



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:46 AM UTC

PDB ID : 3KJS / pdb_00003kjs
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 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

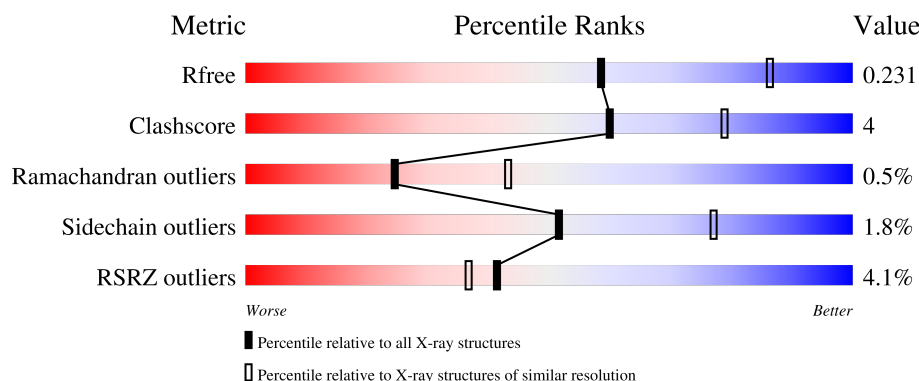
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	521	4% 86% 9% ..
1	B	521	3% 87% 8% ..
1	C	521	5% 87% 9% ..
1	D	521	3% 88% 9% .

2 Entry composition [i](#)

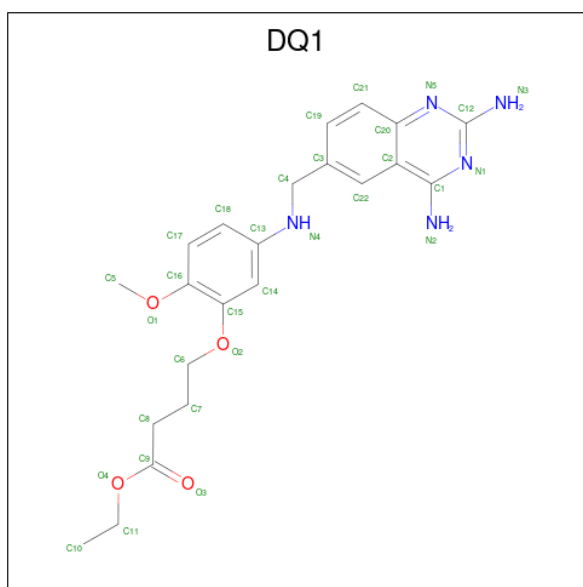
There are 6 unique types of molecules in this entry. The entry contains 17053 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: DQ1) (formula: C₂₂H₂₇N₅O₄).



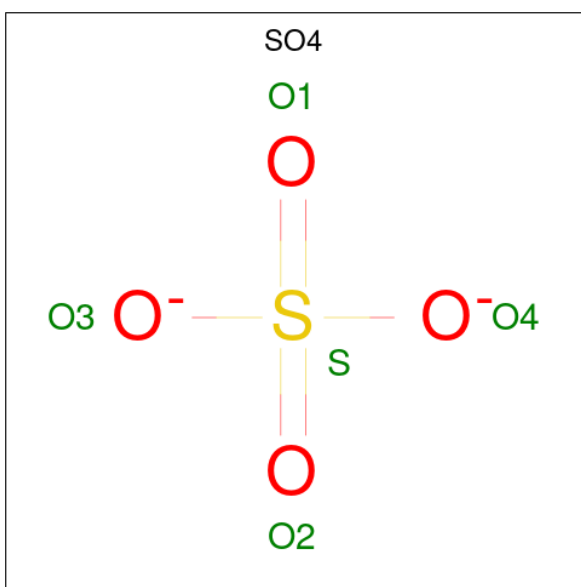
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	22	5	4		
2	B	1	Total	C	N	O	0	0
			31	22	5	4		

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

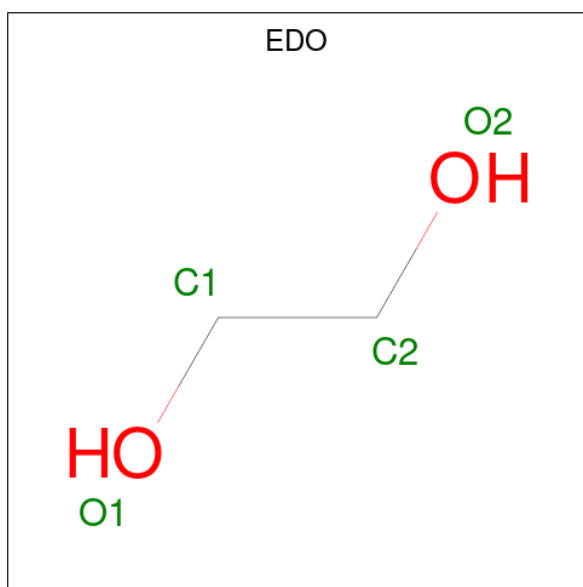
- # NAP

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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		

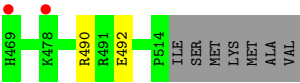
- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



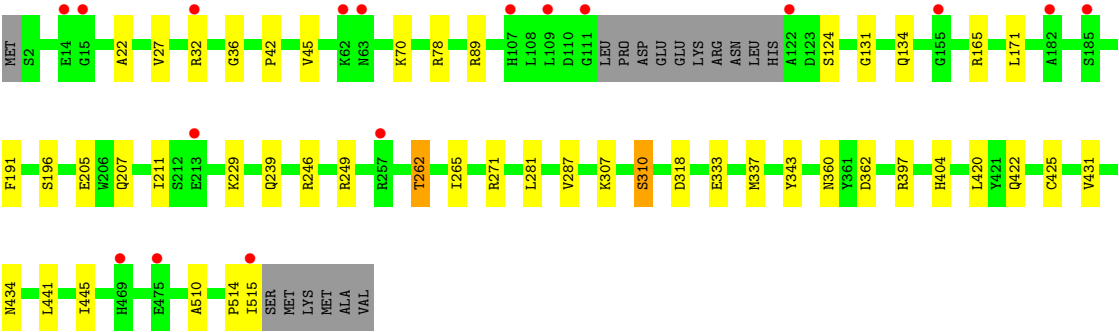
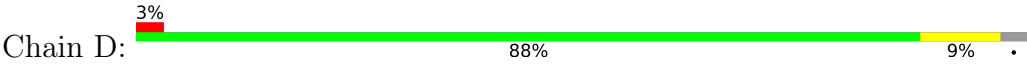
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total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



● 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 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.50) 99.3 (20.00-2.50)	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 (5.01%)	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 , 36.7	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	0.49	0/4045	0.77	4/5492 (0.1%)
1	B	0.48	0/4050	0.77	1/5496 (0.0%)
1	C	0.49	0/4110	0.76	0/5579
1	D	0.48	0/4086	0.76	0/5545
All	All	0.49	0/16291	0.77	5/22112 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	ASP	N-CA-C	6.00	119.87	112.54
1	A	155	GLY	N-CA-C	5.43	118.36	111.85
1	B	61	GLY	N-CA-C	5.38	120.25	112.82
1	A	91	LEU	CA-C-N	5.10	125.04	119.78
1	A	91	LEU	C-N-CA	5.10	125.04	119.78

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	31	0
1	B	3956	0	3906	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4011	0	3956	44	0
1	D	3991	0	3947	37	0
2	A	31	0	27	4	0
2	B	31	0	27	2	0
2	C	31	0	27	8	0
2	D	31	0	27	4	0
3	A	48	0	25	3	0
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	5	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	137	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 (137) 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:49:MET:HE1	2:C:602:DQ1:H21	1.26	1.11
1:C:45:VAL:H	2:C:602:DQ1:H10A	1.37	0.88
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	0.79
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:C:49:MET:HE1	2:C:602:DQ1:C21	2.15	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:109:LEU:C	1:B:110:ASP:OD1	2.41	0.63
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
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: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: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:C:49:MET:HE3	2:C:602:DQ1:H10B	1.91	0.53
1:A:31:GLU:OE2	1:A:181:ARG:HD2	2.07	0.53
1:A:95:LEU:HD22	1:A:148:ILE:HD11	1.90	0.53
1:A:108:LEU:HD12	1:A:125:ILE:HD12	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: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:A:76:MET:HE2	1:A:154:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H14	2:C:602:DQ1:H6	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:99:LEU:O	3:A:702:NAP:H1B	2.18	0.44
1:A:228:GLU:HG2	6:A:522:HOH:O	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLN:HE22	1:B:271:ARG:H	1.66	0.43
1:C:265:ILE:C	1:C:265:ILE:HD12	2.44	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:H6	2:D:602:DQ1:H14	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
1:A:91:LEU:HB3	1:A:94:ARG:NH2	2.33	0.43
1:A:407:ALA:HA	1:A:419:MET:O	2.19	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:D:265:ILE:C	1:D:265:ILE:HD12	2.43	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:35:ILE:O	3:A:702:NAP:H2N	2.20	0.41
1:A:295:GLU:O	1:A:298:TRP:HB3	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:B:236:GLU:CD	1:B:278:ARG:NH2	2.79	0.41
1:B:236:GLU:CD	1:B:278:ARG:HH22	2.29	0.41
1:C:70:LYS:HE2	6:C:637:HOH:O	2.21	0.41
1:D:510:ALA:CB	5:D:908:EDO:H12	2.50	0.41
1:A:14:GLU:OE1	1:C:190:PHE:CE2	2.74	0.41
1:B:59:LEU:C	1:B:61:GLY:H	2.28	0.41
1:B:155:GLY:HA2	1:B:160:TYR:CZ	2.56	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:41:ILE:HA	1:C:42:PRO:HD3	1.95	0.40
1:C:111:GLY:O	6:C:546:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LEU:H	1:C:64:VAL:CG1	2.33	0.40
1:D:318:ASP:HA	1:D:337:MET:HE1	2.03	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	496/521 (95%)	483 (97%)	12 (2%)	1 (0%)	43	63
1	B	493/521 (95%)	476 (97%)	14 (3%)	3 (1%)	21	38
1	C	504/521 (97%)	486 (96%)	13 (3%)	5 (1%)	12	24
1	D	500/521 (96%)	489 (98%)	10 (2%)	1 (0%)	43	63
All	All	1993/2084 (96%)	1934 (97%)	49 (2%)	10 (0%)	24	43

