:A:59:LYS:HE3	1:A:65:VAL:CG1	2.52	0.40
1:B:7:TYR:O	1:B:8:ASP:C	2.64	0.40
1:B:46:ILE:HD13	1:B:63:PHE:HB3	2.03	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	323/344 (94%)	309 (96%)	14 (4%)	0	100	100
1	B	325/344 (94%)	309 (95%)	15 (5%)	1 (0%)	36	58
1	C	322/344 (94%)	307 (95%)	15 (5%)	0	100	100
1	D	320/344 (93%)	301 (94%)	18 (6%)	1 (0%)	36	58
All	All	1290/1376 (94%)	1226 (95%)	62 (5%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	116	ASP
1	B	51	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	256/271 (94%)	246 (96%)	10 (4%)	28	55
1	B	258/271 (95%)	251 (97%)	7 (3%)	39	67
1	C	254/271 (94%)	241 (95%)	13 (5%)	21	45
1	D	253/271 (93%)	241 (95%)	12 (5%)	23	48
All	All	1021/1084 (94%)	979 (96%)	42 (4%)	27	54

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	31	HIS
1	A	64	GLU
1	A	100	ASN
1	A	208	VAL
1	A	223	GLU
1	A	229	VAL
1	A	296	VAL
1	A	310	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	325	LEU
1	B	4	GLU
1	B	50	GLU
1	B	84	ASP
1	B	100	ASN
1	B	190	VAL
1	B	223	GLU
1	B	229	VAL
1	C	15	LEU
1	C	80	LEU
1	C	137	LEU
1	C	146	LYS
1	C	177	ARG
1	C	208	VAL
1	C	223	GLU
1	C	235	LEU
1	C	252	VAL
1	C	303	LEU
1	C	321	LYS
1	C	322	LEU
1	C	325	LEU
1	D	4	GLU
1	D	57	LYS
1	D	59	LYS
1	D	67	THR
1	D	85	THR
1	D	143	VAL
1	D	177	ARG
1	D	208	VAL
1	D	223	GLU
1	D	234	LYS
1	D	235	LEU
1	D	290	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	136	HIS
1	A	156	GLN
1	A	197	GLN
1	A	295	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	313	HIS
1	B	87	GLN
1	B	109	HIS
1	B	114	HIS
1	B	141	GLN
1	B	197	GLN
1	B	249	ASN
1	B	313	HIS
1	C	29	GLN
1	C	31	HIS
1	C	109	HIS
1	C	114	HIS
1	C	197	GLN
1	C	231	HIS
1	C	249	ASN
1	C	284	GLN
1	C	313	HIS
1	D	29	GLN
1	D	35	GLN
1	D	100	ASN
1	D	109	HIS
1	D	156	GLN
1	D	197	GLN
1	D	249	ASN
1	D	313	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 13 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	EDO	B	408	-	3,3,3	0.49	0	2,2,2	0.34	0
4	EDO	B	407	-	3,3,3	0.44	0	2,2,2	0.44	0
4	EDO	B	406	-	3,3,3	0.58	0	2,2,2	0.36	0
4	EDO	A	406	-	3,3,3	0.50	0	2,2,2	0.30	0
4	EDO	A	407	-	3,3,3	0.43	0	2,2,2	0.47	0
3	NAP	A	405	-	32,33,52	1.55	6 (18%)	50,52,80	1.86	9 (18%)
3	NAP	D	403	-	32,33,52	1.54	6 (18%)	50,52,80	1.83	10 (20%)
3	NAP	C	403	-	50,52,52	1.43	8 (16%)	71,80,80	1.67	14 (19%)

