



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:14 PM BST

PDB ID : 3KJS
Title : Crystal Structure of T. cruzi DHFR-TS with 3 high affinity DHFR inhibitors:
DQ1 inhibitor complex
Authors : Schormann, N.; Senkovich, O.; Chattopadhyay, D.
Deposited on : 2009-11-03
Resolution : 2.50 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 : 2.13.1
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) : 2.13.1

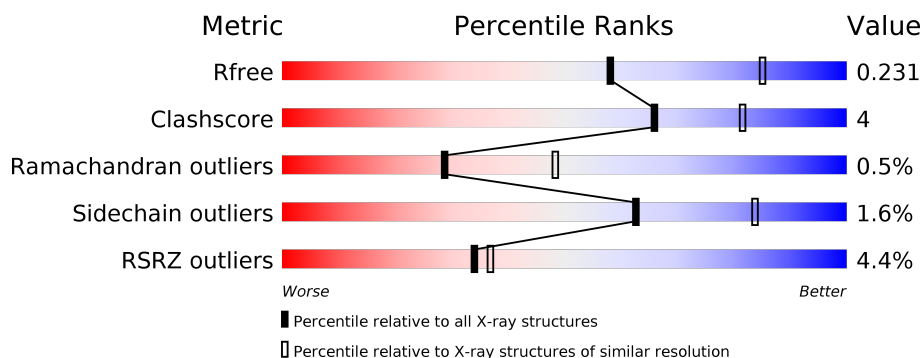
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	521	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div></div> </div> <div>.</div> </div>
1	B	521	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div></div> </div> <div>..</div> </div>
1	C	521	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div></div> </div> <div>..</div> </div>
1	D	521	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div></div> </div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	D	908	-	-	X	-

2 Entry composition [i](#)

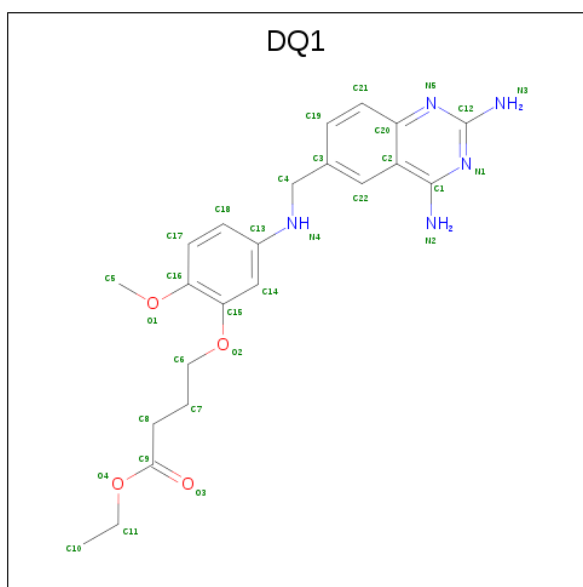
There are 6 unique types of molecules in this entry. The entry contains 17053 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	0	0
			3950	2512	695	725	18			
1	B	499	Total	C	N	O	S	0	0	0
			3956	2515	696	727	18			
1	C	507	Total	C	N	O	S	0	1	0
			4011	2546	707	739	19			
1	D	504	Total	C	N	O	S	0	0	0
			3991	2535	704	734	18			

- Molecule 2 is ethyl 4-(5-[[[(2,4-diaminoquinazolin-6-yl)methyl]amino}-2-methoxyphenoxy]butanoate (three-letter code: DQ1) (formula: C₂₂H₂₇N₅O₄).



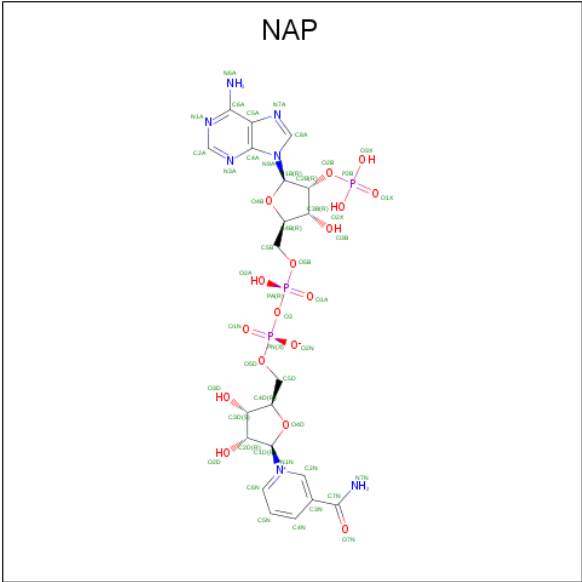
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	22	5	4		
2	B	1	Total	C	N	O	0	0
			31	22	5	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			31	22	5	4		
2	D	1	Total	C	N	O	0	0
			31	22	5	4		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	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
			48	21	7	17	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

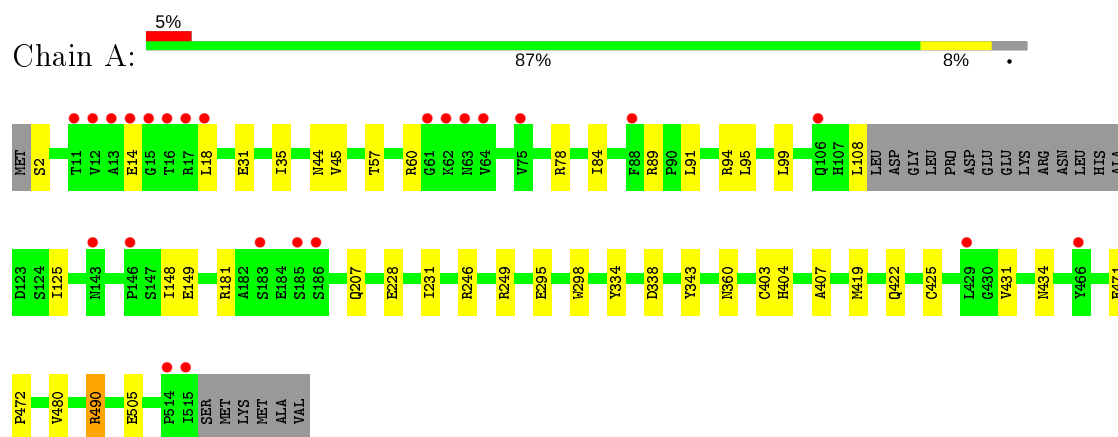
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	157	Total 157	O 157	0	0
6	B	168	Total 168	O 168	0	0
6	C	204	Total 204	O 204	0	0
6	D	208	Total 208	O 208	0	0

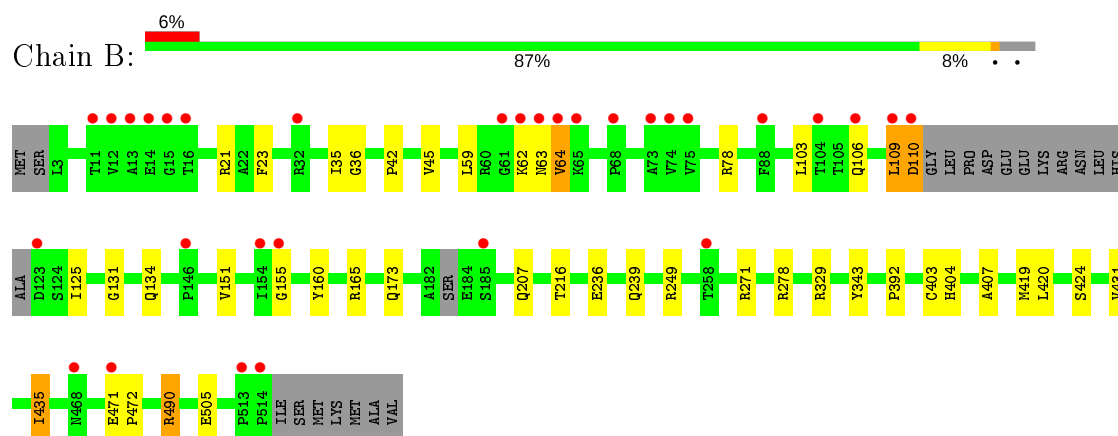
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

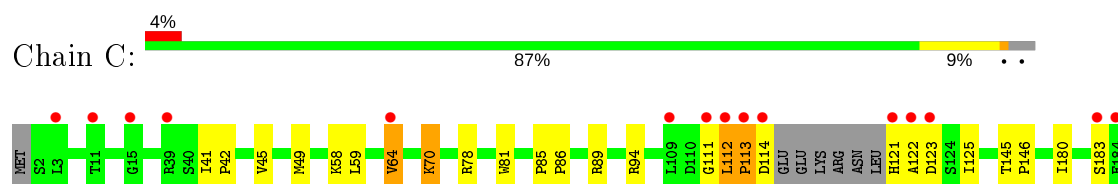
- Molecule 1: Dihydrofolate reductase-thymidylate synthase

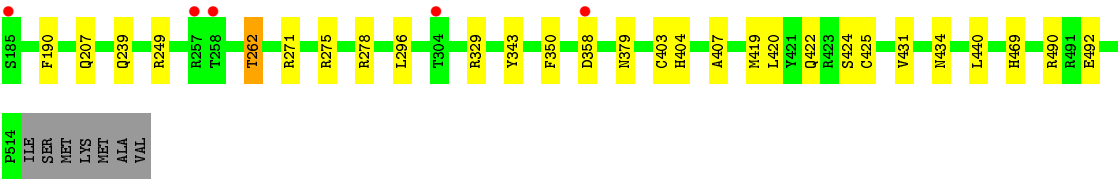


- Molecule 1: Dihydrofolate reductase-thymidylate synthase

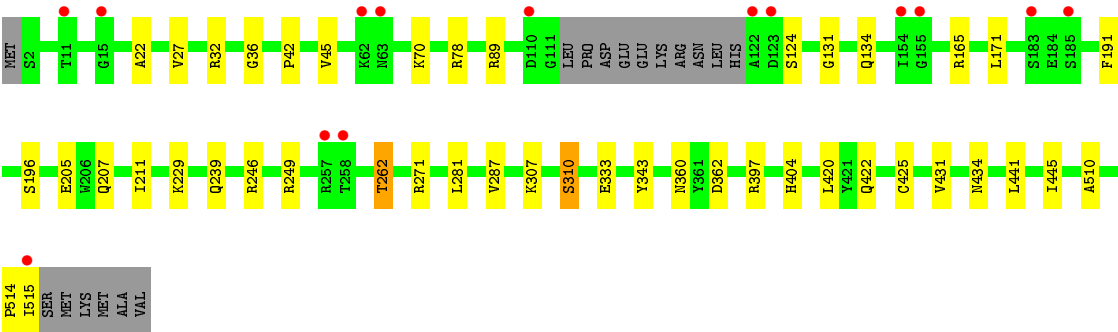
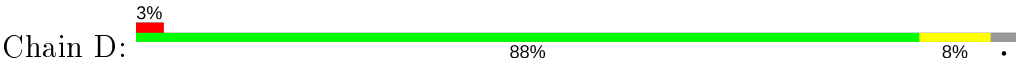


- Molecule 1: Dihydrofolate reductase-thymidylate synthase





● Molecule 1: Dihydrofolate reductase-thymidylate synthase



●



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	175.62Å 175.62Å 249.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.50) 99.6 (19.99-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.200 , 0.234 0.201 , 0.231	Depositor DCC
R_{free} test set	6726 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17053	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.14% 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: NAP, DQ1, EDO, SO4