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%)	415 (99%)	6 (1%)	59	81
1	B	423/446 (95%)	412 (97%)	11 (3%)	40	68
1	C	429/446 (96%)	422 (98%)	7 (2%)	55	79
1	D	427/446 (96%)	421 (99%)	6 (1%)	59	81
All	All	1700/1784 (95%)	1670 (98%)	30 (2%)	51	77

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	239	GLN
1	A	360	ASN
1	A	403	CYS
1	A	419	MET
1	A	490	ARG
1	B	18	LEU
1	B	26	VAL
1	B	63	ASN
1	B	65	LYS
1	B	110	ASP
1	B	125	ILE
1	B	216	THR
1	B	239	GLN
1	B	329	ARG
1	B	435	ILE
1	B	490	ARG
1	C	89	ARG
1	C	94	ARG
1	C	183	SER
1	C	262	THR
1	C	303	GLU
1	C	490	ARG
1	C	492	GLU

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Mol	Chain	Res	Type
1	D	32	ARG
1	D	70	LYS
1	D	89	ARG
1	D	124	SER
1	D	262	THR
1	D	310	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	134	GLN
1	A	221	ASN
1	A	239	GLN
1	A	315	HIS
1	A	320	ASN
1	A	346	GLN
1	A	360	ASN
1	A	364	GLN
1	A	391	ASN
1	A	434	ASN
1	A	469	HIS
1	B	134	GLN
1	B	239	GLN
1	B	315	HIS
1	B	346	GLN
1	B	364	GLN
1	B	391	ASN
1	B	422	GLN
1	B	434	ASN
1	C	106	GLN
1	C	170	HIS
1	C	173	GLN
1	C	207	GLN
1	C	239	GLN
1	C	269	GLN
1	C	346	GLN
1	C	360	ASN
1	C	379	ASN
1	C	434	ASN
1	D	134	GLN
1	D	143	ASN

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Mol	Chain	Res	Type
1	D	173	GLN
1	D	207	GLN
1	D	239	GLN
1	D	277	ASN
1	D	315	HIS
1	D	360	ASN
1	D	364	GLN
1	D	391	ASN
1	D	413	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 oligosaccharides 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	$\# Z > 2$
4	SO4	B	701	-	4,4,4	0.22	0	6,6,6	0.09	0
5	EDO	B	904	-	3,3,3	0.43	0	2,2,2	0.39	0
5	EDO	D	903	-	3,3,3	0.38	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DQ1	C	602	-	33,33,33	1.30	1 (3%)	43,44,44	1.44	5 (11%)
4	SO4	C	701	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	C	801	-	4,4,4	0.23	0	6,6,6	0.15	0
2	DQ1	A	602	-	33,33,33	1.25	1 (3%)	43,44,44	1.53	6 (13%)
5	EDO	B	905	-	3,3,3	0.45	0	2,2,2	0.43	0
5	EDO	C	909	-	3,3,3	0.40	0	2,2,2	0.35	0
5	EDO	A	906	-	3,3,3	0.46	0	2,2,2	0.24	0
2	DQ1	D	602	-	33,33,33	1.34	1 (3%)	43,44,44	1.59	7 (16%)
5	EDO	B	912	-	3,3,3	0.41	0	2,2,2	0.46	0
5	EDO	A	902	-	3,3,3	0.38	0	2,2,2	0.52	0
5	EDO	C	913	-	3,3,3	0.43	0	2,2,2	0.36	0
5	EDO	D	910	-	3,3,3	0.46	0	2,2,2	0.28	0
5	EDO	D	911	-	3,3,3	0.41	0	2,2,2	0.42	0
3	NAP	A	702	-	50,52,52	1.80	10 (20%)	71,80,80	2.10	17 (23%)
5	EDO	A	907	-	3,3,3	0.42	0	2,2,2	0.42	0
5	EDO	A	901	-	3,3,3	0.46	0	2,2,2	0.39	0
4	SO4	D	601	-	4,4,4	0.24	0	6,6,6	0.21	0
3	NAP	D	702	-	50,52,52	2.04	10 (20%)	71,80,80	2.09	17 (23%)
4	SO4	A	701	-	4,4,4	0.24	0	6,6,6	0.12	0
3	NAP	B	702	-	50,52,52	1.92	10 (20%)	71,80,80	2.17	18 (25%)
5	EDO	D	908	-	3,3,3	0.39	0	2,2,2	0.51	0
4	SO4	D	522	-	4,4,4	0.25	0	6,6,6	0.22	0
3	NAP	C	702	-	50,52,52	1.96	10 (20%)	71,80,80	2.05	18 (25%)
4	SO4	B	601	-	4,4,4	0.21	0	6,6,6	0.24	0
2	DQ1	B	602	-	33,33,33	1.27	1 (3%)	43,44,44	1.56	7 (16%)
4	SO4	D	701	-	4,4,4	0.26	0	6,6,6	0.11	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	B	904	-	-	1/1/1/1	-
5	EDO	D	903	-	-	1/1/1/1	-
2	DQ1	C	602	-	-	5/17/17/17	0/3/3/3
2	DQ1	A	602	-	-	8/17/17/17	0/3/3/3
5	EDO	B	905	-	-	1/1/1/1	-
5	EDO	C	909	-	-	0/1/1/1	-
5	EDO	A	906	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DQ1	D	602	-	-	6/17/17/17	0/3/3/3
5	EDO	B	912	-	-	0/1/1/1	-
5	EDO	A	902	-	-	1/1/1/1	-
5	EDO	C	913	-	-	0/1/1/1	-
5	EDO	D	910	-	-	1/1/1/1	-
5	EDO	D	911	-	-	0/1/1/1	-
3	NAP	A	702	-	-	8/35/67/67	0/5/5/5
5	EDO	A	907	-	-	1/1/1/1	-
5	EDO	A	901	-	-	1/1/1/1	-
3	NAP	D	702	-	-	5/35/67/67	0/5/5/5
3	NAP	B	702	-	-	7/35/67/67	0/5/5/5
5	EDO	D	908	-	-	1/1/1/1	-
3	NAP	C	702	-	-	7/35/67/67	0/5/5/5
2	DQ1	B	602	-	-	7/17/17/17	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	NAP	PA-O3	7.48	1.67	1.59
3	D	702	NAP	PN-O3	7.27	1.67	1.59
3	C	702	NAP	PA-O3	7.26	1.67	1.59
3	C	702	NAP	PN-O3	6.68	1.66	1.59
3	B	702	NAP	PN-O3	6.40	1.66	1.59
3	A	702	NAP	PA-O3	6.11	1.66	1.59
3	B	702	NAP	C2N-N1N	6.08	1.41	1.35
3	B	702	NAP	PA-O3	5.98	1.66	1.59
2	D	602	DQ1	C1-C2	-5.81	1.39	1.45
2	C	602	DQ1	C1-C2	-5.50	1.40	1.45
3	A	702	NAP	C2N-N1N	5.38	1.40	1.35
3	D	702	NAP	C2N-N1N	5.33	1.40	1.35
2	B	602	DQ1	C1-C2	-5.27	1.40	1.45
2	A	602	DQ1	C1-C2	-5.08	1.40	1.45
3	A	702	NAP	PN-O3	4.95	1.64	1.59
3	C	702	NAP	C2N-N1N	4.91	1.40	1.35
3	D	702	NAP	O4D-C1D	3.11	1.45	1.40
3	C	702	NAP	O4D-C1D	3.06	1.44	1.40
3	A	702	NAP	C5A-N7A	-3.02	1.33	1.39
3	B	702	NAP	C5A-N7A	-3.00	1.33	1.39
3	B	702	NAP	C6N-N1N	2.94	1.42	1.35
3	C	702	NAP	C5A-N7A	-2.92	1.33	1.39
3	A	702	NAP	O4D-C1D	2.90	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	NAP	C5A-N7A	-2.86	1.33	1.39
3	B	702	NAP	O4D-C1D	2.80	1.44	1.40
3	D	702	NAP	C6N-N1N	2.60	1.41	1.35
3	C	702	NAP	C6N-N1N	2.56	1.41	1.35
3	D	702	NAP	O4B-C1B	2.52	1.47	1.42
3	A	702	NAP	C3N-C7N	2.46	1.54	1.50
3	A	702	NAP	C6N-N1N	2.46	1.40	1.35
3	C	702	NAP	O4B-C1B	2.33	1.47	1.42
3	A	702	NAP	P2B-O3X	2.28	1.63	1.54
3	B	702	NAP	C3N-C7N	2.26	1.54	1.50
3	C	702	NAP	P2B-O2B	2.26	1.63	1.59
3	C	702	NAP	P2B-O2X	2.21	1.63	1.54
3	B	702	NAP	O4B-C1B	2.20	1.47	1.42
3	C	702	NAP	P2B-O3X	2.20	1.63	1.54
3	D	702	NAP	P2B-O2X	2.12	1.62	1.54
3	D	702	NAP	C3N-C7N	2.12	1.53	1.50
3	D	702	NAP	C8A-N9A	-2.08	1.34	1.37
3	B	702	NAP	P2B-O2B	2.07	1.63	1.59
3	A	702	NAP	C8A-N9A	-2.04	1.34	1.37
3	A	702	NAP	O4B-C1B	2.04	1.46	1.42
3	B	702	NAP	C8A-N9A	-2.02	1.34	1.37

