Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:26 am BST

PDB ID	:	3BXX
Title	:	Binding of two substrate analogue molecules to dihydroflavonol 4-reductase alters the functional geometry of the catalytic site
Authors	:	Trabelsi, N.; Petit, P.; Granier, T.; Langlois d'Estaintot, B.; Delrot, S.; Gallois, B.
Deposited on	:	2008-01-15
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

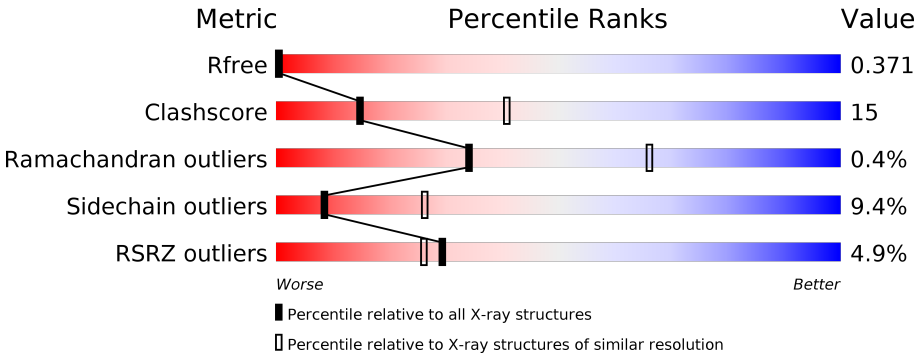
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	337	3% 65% 29%
1	B	337	70% 24%
1	C	337	% 66% 28%
1	D	337	10% 56% 35% 5%
1	E	337	12% 56% 36%
1	F	337	2% 63% 29%

2 Entry composition (i)

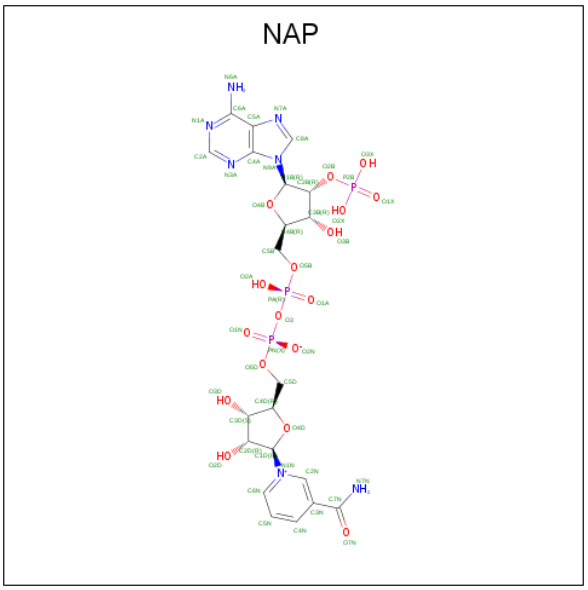
There are 4 unique types of molecules in this entry. The entry contains 15797 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 dihydroflavonol 4-reductase.

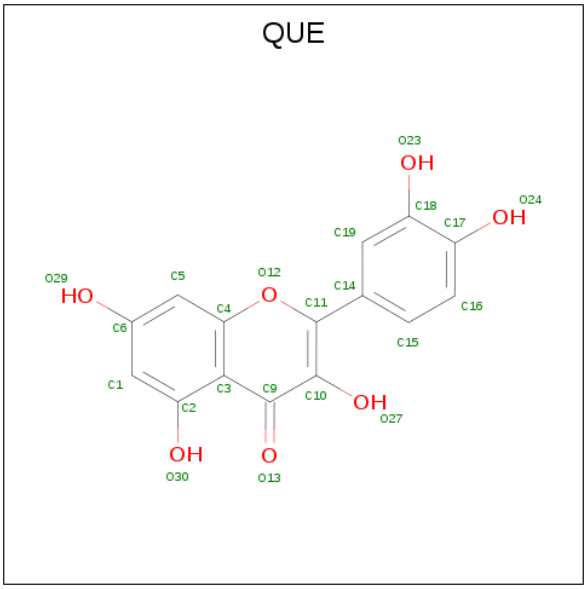
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2531	1621	417	473	20			
1	B	324	Total	C	N	O	S	0	0	0
			2531	1621	417	473	20			
1	C	324	Total	C	N	O	S	0	0	0
			2531	1621	417	473	20			
1	D	324	Total	C	N	O	S	0	0	0
			2531	1621	417	473	20			
1	E	324	Total	C	N	O	S	0	0	0
			2531	1621	417	473	20			
1	F	324	Total	C	N	O	S	0	0	0
			2527	1619	417	471	20			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 3 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (three-letter code: QUE) (formula: $C_{15}H_{10}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	15	7		
3	B	1	Total	C	O	0	0
			22	15	7		
3	B	1	Total	C	O	0	0
			22	15	7		
3	C	1	Total	C	O	0	0
			22	15	7		
3	C	1	Total	C	O	0	0
			22	15	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 22 15 7	0	0
3	D	1	Total C O 22 15 7	0	0
3	F	1	Total C O 22 15 7	0	0
3	F	1	Total C O 22 15 7	0	0

- Molecule 4 is water.

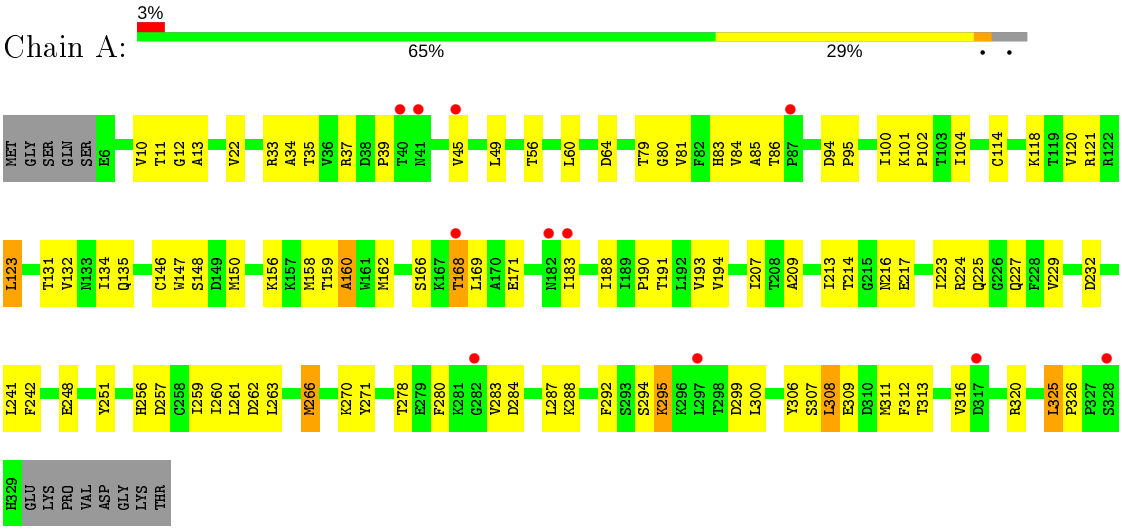
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	B	15	Total O 15 15	0	0
4	C	16	Total O 16 16	0	0
4	D	29	Total O 29 29	0	0
4	E	33	Total O 33 33	0	0
4	F	17	Total O 17 17	0	0

3 Residue-property plots (i)

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

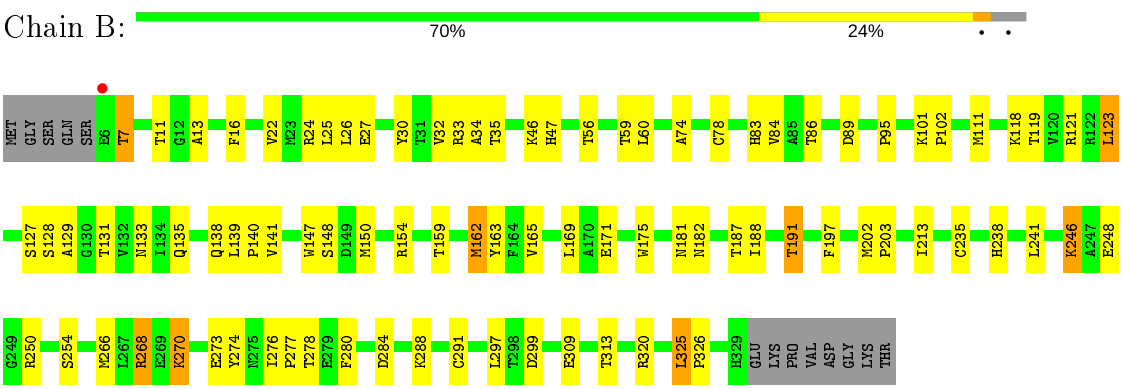
- Molecule 1: dihydroflavonol 4-reductase

Chain A:



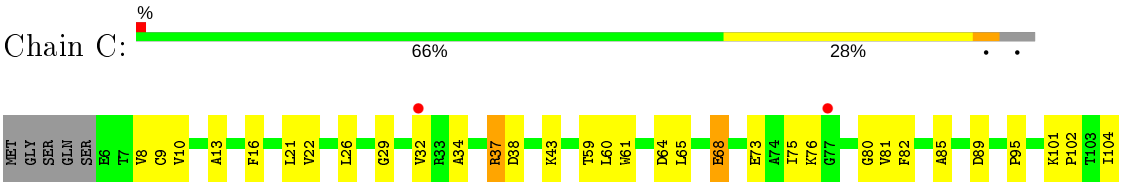
- Molecule 1: dihydroflavonol 4-reductase