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	0.39	0/4045	0.53	0/5492
1	B	0.39	0/4050	0.54	0/5496
1	C	0.39	0/4110	0.54	0/5579
1	D	0.38	0/4086	0.53	0/5545
All	All	0.39	0/16291	0.54	0/22112

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	3950	0	3896	30	0
1	B	3956	0	3906	29	0
1	C	4011	0	3956	42	0
1	D	3991	0	3947	36	0
2	A	31	0	27	4	0
2	B	31	0	27	2	0
2	C	31	0	27	7	0
2	D	31	0	27	4	0
3	A	48	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	25	1	0
3	C	48	0	25	1	0
3	D	48	0	25	1	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	15	0	0	0	0
5	A	16	0	24	0	0
5	B	12	0	18	0	0
5	C	8	0	12	0	0
5	D	16	0	24	6	0
6	A	157	0	0	4	0
6	B	168	0	0	1	0
6	C	204	0	0	3	0
6	D	208	0	0	2	0
All	All	17053	0	15991	130	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 (130) 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:45:VAL:H	2:C:602:DQ1:H10A	1.37	0.88
1:C:49:MET:HE2	2:C:602:DQ1:H21	1.59	0.85
1:A:60:ARG:HG3	1:A:149:GLU:OE2	1.78	0.84
1:C:49:MET:CE	2:C:602:DQ1:H21	2.10	0.82
1:D:45:VAL:H	2:D:602:DQ1:H10A	1.47	0.78
1:B:471:GLU:HB3	1:B:472:PRO:HD3	1.70	0.73
1:C:112:LEU:CB	1:C:113:PRO:HA	2.20	0.70
1:B:106:GLN:HA	1:B:109:LEU:HD12	1.75	0.69
1:C:404:HIS:HB2	1:C:420:LEU:HD11	1.74	0.69
1:A:231:ILE:HD11	1:A:480:VAL:HG11	1.75	0.68
1:B:404:HIS:HB2	1:B:420:LEU:HD11	1.77	0.67
1:A:2:SER:HB3	6:A:524:HOH:O	1.93	0.66
1:C:121:HIS:O	1:C:123:ASP:N	2.30	0.65
1:D:78:ARG:HD3	3:D:702:NAP:O2X	1.97	0.64
1:C:113:PRO:O	1:C:114:ASP:CB	2.45	0.63
1:B:59:LEU:H	1:B:64:VAL:HG13	1.64	0.63
1:D:131:GLY:H	1:D:134:GLN:HE21	1.46	0.63
1:C:45:VAL:H	2:C:602:DQ1:C10	2.11	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:GLN:HE22	1:C:271:ARG:H	1.48	0.60
1:D:514:PRO:O	1:D:515:ILE:HB	2.02	0.59
1:B:59:LEU:H	1:B:64:VAL:CG1	2.15	0.59
1:B:109:LEU:C	1:B:110:ASP:OD1	2.41	0.58
1:C:113:PRO:O	1:C:114:ASP:HB2	2.02	0.58
1:B:236:GLU:OE1	1:B:278:ARG:NH2	2.37	0.58
1:C:112:LEU:H	1:C:113:PRO:HA	1.68	0.58
1:C:112:LEU:CB	1:C:113:PRO:CA	2.82	0.57
6:A:525:HOH:O	1:D:262:THR:HG21	2.04	0.56
1:C:59:LEU:H	1:C:64:VAL:HG13	1.70	0.56
1:D:404:HIS:HB2	1:D:420:LEU:HD11	1.87	0.56
1:A:471:GLU:HB3	1:A:472:PRO:HD3	1.88	0.55
1:B:36:GLY:HA2	1:B:42:PRO:HD3	1.88	0.55
1:C:49:MET:HE1	2:C:602:DQ1:H21	1.88	0.55
1:C:403[B]:CYS:SG	1:C:424:SER:O	2.65	0.54
1:C:78:ARG:HD3	3:C:702:NAP:O2X	2.07	0.54
1:C:207:GLN:NE2	1:D:249:ARG:HH11	2.04	0.54
1:A:78:ARG:HD3	3:A:702:NAP:O2X	2.07	0.54
1:D:36:GLY:HA2	1:D:42:PRO:HD3	1.90	0.54
1:A:14:GLU:OE1	1:C:190:PHE:CZ	2.61	0.53
1:D:45:VAL:H	2:D:602:DQ1:C10	2.18	0.53
1:A:31:GLU:OE2	1:A:181:ARG:HD2	2.07	0.53
1:A:108:LEU:HD12	1:A:125:ILE:HD12	1.90	0.53
1:A:95:LEU:HD22	1:A:148:ILE:HD11	1.90	0.53
1:A:45:VAL:H	2:A:602:DQ1:H10A	1.74	0.52
1:A:246:ARG:NH2	6:A:575:HOH:O	2.43	0.52
1:A:91:LEU:HB3	1:A:94:ARG:HH21	1.75	0.52
1:D:229:LYS:HZ1	5:D:908:EDO:H11	1.75	0.52
1:A:84:ILE:O	1:A:89:ARG:NH1	2.37	0.51
1:C:207:GLN:HE22	1:D:249:ARG:HH11	1.56	0.51
1:B:490:ARG:HD2	1:B:505:GLU:OE1	2.10	0.51
1:B:109:LEU:O	1:B:110:ASP:OD1	2.30	0.50
1:C:407:ALA:HA	1:C:419:MET:O	2.11	0.50
1:C:422:GLN:HE22	1:C:434:ASN:HD22	1.59	0.49
1:D:510:ALA:HB1	5:D:908:EDO:H12	1.94	0.49
1:A:334:TYR:HB3	1:A:338:ASP:HB3	1.93	0.49
1:B:431:VAL:O	1:B:435:ILE:HG12	2.12	0.49
1:C:379:ASN:ND2	6:C:556:HOH:O	2.44	0.49
1:A:425:CYS:HB3	1:A:431:VAL:CG2	2.42	0.49
1:B:165:ARG:NH2	1:D:165:ARG:HE	2.10	0.49
1:B:407:ALA:HA	1:B:419:MET:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:LYS:HA	1:C:64:VAL:HG11	1.95	0.48
1:B:59:LEU:HB2	1:B:64:VAL:HG13	1.94	0.48
1:D:422:GLN:HE22	1:D:434:ASN:ND2	2.11	0.48
6:B:572:HOH:O	1:C:262:THR:HG21	2.13	0.48
2:C:602:DQ1:H6	2:C:602:DQ1:H14	1.66	0.48
1:B:165:ARG:HH21	1:D:165:ARG:HE	1.62	0.48
1:D:360:ASN:HD21	1:D:362:ASP:HB2	1.79	0.48
1:A:422:GLN:HE22	1:A:434:ASN:ND2	2.13	0.47
1:D:211:ILE:HD11	5:D:903:EDO:H12	1.96	0.47
1:D:239:GLN:HE22	1:D:271:ARG:H	1.62	0.47
1:A:44:ASN:HA	2:A:602:DQ1:H10A	1.97	0.47
1:C:249:ARG:HD2	1:D:207:GLN:NE2	2.30	0.47
1:D:425:CYS:HB3	1:D:431:VAL:CG2	2.45	0.46
1:D:441:LEU:O	1:D:445:ILE:HG12	2.14	0.46
1:D:422:GLN:HE22	1:D:434:ASN:HD22	1.64	0.46
1:D:333:GLU:OE2	1:D:397:ARG:NH2	2.32	0.46
1:D:246:ARG:NH2	6:D:588:HOH:O	2.50	0.45
1:C:249:ARG:HH11	1:D:207:GLN:NE2	2.13	0.45
1:D:27:VAL:HG11	1:D:191:PHE:CE2	2.52	0.45
1:B:131:GLY:N	1:B:134:GLN:HE21	2.15	0.45
1:A:249:ARG:NH1	1:B:207:GLN:OE1	2.49	0.45
1:A:490:ARG:HD2	1:A:505:GLU:OE1	2.17	0.44
1:C:275:ARG:O	1:C:278:ARG:HD2	2.17	0.44
1:B:23:PHE:O	1:B:173:GLN:HG2	2.18	0.44
1:D:229:LYS:NZ	5:D:908:EDO:H11	2.32	0.44
1:A:45:VAL:H	2:A:602:DQ1:C10	2.31	0.44
1:B:35:ILE:O	3:B:702:NAP:H2N	2.18	0.44
1:A:228:GLU:HG2	6:A:522:HOH:O	2.17	0.44
1:A:99:LEU:O	3:A:702:NAP:H1B	2.18	0.44
1:B:131:GLY:H	1:B:134:GLN:HE21	1.65	0.44
1:B:392:PRO:HD2	1:C:350:PHE:CZ	2.53	0.44
1:D:131:GLY:N	1:D:134:GLN:HE21	2.15	0.44
2:B:602:DQ1:H14	2:B:602:DQ1:H6	1.62	0.44
1:B:239:GLN:HE22	1:B:271:ARG:H	1.66	0.43
1:D:249:ARG:NH2	6:D:590:HOH:O	2.51	0.43
1:A:57:THR:OG1	1:A:94:ARG:NH1	2.51	0.43
2:D:602:DQ1:H14	2:D:602:DQ1:H6	1.62	0.43
1:B:403:CYS:SG	1:B:424:SER:O	2.77	0.43
1:C:145:THR:HA	1:C:146:PRO:HA	1.88	0.43
1:C:422:GLN:HE22	1:C:434:ASN:ND2	2.16	0.43
1:B:78:ARG:HG3	1:B:103:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ALA:HA	1:A:419:MET:O	2.19	0.43
1:A:91:LEU:HB3	1:A:94:ARG:NH2	2.33	0.43
1:C:425:CYS:HB3	1:C:431:VAL:CG2	2.49	0.43
1:D:211:ILE:CD1	5:D:903:EDO:H12	2.49	0.43
1:C:81:TRP:CH2	1:C:125:ILE:HD12	2.54	0.42
1:B:131:GLY:H	1:B:134:GLN:NE2	2.17	0.42
1:C:112:LEU:N	1:C:113:PRO:HA	2.25	0.42
1:A:207:GLN:OE1	1:B:249:ARG:HD2	2.19	0.42
1:D:22:ALA:HA	1:D:171:LEU:HB3	2.01	0.42
2:A:602:DQ1:H6	2:A:602:DQ1:H14	1.62	0.41
1:A:295:GLU:O	1:A:298:TRP:HB3	2.20	0.41
1:A:35:ILE:O	3:A:702:NAP:H2N	2.20	0.41
1:C:45:VAL:N	2:C:602:DQ1:H10A	2.20	0.41
1:D:307:LYS:HA	1:D:310:SER:HB2	2.02	0.41
1:D:281:LEU:HD22	1:D:287:VAL:HB	2.02	0.41
1:C:45:VAL:HG21	1:C:180:ILE:HD12	2.02	0.41
1:D:196:SER:OG	1:D:205:GLU:HG3	2.20	0.41
1:B:21:ARG:HG2	1:B:151:VAL:HG21	2.02	0.41
1:D:45:VAL:N	2:D:602:DQ1:H10A	2.25	0.41
1:A:404:HIS:CD2	1:A:404:HIS:H	2.39	0.41
1:D:510:ALA:CB	5:D:908:EDO:H12	2.50	0.41
1:C:70:LYS:HE2	6:C:637:HOH:O	2.21	0.41
1:B:155:GLY:HA2	1:B:160:TYR:CZ	2.56	0.41
1:A:14:GLU:OE1	1:C:190:PHE:CE2	2.74	0.41
1:C:85:PRO:HA	1:C:86:PRO:HD3	1.95	0.40
1:B:45:VAL:H	2:B:602:DQ1:H10A	1.85	0.40
1:C:111:GLY:O	6:C:546:HOH:O	2.22	0.40
1:C:41:ILE:HA	1:C:42:PRO:HD3	1.95	0.40
1:C:59:LEU:H	1:C:64:VAL:CG1	2.33	0.40
1:C:296:LEU:HD22	1:C:440:LEU:HG	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	496/521 (95%)	483 (97%)	12 (2%)	1 (0%)	47	68
1	B	493/521 (95%)	476 (97%)	14 (3%)	3 (1%)	25	43
1	C	504/521 (97%)	486 (96%)	13 (3%)	5 (1%)	15	28
1	D	500/521 (96%)	489 (98%)	10 (2%)	1 (0%)	47	68
All	All	1993/2084 (96%)	1934 (97%)	49 (2%)	10 (0%)	29	48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	122	ALA
1	B	64	VAL
1	D	343	TYR
1	B	109	LEU
1	B	343	TYR
1	C	343	TYR
1	A	343	TYR
1	C	112	LEU
1	C	113	PRO
1	C	64	VAL