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NAP	O3-PN-O1N	-8.66	84.65	110.70
3	A	702	NAP	O3-PN-O1N	-8.05	86.50	110.70
3	C	702	NAP	O3-PN-O1N	-8.04	86.52	110.70
3	D	702	NAP	O3-PN-O1N	-7.34	88.62	110.70
3	D	702	NAP	O2N-PN-O3	-6.56	89.53	107.27
3	A	702	NAP	O2N-PN-O3	-6.35	90.10	107.27
3	B	702	NAP	O2N-PN-O3	-6.05	90.93	107.27
3	C	702	NAP	O2N-PN-O3	-5.63	92.06	107.27
3	C	702	NAP	C5A-C4A-N3A	-5.38	119.31	126.72
2	B	602	DQ1	N5-C12-N1	-5.36	120.40	127.21
2	A	602	DQ1	N5-C12-N1	-5.33	120.44	127.21
3	B	702	NAP	C5A-C4A-N3A	-5.32	119.39	126.72
3	D	702	NAP	C5A-C4A-N3A	-5.29	119.43	126.72
2	C	602	DQ1	N5-C12-N1	-5.18	120.62	127.21
3	A	702	NAP	C5A-C4A-N3A	-5.12	119.67	126.72
2	D	602	DQ1	N5-C12-N1	-5.09	120.74	127.21
3	B	702	NAP	C2B-C1B-N9A	-4.91	105.67	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NAP	N3A-C2A-N1A	-4.90	121.17	128.58
3	B	702	NAP	N3A-C2A-N1A	-4.75	121.40	128.58
3	D	702	NAP	N3A-C2A-N1A	-4.72	121.44	128.58
3	C	702	NAP	N3A-C2A-N1A	-4.70	121.47	128.58
3	D	702	NAP	C4D-O4D-C1D	-4.70	105.62	109.92
3	C	702	NAP	C4D-O4D-C1D	-4.16	106.12	109.92
3	B	702	NAP	C4D-O4D-C1D	-4.12	106.16	109.92
3	A	702	NAP	C4D-O4D-C1D	-3.87	106.38	109.92
2	D	602	DQ1	C22-C2-C1	-3.79	121.32	124.75
3	C	702	NAP	N3A-C4A-N9A	3.69	133.44	127.17
3	A	702	NAP	C2B-C1B-N9A	-3.68	107.70	113.75
3	B	702	NAP	N3A-C4A-N9A	3.67	133.41	127.17
3	D	702	NAP	C2A-N3A-C4A	3.66	120.78	111.83
3	B	702	NAP	C2A-N3A-C4A	3.66	120.77	111.83
3	D	702	NAP	N3A-C4A-N9A	3.65	133.38	127.17
3	A	702	NAP	N3A-C4A-N9A	3.65	133.37	127.17
3	C	702	NAP	C2A-N3A-C4A	3.63	120.69	111.83
3	A	702	NAP	C2A-N3A-C4A	3.62	120.67	111.83
3	D	702	NAP	C2B-C1B-N9A	-3.57	107.88	113.75
3	A	702	NAP	N9A-C8A-N7A	-3.52	108.94	113.94
3	D	702	NAP	O4B-C1B-N9A	3.46	114.74	108.09
3	B	702	NAP	N9A-C8A-N7A	-3.36	109.17	113.94
3	B	702	NAP	O4B-C1B-N9A	3.32	114.46	108.09
3	C	702	NAP	N9A-C8A-N7A	-3.25	109.33	113.94
3	C	702	NAP	C2B-C1B-N9A	-3.24	108.42	113.75
3	D	702	NAP	N9A-C8A-N7A	-3.23	109.36	113.94
3	A	702	NAP	O4B-C1B-N9A	3.20	114.23	108.09
2	B	602	DQ1	O1-C16-C15	3.07	119.56	115.40
3	A	702	NAP	C5A-N7A-C8A	3.01	108.18	103.45
3	C	702	NAP	O4B-C1B-N9A	2.96	113.78	108.09
3	C	702	NAP	C5A-N7A-C8A	2.95	108.09	103.45
3	D	702	NAP	C5A-N7A-C8A	2.95	108.08	103.45
2	C	602	DQ1	C22-C2-C1	-2.95	122.09	124.75
2	B	602	DQ1	C22-C2-C1	-2.93	122.10	124.75
3	B	702	NAP	C5A-N7A-C8A	2.92	108.03	103.45
2	A	602	DQ1	C2-C20-N5	-2.91	119.71	122.80
2	B	602	DQ1	C2-C20-N5	-2.91	119.72	122.80
2	A	602	DQ1	C22-C2-C1	-2.91	122.12	124.75
3	D	702	NAP	C4A-C5A-N7A	-2.89	107.27	110.58
3	C	702	NAP	C4A-C5A-N7A	-2.82	107.36	110.58
2	D	602	DQ1	C2-C1-N1	-2.80	118.96	121.97
2	D	602	DQ1	C2-C20-N5	-2.75	119.89	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NAP	C4A-C5A-N7A	-2.71	107.48	110.58
3	D	702	NAP	O2N-PN-O5D	2.68	119.72	107.57
3	A	702	NAP	C4A-C5A-N7A	-2.67	107.53	110.58
2	C	602	DQ1	C2-C1-N1	-2.61	119.17	121.97
3	B	702	NAP	C5D-C4D-C3D	-2.59	105.91	115.21
2	A	602	DQ1	C2-C1-N1	-2.58	119.20	121.97
2	D	602	DQ1	O1-C16-C15	2.55	118.87	115.40
3	A	702	NAP	O2N-PN-O5D	2.53	119.06	107.57
3	A	702	NAP	C4A-N9A-C8A	2.53	108.39	105.74
3	D	702	NAP	C6N-N1N-C2N	-2.52	119.73	121.88
3	B	702	NAP	C6N-N1N-C2N	-2.49	119.76	121.88
2	C	602	DQ1	C2-C20-N5	-2.47	120.18	122.80
2	B	602	DQ1	O4-C9-C8	2.47	119.36	111.83
2	A	602	DQ1	O4-C9-C8	2.42	119.22	111.83
3	C	702	NAP	O2N-PN-O5D	2.41	118.48	107.57
3	B	702	NAP	O5D-PN-O1N	2.40	118.44	108.94
2	A	602	DQ1	O1-C16-C15	2.33	118.57	115.40
3	A	702	NAP	C6N-N1N-C2N	-2.33	119.90	121.88
2	D	602	DQ1	O4-C9-C8	2.32	118.90	111.83
3	C	702	NAP	O5D-PN-O1N	2.30	118.05	108.94
3	B	702	NAP	C4A-N9A-C8A	2.27	108.12	105.74
3	C	702	NAP	C5D-C4D-C3D	-2.26	107.07	115.21
3	D	702	NAP	C4A-N9A-C8A	2.24	108.09	105.74
3	B	702	NAP	O2N-PN-O1N	2.24	122.87	112.44
2	B	602	DQ1	C2-C1-N1	-2.20	119.61	121.97
3	B	702	NAP	O2N-PN-O5D	2.19	117.49	107.57
2	C	602	DQ1	O4-C9-C8	2.19	118.51	111.83
3	C	702	NAP	C6N-N1N-C2N	-2.18	120.02	121.88
3	C	702	NAP	C4A-N9A-C8A	2.13	107.97	105.74
2	D	602	DQ1	C11-O4-C9	-2.13	110.62	116.67
2	B	602	DQ1	O1-C16-C17	-2.11	120.75	124.30
3	C	702	NAP	O2N-PN-O1N	2.10	122.20	112.44
3	A	702	NAP	O5D-PN-O1N	2.09	117.21	108.94
3	D	702	NAP	O5D-PN-O1N	2.07	117.13	108.94
3	A	702	NAP	O2N-PN-O1N	2.03	121.90	112.44
3	D	702	NAP	O2N-PN-O1N	2.01	121.78	112.44

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	602	DQ1	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	D	602	DQ1	C6-C7-C8-C9
3	A	702	NAP	C5D-O5D-PN-O1N
3	A	702	NAP	O4D-C1D-N1N-C6N
3	B	702	NAP	C5D-O5D-PN-O1N
3	B	702	NAP	O4D-C1D-N1N-C6N
3	C	702	NAP	C5D-O5D-PN-O1N
3	C	702	NAP	O4D-C1D-N1N-C6N
3	D	702	NAP	C5D-O5D-PN-O1N
3	D	702	NAP	O4D-C1D-N1N-C6N
2	B	602	DQ1	C15-C16-O1-C5
2	A	602	DQ1	C8-C9-O4-C11
2	B	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
3	C	702	NAP	C3D-C4D-C5D-O5D
3	D	702	NAP	C3D-C4D-C5D-O5D
2	D	602	DQ1	O3-C9-O4-C11
5	A	906	EDO	O1-C1-C2-O2
5	B	904	EDO	O1-C1-C2-O2
3	B	702	NAP	C3D-C4D-C5D-O5D
2	D	602	DQ1	C7-C6-O2-C15
2	C	602	DQ1	C7-C6-O2-C15
2	A	602	DQ1	C7-C6-O2-C15
2	B	602	DQ1	C7-C6-O2-C15
2	A	602	DQ1	C17-C16-O1-C5
2	C	602	DQ1	C8-C9-O4-C11
5	D	910	EDO	O1-C1-C2-O2
2	D	602	DQ1	C15-C16-O1-C5
2	A	602	DQ1	C6-C7-C8-C9
3	D	702	NAP	O4D-C4D-C5D-O5D
2	C	602	DQ1	O3-C9-O4-C11
5	A	901	EDO	O1-C1-C2-O2
5	D	908	EDO	O1-C1-C2-O2
2	D	602	DQ1	C17-C16-O1-C5
5	A	907	EDO	O1-C1-C2-O2
3	C	702	NAP	O4D-C4D-C5D-O5D
3	A	702	NAP	C5B-O5B-PA-O1A
3	B	702	NAP	C5D-O5D-PN-O3
3	C	702	NAP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	C	702	NAP	C5D-O5D-PN-O3
3	A	702	NAP	C3D-C4D-C5D-O5D
3	A	702	NAP	C2D-C1D-N1N-C2N
3	A	702	NAP	C2D-C1D-N1N-C6N
5	A	902	EDO	O1-C1-C2-O2
3	B	702	NAP	C4D-C5D-O5D-PN
3	A	702	NAP	O4D-C1D-N1N-C2N
3	B	702	NAP	O4D-C4D-C5D-O5D
3	B	702	NAP	O4D-C1D-N1N-C2N
3	C	702	NAP	O4D-C1D-N1N-C2N
3	D	702	NAP	O4D-C1D-N1N-C2N
2	A	602	DQ1	C10-C11-O4-C9
5	B	905	EDO	O1-C1-C2-O2
2	B	602	DQ1	C10-C11-O4-C9
2	C	602	DQ1	C10-C11-O4-C9
2	B	602	DQ1	C6-C7-C8-C9
5	D	903	EDO	O1-C1-C2-O2
2	A	602	DQ1	C7-C8-C9-O4
3	A	702	NAP	O4D-C4D-C5D-O5D