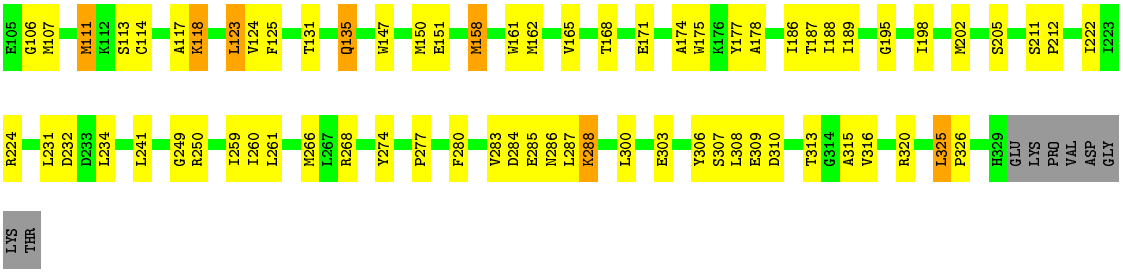
Chain B:



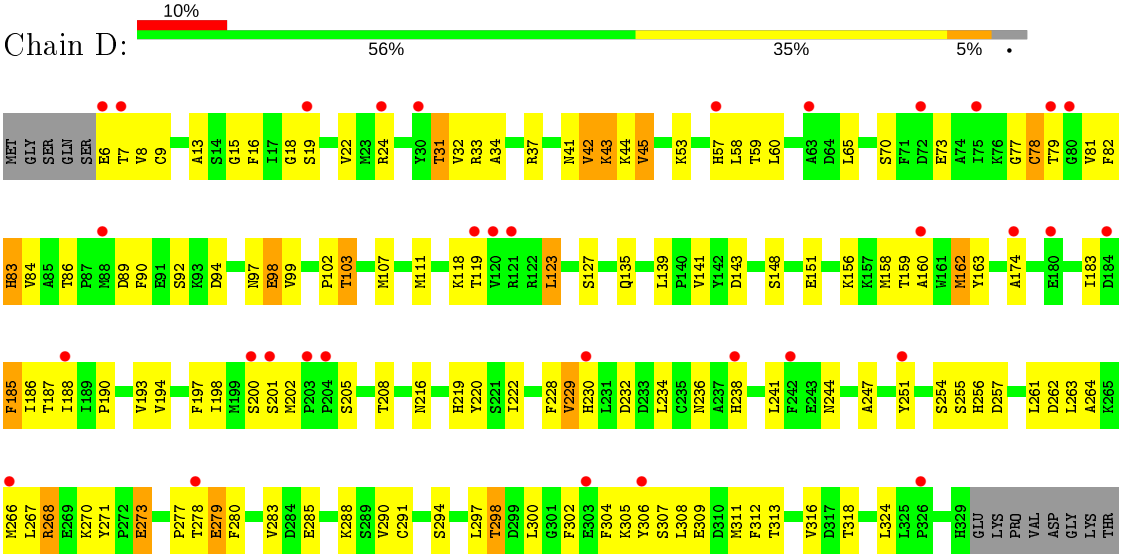
- Molecule 1: dihydroflavonol 4-reductase

Chain C:

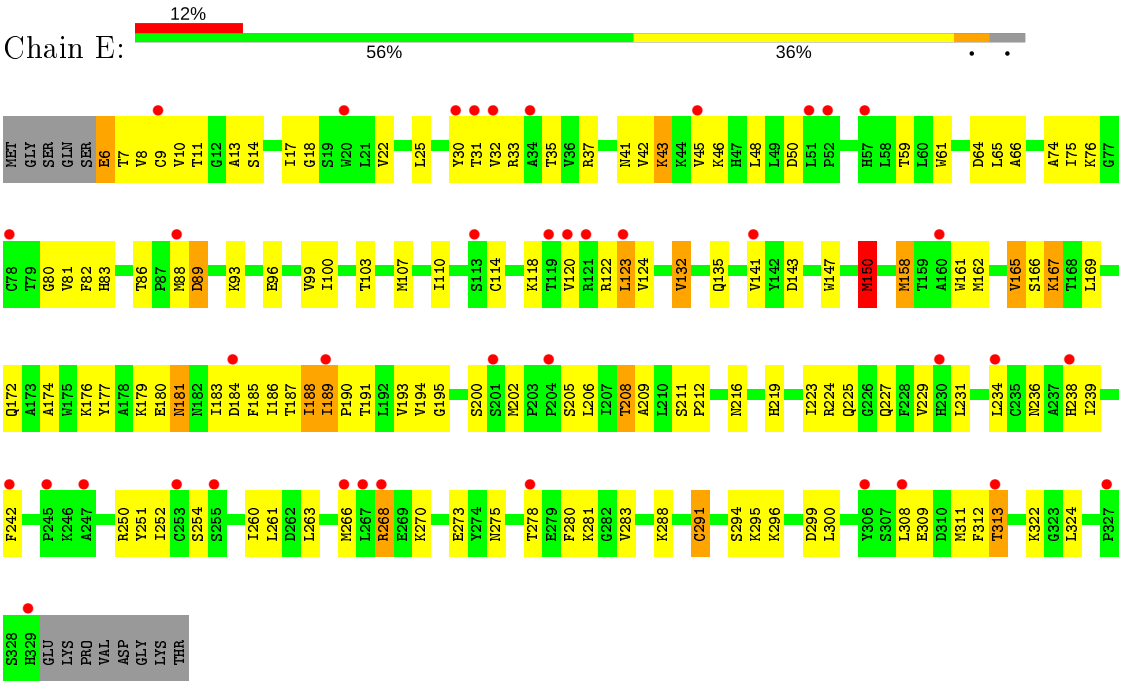




• Molecule 1: dihydroflavonol 4-reductase

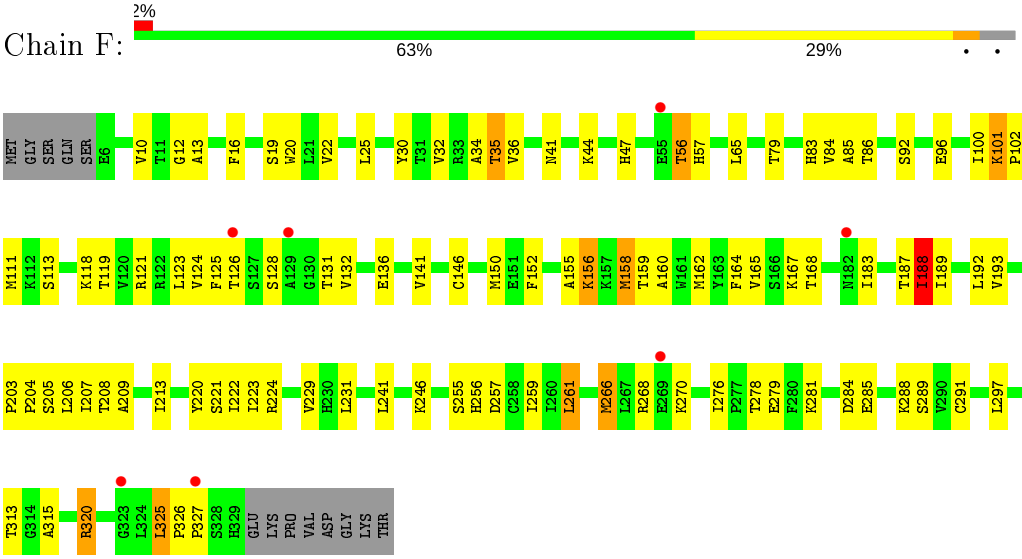


• Molecule 1: dihydroflavonol 4-reductase



• Molecule 1: dihydroflavonol 4-reductase

Chain F:


2%
63%
29%
MET GLY SER GLN SER E6 V10 T11 G12 A13 F16 S19 W20 L21 V22 L25 Y30 T31 V32 R33 A34 T35 V36 N41 K44 H47 E55 T56 H57 L65 T79 H83 V84 A85 T86 S92 E96 I100 K101 P102 T103 I104 M107
M111 K112 S113 K118 T119 V120 R121 R122 L123 V124 F125 T126 S127 S128 A129 G130 T131 V132 E136 V141 C146 M150 E151 F152 A155 K156 K157 M158 T159 A160 W161 M162 Y163 F164 V165 S166 K167 T168 N182 I183 T187 I188 I189 L192 V193 P196 M199 S200
P203 P204 S205 L206 I207 T208 A209 I213 Y220 S221 I222 I223 R224 V229 H230 L231 L241 K246 S255 H256 D257 C258 I259 I260 L261 M266 L267 R268 E269 K270 I276 P277 T278 E279 F280 K281 D284 E285 K288 S289 V290 C291 L297 F302 E303 M311 F312
T313 G314 A315 R320 G323 L324 L325 P326 P327 S328 H329 GLU LYS PRO VAL ASP GLY LYS THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	174.94Å 174.94Å 290.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.81 – 2.90 75.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (75.81-2.90) 100.0 (75.75-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	5.65 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.288 , 0.366 0.292 , 0.371	Depositor DCC
R_{free} test set	2967 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	15797	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7460e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAP, QUE