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	421/446 (94%)	417 (99%)	4 (1%)	76	90
1	B	423/446 (95%)	415 (98%)	8 (2%)	57	80
1	C	429/446 (96%)	419 (98%)	10 (2%)	50	76
1	D	427/446 (96%)	421 (99%)	6 (1%)	67	86
All	All	1700/1784 (95%)	1672 (98%)	28 (2%)	62	84

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	360	ASN
1	A	403	CYS
1	A	490	ARG
1	B	62	LYS
1	B	63	ASN
1	B	110	ASP
1	B	125	ILE
1	B	216	THR
1	B	329	ARG
1	B	435	ILE
1	B	490	ARG
1	C	70	LYS
1	C	89	ARG
1	C	94	ARG
1	C	183	SER
1	C	262	THR
1	C	329	ARG
1	C	358	ASP
1	C	469	HIS
1	C	490	ARG
1	C	492	GLU
1	D	32	ARG
1	D	70	LYS
1	D	89	ARG
1	D	124	SER
1	D	262	THR
1	D	310	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	239	GLN
1	A	315	HIS
1	A	360	ASN
1	A	434	ASN
1	A	469	HIS
1	B	134	GLN
1	B	239	GLN
1	B	315	HIS
1	B	320	ASN
1	B	422	GLN

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Mol	Chain	Res	Type
1	B	434	ASN
1	B	469	HIS
1	C	173	GLN
1	C	207	GLN
1	C	239	GLN
1	C	269	GLN
1	C	315	HIS
1	C	320	ASN
1	C	346	GLN
1	C	360	ASN
1	C	379	ASN
1	C	434	ASN
1	D	134	GLN
1	D	207	GLN
1	D	239	GLN
1	D	315	HIS
1	D	346	GLN
1	D	360	ASN
1	D	434	ASN
1	D	469	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

29 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
5	EDO	D	911	-	3,3,3	0.45	0	2,2,2	0.38	0
3	NAP	C	702	-	45,52,52	1.38	7 (15%)	56,80,80	1.20	7 (12%)
5	EDO	A	901	-	3,3,3	0.50	0	2,2,2	0.35	0
4	SO4	B	701	-	4,4,4	0.12	0	6,6,6	0.09	0
4	SO4	C	701	-	4,4,4	0.13	0	6,6,6	0.08	0
2	DQ1	D	602	-	33,33,33	1.32	1 (3%)	43,44,44	1.54	7 (16%)
4	SO4	C	801	-	4,4,4	0.15	0	6,6,6	0.12	0
2	DQ1	B	602	-	33,33,33	1.24	1 (3%)	43,44,44	1.51	7 (16%)
4	SO4	D	522	-	4,4,4	0.15	0	6,6,6	0.20	0
3	NAP	B	702	-	45,52,52	1.46	6 (13%)	56,80,80	1.27	7 (12%)
5	EDO	D	908	-	3,3,3	0.42	0	2,2,2	0.48	0
5	EDO	A	902	-	3,3,3	0.40	0	2,2,2	0.49	0
4	SO4	D	601	-	4,4,4	0.16	0	6,6,6	0.16	0
5	EDO	A	906	-	3,3,3	0.49	0	2,2,2	0.20	0
5	EDO	D	910	-	3,3,3	0.50	0	2,2,2	0.23	0
4	SO4	D	701	-	4,4,4	0.16	0	6,6,6	0.10	0
3	NAP	D	702	-	45,52,52	1.43	6 (13%)	56,80,80	1.22	6 (10%)
2	DQ1	C	602	-	33,33,33	1.28	1 (3%)	43,44,44	1.39	5 (11%)
2	DQ1	A	602	-	33,33,33	1.23	1 (3%)	43,44,44	1.49	6 (13%)
5	EDO	C	913	-	3,3,3	0.46	0	2,2,2	0.31	0
4	SO4	A	701	-	4,4,4	0.14	0	6,6,6	0.08	0
3	NAP	A	702	-	45,52,52	1.40	6 (13%)	56,80,80	1.25	5 (8%)
5	EDO	C	909	-	3,3,3	0.43	0	2,2,2	0.30	0
5	EDO	B	905	-	3,3,3	0.48	0	2,2,2	0.39	0
4	SO4	B	601	-	4,4,4	0.13	0	6,6,6	0.23	0
5	EDO	B	904	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	B	912	-	3,3,3	0.43	0	2,2,2	0.42	0
5	EDO	A	907	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	D	903	-	3,3,3	0.41	0	2,2,2	0.37	0

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	EDO	D	910	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	911	-	-	0/1/1/1	-
2	DQ1	B	602	-	-	8/17/17/17	0/3/3/3
3	NAP	A	702	-	-	6/31/67/67	0/5/5/5
3	NAP	C	702	-	-	6/31/67/67	0/5/5/5
5	EDO	A	901	-	-	1/1/1/1	-
3	NAP	D	702	-	-	5/31/67/67	0/5/5/5
5	EDO	C	909	-	-	0/1/1/1	-
3	NAP	B	702	-	-	7/31/67/67	0/5/5/5
5	EDO	D	908	-	-	1/1/1/1	-
2	DQ1	C	602	-	-	5/17/17/17	0/3/3/3
5	EDO	A	902	-	-	1/1/1/1	-
5	EDO	B	905	-	-	1/1/1/1	-
5	EDO	B	912	-	-	0/1/1/1	-
2	DQ1	A	602	-	-	8/17/17/17	0/3/3/3
5	EDO	A	907	-	-	1/1/1/1	-
5	EDO	C	913	-	-	0/1/1/1	-
5	EDO	A	906	-	-	1/1/1/1	-
5	EDO	B	904	-	-	1/1/1/1	-
5	EDO	D	903	-	-	1/1/1/1	-
2	DQ1	D	602	-	-	6/17/17/17	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	DQ1	C1-C2	-5.68	1.39	1.45
3	B	702	NAP	C2N-N1N	5.50	1.41	1.35
2	C	602	DQ1	C1-C2	-5.37	1.40	1.45
2	B	602	DQ1	C1-C2	-5.15	1.40	1.45
2	A	602	DQ1	C1-C2	-4.95	1.40	1.45
3	A	702	NAP	C2N-N1N	4.87	1.40	1.35
3	D	702	NAP	O4B-C1B	4.84	1.47	1.41
3	D	702	NAP	C2N-N1N	4.82	1.40	1.35
3	C	702	NAP	O4B-C1B	4.52	1.47	1.41
3	C	702	NAP	C2N-N1N	4.45	1.40	1.35
3	B	702	NAP	O4B-C1B	4.31	1.47	1.41
3	A	702	NAP	O4B-C1B	4.04	1.46	1.41
3	D	702	NAP	O4D-C1D	2.79	1.45	1.41
3	C	702	NAP	O4D-C1D	2.74	1.44	1.41
3	B	702	NAP	C6N-N1N	2.72	1.42	1.35
3	A	702	NAP	O4D-C1D	2.59	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NAP	O4D-C1D	2.50	1.44	1.41
3	A	702	NAP	C3N-C7N	2.45	1.54	1.50
3	D	702	NAP	C6N-N1N	2.39	1.41	1.35
3	C	702	NAP	C6N-N1N	2.35	1.41	1.35
3	A	702	NAP	C6N-N1N	2.26	1.40	1.35
3	B	702	NAP	C3N-C7N	2.26	1.54	1.50
3	C	702	NAP	P2B-O2B	2.21	1.63	1.59
3	A	702	NAP	P2B-O3X	2.19	1.63	1.54
3	C	702	NAP	P2B-O2X	2.12	1.63	1.54
3	D	702	NAP	C3N-C7N	2.11	1.53	1.50
3	C	702	NAP	P2B-O3X	2.11	1.63	1.54
3	B	702	NAP	P2B-O2B	2.04	1.63	1.59
3	D	702	NAP	P2B-O2X	2.04	1.62	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	DQ1	N5-C12-N1	-5.11	120.40	127.22
2	A	602	DQ1	N5-C12-N1	-5.08	120.44	127.22
2	C	602	DQ1	N5-C12-N1	-4.95	120.62	127.22
2	D	602	DQ1	N5-C12-N1	-4.86	120.74	127.22
3	A	702	NAP	N3A-C2A-N1A	-4.81	121.17	128.68
3	B	702	NAP	N3A-C2A-N1A	-4.66	121.40	128.68
3	D	702	NAP	N3A-C2A-N1A	-4.63	121.44	128.68
3	C	702	NAP	N3A-C2A-N1A	-4.61	121.47	128.68
3	A	702	NAP	O4D-C1D-C2D	-3.46	101.87	106.93
2	D	602	DQ1	C22-C2-C1	-3.40	121.32	124.76
3	B	702	NAP	O4D-C1D-C2D	-3.39	101.97	106.93
3	D	702	NAP	O4D-C1D-C2D	-3.12	102.37	106.93
2	B	602	DQ1	O1-C16-C15	2.98	119.56	115.41
2	A	602	DQ1	C2-C20-N5	-2.92	119.71	122.81
2	B	602	DQ1	C2-C20-N5	-2.92	119.72	122.81
2	D	602	DQ1	C2-C1-N1	-2.85	118.96	121.93
2	D	602	DQ1	C2-C20-N5	-2.76	119.89	122.81
2	C	602	DQ1	C2-C1-N1	-2.65	119.17	121.93
2	C	602	DQ1	C22-C2-C1	-2.65	122.09	124.76
2	B	602	DQ1	C22-C2-C1	-2.63	122.10	124.76
2	A	602	DQ1	C2-C1-N1	-2.62	119.20	121.93
2	A	602	DQ1	C22-C2-C1	-2.62	122.12	124.76
3	C	702	NAP	O4D-C1D-C2D	-2.61	103.12	106.93
3	D	702	NAP	O2N-PN-O5D	2.58	119.72	107.75
2	D	602	DQ1	O1-C16-C15	2.48	118.87	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	602	DQ1	C2-C20-N5	-2.48	120.18	122.81
3	B	702	NAP	C5D-C4D-C3D	-2.48	105.91	115.18
3	D	702	NAP	C6N-N1N-C2N	-2.46	119.73	121.97
3	A	702	NAP	O2N-PN-O5D	2.44	119.06	107.75
3	B	702	NAP	C6N-N1N-C2N	-2.43	119.76	121.97
3	B	702	NAP	O5D-PN-O1N	2.40	118.44	109.07
2	B	602	DQ1	O4-C9-C8	2.38	119.36	111.91
2	A	602	DQ1	O4-C9-C8	2.33	119.22	111.91
3	C	702	NAP	O2N-PN-O5D	2.31	118.48	107.75
3	C	702	NAP	O5D-PN-O1N	2.30	118.05	109.07
3	A	702	NAP	C6N-N1N-C2N	-2.28	119.90	121.97
2	A	602	DQ1	O1-C16-C15	2.27	118.57	115.41
2	B	602	DQ1	C2-C1-N1	-2.23	119.61	121.93
2	D	602	DQ1	O4-C9-C8	2.23	118.90	111.91
3	C	702	NAP	C5D-C4D-C3D	-2.16	107.07	115.18
3	B	702	NAP	O2N-PN-O1N	2.15	122.87	112.24
3	C	702	NAP	C6N-N1N-C2N	-2.14	120.02	121.97
2	B	602	DQ1	O1-C16-C17	-2.11	120.75	124.37
2	C	602	DQ1	O4-C9-C8	2.10	118.51	111.91
2	D	602	DQ1	C11-O4-C9	-2.10	110.62	116.73
3	B	702	NAP	O2N-PN-O5D	2.10	117.49	107.75
3	A	702	NAP	O5D-PN-O1N	2.08	117.21	109.07
3	D	702	NAP	O5D-PN-O1N	2.06	117.13	109.07
3	D	702	NAP	C4A-C5A-N7A	-2.04	107.27	109.40
3	C	702	NAP	O2N-PN-O1N	2.02	122.20	112.24