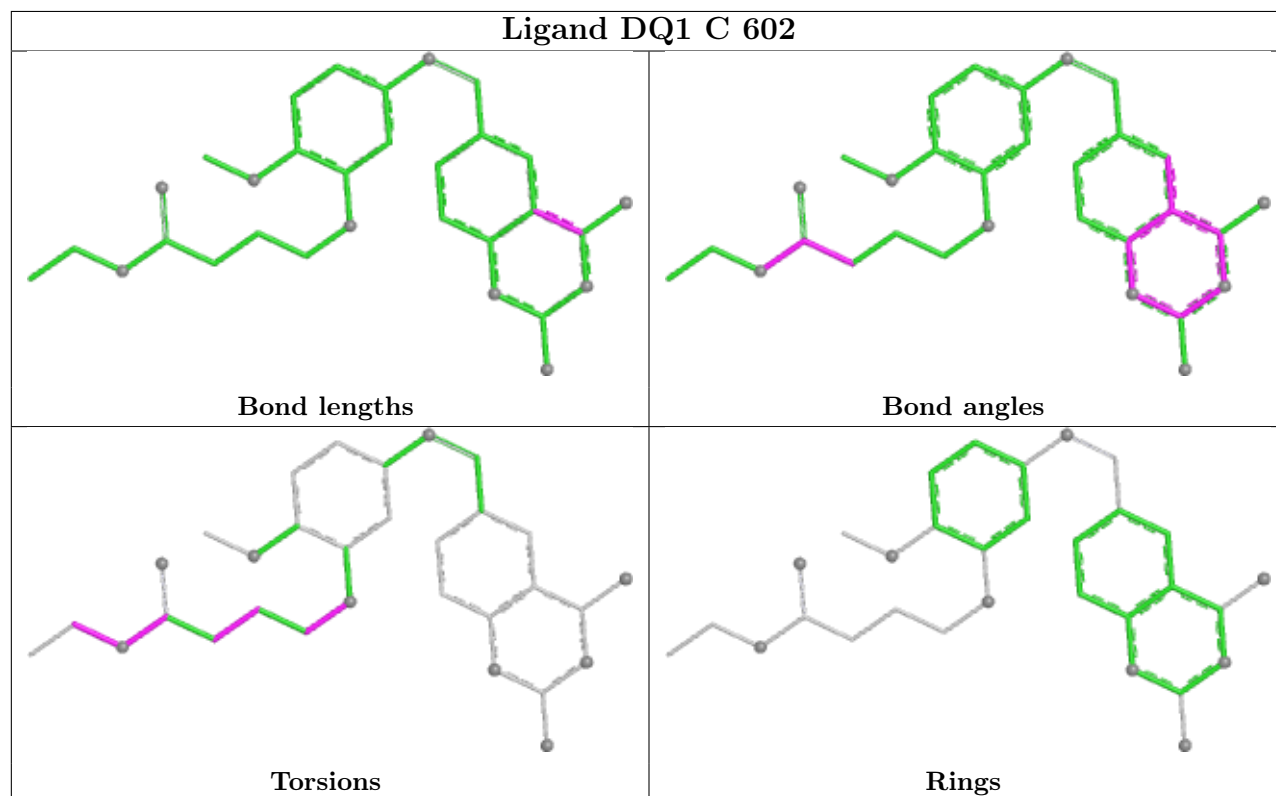
There are no ring outliers.

10 monomers are involved in 29 short contacts:

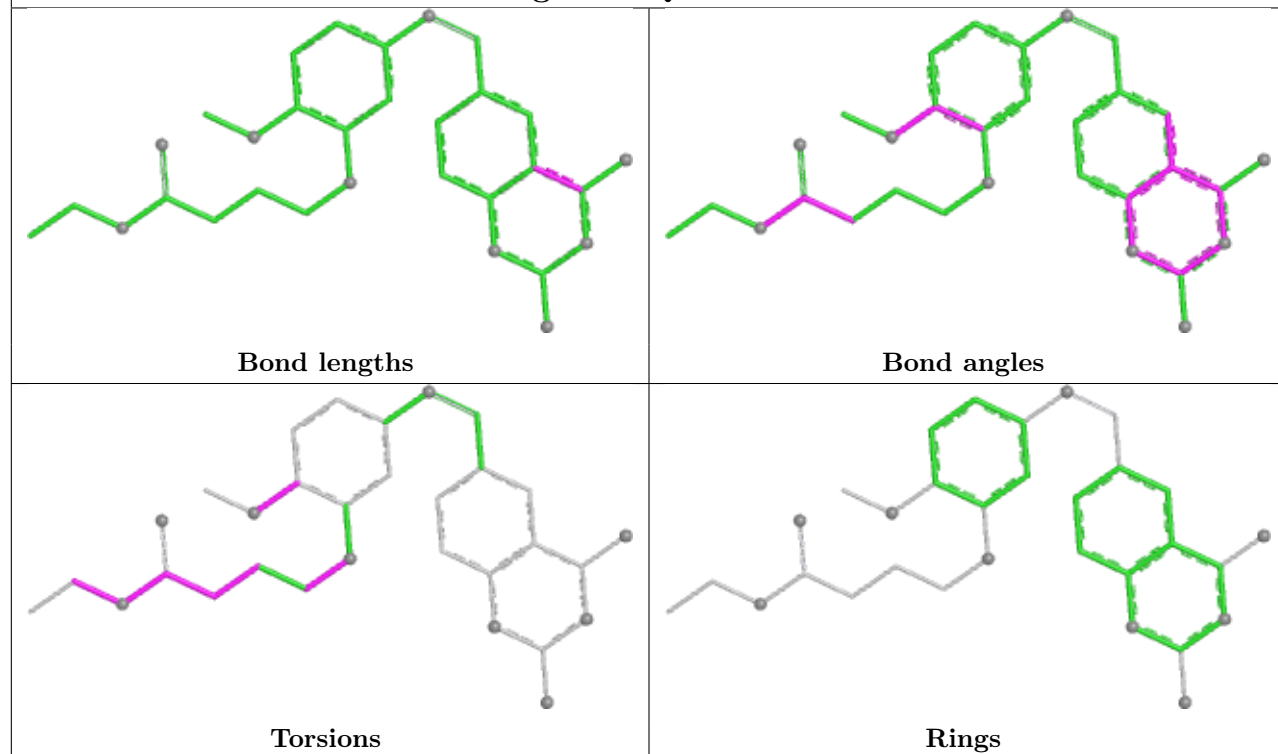
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	903	EDO	2	0
2	C	602	DQ1	8	0
2	A	602	DQ1	4	0
2	D	602	DQ1	4	0
3	A	702	NAP	3	0
3	D	702	NAP	1	0
3	B	702	NAP	1	0
5	D	908	EDO	3	0
3	C	702	NAP	1	0
2	B	602	DQ1	2	0

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

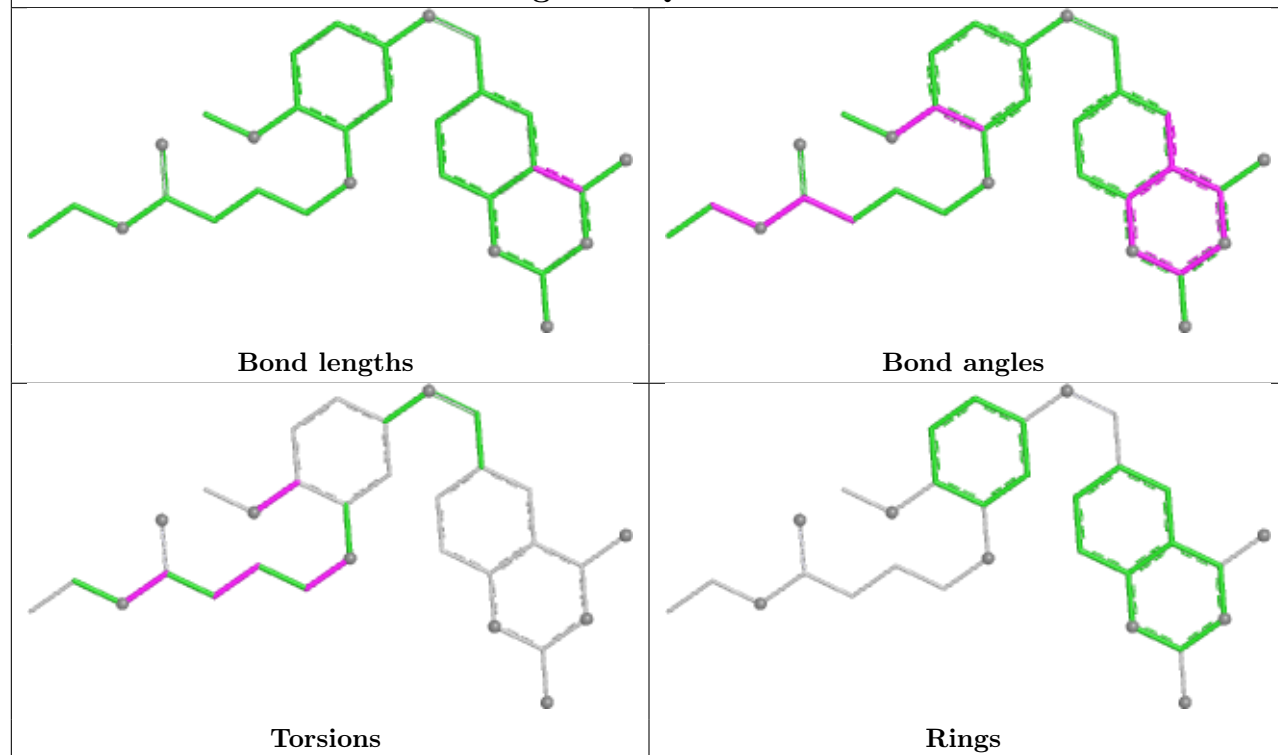
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