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	0.63	0/2591	1.03	7/3513 (0.2%)
1	B	0.62	0/2591	1.10	10/3513 (0.3%)
1	C	0.64	0/2591	1.10	5/3513 (0.1%)
1	D	0.62	0/2591	1.08	5/3513 (0.1%)
1	E	0.66	0/2591	1.13	1/3513 (0.0%)
1	F	0.62	0/2587	1.09	6/3508 (0.2%)
All	All	0.63	0/15542	1.09	34/21073 (0.2%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	320	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	D	60	LEU	CA-CB-CG	5.86	128.78	115.30
1	B	299	ASP	CB-CG-OD1	5.85	123.57	118.30
1	C	64	ASP	CB-CG-OD1	5.71	123.44	118.30
1	D	162	MET	CG-SD-CE	5.70	109.32	100.20
1	B	24	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	F	200	SER	N-CA-CB	-5.62	102.06	110.50
1	A	217	GLU	OE1-CD-OE2	-5.62	116.56	123.30
1	D	37	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	89	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	24	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	320	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	121	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	38	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	E	150	MET	CG-SD-CE	5.39	108.82	100.20
1	C	232	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	94	ASP	CB-CG-OD1	5.32	123.08	118.30
1	F	188	ILE	CB-CA-C	-5.27	101.06	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	320	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	284	ASP	N-CA-CB	-5.26	101.13	110.60
1	A	49	LEU	CB-CG-CD2	5.26	119.94	111.00
1	B	150	MET	CG-SD-CE	5.22	108.56	100.20
1	D	262	ASP	CB-CG-OD2	-5.22	113.61	118.30
1	F	220	TYR	CB-CG-CD1	5.21	124.13	121.00
1	A	60	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	202	MET	CG-SD-CE	5.13	108.41	100.20
1	F	220	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	160	ALA	CB-CA-C	-5.09	102.47	110.10
1	F	261	LEU	CA-CB-CG	5.08	126.98	115.30
1	B	191	THR	N-CA-C	-5.05	97.36	111.00
1	A	33	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	D	232	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	284	ASP	CB-CG-OD1	-5.03	113.78	118.30
1	C	37	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	2531	0	2508	62	0
1	B	2531	0	2508	68	0
1	C	2531	0	2508	67	0
1	D	2531	0	2508	101	0
1	E	2531	0	2508	114	0
1	F	2527	0	2504	68	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	5	0
2	D	48	0	25	3	0
2	E	48	0	25	6	0
2	F	48	0	25	2	0
3	A	22	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	11	4	0
3	C	44	0	14	0	0
3	D	44	0	13	2	0
3	F	44	0	17	5	0
4	A	19	0	0	2	0
4	B	15	0	0	3	0
4	C	16	0	0	2	0
4	D	29	0	0	9	0
4	E	33	0	0	4	0
4	F	17	0	0	0	0
All	All	15797	0	15255	469	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 15.