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	702	NAP	C5D-O5D-PN-O1N
3	C	702	NAP	O4D-C1D-N1N-C6N
2	D	602	DQ1	C6-C7-C8-C9
3	B	702	NAP	C5D-O5D-PN-O1N
3	B	702	NAP	O4D-C1D-N1N-C6N
3	D	702	NAP	C5D-O5D-PN-O1N
3	D	702	NAP	O4D-C1D-N1N-C6N
2	C	602	DQ1	C6-C7-C8-C9
2	A	602	DQ1	C6-C7-C8-C9
3	A	702	NAP	C5D-O5D-PN-O1N
3	A	702	NAP	O4D-C1D-N1N-C6N
2	B	602	DQ1	C15-C16-O1-C5

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Mol	Chain	Res	Type	Atoms
2	B	602	DQ1	C8-C9-O4-C11
2	A	602	DQ1	C8-C9-O4-C11
2	B	602	DQ1	O3-C9-O4-C11
2	A	602	DQ1	O3-C9-O4-C11
2	B	602	DQ1	C17-C16-O1-C5
2	D	602	DQ1	C8-C9-O4-C11
2	A	602	DQ1	C15-C16-O1-C5
2	D	602	DQ1	O3-C9-O4-C11
3	C	702	NAP	C3D-C4D-C5D-O5D
3	D	702	NAP	C3D-C4D-C5D-O5D
5	A	906	EDO	O1-C1-C2-O2
5	B	904	EDO	O1-C1-C2-O2
2	D	602	DQ1	C7-C6-O2-C15
2	C	602	DQ1	C7-C6-O2-C15
3	B	702	NAP	C3D-C4D-C5D-O5D
2	A	602	DQ1	C17-C16-O1-C5
2	B	602	DQ1	C7-C6-O2-C15
2	A	602	DQ1	C7-C6-O2-C15
2	D	602	DQ1	C15-C16-O1-C5
2	C	602	DQ1	C8-C9-O4-C11
5	D	910	EDO	O1-C1-C2-O2
2	C	602	DQ1	O3-C9-O4-C11
3	D	702	NAP	O4D-C4D-C5D-O5D
5	A	901	EDO	O1-C1-C2-O2
5	D	908	EDO	O1-C1-C2-O2
2	D	602	DQ1	C17-C16-O1-C5
3	C	702	NAP	C5D-O5D-PN-O3
3	B	702	NAP	C5D-O5D-PN-O3
5	A	902	EDO	O1-C1-C2-O2
5	A	907	EDO	O1-C1-C2-O2
3	C	702	NAP	O4D-C4D-C5D-O5D
3	A	702	NAP	C3D-C4D-C5D-O5D
2	B	602	DQ1	C6-C7-C8-C9
3	B	702	NAP	C4D-C5D-O5D-PN
2	A	602	DQ1	C10-C11-O4-C9
5	D	903	EDO	O1-C1-C2-O2
3	B	702	NAP	O4D-C4D-C5D-O5D
2	B	602	DQ1	C10-C11-O4-C9
2	C	602	DQ1	C10-C11-O4-C9
5	B	905	EDO	O1-C1-C2-O2
3	B	702	NAP	C2B-O2B-P2B-O2X
3	D	702	NAP	C5D-O5D-PN-O3

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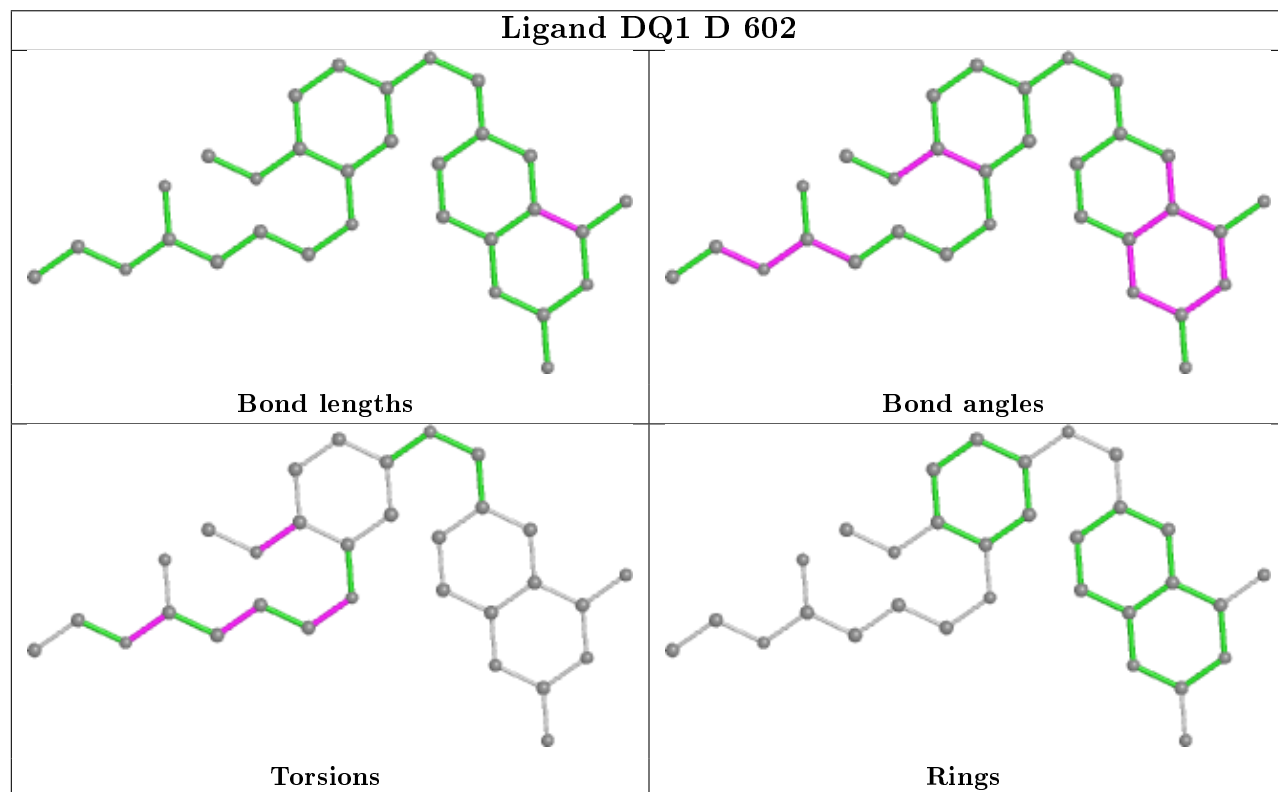
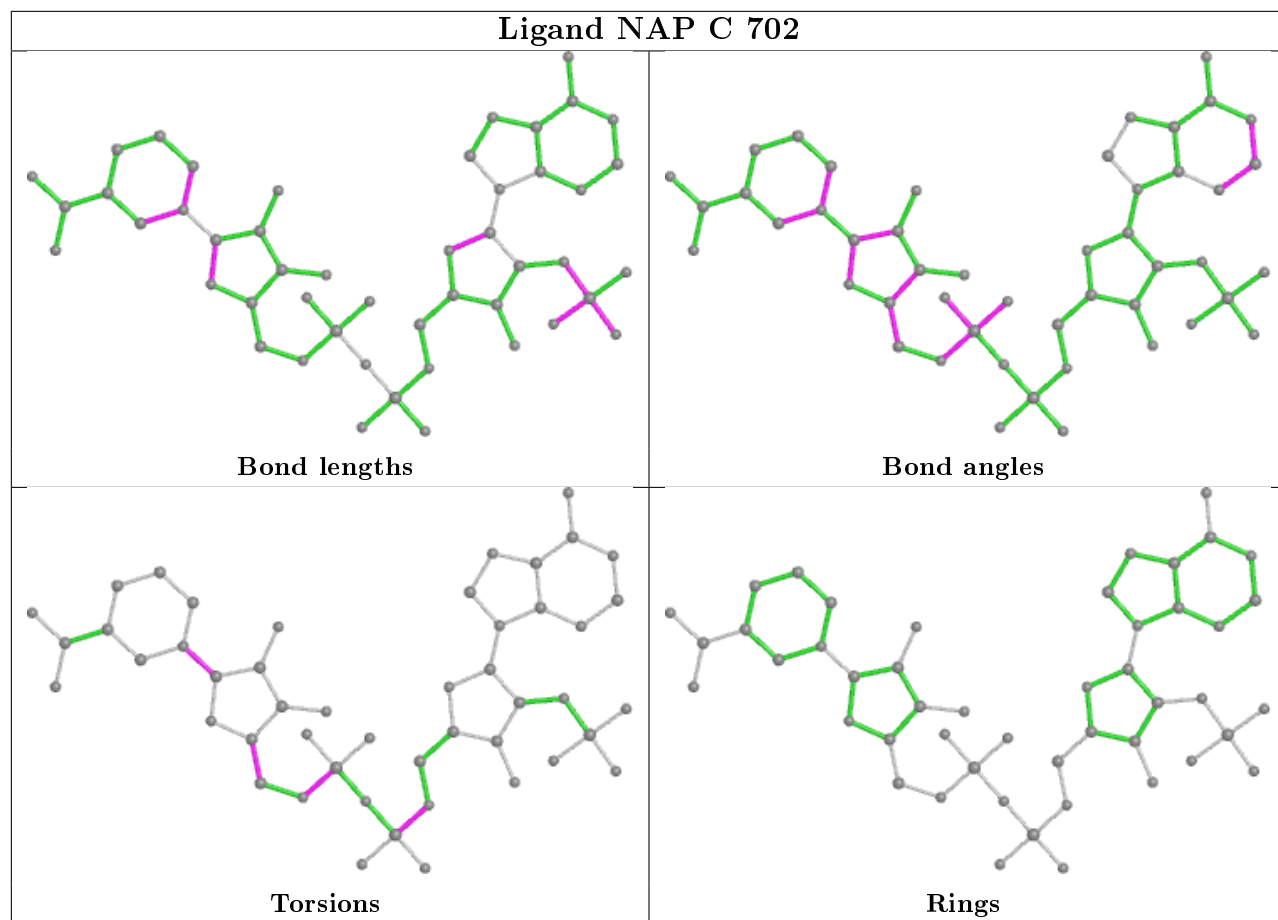
Mol	Chain	Res	Type	Atoms
3	A	702	NAP	C2D-C1D-N1N-C2N
3	A	702	NAP	C2D-C1D-N1N-C6N
3	C	702	NAP	C5B-O5B-PA-O1A
3	A	702	NAP	C5B-O5B-PA-O1A
2	B	602	DQ1	C7-C8-C9-O4
2	A	602	DQ1	C7-C8-C9-O4