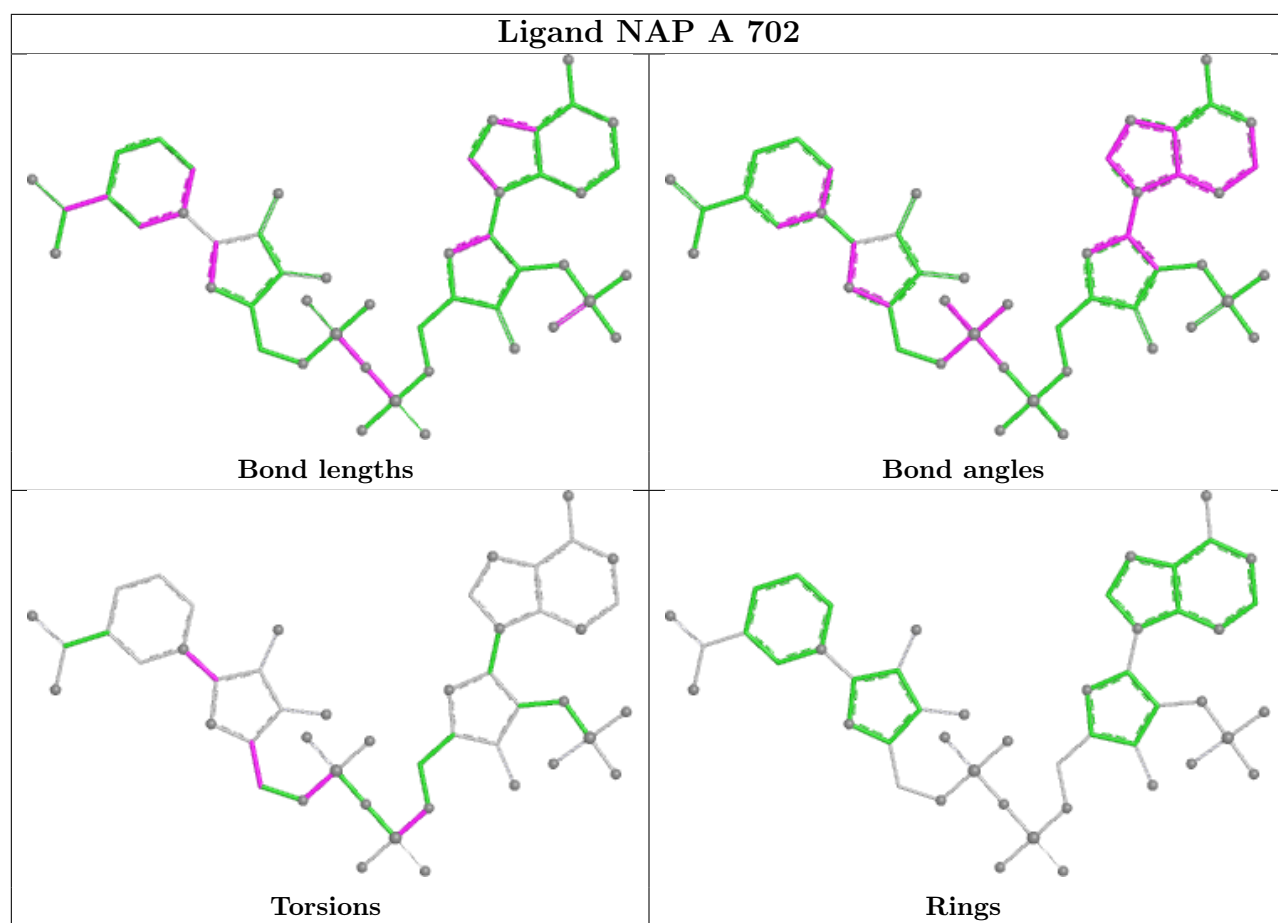


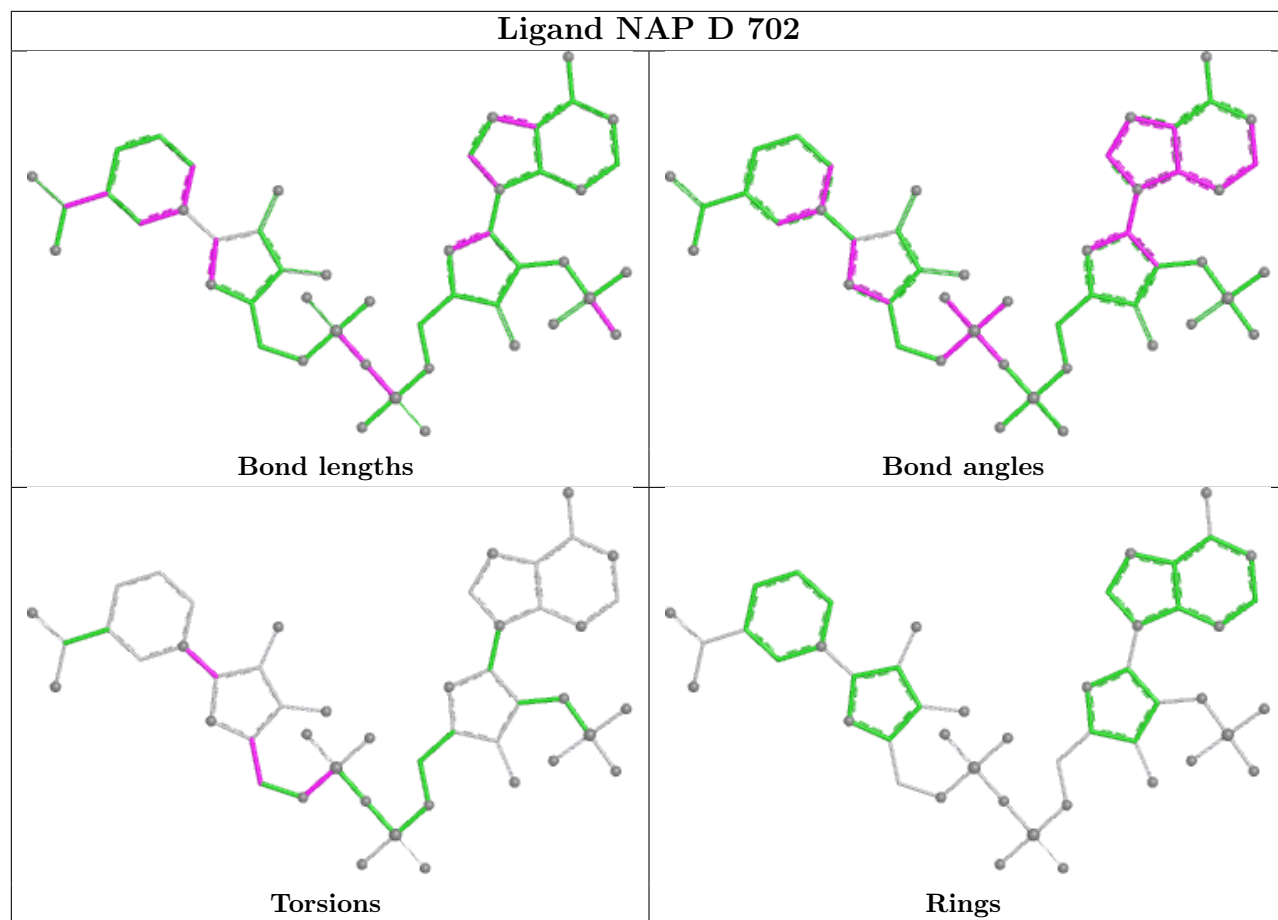
Ligand DQ1 A 602

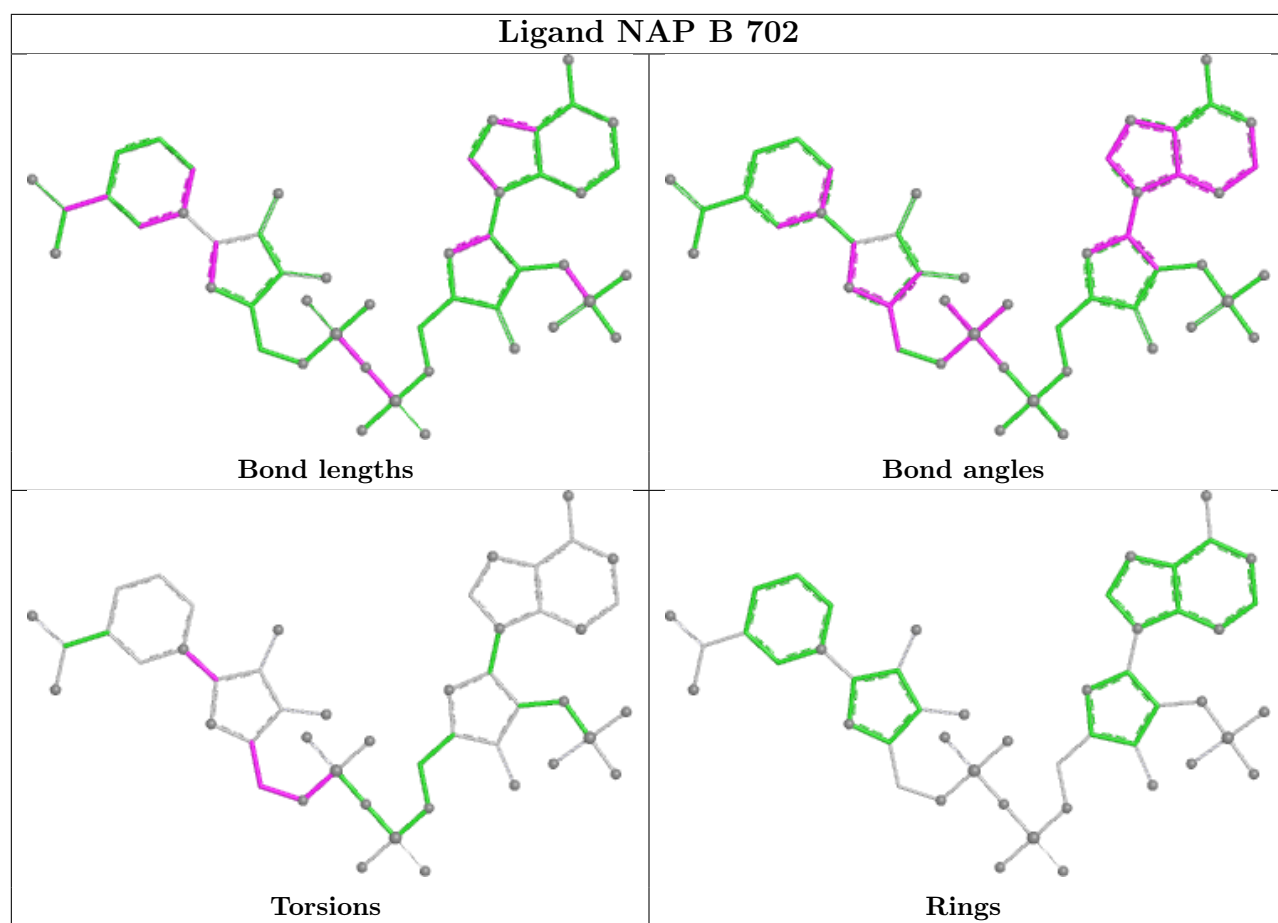