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
4	EDO	B	408	-	-	1/1/1/1	-
4	EDO	B	407	-	-	1/1/1/1	-
4	EDO	B	406	-	-	1/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-
4	EDO	A	407	-	-	0/1/1/1	-
3	NAP	A	405	-	-	1/21/37/67	0/3/3/5
3	NAP	D	403	-	-	1/21/37/67	0/3/3/5
3	NAP	C	403	-	-	9/35/67/67	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	NAP	C5A-C4A	4.89	1.47	1.39
3	C	403	NAP	C5A-C4A	4.84	1.47	1.39
3	D	403	NAP	C5A-C4A	4.64	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	NAP	PA-O3	4.60	1.64	1.59
3	D	403	NAP	PA-O3	3.66	1.63	1.59
3	A	405	NAP	PA-O3	3.25	1.63	1.59
3	A	405	NAP	C5A-C6A	3.22	1.49	1.41
3	C	403	NAP	C5A-C6A	3.03	1.49	1.41
3	D	403	NAP	C5A-C6A	2.90	1.49	1.41
3	C	403	NAP	O4D-C1D	2.53	1.44	1.40
3	C	403	NAP	C8A-N7A	2.45	1.36	1.31
3	A	405	NAP	C8A-N7A	2.44	1.36	1.31
3	D	403	NAP	C8A-N7A	2.34	1.36	1.31
3	D	403	NAP	PN-O5D	2.16	1.62	1.54
3	C	403	NAP	C5A-N7A	-2.15	1.35	1.39
3	D	403	NAP	C5A-N7A	-2.15	1.35	1.39
3	A	405	NAP	PN-O5D	2.11	1.62	1.54
3	C	403	NAP	C4A-N9A	-2.08	1.33	1.37
3	C	403	NAP	PN-O3	2.06	1.61	1.59
3	A	405	NAP	C5A-N7A	-2.03	1.35	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	405	NAP	C5A-C4A-N3A	-6.15	118.24	126.72
3	D	403	NAP	C5A-C4A-N3A	-5.54	119.09	126.72
3	C	403	NAP	C5A-C4A-N3A	-5.33	119.38	126.72
3	A	405	NAP	N3A-C4A-N9A	4.95	135.59	127.17
3	D	403	NAP	N3A-C4A-N9A	4.59	134.97	127.17
3	C	403	NAP	N3A-C4A-N9A	4.30	134.49	127.17
3	A	405	NAP	C2A-N3A-C4A	3.98	121.54	111.83
3	D	403	NAP	C2A-N3A-C4A	3.91	121.38	111.83
3	C	403	NAP	C2A-N3A-C4A	3.90	121.36	111.83
3	A	405	NAP	C4A-C5A-N7A	-3.89	106.13	110.58
3	D	403	NAP	N3A-C2A-N1A	-3.84	122.77	128.58
3	D	403	NAP	C4A-C5A-N7A	-3.75	106.29	110.58
3	C	403	NAP	N3A-C2A-N1A	-3.73	122.94	128.58
3	D	403	NAP	C4A-N9A-C8A	3.60	109.52	105.74
3	A	405	NAP	C5A-N7A-C8A	3.17	108.43	103.45
3	A	405	NAP	C4A-N9A-C8A	3.15	109.05	105.74
3	A	405	NAP	N3A-C2A-N1A	-3.11	123.88	128.58
3	D	403	NAP	C5A-N7A-C8A	3.09	108.31	103.45
3	C	403	NAP	C4A-C5A-N7A	-3.08	107.06	110.58
3	C	403	NAP	O4B-C1B-N9A	3.02	113.90	108.09
3	C	403	NAP	O7N-C7N-N7N	-3.02	118.25	122.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	NAP	C4A-N9A-C8A	2.85	108.73	105.74
3	D	403	NAP	N9A-C8A-N7A	-2.82	109.93	113.94
3	C	403	NAP	C3N-C7N-N7N	2.82	121.21	117.74
3	C	403	NAP	O2A-PA-O3	2.71	114.61	107.27
3	A	405	NAP	N9A-C8A-N7A	-2.62	110.22	113.94
3	D	403	NAP	C6A-C5A-N7A	2.58	137.07	132.09
3	C	403	NAP	C6N-N1N-C2N	-2.55	119.71	121.88
3	C	403	NAP	C6A-C5A-N7A	2.41	136.74	132.09
3	A	405	NAP	C6A-C5A-N7A	2.38	136.68	132.09
3	C	403	NAP	C5A-N7A-C8A	2.38	107.19	103.45
3	D	403	NAP	O4B-C1B-N9A	2.21	112.34	108.09
3	C	403	NAP	N9A-C8A-N7A	-2.15	110.88	113.94