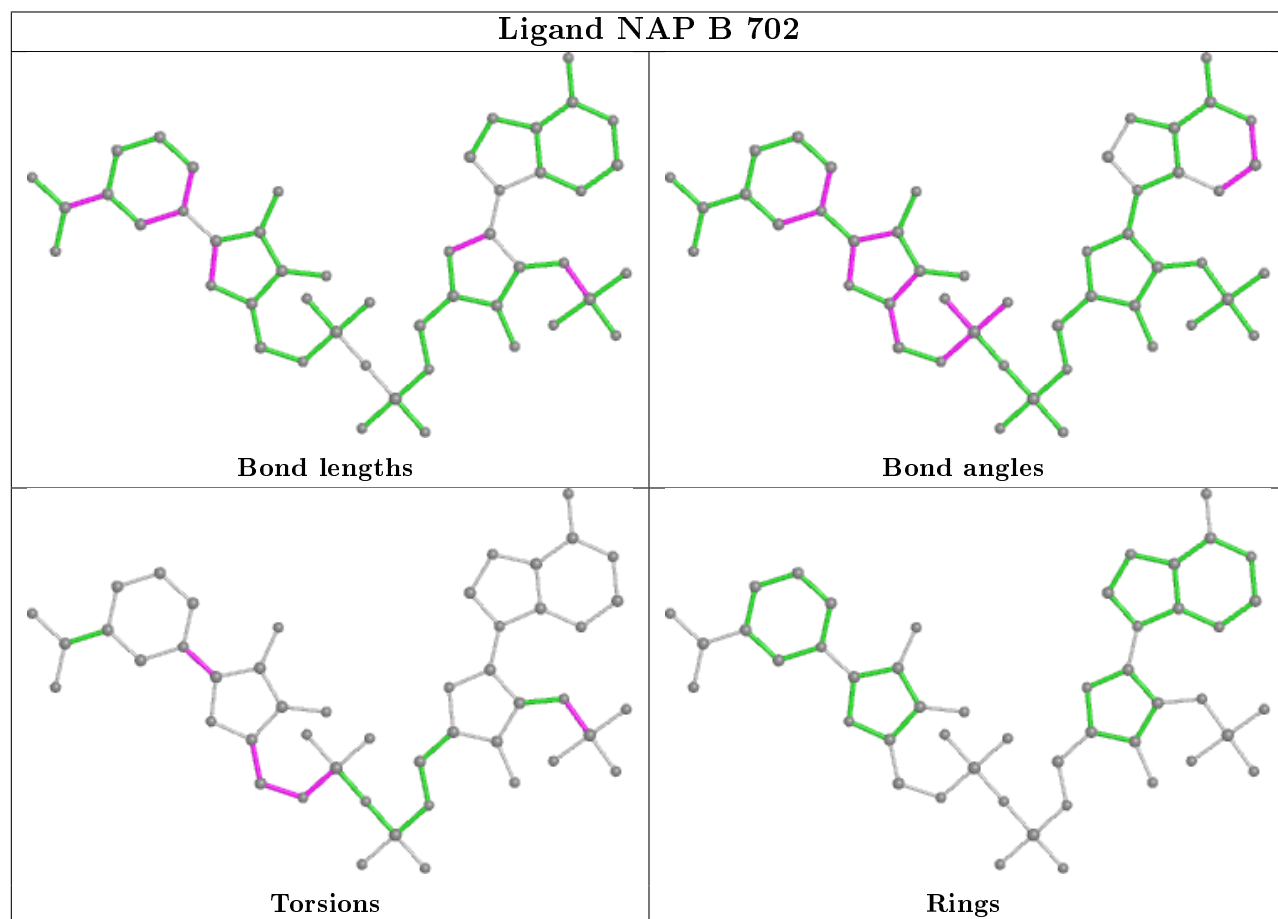
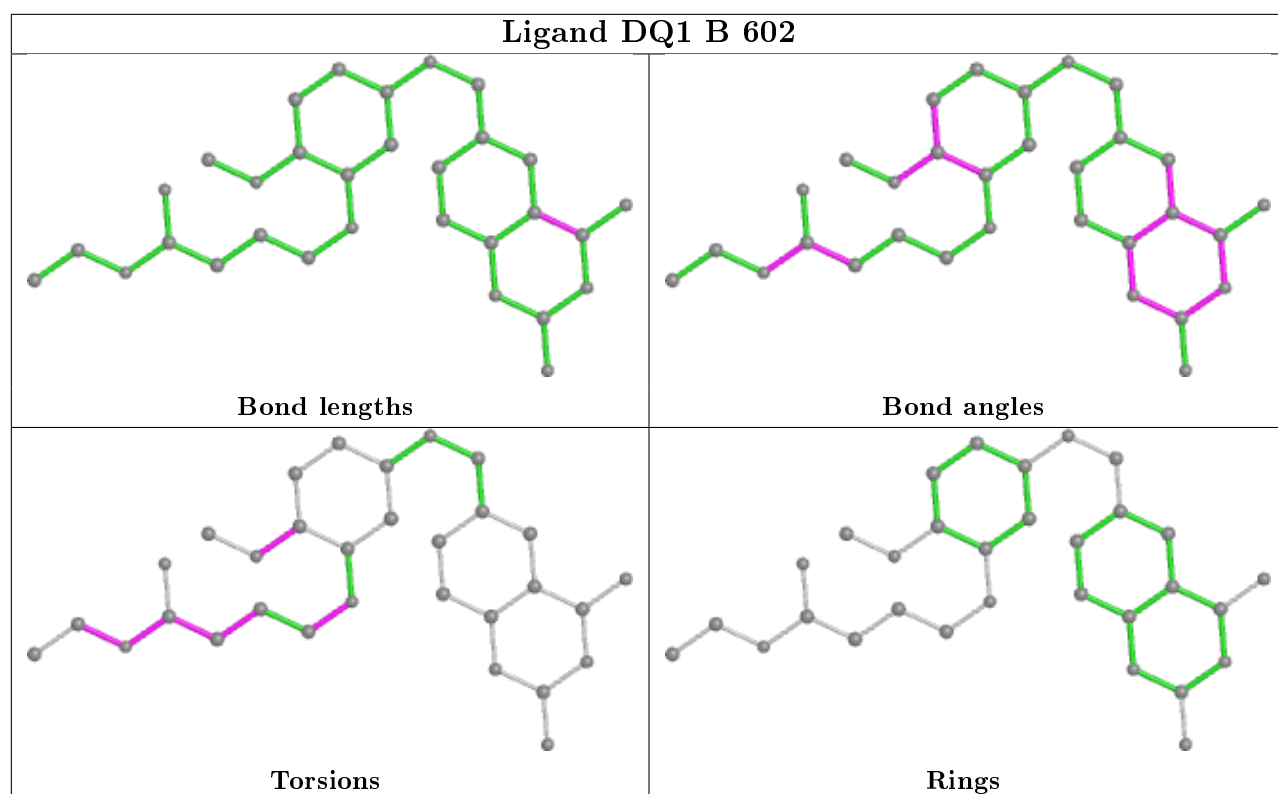
There are no ring outliers.

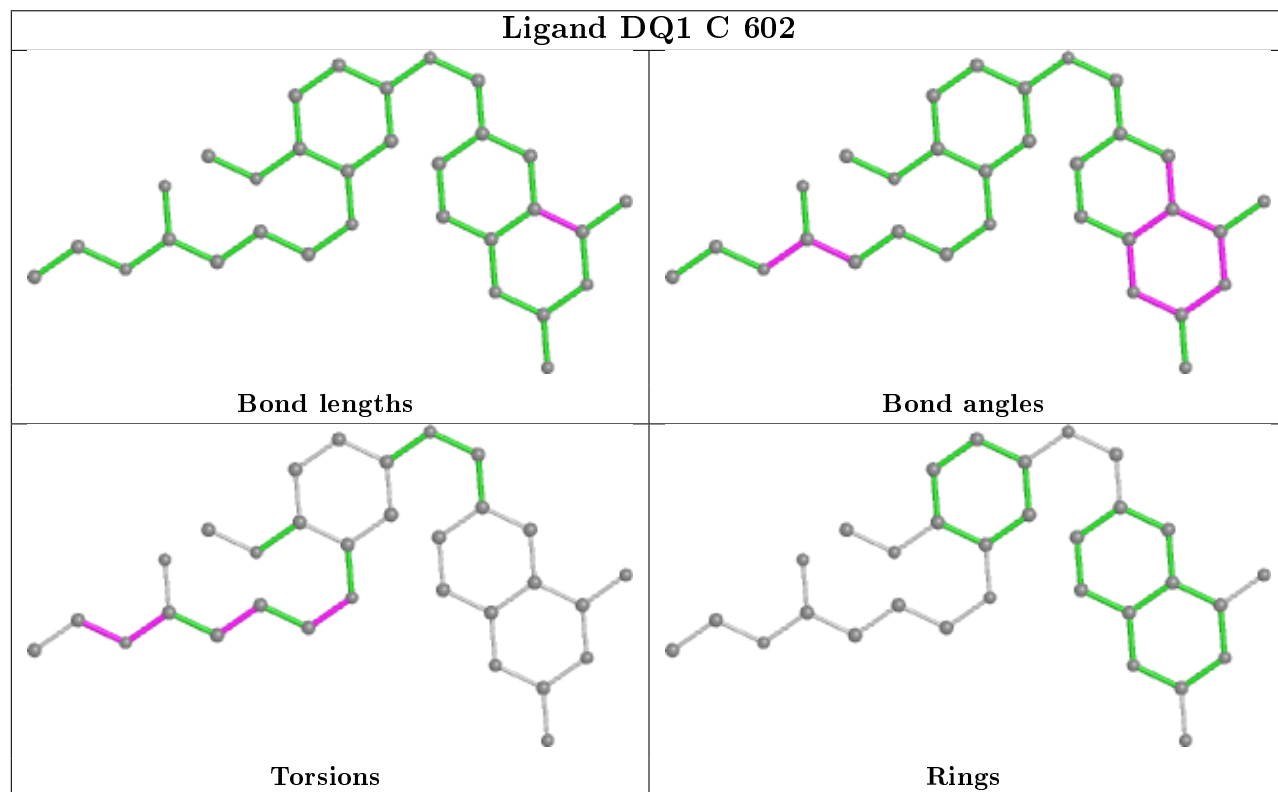
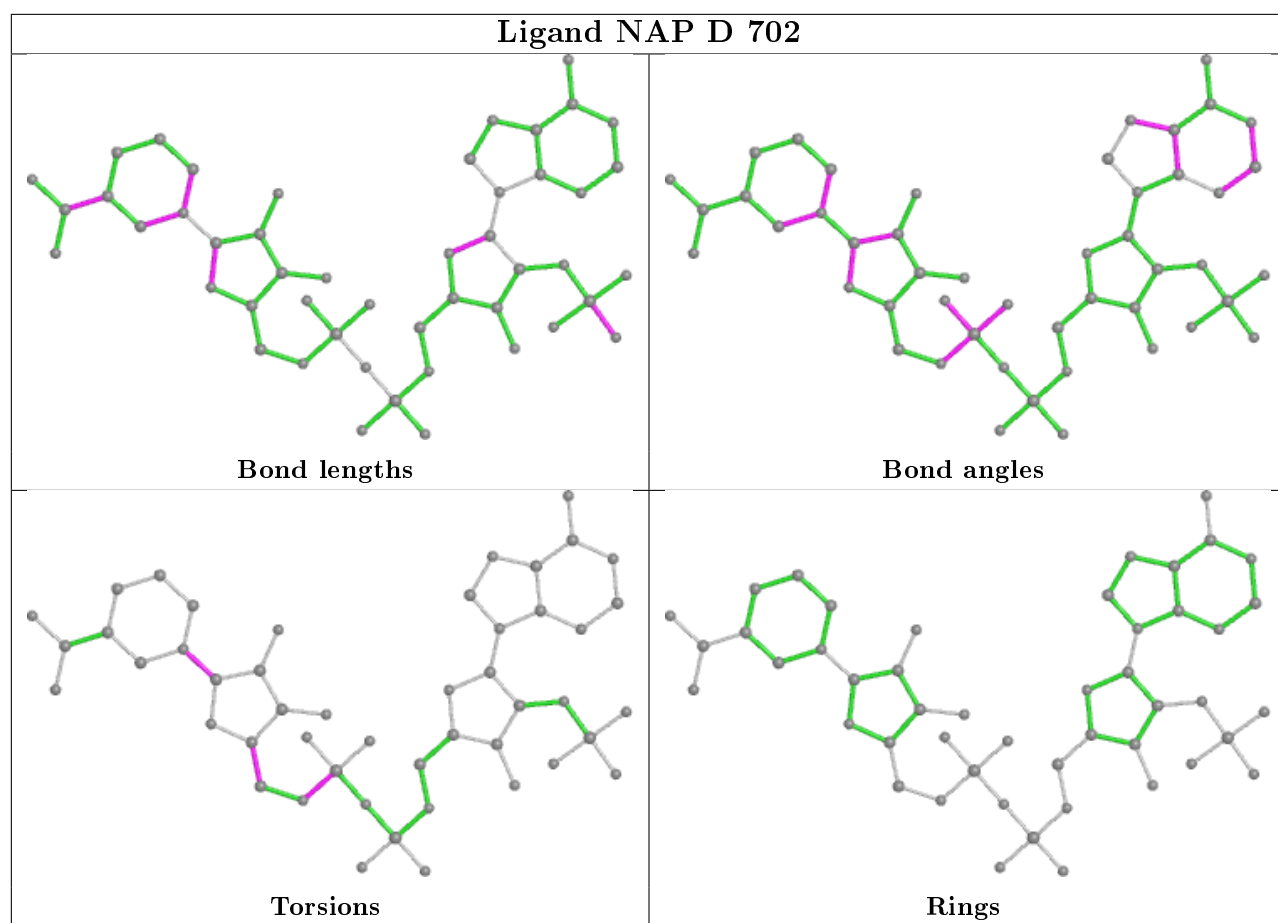
10 monomers are involved in 29 short contacts:

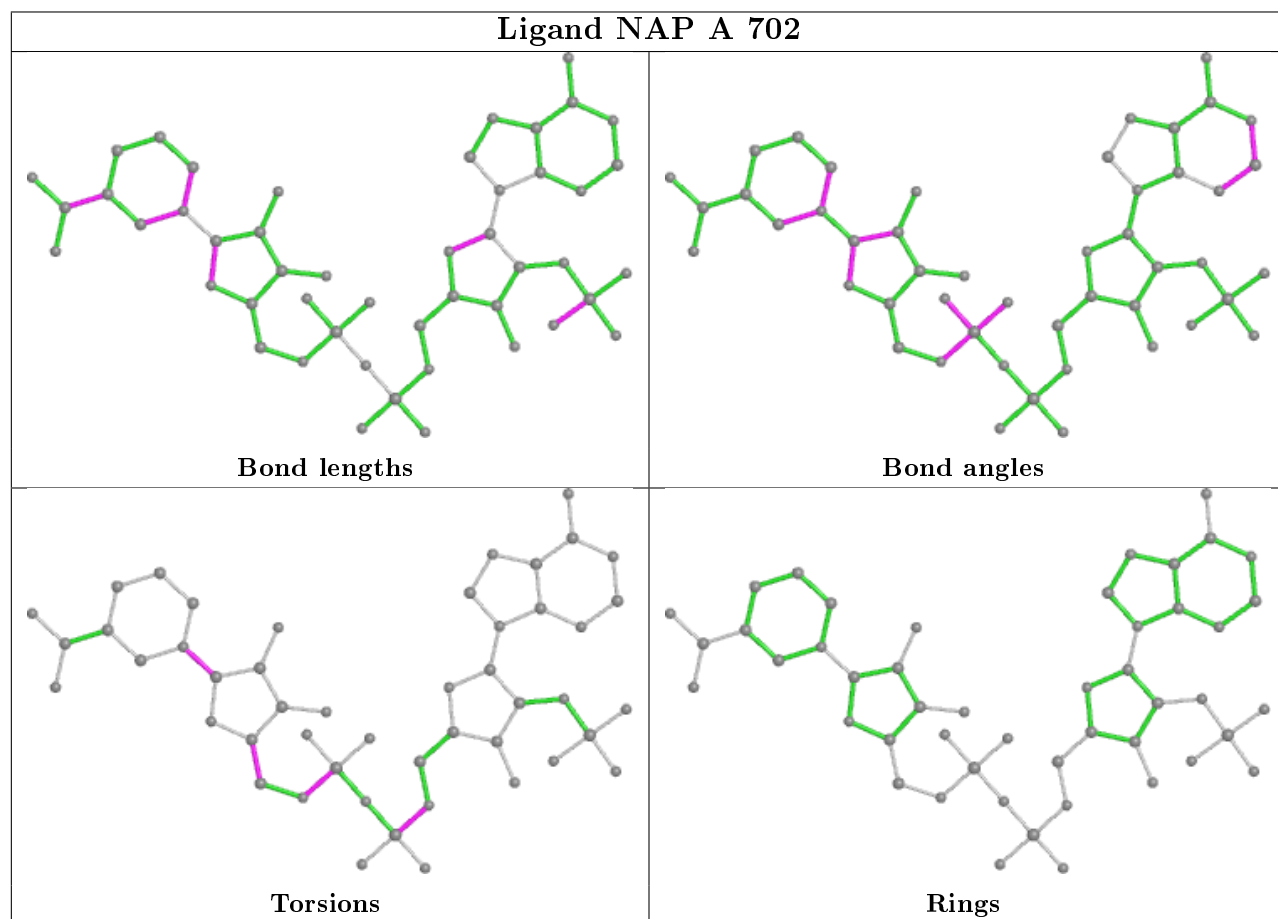
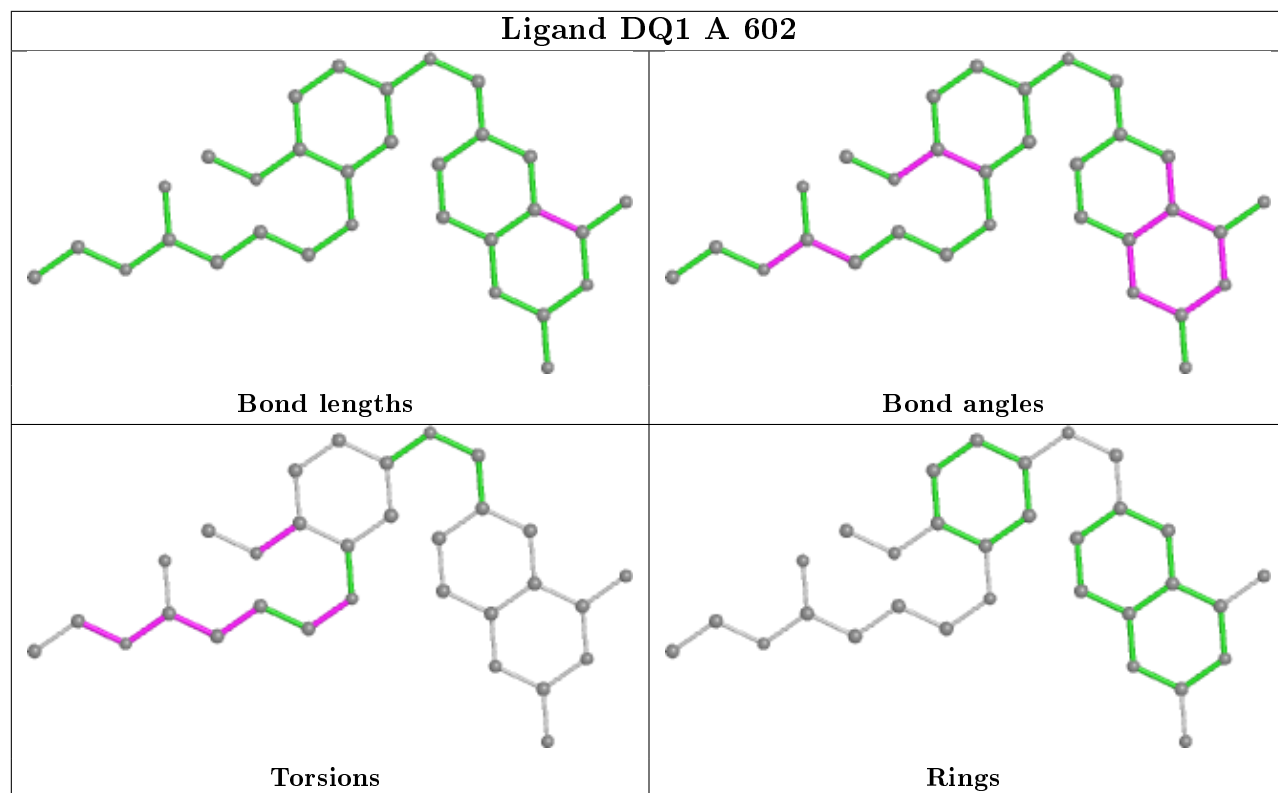
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	NAP	1	0
2	D	602	DQ1	4	0
2	B	602	DQ1	2	0
3	B	702	NAP	1	0
5	D	908	EDO	4	0
3	D	702	NAP	1	0
2	C	602	DQ1	7	0
2	A	602	DQ1	4	0
3	A	702	NAP	3	0
5	D	903	EDO	2	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	500/521 (95%)	-0.01	24 (4%)	30 32	26, 42, 68, 92	3 (0%)
1	B	499/521 (95%)	0.01	31 (6%)	20 21	25, 41, 71, 96	4 (0%)
1	C	507/521 (97%)	-0.07	20 (3%)	39 42	25, 38, 61, 103	4 (0%)
1	D	504/521 (96%)	-0.12	14 (2%)	53 56	25, 38, 59, 83	1 (0%)
All	All	2010/2084 (96%)	-0.05	89 (4%)	34 37	25, 39, 66, 103	12 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	SER	8.5
1	B	13	ALA	6.0
1	B	63	ASN	5.7
1	A	14	GLU	4.9
1	B	62	LYS	4.8
1	B	185	SER	4.8
1	A	63	ASN	4.6
1	C	113	PRO	4.6
1	A	185	SER	4.6
1	B	12	VAL	4.5
1	D	515	ILE	4.4
1	D	185	SER	4.3
1	C	185	SER	4.3
1	D	62	LYS	4.3
1	D	63	ASN	4.3
1	A	16	THR	4.2
1	D	257	ARG	4.1
1	C	121	HIS	4.1
1	C	122	ALA	4.0
1	D	122	ALA	4.0
1	A	64	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	183	SER	3.8
1	B	61	GLY	3.6
1	C	64	VAL	3.6
1	A	13	ALA	3.6
1	A	11	THR	3.5
1	B	64	VAL	3.4
1	A	61	GLY	3.3
1	C	111	GLY	3.3
1	C	114	ASP	3.3
1	B	16	THR	3.3
1	C	112	LEU	3.2
1	C	184	GLU	3.2
1	A	15	GLY	3.2
1	B	65	LYS	3.1
1	D	110	ASP	3.1
1	B	11	THR	3.1
1	A	514	PRO	3.1
1	B	68	PRO	3.0
1	D	258	THR	3.0
1	A	17	ARG	3.0
1	B	146	PRO	2.9
1	A	106	GLN	2.9
1	B	15	GLY	2.9
1	B	74	VAL	2.9
1	B	14	GLU	2.9
1	B	514	PRO	2.9
1	C	304	THR	2.8
1	B	110	ASP	2.8
1	C	257	ARG	2.8
1	B	123	ASP	2.7
1	C	258	THR	2.7
1	D	11	THR	2.7
1	B	106	GLN	2.6
1	C	3	LEU	2.6
1	A	75	VAL	2.6
1	B	109	LEU	2.6
1	B	104	THR	2.6
1	B	75	VAL	2.5
1	A	12	VAL	2.5
1	B	468	ASN	2.5
1	A	62	LYS	2.5
1	A	515	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	123	ASP	2.4
1	B	88	PHE	2.4
1	B	32	ARG	2.4
1	A	466	TYR	2.3
1	B	154	ILE	2.3
1	A	186	SER	2.3
1	B	258	THR	2.3
1	B	471	GLU	2.3
1	C	39	ARG	2.3
1	D	183	SER	2.3
1	D	123	ASP	2.3
1	A	429	LEU	2.2
1	B	513	PRO	2.2
1	C	11	THR	2.2
1	D	155	GLY	2.2
1	D	154	ILE	2.2
1	A	143	ASN	2.2
1	C	15	GLY	2.1
1	B	73	ALA	2.1
1	C	358	ASP	2.0
1	C	109	LEU	2.0
1	A	146	PRO	2.0
1	D	15	GLY	2.0
1	A	88	PHE	2.0
1	B	155	GLY	2.0
1	A	18	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