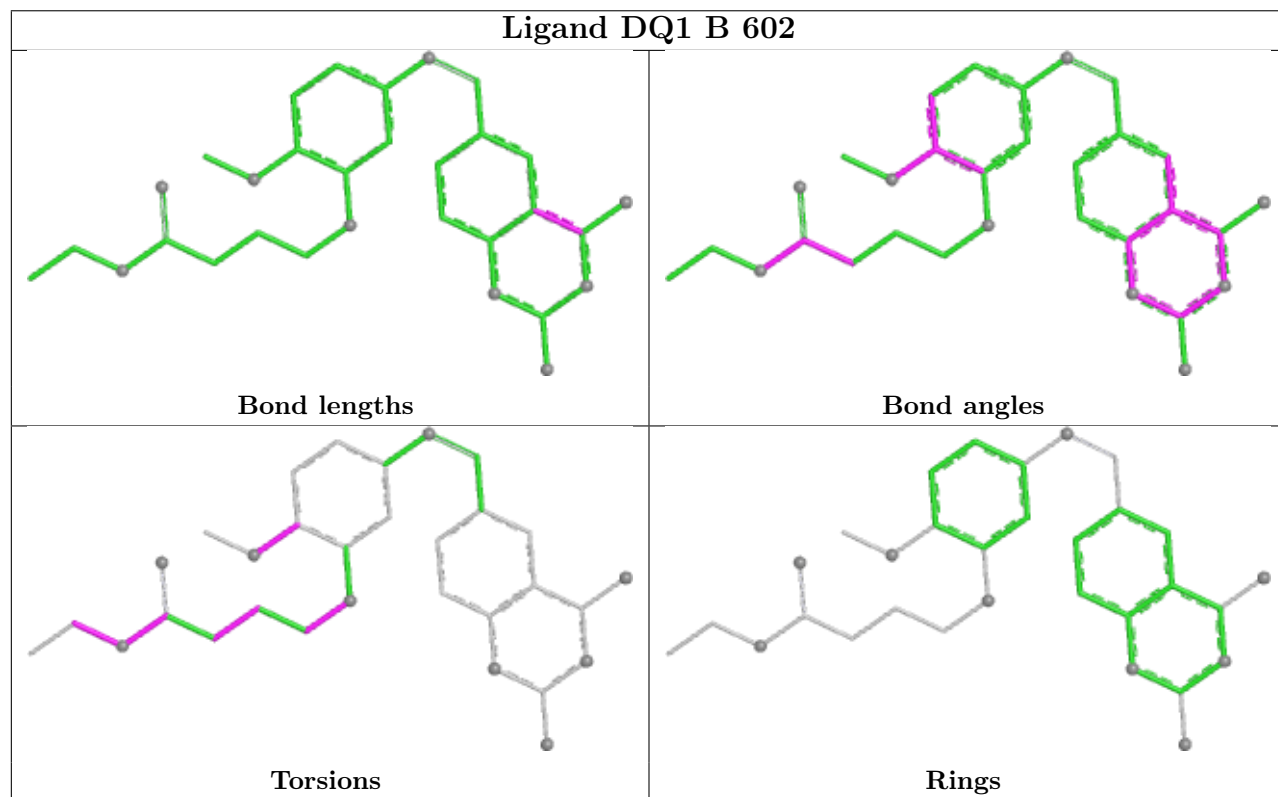
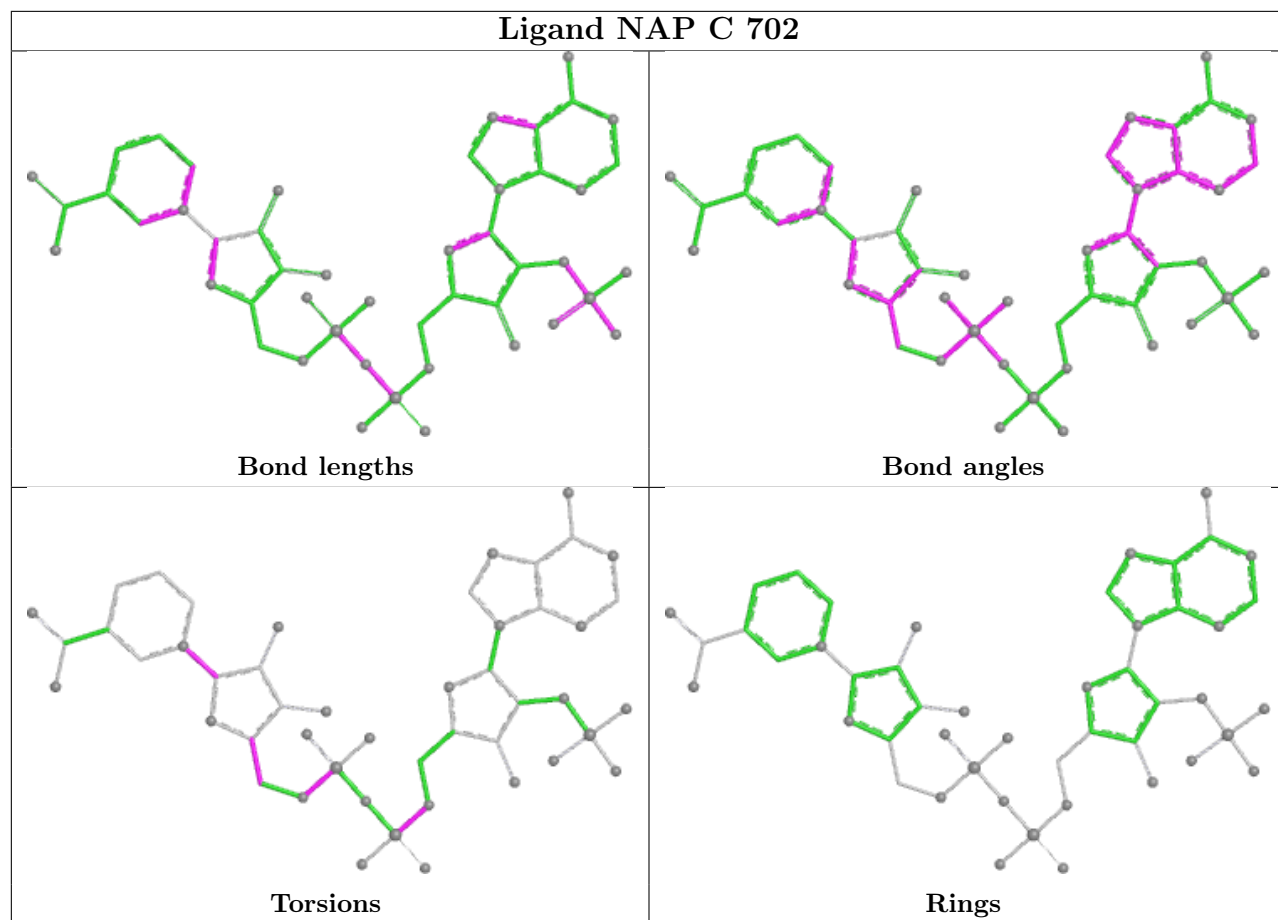
Ligand DQ1 D 602