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	403	NAP	C5D-O5D-PN-O2N
3	C	403	NAP	O4D-C1D-N1N-C2N
3	C	403	NAP	O4D-C1D-N1N-C6N
3	C	403	NAP	C2D-C1D-N1N-C6N
3	C	403	NAP	O4D-C4D-C5D-O5D
4	B	406	EDO	O1-C1-C2-O2
4	B	407	EDO	O1-C1-C2-O2
4	B	408	EDO	O1-C1-C2-O2
3	C	403	NAP	C3D-C4D-C5D-O5D
4	A	406	EDO	O1-C1-C2-O2
3	C	403	NAP	C2B-O2B-P2B-O2X
3	C	403	NAP	C2D-C1D-N1N-C2N
3	A	405	NAP	PN-O3-PA-O1A
3	C	403	NAP	PN-O3-PA-O1A
3	D	403	NAP	O4B-C4B-C5B-O5B

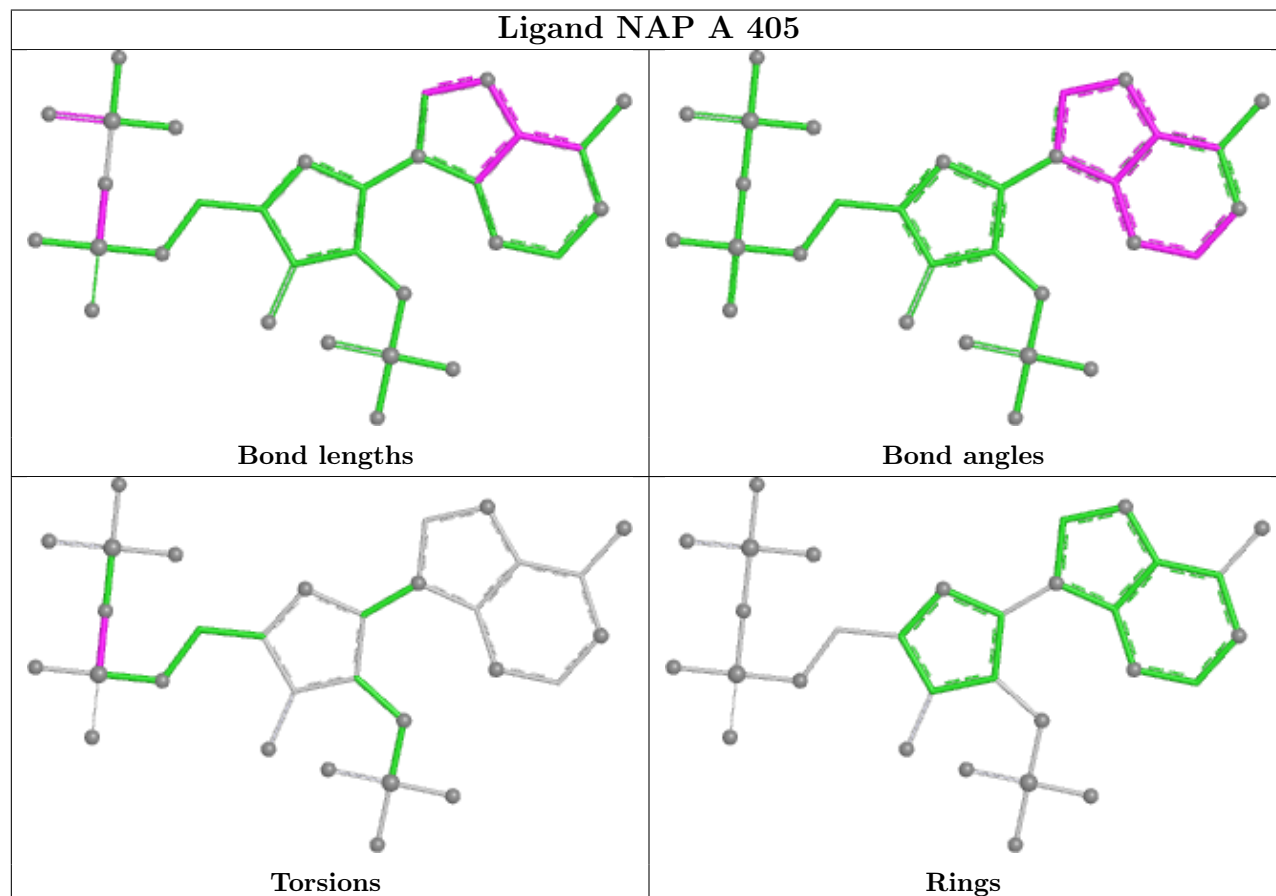
There are no ring outliers.