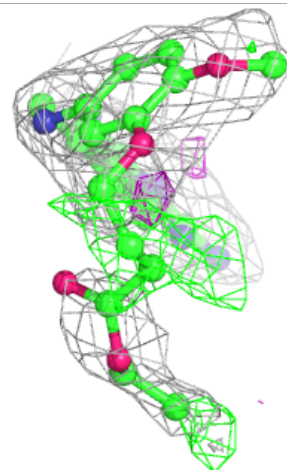
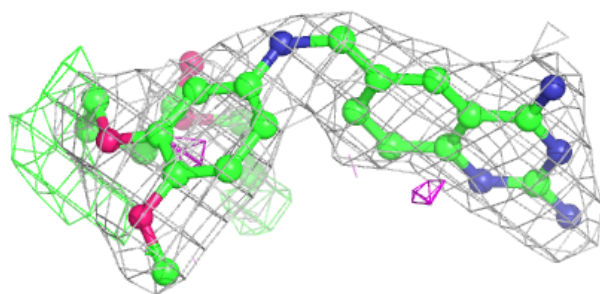
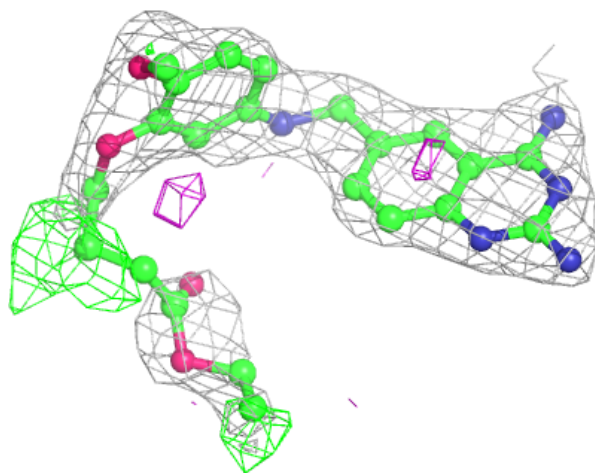
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	A	906	4/4	0.73	0.24	59,59,60,60	0
4	SO4	C	701	5/5	0.82	0.58	112,112,112,113	0
5	EDO	D	910	4/4	0.83	0.33	58,59,59,59	0
5	EDO	B	905	4/4	0.83	0.24	64,64,64,64	0
2	DQ1	B	602	31/31	0.84	0.29	76,89,98,98	2
4	SO4	D	701	5/5	0.87	0.45	98,98,98,98	0
4	SO4	A	701	5/5	0.88	0.43	100,100,100,100	0
5	EDO	A	901	4/4	0.88	0.11	50,51,52,52	0
5	EDO	D	908	4/4	0.90	0.26	49,50,50,52	0
2	DQ1	C	602	31/31	0.91	0.26	51,65,81,82	2
2	DQ1	A	602	31/31	0.91	0.20	45,51,58,59	2
3	NAP	C	702	48/48	0.91	0.17	51,59,65,66	0
4	SO4	B	701	5/5	0.91	0.56	114,115,115,115	0
5	EDO	A	907	4/4	0.91	0.15	77,77,77,77	0
2	DQ1	D	602	31/31	0.92	0.16	35,44,57,57	2
3	NAP	B	702	48/48	0.92	0.16	57,66,76,77	0
5	EDO	C	913	4/4	0.92	0.17	67,67,67,67	0
3	NAP	A	702	48/48	0.93	0.16	34,41,46,46	0
5	EDO	D	911	4/4	0.93	0.15	67,67,67,68	0
3	NAP	D	702	48/48	0.93	0.18	38,42,44,45	0
5	EDO	B	904	4/4	0.94	0.14	63,63,63,64	0
5	EDO	D	903	4/4	0.94	0.20	40,40,41,42	0
5	EDO	A	902	4/4	0.95	0.19	39,39,39,40	0
5	EDO	B	912	4/4	0.95	0.14	42,42,43,45	0
4	SO4	D	522	5/5	0.96	0.11	65,66,66,66	0
5	EDO	C	909	4/4	0.96	0.16	41,41,41,43	0
4	SO4	D	601	5/5	0.96	0.12	56,56,57,57	0
4	SO4	B	601	5/5	0.96	0.12	69,69,70,71	0
4	SO4	C	801	5/5	0.98	0.10	66,67,68,69	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.

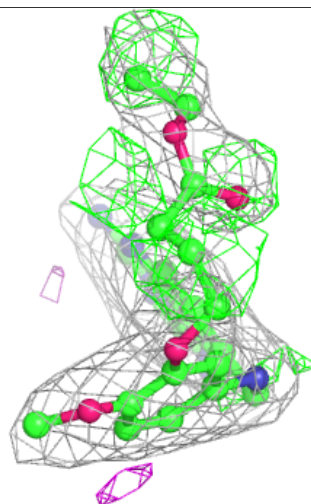
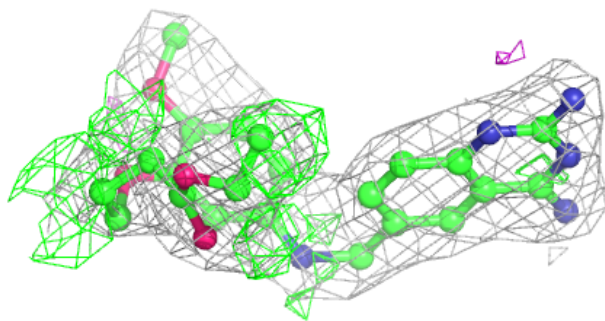
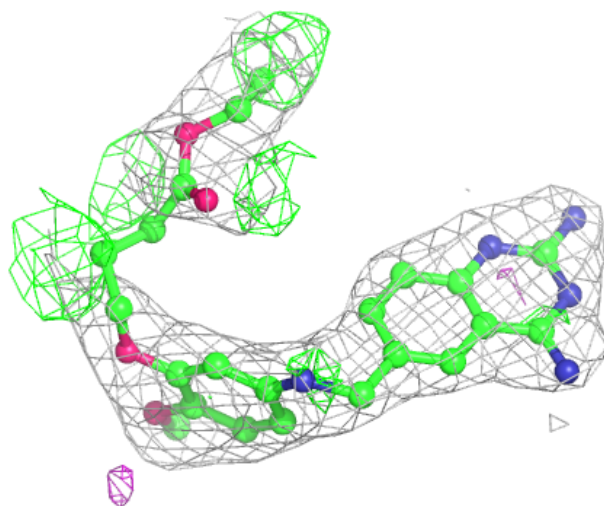
Electron density around DQ1 B 602:

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



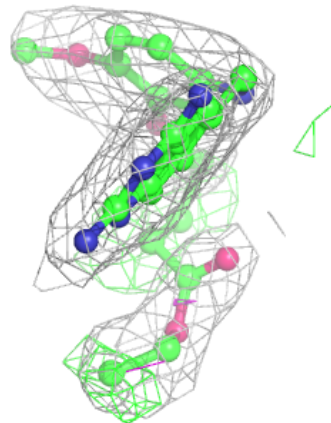
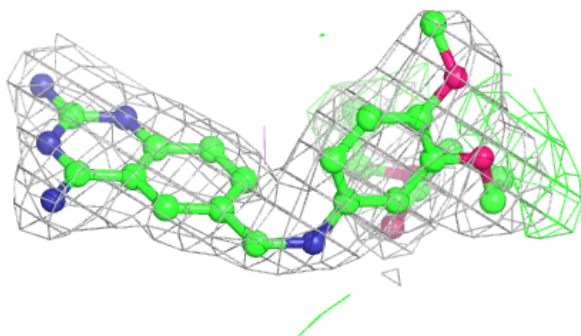
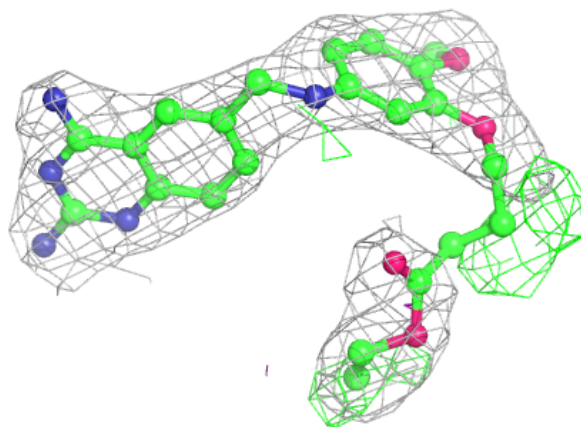
Electron density around DQ1 C 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