All (469) 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:E:236:ASN:HA	1:E:239:ILE:HD12	1.36	1.06
1:F:132:VAL:HG22	1:F:146:CYS:O	1.57	1.02
1:E:193:VAL:HG21	1:E:234:LEU:HD22	1.41	0.99
1:B:141:VAL:HG22	1:B:291:CYS:HB3	1.44	0.99
1:B:95:PRO:HB3	1:B:162:MET:HE2	1.46	0.95
1:B:95:PRO:HB3	1:B:162:MET:CE	2.00	0.92
1:B:95:PRO:CB	1:B:162:MET:HE2	2.00	0.91
1:D:270:LYS:HE2	1:D:313:THR:HG22	1.51	0.91
1:B:95:PRO:CB	1:B:162:MET:CE	2.49	0.90
1:C:171:GLU:O	1:C:174:ALA:HB3	1.70	0.90
1:F:204:PRO:HA	1:F:207:ILE:HD12	1.52	0.90
1:D:31:THR:HG23	1:D:57:HIS:ND1	1.88	0.89
1:F:10:VAL:HG11	1:F:22:VAL:HG23	1.55	0.88
1:D:7:THR:HG22	1:D:78:CYS:HB3	1.60	0.83
1:E:35:THR:HG22	1:E:61:TRP:HB2	1.58	0.83
1:B:325:LEU:HD23	1:B:326:PRO:HD2	1.62	0.81
1:A:168:THR:HG22	1:A:169:LEU:HD23	1.61	0.81
1:C:288:LYS:HE3	1:D:139:LEU:HD22	1.60	0.81
1:E:141:VAL:HG22	1:E:291:CYS:HB3	1.64	0.80
1:D:77:GLY:O	1:D:119:THR:HG21	1.81	0.79
1:E:174:ALA:HB1	1:E:185:PHE:CZ	2.19	0.78
1:E:193:VAL:CG2	1:E:234:LEU:HD22	2.13	0.77
1:F:132:VAL:HG13	1:F:146:CYS:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:ASN:CA	1:E:239:ILE:HD12	2.15	0.77
1:E:309:GLU:O	1:E:313:THR:HG23	1.86	0.76
1:B:11:THR:OG1	1:B:83:HIS:HA	1.85	0.76
1:B:188:ILE:HD12	1:B:238:HIS:CD2	2.22	0.74
1:A:325:LEU:HD23	1:A:326:PRO:HD2	1.70	0.74
1:E:225:GLN:O	1:E:227:GLN:NE2	2.21	0.74
1:B:268:ARG:CZ	1:B:278:THR:HG22	2.18	0.73
1:F:203:PRO:HG2	1:F:206:LEU:HD12	1.69	0.73
1:B:165:VAL:HG12	1:B:169:LEU:HD12	1.71	0.73
1:F:22:VAL:HG22	1:F:32:VAL:HG11	1.70	0.73
1:A:261:LEU:HD13	1:A:283:VAL:HG12	1.72	0.71
1:D:89:ASP:HB3	4:D:351:HOH:O	1.90	0.70
1:C:125:PHE:HB3	1:C:187:THR:HG22	1.71	0.70
1:C:22:VAL:HG22	1:C:32:VAL:HG11	1.74	0.69
1:D:279:GLU:HB3	4:D:366:HOH:O	1.91	0.69
1:E:193:VAL:HG21	1:E:234:LEU:CD2	2.19	0.69
1:B:191:THR:HG21	1:B:254:SER:HB2	1.74	0.69
1:C:158:MET:HE2	1:C:161:TRP:HB3	1.73	0.69
1:E:273:GLU:OE1	1:E:273:GLU:N	2.25	0.69
1:C:325:LEU:HD22	1:C:326:PRO:HD2	1.73	0.69
1:E:188:ILE:HD12	1:E:238:HIS:CD2	2.27	0.69
1:A:260:ILE:HG23	1:A:280:PHE:CD2	2.27	0.68
1:D:244:ASN:HD21	1:D:300:LEU:HD22	1.59	0.68
1:E:236:ASN:HA	1:E:239:ILE:CD1	2.20	0.68
1:E:64:ASP:OD1	1:E:66:ALA:N	2.26	0.68
1:C:284:ASP:OD1	1:C:286:ASN:N	2.27	0.68
1:F:125:PHE:HB3	1:F:187:THR:HG22	1.76	0.67
1:F:111:MET:HE2	1:F:183:ILE:HD12	1.77	0.67
1:D:306:TYR:HA	4:D:361:HOH:O	1.95	0.66
1:B:129:ALA:HB3	3:B:341:QUE:C19	2.24	0.66
1:D:244:ASN:ND2	1:D:300:LEU:HD22	2.12	0.65
1:B:309:GLU:O	1:B:313:THR:HG23	1.96	0.65
1:E:275:ASN:CB	4:E:366:HOH:O	2.44	0.65
1:C:81:VAL:HG21	1:C:114:CYS:SG	2.36	0.64
1:E:89:ASP:CG	1:E:89:ASP:O	2.36	0.64
1:C:288:LYS:HE2	1:D:139:LEU:HD13	1.79	0.63
1:A:188:ILE:HD11	1:A:241:LEU:HD12	1.81	0.63
1:D:111:MET:HE2	1:D:183:ILE:HD12	1.81	0.63
1:E:75:ILE:HD11	1:E:110:ILE:HG23	1.80	0.62
1:C:189:ILE:HD11	1:C:250:ARG:NH2	2.13	0.62
1:A:193:VAL:HG13	1:A:229:VAL:HG13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:MET:HA	1:E:150:MET:CE	2.30	0.62
1:A:309:GLU:O	1:A:313:THR:HG23	1.99	0.62
1:B:141:VAL:HG22	1:B:291:CYS:CB	2.24	0.62
1:E:17:ILE:HD12	2:E:338:NAP:H51N	1.82	0.62
1:D:174:ALA:HB1	1:D:185:PHE:CE2	2.36	0.61
1:D:270:LYS:CE	1:D:313:THR:HG22	2.26	0.61
1:E:208:THR:HG23	1:E:219:HIS:HB3	1.82	0.61
1:E:96:GLU:HA	1:E:100:ILE:HD12	1.82	0.61
1:E:174:ALA:HB1	1:E:185:PHE:CE2	2.35	0.61
1:B:191:THR:CG2	1:B:254:SER:HB2	2.30	0.61
1:E:167:LYS:NZ	2:E:338:NAP:O3D	2.34	0.61
1:D:186:ILE:HG22	1:D:187:THR:N	2.15	0.61
1:D:229:VAL:HG11	1:D:234:LEU:HB2	1.83	0.61
1:D:222:ILE:O	1:D:222:ILE:HG22	2.00	0.60
1:A:12:GLY:HA3	1:A:85:ALA:HB2	1.84	0.60
1:F:96:GLU:HA	1:F:100:ILE:HD12	1.83	0.60
1:C:158:MET:CE	1:C:158:MET:H	2.15	0.60
1:E:75:ILE:O	1:E:75:ILE:CG2	2.48	0.60
1:D:98:GLU:HG2	4:D:353:HOH:O	2.01	0.60
1:A:100:ILE:HG23	1:A:166:SER:HA	1.84	0.59
1:B:141:VAL:CG2	1:B:291:CYS:HB3	2.26	0.59
1:E:180:GLU:C	1:E:181:ASN:HD22	2.05	0.59
1:F:141:VAL:HG22	1:F:291:CYS:HB3	1.83	0.59
1:B:33:ARG:CZ	4:B:348:HOH:O	2.50	0.59
1:F:325:LEU:HD23	1:F:326:PRO:HD2	1.84	0.59
1:B:213:ILE:HG12	1:B:276:ILE:HD11	1.85	0.59
1:C:101:LYS:HB3	1:C:102:PRO:HD3	1.85	0.59
1:D:94:ASP:CG	1:D:97:ASN:HD22	2.04	0.59
1:E:81:VAL:HG21	1:E:114:CYS:SG	2.43	0.59
1:E:191:THR:HG21	1:E:254:SER:HB2	1.83	0.59
1:A:261:LEU:HD13	1:A:283:VAL:CG1	2.33	0.58
1:A:295:LYS:NZ	1:A:299:ASP:OD2	2.36	0.58
1:E:33:ARG:HD2	1:E:74:ALA:O	2.02	0.58
1:F:189:ILE:N	1:F:189:ILE:HD12	2.18	0.58
1:E:93:LYS:O	1:F:156:LYS:HG2	2.03	0.58
1:A:194:VAL:HG11	1:A:312:PHE:CE1	2.39	0.58
1:A:84:VAL:HG12	2:A:338:NAP:H4D	1.85	0.58
1:F:123:LEU:HD23	1:F:124:VAL:N	2.19	0.58
1:F:266:MET:HE1	1:F:270:LYS:HG3	1.84	0.58
1:A:194:VAL:HG11	1:A:312:PHE:CD1	2.38	0.58
1:C:75:ILE:HD12	1:C:113:SER:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:VAL:HB	1:D:123:LEU:HD23	1.86	0.58
1:F:128:SER:OG	3:F:342:QUE:O24	2.21	0.58
1:C:13:ALA:CB	1:C:34:ALA:HB1	2.34	0.58
1:A:13:ALA:CB	1:A:34:ALA:HB1	2.34	0.57
1:F:188:ILE:HD11	1:F:241:LEU:HD12	1.85	0.57
1:D:263:LEU:HD11	1:D:312:PHE:CZ	2.39	0.57
1:D:186:ILE:CG2	1:D:187:THR:N	2.68	0.57
1:E:13:ALA:CB	1:E:48:LEU:HD11	2.34	0.57
1:E:64:ASP:C	1:E:64:ASP:OD1	2.43	0.57
1:B:128:SER:OG	3:B:342:QUE:O24	2.23	0.56
1:D:8:VAL:HG23	1:D:9:CYS:O	2.05	0.56
1:E:75:ILE:O	1:E:75:ILE:HG22	2.05	0.56
1:E:13:ALA:HB1	1:E:48:LEU:HD11	1.86	0.56
1:F:111:MET:CE	1:F:183:ILE:HD12	2.35	0.56
1:E:165:VAL:HG13	1:E:169:LEU:HD11	1.87	0.56
1:E:322:LYS:HB2	1:E:324:LEU:HD12	1.88	0.56
1:E:11:THR:HA	1:E:35:THR:OG1	2.05	0.56
1:C:65:LEU:HD22	1:C:106:GLY:HA3	1.87	0.56
1:D:261:LEU:HD13	1:D:283:VAL:CG1	2.36	0.56
1:E:123:LEU:HD13	1:E:185:PHE:CD1	2.41	0.56
1:E:8:VAL:HG21	1:E:82:PHE:CE2	2.40	0.55
1:B:277:PRO:HG2	1:B:280:PHE:CZ	2.41	0.55
1:E:189:ILE:HD12	1:E:252:ILE:HA	1.87	0.55
1:E:194:VAL:HG22	1:E:209:ALA:HB2	1.88	0.55
1:B:140:PRO:O	1:B:141:VAL:HG23	2.07	0.55
1:B:95:PRO:HB2	1:B:162:MET:HE2	1.85	0.55
1:C:75:ILE:HD12	1:C:113:SER:CB	2.37	0.55
1:D:41:ASN:O	1:D:44:LYS:N	2.38	0.55
1:E:17:ILE:HD12	2:E:338:NAP:C5D	2.35	0.55
1:E:100:ILE:HG23	1:E:166:SER:HA	1.89	0.55
1:D:24:ARG:HD2	1:D:236:ASN:HD21	1.71	0.55
1:D:267:LEU:HD21	1:D:312:PHE:CD2	2.42	0.55
1:E:252:ILE:HG22	1:E:294:SER:OG	2.07	0.55
1:D:53:LYS:HB3	4:D:360:HOH:O	2.05	0.54
1:E:194:VAL:HG12	1:E:195:GLY:H	1.71	0.54
1:A:10:VAL:HG11	1:A:22:VAL:HG23	1.88	0.54
1:E:65:LEU:HD21	1:E:83:HIS:HE1	1.72	0.54
1:B:95:PRO:CG	1:B:162:MET:CE	2.85	0.54
1:E:65:LEU:HD21	1:E:83:HIS:CE1	2.43	0.54
1:D:229:VAL:HG13	1:D:230:HIS:O	2.07	0.54
1:F:164:PHE:HE1	3:F:342:QUE:H16	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:MET:HE1	1:C:178:ALA:HB2	1.90	0.54
1:E:150:MET:CE	1:E:165:VAL:HG22	2.38	0.53
1:E:188:ILE:HD12	1:E:238:HIS:NE2	2.23	0.53
2:F:338:NAP:O5D	2:F:338:NAP:H2N	2.09	0.53
1:B:165:VAL:CG1	1:B:169:LEU:CD1	2.87	0.53
1:E:123:LEU:HD13	1:E:185:PHE:CE1	2.43	0.53
1:C:131:THR:HA	1:C:168:THR:OG1	2.09	0.53
1:A:251:TYR:OH	1:A:300:LEU:HD11	2.08	0.53
1:C:309:GLU:O	1:C:313:THR:HG23	2.08	0.53
1:C:111:MET:CE	1:C:178:ALA:HB2	2.39	0.53
1:C:288:LYS:CE	1:D:139:LEU:HD13	2.39	0.53
1:E:280:PHE:HB3	4:E:339:HOH:O	2.08	0.53
1:C:277:PRO:HG2	1:C:280:PHE:CZ	2.44	0.53
1:D:159:THR:O	1:D:160:ALA:HB3	2.09	0.53
1:E:180:GLU:C	1:E:181:ASN:ND2	2.62	0.53
1:C:316:VAL:O	1:C:320:ARG:HG3	2.09	0.53
1:F:119:THR:O	1:F:119:THR:HG22	2.08	0.53
1:A:271:TYR:CE2	1:A:316:VAL:HG21	2.45	0.52
1:B:246:LYS:HB2	1:B:246:LYS:NZ	2.24	0.52
1:E:147:TRP:CZ3	1:E:172:GLN:HG3	2.44	0.52
1:E:189:ILE:CD1	1:E:252:ILE:HG13	2.39	0.52
1:E:189:ILE:HD12	1:E:252:ILE:CG1	2.40	0.52
1:E:141:VAL:HG22	1:E:291:CYS:CB	2.38	0.52
1:B:309:GLU:OE1	1:B:309:GLU:N	2.42	0.52
1:C:150:MET:HE3	1:C:168:THR:HG21	1.92	0.52
1:A:101:LYS:HB3	1:A:102:PRO:HD3	1.91	0.52
1:B:95:PRO:HG3	1:B:162:MET:CE	2.40	0.52
1:A:225:GLN:CG	1:A:287:LEU:HD21	2.39	0.52
1:B:26:LEU:HD23	1:B:32:VAL:HG23	1.92	0.52
1:B:163:TYR:HB3	3:B:342:QUE:C19	2.40	0.52
1:C:37:ARG:HB2	2:C:338:NAP:O3X	2.09	0.52
1:C:259:ILE:HG21	1:C:287:LEU:O	2.09	0.52
1:D:271:TYR:CE2	1:D:316:VAL:HG21	2.44	0.52
1:E:46:LYS:NZ	1:E:50:ASP:OD2	2.40	0.52
1:C:307:SER:O	1:C:308:LEU:C	2.46	0.51
1:B:165:VAL:CG1	1:B:169:LEU:HD12	2.40	0.51
1:B:33:ARG:HD2	1:B:74:ALA:O	2.11	0.51
1:C:325:LEU:HD22	1:C:326:PRO:CD	2.39	0.51
1:E:224:ARG:HA	1:E:260:ILE:HB	1.93	0.51
1:D:107:MET:HE3	1:D:107:MET:HA	1.91	0.51
1:C:10:VAL:HG11	1:C:22:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:THR:HG22	1:B:78:CYS:HA	1.92	0.51
1:A:312:PHE:O	1:A:316:VAL:HG23	2.11	0.51
1:D:188:ILE:HD11	1:D:238:HIS:HA	1.93	0.51
1:E:150:MET:HE1	1:E:165:VAL:HG22	1.93	0.51
1:D:53:LYS:CB	4:D:360:HOH:O	2.59	0.50
1:E:194:VAL:HG12	1:E:195:GLY:N	2.26	0.50
1:E:14:SER:OG	2:E:338:NAP:O2X	2.20	0.50
1:F:101:LYS:HB3	1:F:102:PRO:HD3	1.93	0.50
1:F:126:THR:O	1:F:167:LYS:NZ	2.41	0.50
1:B:268:ARG:NE	1:B:278:THR:HG22	2.25	0.50
1:F:131:THR:HG22	1:F:168:THR:N	2.27	0.50
1:F:213:ILE:HG21	1:F:325:LEU:HD21	1.92	0.50
1:D:99:VAL:O	1:D:103:THR:OG1	2.23	0.50
1:F:65:LEU:HD21	1:F:83:HIS:CE1	2.46	0.50
1:E:190:PRO:HB2	2:E:338:NAP:H5N	1.93	0.50
1:A:188:ILE:O	1:A:190:PRO:HD3	2.11	0.50
1:D:18:GLY:O	1:D:22:VAL:HG23	2.12	0.50
1:D:77:GLY:HA3	4:D:369:HOH:O	2.10	0.50
1:E:80:GLY:HA3	1:E:242:PHE:CZ	2.46	0.50
1:D:111:MET:CE	1:D:183:ILE:HD12	2.42	0.50
1:A:188:ILE:CD1	1:A:241:LEU:HD12	2.41	0.50
1:C:261:LEU:HD13	1:C:283:VAL:CG1	2.41	0.50
1:D:94:ASP:OD1	1:D:97:ASN:ND2	2.41	0.50
1:A:37:ARG:HD2	1:A:64:ASP:OD2	2.12	0.49
1:A:214:THR:OG1	1:A:216:ASN:ND2	2.44	0.49
1:A:263:LEU:HD21	1:A:312:PHE:CE2	2.47	0.49
1:D:257:ASP:OD1	1:D:257:ASP:O	2.30	0.49
1:E:165:VAL:HG13	1:E:169:LEU:CD1	2.42	0.49
1:F:192:LEU:HD21	1:F:209:ALA:HB2	1.93	0.49
1:A:213:ILE:HG21	1:A:325:LEU:HD21	1.93	0.49
1:C:95:PRO:HD2	4:C:346:HOH:O	2.11	0.49
1:D:174:ALA:HB1	1:D:185:PHE:CZ	2.46	0.49
1:E:31:THR:HG22	1:E:32:VAL:N	2.27	0.49
1:A:223:ILE:HD12	1:A:260:ILE:HG13	1.95	0.49
1:A:95:PRO:HD2	4:A:350:HOH:O	2.13	0.49
1:F:16:PHE:CZ	1:F:231:LEU:HD22	2.47	0.49
1:A:270:LYS:HD3	1:A:313:THR:CG2	2.43	0.49
1:E:124:VAL:CG1	1:E:188:ILE:HD11	2.43	0.49
1:E:124:VAL:HG11	1:E:188:ILE:HD11	1.95	0.49
1:E:7:THR:O	1:E:7:THR:HG22	2.13	0.49
1:E:88:MET:O	1:E:99:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:SER:OG	3:B:342:QUE:O23	2.23	0.48
1:D:163:TYR:HB3	3:D:342:QUE:C19	2.42	0.48
1:B:95:PRO:HB3	1:B:162:MET:HE1	1.93	0.48
1:C:26:LEU:O	1:C:29:GLY:N	2.46	0.48
1:D:127:SER:O	2:D:338:NAP:H6N	2.12	0.48
1:D:268:ARG:CZ	1:D:278:THR:HG22	2.43	0.48
1:F:152:PHE:O	1:F:155:ALA:HB3	2.13	0.48
1:A:261:LEU:CD1	1:A:283:VAL:HG12	2.42	0.48
1:B:101:LYS:HB3	1:B:102:PRO:HD3	1.96	0.48
1:E:96:GLU:HA	1:E:100:ILE:CD1	2.43	0.48
1:F:257:ASP:OD2	1:F:289:SER:OG	2.30	0.48
1:E:205:SER:HB3	2:E:338:NAP:O7N	2.13	0.48
1:E:93:LYS:O	1:F:156:LYS:CG	2.61	0.48
1:E:99:VAL:O	1:E:103:THR:OG1	2.24	0.48