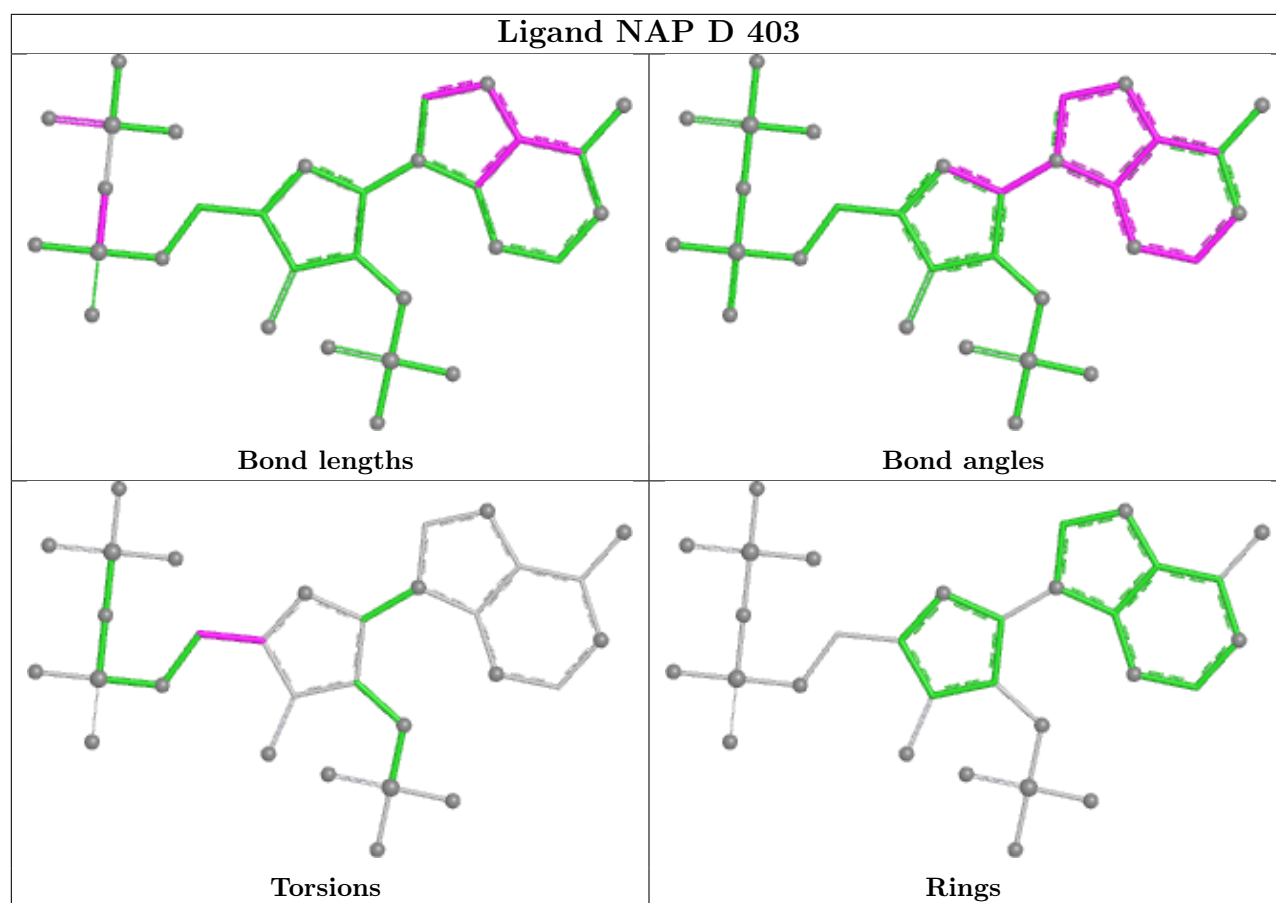
1 monomer is involved in 1 short contact:

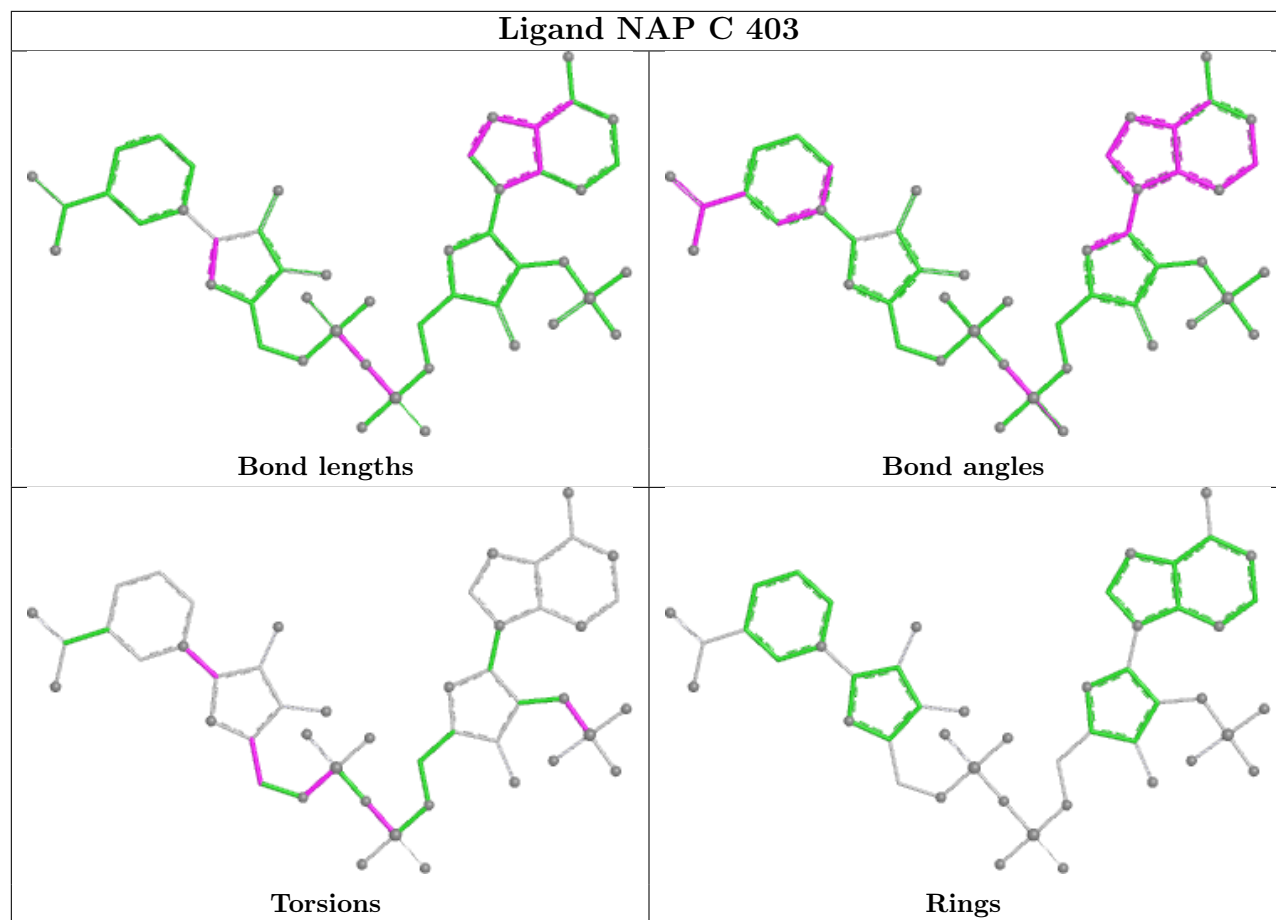
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	NAP	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	325/344 (94%)	-0.61	0 100 100	27, 41, 69, 116	0
1	B	327/344 (95%)	-0.51	1 (0%) 90 88	26, 46, 70, 99	0
1	C	324/344 (94%)	-0.28	0 100 100	38, 62, 83, 97	0
1	D	322/344 (93%)	-0.25	0 100 100	45, 62, 83, 94	0
All	All	1298/1376 (94%)	-0.41	1 (0%) 92 90	26, 54, 80, 116	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	VAL	3.0