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	500/521 (95%)	0.10	21 (4%)	40 36	1, 41, 68, 92	3 (0%)
1	B	499/521 (95%)	0.06	17 (3%)	48 43	1, 41, 71, 96	4 (0%)
1	C	507/521 (97%)	-0.05	27 (5%)	32 28	19, 37, 61, 103	5 (0%)
1	D	504/521 (96%)	-0.14	17 (3%)	48 43	25, 38, 59, 83	1 (0%)
All	All	2010/2084 (96%)	-0.01	82 (4%)	41 37	1, 39, 66, 103	13 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	SER	64.0
1	B	13	ALA	35.4
1	C	62	LYS	9.7
1	C	63	ASN	8.8
1	B	3	LEU	7.2
1	C	3	LEU	6.8
1	A	14	GLU	6.0
1	D	155	GLY	6.0
1	B	32	ARG	5.9
1	A	3	LEU	5.6
1	D	122	ALA	5.0
1	A	32	ARG	4.9
1	A	108	LEU	4.8
1	C	32	ARG	4.5
1	B	110	ASP	4.5
1	C	64	VAL	4.4
1	C	113	PRO	4.3
1	D	32	ARG	4.2
1	C	111	GLY	4.0
1	A	123	ASP	4.0
1	C	112	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	452	ARG	3.9
1	B	184	GLU	3.8
1	C	122	ALA	3.6
1	D	62	LYS	3.6
1	B	64	VAL	3.5
1	C	183	SER	3.5
1	A	184	GLU	3.4
1	A	107	HIS	3.4
1	A	12	VAL	3.4
1	C	121	HIS	3.4
1	A	13	ALA	3.3
1	A	185	SER	3.3
1	C	114	ASP	3.3
1	D	515	ILE	3.2
1	B	14	GLU	3.2
1	B	63	ASN	3.1
1	D	111	GLY	3.1
1	A	63	ASN	3.1
1	C	109	LEU	3.0
1	C	14	GLU	3.0
1	B	123	ASP	3.0
1	C	40	SER	3.0
1	C	123	ASP	2.9
1	A	39	ARG	2.9
1	D	257	ARG	2.9
1	D	185	SER	2.9
1	C	469	HIS	2.8
1	C	184	GLU	2.8
1	B	12	VAL	2.7
1	C	257	ARG	2.7
1	D	63	ASN	2.7
1	A	64	VAL	2.6
1	D	213	GLU	2.6
1	C	15	GLY	2.6
1	B	17	ARG	2.5
1	A	38	GLY	2.5
1	D	107	HIS	2.4
1	C	44	ASN	2.4
1	D	109	LEU	2.4
1	C	39	ARG	2.4
1	A	17	ARG	2.3
1	A	277	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	220	GLY	2.3
1	B	61	GLY	2.3
1	D	469	HIS	2.3
1	C	182	ALA	2.2
1	A	466	TYR	2.2
1	B	62	LYS	2.2
1	C	105	THR	2.2
1	D	475	GLU	2.2
1	D	182	ALA	2.1
1	C	16	THR	2.1
1	C	358	ASP	2.1
1	C	478	LYS	2.1
1	B	16	THR	2.1
1	D	14	GLU	2.0
1	D	15	GLY	2.0
1	A	515	ILE	2.0
1	A	16	THR	2.0
1	A	102	THR	2.0
1	B	216	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	701	5/5	0.61	0.21	114,115,115,115	0
4	SO4	A	701	5/5	0.65	0.17	100,100,100,100	0
4	SO4	C	701	5/5	0.70	0.23	112,112,112,113	0
4	SO4	D	701	5/5	0.74	0.20	98,98,98,98	0

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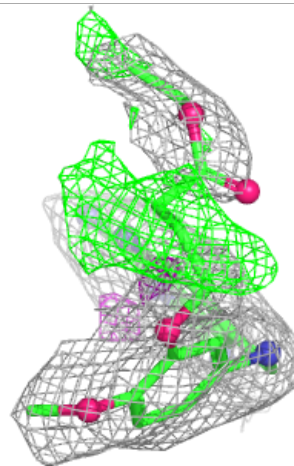
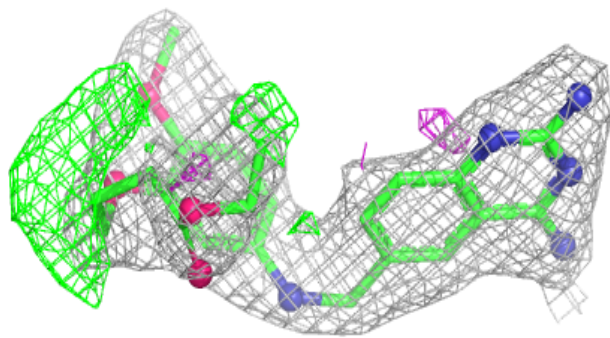
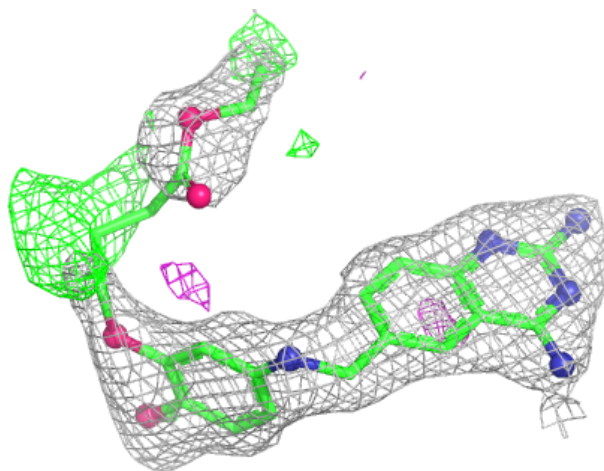
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	905	4/4	0.74	0.26	64,64,64,64	0
5	EDO	A	901	4/4	0.78	0.19	50,51,52,52	0
5	EDO	A	907	4/4	0.79	0.26	77,77,77,77	0
2	DQ1	B	602	31/31	0.82	0.24	76,89,98,98	2
5	EDO	A	906	4/4	0.82	0.19	59,59,60,60	0
5	EDO	D	910	4/4	0.83	0.16	58,59,59,59	0
5	EDO	C	913	4/4	0.85	0.22	67,67,67,67	0
2	DQ1	A	602	31/31	0.87	0.14	45,51,58,59	2
2	DQ1	C	602	31/31	0.87	0.19	51,65,81,82	2
2	DQ1	D	602	31/31	0.88	0.13	35,44,57,57	2
5	EDO	D	911	4/4	0.88	0.19	67,67,67,68	0
4	SO4	D	522	5/5	0.89	0.12	65,66,66,66	0
5	EDO	D	908	4/4	0.89	0.16	49,50,50,52	0
4	SO4	B	601	5/5	0.91	0.14	69,69,70,71	0
5	EDO	B	904	4/4	0.92	0.15	63,63,63,64	0
3	NAP	C	702	48/48	0.93	0.11	51,59,65,66	0
3	NAP	A	702	48/48	0.93	0.09	34,41,46,46	0
3	NAP	B	702	48/48	0.94	0.11	57,66,76,77	0
3	NAP	D	702	48/48	0.94	0.09	38,42,44,45	0
5	EDO	D	903	4/4	0.94	0.10	40,40,41,42	0
5	EDO	C	909	4/4	0.95	0.09	41,41,41,43	0
4	SO4	D	601	5/5	0.95	0.10	56,56,57,57	0
5	EDO	B	912	4/4	0.95	0.09	42,42,43,45	0
5	EDO	A	902	4/4	0.96	0.10	39,39,39,40	0
4	SO4	C	801	5/5	0.98	0.08	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.

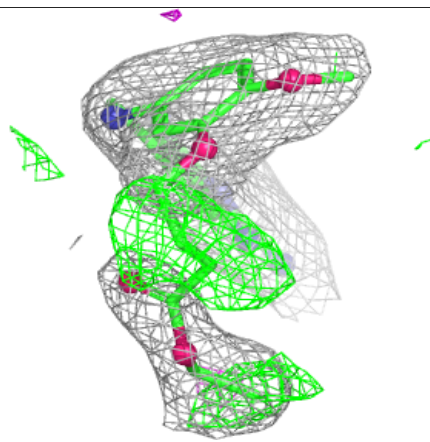
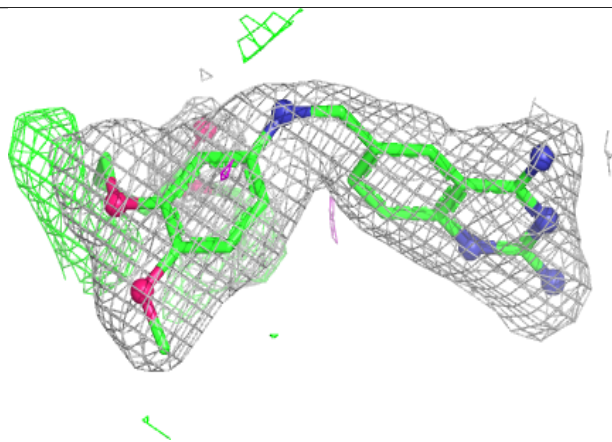
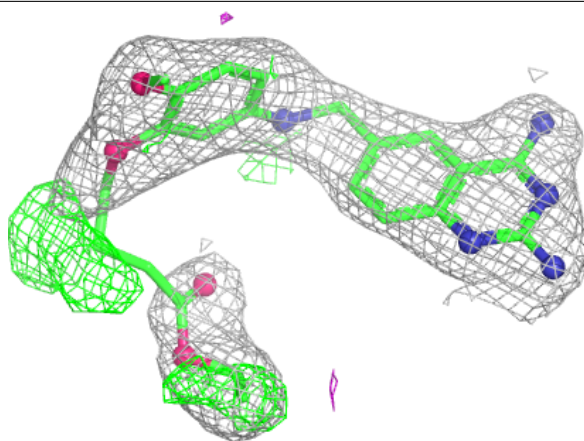
Electron density around DQ1 B 602:

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



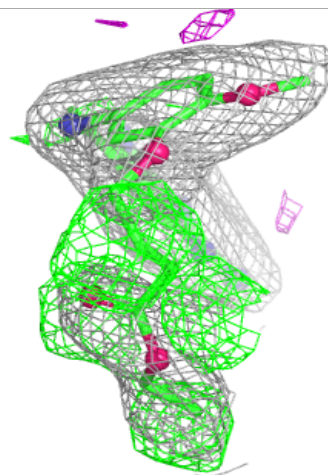
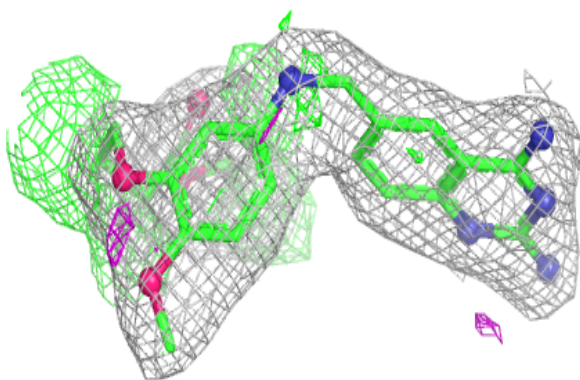
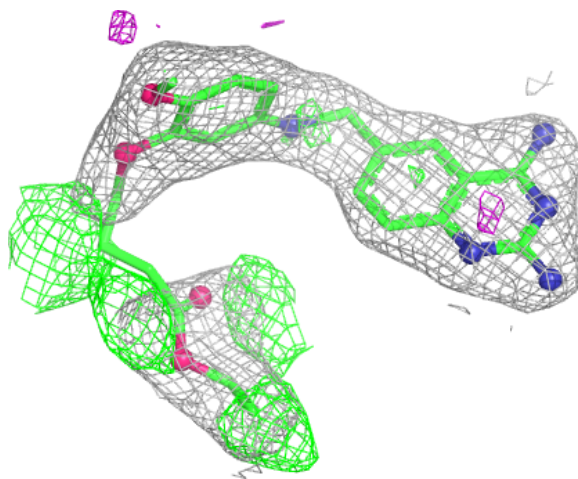
Electron density around DQ1 A 602:

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



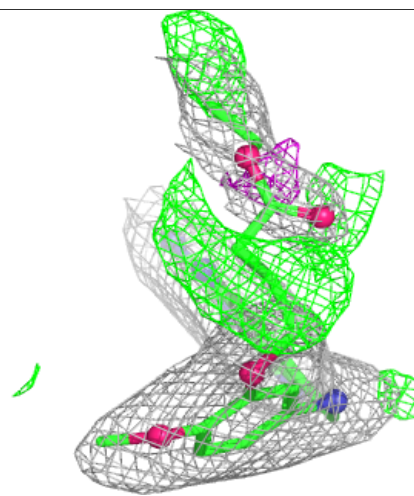
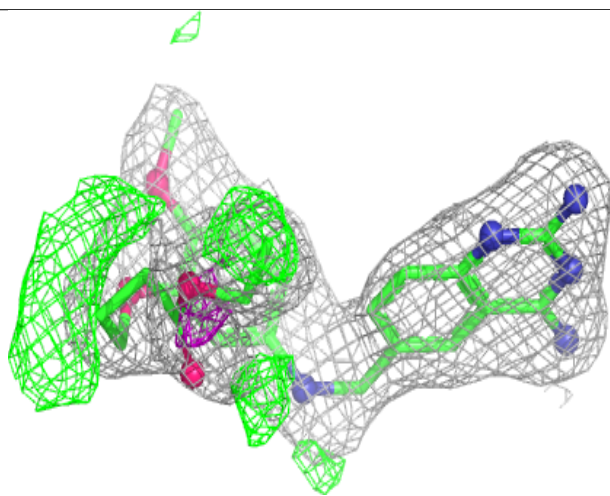
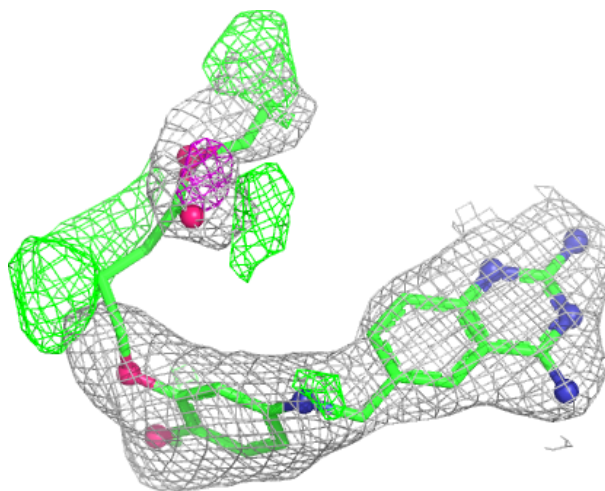
Electron density around DQ1 C 602:

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



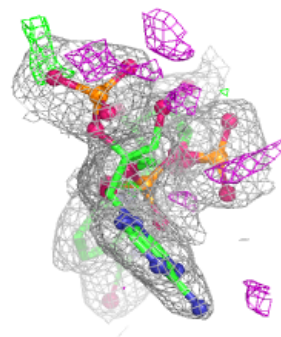
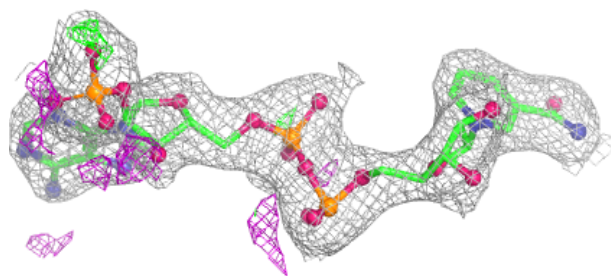
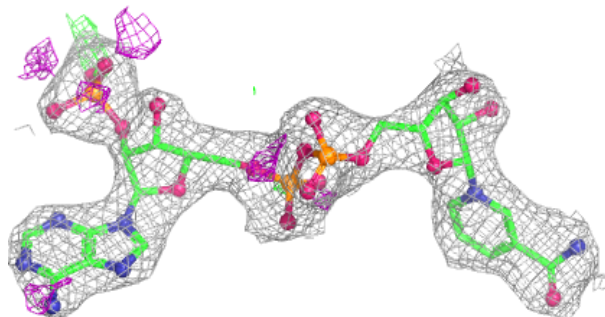
Electron density around DQ1 D 602:

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

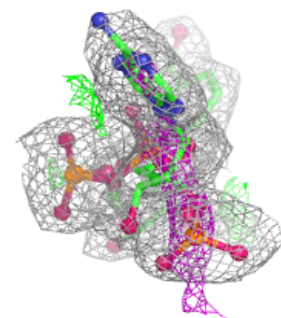
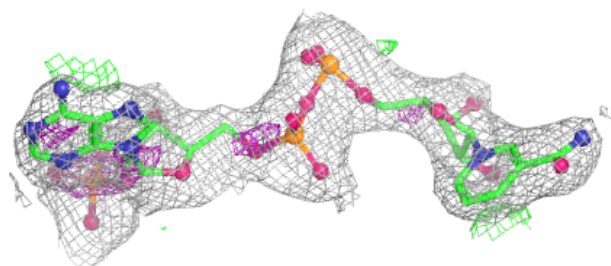
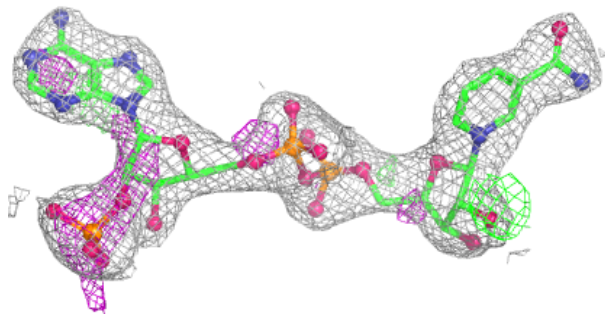


Electron density around NAP C 702:

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

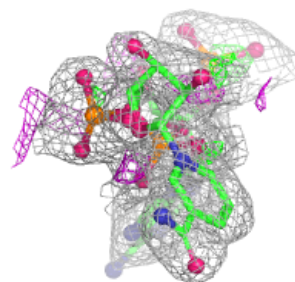
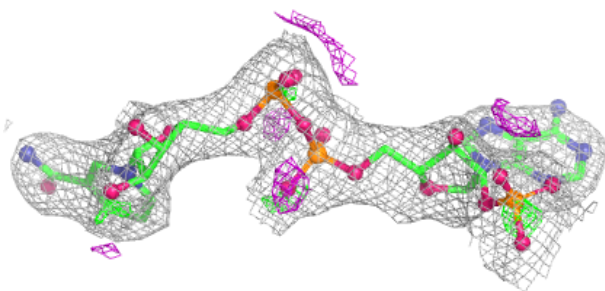
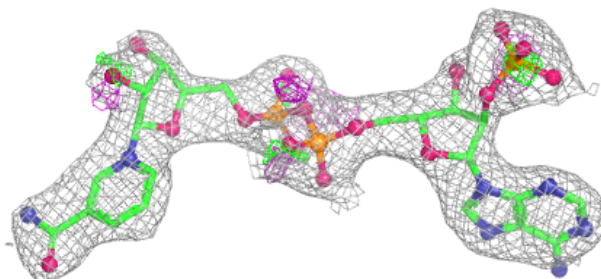
**Electron density around NAP A 702:**

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

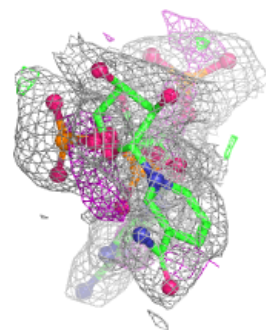
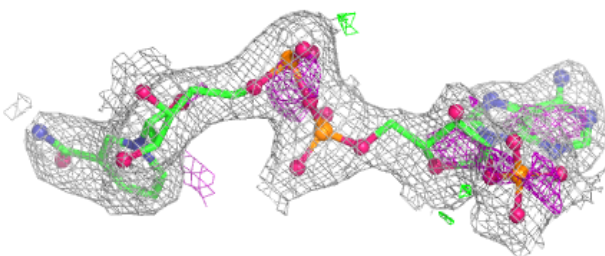
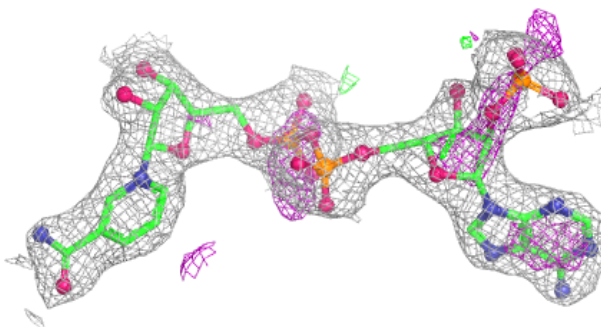


Electron density around NAP B 702:

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

**Electron density around NAP D 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.