1:D:185:PHE:O	1:D:186:ILE:HD13	2.12	0.48
1:A:81:VAL:O	1:A:123:LEU:HD23	2.14	0.48
1:B:175:TRP:CZ2	1:B:187:THR:HG23	2.49	0.48
1:C:81:VAL:HG12	1:C:81:VAL:O	2.13	0.48
1:F:266:MET:O	1:F:266:MET:HE1	2.14	0.48
1:D:255:SER:HB3	1:D:304:PHE:CD1	2.49	0.47
1:D:41:ASN:O	1:D:43:LYS:N	2.47	0.47
1:D:256:HIS:CE1	1:D:307:SER:HA	2.49	0.47
1:E:188:ILE:CD1	1:E:238:HIS:CD2	2.97	0.47
1:E:268:ARG:CZ	1:E:278:THR:HG22	2.44	0.47
1:A:225:GLN:HG3	1:A:287:LEU:HD21	1.96	0.47
1:C:211:SER:N	1:C:212:PRO:CD	2.77	0.47
1:E:268:ARG:NE	1:E:278:THR:HG22	2.30	0.47
1:E:25:LEU:O	1:E:30:TYR:HB2	2.15	0.47
1:F:266:MET:O	1:F:266:MET:CE	2.63	0.47
1:A:270:LYS:HD3	1:A:313:THR:HG22	1.97	0.47
1:A:224:ARG:CZ	1:A:287:LEU:HD11	2.45	0.47
1:D:58:LEU:HD12	1:D:59:THR:H	1.79	0.47
1:F:19:SER:OG	1:F:20:TRP:N	2.48	0.47
1:B:119:THR:HG22	1:B:119:THR:O	2.14	0.47
1:B:127:SER:O	2:B:338:NAP:H6N	2.15	0.47
1:C:165:VAL:O	1:C:165:VAL:HG12	2.13	0.47
1:C:231:LEU:O	1:C:234:LEU:HB3	2.14	0.47
1:C:205:SER:CB	2:C:338:NAP:H72N	2.28	0.46
1:E:37:ARG:NH1	1:F:281:LYS:NZ	2.64	0.46
1:A:100:ILE:HG22	1:A:104:ILE:HD12	1.97	0.46
1:C:81:VAL:O	1:C:123:LEU:HD23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:VAL:HG22	1:F:229:VAL:HG13	1.97	0.46
1:A:11:THR:OG1	1:A:84:VAL:N	2.49	0.46
1:A:227:GLN:OE1	1:A:292:PHE:CE1	2.69	0.46
1:C:195:GLY:O	1:C:315:ALA:CA	2.64	0.46
1:D:141:VAL:HG13	1:D:291:CYS:HB3	1.97	0.46
1:D:31:THR:HG23	1:D:57:HIS:CG	2.50	0.46
1:B:34:ALA:HB3	1:B:60:LEU:HD22	1.98	0.46
1:C:37:ARG:HD3	2:C:338:NAP:C6A	2.46	0.46
1:E:181:ASN:N	1:E:181:ASN:HD22	2.14	0.46
1:E:25:LEU:HD11	1:E:82:PHE:CE2	2.50	0.46
1:C:261:LEU:HD13	1:C:283:VAL:HG12	1.96	0.46
1:E:194:VAL:HA	1:E:206:LEU:HD21	1.98	0.46
1:E:191:THR:CG2	1:E:254:SER:HB2	2.44	0.46
1:F:192:LEU:HD22	1:F:223:ILE:HG22	1.97	0.46
1:D:82:PHE:O	1:D:84:VAL:HG23	2.16	0.46
1:E:251:TYR:OH	1:E:300:LEU:HD11	2.16	0.46
1:A:12:GLY:CA	1:A:85:ALA:HB2	2.45	0.46
1:B:22:VAL:HG22	1:B:32:VAL:HG11	1.98	0.46
1:D:241:LEU:HD21	1:D:251:TYR:CE2	2.51	0.46
1:E:8:VAL:HG21	1:E:82:PHE:HE2	1.79	0.46
1:E:216:ASN:ND2	1:F:207:ILE:HD13	2.31	0.46
1:A:147:TRP:CH2	1:A:171:GLU:OE1	2.69	0.45
1:B:325:LEU:CD2	1:B:326:PRO:HD2	2.40	0.45
1:C:307:SER:O	1:C:310:ASP:N	2.49	0.45
1:E:122:ARG:NE	1:E:184:ASP:OD2	2.48	0.45
1:F:128:SER:HG	3:F:342:QUE:C17	2.29	0.45
1:A:232:ASP:OD2	1:A:306:TYR:OH	2.25	0.45
1:B:274:TYR:OH	1:B:326:PRO:O	2.24	0.45
1:D:31:THR:CG2	1:D:57:HIS:ND1	2.72	0.45
1:A:150:MET:SD	1:A:168:THR:HG21	2.56	0.45
1:C:188:ILE:CD1	1:C:241:LEU:HD12	2.46	0.45
1:E:8:VAL:HG23	1:E:80:GLY:O	2.16	0.45
1:B:13:ALA:HB3	1:B:34:ALA:HB1	1.97	0.45
1:F:44:LYS:O	1:F:47:HIS:CE1	2.70	0.45
1:A:147:TRP:HH2	1:A:171:GLU:OE1	1.99	0.45
1:B:147:TRP:CH2	1:B:250:ARG:CZ	3.00	0.45
1:E:296:LYS:O	1:E:299:ASP:HB2	2.16	0.45
1:F:266:MET:CE	1:F:270:LYS:HG3	2.47	0.45
1:A:207:ILE:HG21	1:D:216:ASN:HD21	1.81	0.45
1:D:94:ASP:CG	1:D:97:ASN:ND2	2.70	0.45
1:A:207:ILE:HD13	1:D:216:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LEU:C	1:C:61:TRP:CD1	2.90	0.45
1:D:16:PHE:HE1	1:D:197:PHE:HB3	1.81	0.45
1:B:138:GLN:HG2	4:B:349:HOH:O	2.16	0.45
1:B:202:MET:HA	1:B:203:PRO:HD3	1.84	0.45
1:B:270:LYS:HD3	1:B:313:THR:HG22	1.99	0.45
1:B:84:VAL:HG12	1:B:84:VAL:O	2.17	0.45
1:D:197:PHE:CZ	1:D:318:THR:HG22	2.52	0.45
1:D:297:LEU:CD2	1:D:302:PHE:CD2	3.00	0.45
1:F:13:ALA:CB	1:F:34:ALA:HB1	2.47	0.45
1:C:147:TRP:CH2	1:C:250:ARG:CZ	2.99	0.45
1:B:139:LEU:HA	1:B:139:LEU:HD23	1.83	0.44
1:E:33:ARG:NH1	1:E:61:TRP:CZ2	2.85	0.44
1:B:159:THR:OG1	1:C:89:ASP:OD2	2.28	0.44
1:D:294:SER:O	1:D:297:LEU:N	2.50	0.44
1:E:150:MET:HA	1:E:150:MET:HE3	1.99	0.44
1:F:206:LEU:HD21	1:F:315:ALA:HB1	2.00	0.44
1:B:111:MET:HG2	1:B:123:LEU:HD12	1.99	0.44
1:C:117:ALA:O	1:C:118:LYS:HB2	2.18	0.44
1:D:41:ASN:O	1:D:42:VAL:C	2.54	0.44
1:E:158:MET:HB2	1:F:92:SER:O	2.17	0.44
1:D:273:GLU:N	1:D:273:GLU:OE1	2.47	0.44
1:F:12:GLY:N	1:F:85:ALA:HB2	2.33	0.44
1:D:15:GLY:O	1:D:19:SER:OG	2.25	0.44
1:E:189:ILE:HD12	1:E:252:ILE:HG13	1.98	0.44
1:E:263:LEU:HD11	1:E:312:PHE:CZ	2.52	0.44
1:B:95:PRO:HB2	1:B:162:MET:CE	2.42	0.44
1:C:158:MET:HE2	1:C:158:MET:H	1.82	0.44
1:E:308:LEU:O	1:E:308:LEU:HD23	2.18	0.44
1:E:6:GLU:HA	4:E:364:HOH:O	2.17	0.44
1:A:11:THR:OG1	1:A:83:HIS:HA	2.18	0.44
1:C:68:GLU:OE1	1:C:68:GLU:N	2.51	0.44
1:D:98:GLU:O	1:D:102:PRO:HG2	2.17	0.44
1:D:309:GLU:O	1:D:313:THR:HG23	2.17	0.44
1:D:6:GLU:HA	4:D:358:HOH:O	2.17	0.44
1:E:186:ILE:HG22	1:E:187:THR:N	2.33	0.44
1:B:241:LEU:HD11	1:B:297:LEU:HD13	2.00	0.43
1:E:9:CYS:SG	1:E:10:VAL:N	2.92	0.43
1:E:37:ARG:HG2	1:E:64:ASP:HB2	1.99	0.43
1:F:159:THR:O	1:F:160:ALA:HB3	2.17	0.43
1:C:9:CYS:O	1:C:82:PHE:N	2.41	0.43
1:D:42:VAL:HA	1:D:45:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:VAL:HG22	1:E:229:VAL:CG1	2.48	0.43
1:B:273:GLU:N	1:B:273:GLU:OE1	2.37	0.43
1:D:65:LEU:HD21	1:D:83:HIS:CE1	2.53	0.43
1:F:193:VAL:HG22	1:F:229:VAL:CG1	2.49	0.43
1:A:39:PRO:HA	1:A:45:VAL:HG11	2.01	0.43
1:D:13:ALA:CB	1:D:34:ALA:HB1	2.49	0.43
1:D:7:THR:HA	1:D:31:THR:O	2.18	0.43
1:E:93:LYS:N	4:E:356:HOH:O	2.51	0.43
1:B:246:LYS:NZ	1:B:246:LYS:CB	2.82	0.43
1:D:222:ILE:O	1:D:222:ILE:CG2	2.66	0.43
1:D:228:PHE:HE2	1:D:263:LEU:HD13	1.83	0.43
1:F:203:PRO:HA	1:F:204:PRO:HD3	1.91	0.43
1:A:259:ILE:HG21	1:A:287:LEU:O	2.18	0.43
1:C:150:MET:CE	1:C:168:THR:HG21	2.49	0.43
1:C:16:PHE:CE1	1:C:231:LEU:HD22	2.54	0.43
1:C:135:GLN:HB3	1:C:135:GLN:HE21	1.67	0.43
1:D:264:ALA:HB2	1:D:280:PHE:CZ	2.54	0.43
1:F:56:THR:HB	1:F:57:HIS:CD2	2.54	0.43
1:A:194:VAL:HG12	1:A:311:MET:CB	2.49	0.43
1:B:270:LYS:HD3	1:B:313:THR:CG2	2.48	0.43
1:B:46:LYS:O	1:B:47:HIS:C	2.57	0.43
1:E:260:ILE:CG2	1:E:283:VAL:HG11	2.48	0.43
1:F:224:ARG:O	1:F:259:ILE:HA	2.19	0.43
1:C:8:VAL:HG12	1:C:80:GLY:H	1.84	0.42
1:F:20:TRP:CH2	1:F:196:PRO:HG2	2.54	0.42
1:A:283:VAL:HG23	4:A:345:HOH:O	2.19	0.42
1:D:261:LEU:HD13	1:D:283:VAL:HG12	2.00	0.42
1:D:58:LEU:HD12	1:D:59:THR:N	2.34	0.42
1:F:104:ILE:O	1:F:107:MET:HB3	2.19	0.42
1:A:262:ASP:O	1:A:266:MET:HB2	2.20	0.42
1:D:257:ASP:HB2	1:D:290:VAL:O	2.20	0.42
1:D:98:GLU:CG	4:D:353:HOH:O	2.65	0.42
1:A:114:CYS:HB3	1:A:120:VAL:HG11	2.01	0.42
1:C:124:VAL:HA	1:C:186:ILE:O	2.20	0.42
1:C:13:ALA:HB3	1:C:34:ALA:HB1	2.01	0.42
1:D:119:THR:HG22	1:D:119:THR:O	2.19	0.42
1:D:261:LEU:HD12	1:D:280:PHE:HD1	1.84	0.42
1:D:32:VAL:HG12	1:D:33:ARG:N	2.34	0.42
1:E:193:VAL:HG13	1:E:231:LEU:HA	2.01	0.42
1:D:89:ASP:HB2	1:D:99:VAL:HG21	2.00	0.42
1:E:260:ILE:HG21	1:E:283:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:209:ALA:HB1	1:F:312:PHE:CZ	2.54	0.42
1:B:154:ARG:NH2	1:B:169:LEU:HD11	2.35	0.42
1:C:195:GLY:O	1:C:315:ALA:HA	2.19	0.42
1:E:31:THR:CG2	1:E:32:VAL:N	2.83	0.42
1:D:228:PHE:CE2	1:D:263:LEU:HD13	2.55	0.42
1:B:248:GLU:HG2	4:B:351:HOH:O	2.20	0.42
1:D:247:ALA:HB1	1:D:251:TYR:OH	2.19	0.42
1:E:132:VAL:HG23	1:E:250:ARG:HH22	1.84	0.42
1:F:35:THR:C	1:F:36:VAL:HG13	2.40	0.42
1:A:266:MET:SD	1:A:308:LEU:HD23	2.59	0.42
1:A:256:HIS:CE1	1:A:307:SER:HA	2.55	0.42
1:C:205:SER:HB3	2:C:338:NAP:H72N	1.85	0.42
1:D:219:HIS:O	1:D:220:TYR:C	2.58	0.42
1:E:114:CYS:SG	1:E:120:VAL:HG11	2.60	0.42
1:B:181:ASN:O	1:B:182:ASN:OD1	2.38	0.41
1:D:254:SER:H	1:D:294:SER:HG	1.64	0.41
1:F:268:ARG:HD3	1:F:278:THR:HG22	2.02	0.41
1:C:10:VAL:HG13	1:C:21:LEU:HD23	2.02	0.41
1:C:175:TRP:CH2	1:C:249:GLY:HA2	2.55	0.41
1:C:68:GLU:N	1:C:68:GLU:CD	2.72	0.41
1:F:136:GLU:HG3	1:F:136:GLU:O	2.19	0.41
1:C:104:ILE:O	1:C:107:MET:HB3	2.20	0.41
1:D:208:THR:HG23	1:D:219:HIS:HB3	2.02	0.41
1:D:261:LEU:HD12	1:D:280:PHE:CD1	2.55	0.41
1:E:161:TRP:CE3	1:E:165:VAL:HG21	2.55	0.41
1:F:150:MET:SD	1:F:165:VAL:HG22	2.60	0.41
1:A:80:GLY:HA3	1:A:242:PHE:CZ	2.55	0.41
1:C:59:THR:HB	4:C:358:HOH:O	2.20	0.41
1:D:127:SER:O	1:D:190:PRO:HD2	2.21	0.41
1:D:193:VAL:C	1:D:194:VAL:HG23	2.40	0.41
1:D:294:SER:O	1:D:298:THR:HG23	2.20	0.41
1:C:85:ALA:HB1	2:C:338:NAP:N3A	2.35	0.41
1:A:150:MET:CE	1:A:168:THR:HG21	2.51	0.41
1:B:16:PHE:HE1	1:B:197:PHE:HB3	1.86	0.41
1:E:165:VAL:CG1	1:E:169:LEU:CD1	2.98	0.41
1:E:211:SER:N	1:E:212:PRO:CD	2.84	0.41
1:F:297:LEU:HD23	1:F:302:PHE:CD1	2.56	0.41
1:D:90:PHE:CD1	1:D:90:PHE:C	2.94	0.41
1:E:42:VAL:O	1:E:43:LYS:C	2.59	0.41
1:F:192:LEU:HD11	1:F:208:THR:HB	2.02	0.41
1:A:134:ILE:HD12	1:A:134:ILE:HG23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ALA:HB1	1:A:312:PHE:CZ	2.56	0.41
1:F:158:MET:O	1:F:159:THR:C	2.59	0.41
1:F:320:ARG:NH1	1:F:327:PRO:O	2.53	0.41
1:B:131:THR:O	1:B:148:SER:N	2.51	0.41
1:A:159:THR:O	1:A:160:ALA:HB3	2.21	0.41
1:B:34:ALA:HB3	1:B:60:LEU:CD2	2.49	0.41
1:C:274:TYR:OH	1:C:326:PRO:O	2.21	0.41
1:D:186:ILE:HD11	1:D:247:ALA:O	2.20	0.41
1:D:193:VAL:HG23	2:D:338:NAP:C7N	2.50	0.41
1:D:202:MET:N	1:D:324:LEU:HD13	2.36	0.41
1:D:205:SER:HB3	2:D:338:NAP:N7N	2.36	0.41
1:A:132:VAL:HG13	1:A:146:CYS:HB2	2.03	0.40
1:C:224:ARG:O	1:C:260:ILE:N	2.51	0.40
1:E:41:ASN:O	1:E:45:VAL:HG22	2.21	0.40
1:B:171:GLU:OE2	1:B:187:THR:HG21	2.21	0.40
1:E:18:GLY:O	1:E:22:VAL:HG23	2.21	0.40
1:F:268:ARG:HG3	1:F:276:ILE:HB	2.03	0.40
1:A:131:THR:O	1:A:148:SER:N	2.52	0.40
1:B:25:LEU:O	1:B:30:TYR:HB2	2.20	0.40
1:D:277:PRO:HG2	1:D:280:PHE:CE2	2.56	0.40
1:E:141:VAL:HG22	1:E:291:CYS:SG	2.62	0.40
1:B:235:CYS:O	1:B:238:HIS:HB2	2.22	0.40
1:B:246:LYS:HZ2	1:B:246:LYS:HB2	1.86	0.40
1:D:163:TYR:HB3	3:D:342:QUE:H19	2.03	0.40
1:D:270:LYS:HG2	1:D:271:TYR:CE2	2.56	0.40
1:D:230:HIS:CD2	1:D:311:MET:HA	2.57	0.40
1:E:107:MET:O	1:E:107:MET:HE2	2.20	0.40
1:F:255:SER:O	1:F:256:HIS:ND1	2.54	0.40
1:F:25:LEU:O	1:F:30:TYR:HB2	2.21	0.40
1:E:37:ARG:NH1	1:F:281:LYS:HZ2	2.19	0.40
1:F:84:VAL:O	2:F:338:NAP:H4D	2.21	0.40
1:F:205:SER:HA	3:F:341:QUE:O29	2.21	0.40
1:F:128:SER:OG	3:F:342:QUE:O23	2.39	0.40
1:A:11:THR:HA	1:A:35:THR:OG1	2.22	0.40
1:C:158:MET:N	1:C:158:MET:HE2	2.37	0.40
1:F:297:LEU:CD2	1:F:302:PHE:CD1	3.05	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	322/337 (96%)	297 (92%)	25 (8%)	0	100 100
1	B	322/337 (96%)	297 (92%)	25 (8%)	0	100 100
1	C	322/337 (96%)	300 (93%)	22 (7%)	0	100 100
1	D	322/337 (96%)	280 (87%)	37 (12%)	5 (2%)	9 32
1	E	322/337 (96%)	278 (86%)	43 (13%)	1 (0%)	41 71
1	F	322/337 (96%)	292 (91%)	29 (9%)	1 (0%)	41 71
All	All	1932/2022 (96%)	1744 (90%)	181 (9%)	7 (0%)	34 66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	70	SER
1	D	42	VAL
1	D	273	GLU
1	D	83	HIS
1	D	148	SER
1	E	165	VAL
1	F	196	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	278/293 (95%)	255 (92%)	23 (8%)	11 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	278/293 (95%)	261 (94%)	17 (6%)	18 48
1	C	278/293 (95%)	256 (92%)	22 (8%)	12 34
1	D	278/293 (95%)	247 (89%)	31 (11%)	6 18
1	E	278/293 (95%)	242 (87%)	36 (13%)	4 13
1	F	277/293 (94%)	250 (90%)	27 (10%)	8 25
All	All	1667/1758 (95%)	1511 (91%)	156 (9%)	8 26