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
4	EDO	B	407	4/4	0.46	0.29	77,78,78,78	0

Continued on next page...

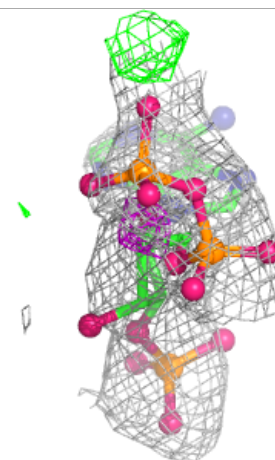
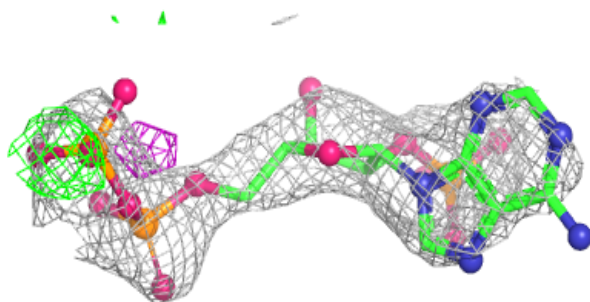
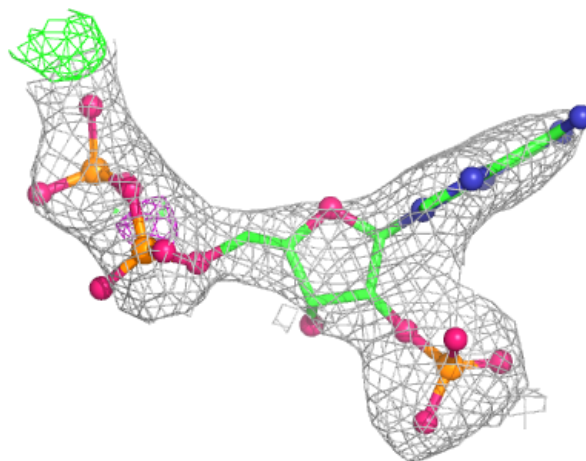
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	406	4/4	0.69	0.30	55,65,69,70	0
4	EDO	A	407	4/4	0.75	0.24	65,67,69,73	0
3	NAP	D	403	31/48	0.77	0.10	87,102,132,134	0
2	MG	A	403	1/1	0.79	0.28	59,59,59,59	0
2	MG	D	402	1/1	0.80	0.24	51,51,51,51	0
2	MG	B	404	1/1	0.80	0.33	56,56,56,56	0
4	EDO	A	406	4/4	0.80	0.20	68,72,75,75	0
2	MG	B	402	1/1	0.83	0.26	45,45,45,45	0
4	EDO	B	408	4/4	0.83	0.14	60,61,64,64	0
3	NAP	A	405	31/48	0.84	0.09	72,85,108,119	0
2	MG	D	401	1/1	0.86	0.16	63,63,63,63	0
2	MG	A	401	1/1	0.86	0.24	46,46,46,46	0
2	MG	A	404	1/1	0.86	0.29	59,59,59,59	0
2	MG	C	401	1/1	0.88	0.26	55,55,55,55	0
2	MG	B	405	1/1	0.89	0.11	47,47,47,47	0
2	MG	B	401	1/1	0.90	0.14	50,50,50,50	0
2	MG	A	402	1/1	0.90	0.13	50,50,50,50	0
3	NAP	C	403	48/48	0.91	0.08	58,71,83,92	0
2	MG	C	402	1/1	0.94	0.09	42,42,42,42	0
2	MG	B	403	1/1	0.96	0.29	56,56,56,56	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.