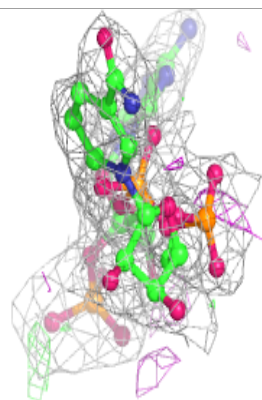
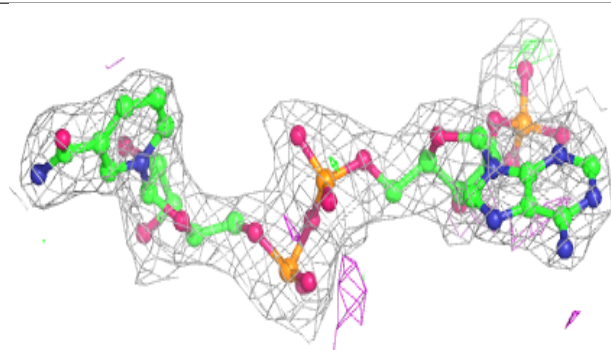
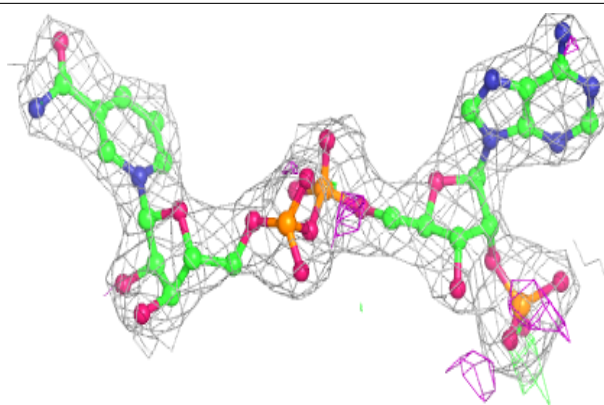
Electron density around DQ1 A 602:

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



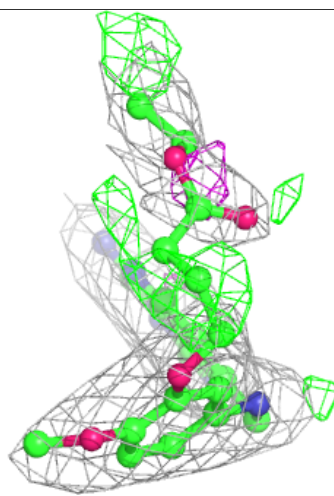
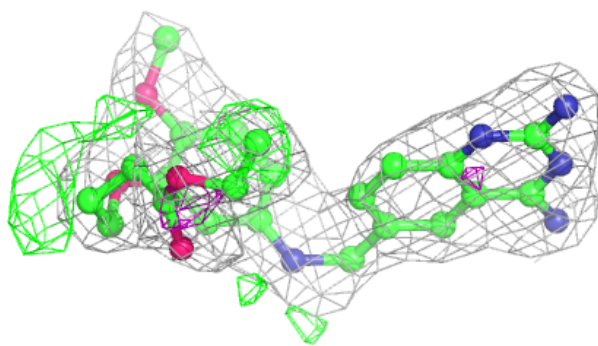
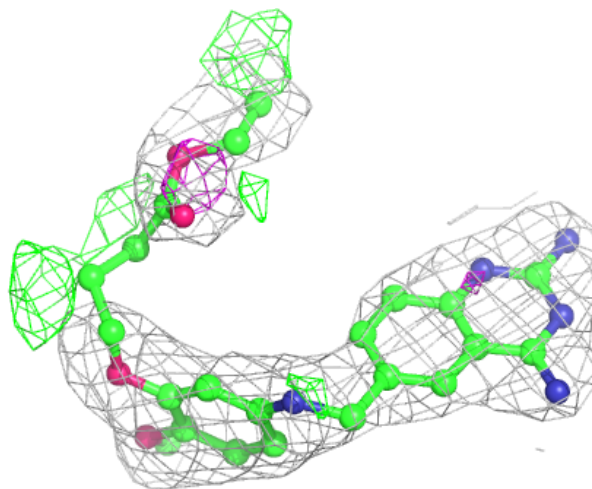
Electron density around NAP C 702:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



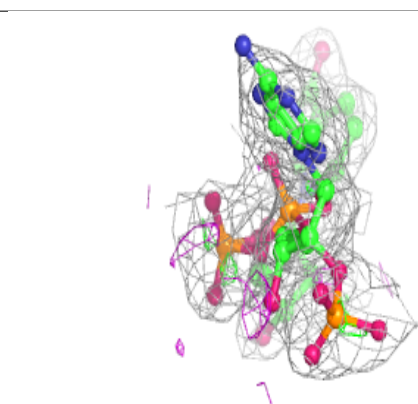
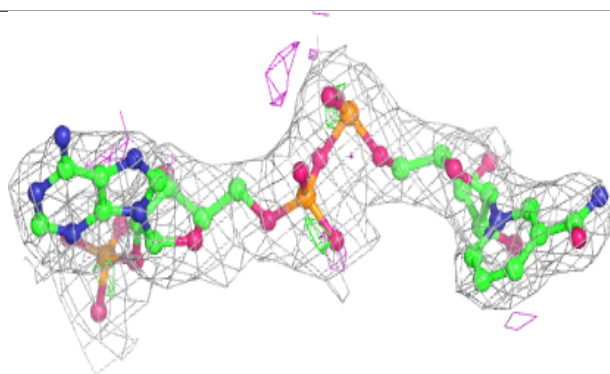
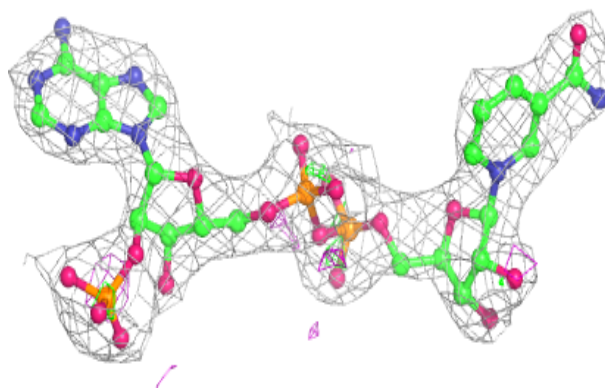
Electron density around DQ1 D 602:

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

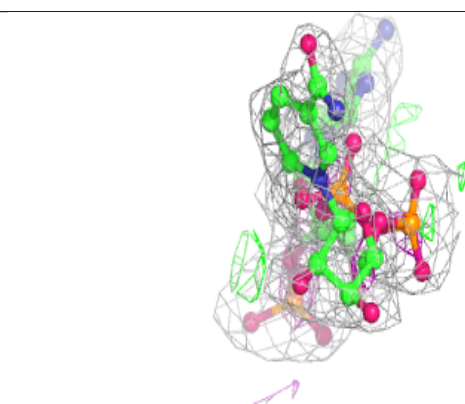
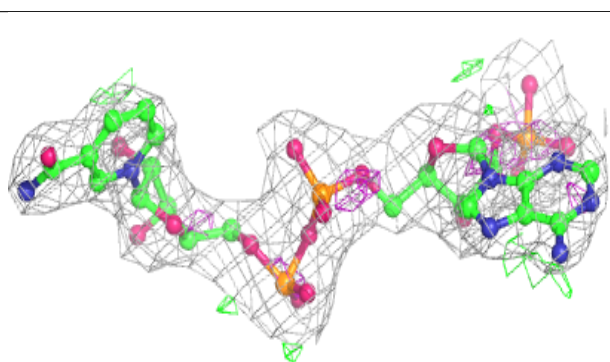
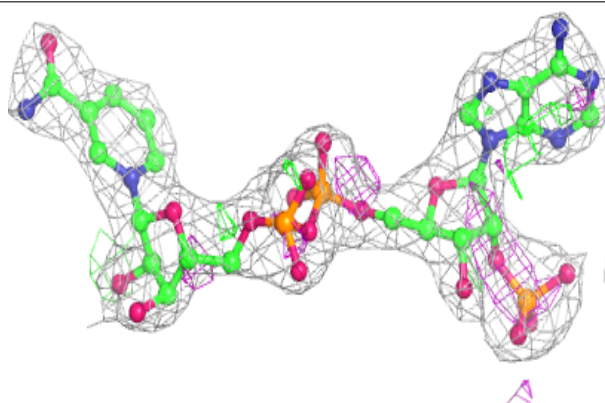


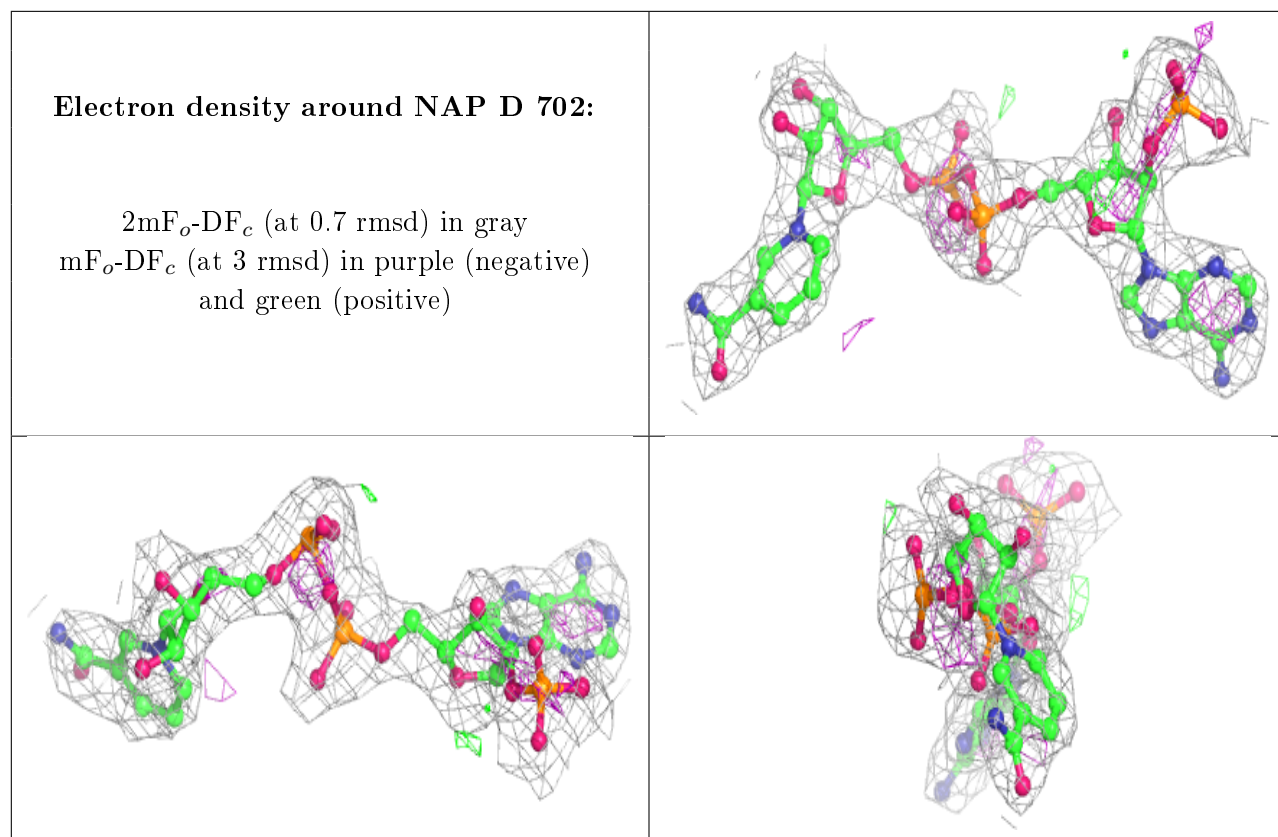
Electron density around NAP B 702:

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

**Electron density around NAP A 702:**

$2mF_o-DF_c$ (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.