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	79	THR
1	A	86	THR
1	A	118	LYS
1	A	121	ARG
1	A	123	LEU
1	A	135	GLN
1	A	156	LYS
1	A	158	MET
1	A	162	MET
1	A	168	THR
1	A	183	ILE
1	A	191	THR
1	A	248	GLU
1	A	257	ASP
1	A	266	MET
1	A	278	THR
1	A	284	ASP
1	A	288	LYS
1	A	294	SER
1	A	295	LYS
1	A	308	LEU
1	A	325	LEU
1	B	7	THR
1	B	27	GLU
1	B	35	THR
1	B	56	THR
1	B	59	THR
1	B	86	THR
1	B	118	LYS

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Mol	Chain	Res	Type
1	B	123	LEU
1	B	133	ASN
1	B	135	GLN
1	B	162	MET
1	B	246	LYS
1	B	266	MET
1	B	268	ARG
1	B	270	LYS
1	B	288	LYS
1	B	325	LEU
1	C	43	LYS
1	C	68	GLU
1	C	73	GLU
1	C	76	LYS
1	C	111	MET
1	C	118	LYS
1	C	123	LEU
1	C	135	GLN
1	C	151	GLU
1	C	158	MET
1	C	162	MET
1	C	177	TYR
1	C	198	ILE
1	C	222	ILE
1	C	266	MET
1	C	268	ARG
1	C	285	GLU
1	C	288	LYS
1	C	300	LEU
1	C	303	GLU
1	C	306	TYR
1	C	325	LEU
1	D	31	THR
1	D	43	LYS
1	D	45	VAL
1	D	73	GLU
1	D	78	CYS
1	D	79	THR
1	D	86	THR
1	D	92	SER
1	D	98	GLU
1	D	103	THR