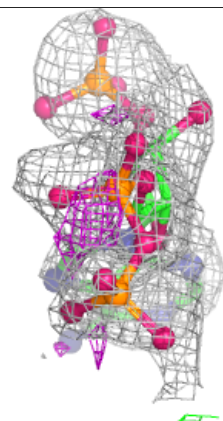
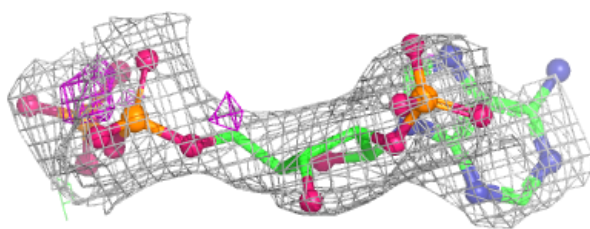
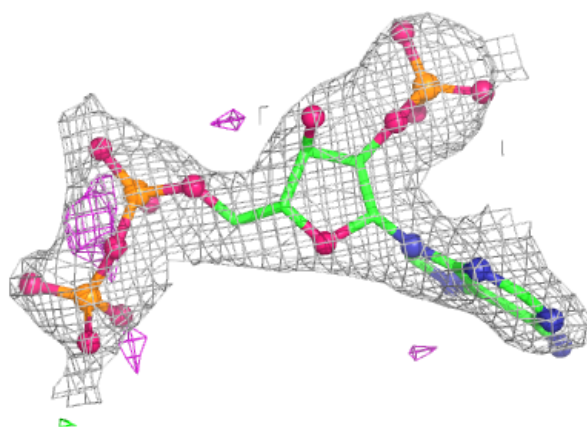
Electron density around NAP D 403:

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

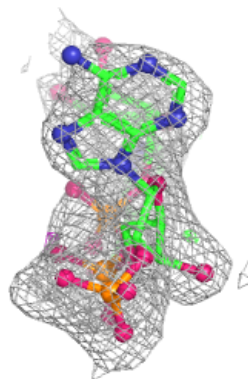
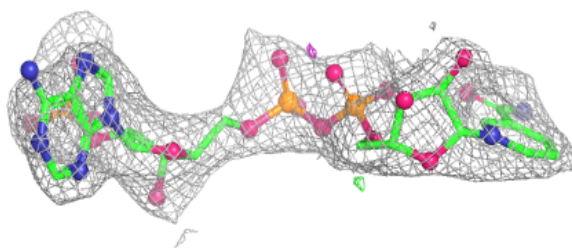
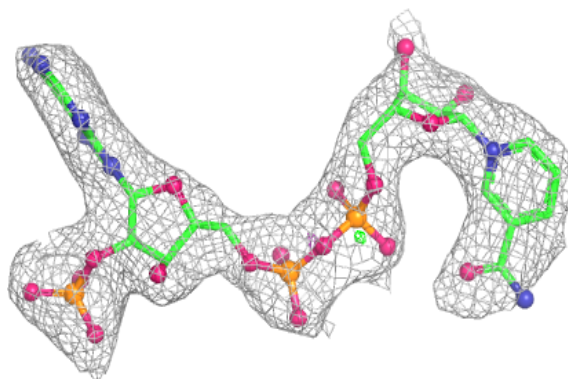


Electron density around NAP A 405:

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

**Electron density around NAP 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.