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Mol	Chain	Res	Type
1	D	118	LYS
1	D	123	LEU
1	D	135	GLN
1	D	143	ASP
1	D	151	GLU
1	D	156	LYS
1	D	158	MET
1	D	162	MET
1	D	185	PHE
1	D	198	ILE
1	D	200	SER
1	D	201	SER
1	D	229	VAL
1	D	266	MET
1	D	268	ARG
1	D	279	GLU
1	D	285	GLU
1	D	288	LYS
1	D	298	THR
1	D	305	LYS
1	D	308	LEU
1	E	6	GLU
1	E	43	LYS
1	E	59	THR
1	E	76	LYS
1	E	86	THR
1	E	89	ASP
1	E	118	LYS
1	E	123	LEU
1	E	132	VAL
1	E	135	GLN
1	E	143	ASP
1	E	150	MET
1	E	158	MET
1	E	162	MET
1	E	167	LYS
1	E	176	LYS
1	E	177	TYR
1	E	179	LYS
1	E	181	ASN
1	E	183	ILE
1	E	188	ILE

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Mol	Chain	Res	Type
1	E	189	ILE
1	E	200	SER
1	E	202	MET
1	E	208	THR
1	E	223	ILE
1	E	261	LEU
1	E	266	MET
1	E	268	ARG
1	E	270	LYS
1	E	281	LYS
1	E	288	LYS
1	E	291	CYS
1	E	295	LYS
1	E	311	MET
1	E	313	THR
1	F	35	THR
1	F	41	ASN
1	F	56	THR
1	F	79	THR
1	F	86	THR
1	F	101	LYS
1	F	113	SER
1	F	118	LYS
1	F	121	ARG
1	F	156	LYS
1	F	158	MET
1	F	162	MET
1	F	188	ILE
1	F	200	SER
1	F	221	SER
1	F	222	ILE
1	F	246	LYS
1	F	261	LEU
1	F	266	MET
1	F	279	GLU
1	F	284	ASP
1	F	285	GLU
1	F	288	LYS
1	F	303	GLU
1	F	311	MET
1	F	313	THR
1	F	325	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	216	ASN
1	B	97	ASN
1	B	133	ASN
1	B	138	GLN
1	B	236	ASN
1	C	181	ASN
1	D	97	ASN
1	D	216	ASN
1	D	219	HIS
1	D	236	ASN
1	D	329	HIS
1	E	181	ASN
1	E	236	ASN
1	F	57	HIS
1	F	329	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 carbohydrates in this entry.

5.6 Ligand geometry

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	QUE	B	342	-	21,24,24	1.91	3 (14%)	28,36,36	2.14	9 (32%)
3	QUE	A	342	-	21,24,24	2.04	6 (28%)	28,36,36	2.50	10 (35%)
3	QUE	C	342	-	21,24,24	1.87	5 (23%)	28,36,36	2.72	9 (32%)
2	NAP	D	338	-	45,52,52	1.63	4 (8%)	56,80,80	1.90	15 (26%)
3	QUE	C	341	-	21,24,24	1.75	5 (23%)	28,36,36	1.84	8 (28%)
2	NAP	F	338	-	45,52,52	1.72	4 (8%)	56,80,80	1.59	13 (23%)
2	NAP	C	338	-	45,52,52	1.73	5 (11%)	56,80,80	1.79	13 (23%)
3	QUE	F	341	-	21,24,24	2.26	4 (19%)	28,36,36	2.11	9 (32%)
2	NAP	E	338	-	45,52,52	1.68	5 (11%)	56,80,80	2.37	21 (37%)
2	NAP	B	338	-	45,52,52	1.80	5 (11%)	56,80,80	1.64	7 (12%)
3	QUE	F	342	-	21,24,24	1.85	5 (23%)	28,36,36	2.25	11 (39%)
2	NAP	A	338	-	45,52,52	1.80	4 (8%)	56,80,80	1.31	7 (12%)
3	QUE	B	341	-	21,24,24	1.65	3 (14%)	28,36,36	1.94	4 (14%)
3	QUE	D	342	-	21,24,24	2.32	5 (23%)	28,36,36	2.02	8 (28%)
3	QUE	D	341	-	21,24,24	2.19	4 (19%)	28,36,36	2.15	8 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	QUE	B	342	-	-	3/4/4/4	0/3/3/3
3	QUE	A	342	-	-	2/4/4/4	0/3/3/3
3	QUE	C	342	-	-	2/4/4/4	0/3/3/3
2	NAP	D	338	-	-	4/31/67/67	0/5/5/5
3	QUE	C	341	-	-	2/4/4/4	0/3/3/3
2	NAP	F	338	-	-	7/31/67/67	0/5/5/5
2	NAP	C	338	-	-	5/31/67/67	0/5/5/5
3	QUE	F	341	-	-	2/4/4/4	0/3/3/3
2	NAP	E	338	-	-	13/31/67/67	0/5/5/5
2	NAP	B	338	-	-	6/31/67/67	0/5/5/5
3	QUE	F	342	-	-	2/4/4/4	0/3/3/3
2	NAP	A	338	-	-	4/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	QUE	B	341	-	-	2/4/4/4	0/3/3/3
3	QUE	D	342	-	-	2/4/4/4	0/3/3/3
3	QUE	D	341	-	-	2/4/4/4	0/3/3/3

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	338	NAP	O7N-C7N	9.12	1.41	1.24
2	A	338	NAP	O7N-C7N	9.01	1.41	1.24
2	F	338	NAP	O7N-C7N	8.86	1.41	1.24
2	D	338	NAP	O7N-C7N	8.41	1.40	1.24
2	E	338	NAP	O7N-C7N	8.22	1.39	1.24
2	C	338	NAP	O7N-C7N	7.40	1.38	1.24
3	D	342	QUE	C3-C4	6.87	1.50	1.41
3	F	341	QUE	C3-C4	6.39	1.50	1.41
3	D	341	QUE	C3-C4	6.09	1.49	1.41
3	F	341	QUE	C18-C17	5.59	1.49	1.40
3	D	341	QUE	C18-C17	5.41	1.48	1.40
3	B	342	QUE	C3-C4	5.36	1.48	1.41
3	A	342	QUE	C3-C4	5.21	1.48	1.41
2	C	338	NAP	C2A-N3A	4.84	1.39	1.32
3	D	342	QUE	C2-C3	4.83	1.52	1.43
2	A	338	NAP	C2A-N3A	4.77	1.39	1.32
3	B	341	QUE	C18-C17	4.68	1.47	1.40
3	A	342	QUE	C18-C17	4.60	1.47	1.40
3	B	342	QUE	C18-C17	4.53	1.47	1.40
3	F	342	QUE	C18-C17	4.46	1.47	1.40
3	F	341	QUE	C2-C3	4.39	1.51	1.43
3	C	341	QUE	C18-C17	4.34	1.47	1.40
3	B	342	QUE	C2-C3	4.31	1.51	1.43
3	D	342	QUE	C18-C17	4.28	1.47	1.40
3	C	342	QUE	C2-C3	4.26	1.50	1.43
3	C	342	QUE	C3-C4	4.24	1.47	1.41
2	E	338	NAP	C2A-N3A	4.19	1.38	1.32
3	B	341	QUE	C3-C4	4.16	1.47	1.41
3	C	341	QUE	C3-C4	4.03	1.46	1.41
3	F	342	QUE	C3-C4	4.02	1.46	1.41
3	C	342	QUE	C18-C17	4.00	1.46	1.40
3	D	341	QUE	C2-C3	3.99	1.50	1.43
2	B	338	NAP	C2A-N3A	3.95	1.38	1.32
2	F	338	NAP	C2A-N3A	3.75	1.38	1.32
2	D	338	NAP	C2A-N3A	3.70	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	342	QUE	C2-C3	3.58	1.49	1.43
3	A	342	QUE	C2-C3	3.40	1.49	1.43
2	A	338	NAP	C2A-N1A	3.31	1.40	1.33
2	F	338	NAP	C2A-N1A	3.17	1.39	1.33
3	C	341	QUE	C14-C11	3.07	1.51	1.46
2	C	338	NAP	C2A-N1A	2.97	1.39	1.33
3	C	341	QUE	C2-C3	2.94	1.48	1.43
2	F	338	NAP	C2N-N1N	2.91	1.38	1.35
3	A	342	QUE	C14-C11	2.86	1.51	1.46
3	F	342	QUE	C14-C11	2.80	1.51	1.46
2	E	338	NAP	C2N-N1N	2.72	1.38	1.35
2	E	338	NAP	C2A-N1A	2.62	1.38	1.33
3	D	342	QUE	C14-C11	2.59	1.50	1.46
2	B	338	NAP	C2A-N1A	2.57	1.38	1.33
3	C	341	QUE	C9-C10	2.55	1.50	1.41
3	D	341	QUE	C9-C10	2.50	1.49	1.41
2	B	338	NAP	O4B-C1B	-2.48	1.37	1.41
3	F	342	QUE	C9-C10	2.45	1.49	1.41
3	C	342	QUE	C9-C10	2.44	1.49	1.41
3	B	341	QUE	C2-C3	2.39	1.47	1.43
2	C	338	NAP	P2B-O2B	2.38	1.63	1.59
2	D	338	NAP	C2A-N1A	2.34	1.38	1.33
3	A	342	QUE	C9-C10	2.26	1.49	1.41
2	B	338	NAP	O4B-C4B	-2.17	1.40	1.45
3	A	342	QUE	C5-C6	2.16	1.41	1.37
2	D	338	NAP	C2N-N1N	2.16	1.37	1.35
3	F	341	QUE	C9-C10	2.15	1.48	1.41
3	C	342	QUE	C14-C11	2.06	1.49	1.46
2	A	338	NAP	O4D-C4D	-2.02	1.40	1.45
2	C	338	NAP	C3B-C2B	-2.01	1.48	1.52
2	E	338	NAP	C2N-C3N	2.01	1.42	1.39
3	D	342	QUE	C9-C10	2.00	1.48	1.41

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	342	QUE	C15-C14-C11	7.49	130.74	120.29
3	A	342	QUE	C15-C14-C11	7.06	130.14	120.29
2	D	338	NAP	N3A-C2A-N1A	-6.89	117.91	128.68
2	E	338	NAP	N3A-C2A-N1A	-6.74	118.14	128.68
3	B	341	QUE	O12-C4-C5	6.32	123.51	116.11
3	C	342	QUE	C19-C14-C11	-6.20	111.64	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	338	NAP	C1B-N9A-C4A	-6.01	116.08	126.64
2	B	338	NAP	N3A-C2A-N1A	-5.92	119.43	128.68
3	B	342	QUE	C5-C4-C3	-5.83	116.60	123.05
3	B	341	QUE	C5-C4-C3	-5.62	116.83	123.05
2	E	338	NAP	C3N-C7N-N7N	5.43	124.26	117.75
3	A	342	QUE	C19-C14-C11	-5.40	112.75	120.29
3	D	341	QUE	C15-C14-C11	-5.27	112.93	120.29
3	D	341	QUE	C5-C4-C3	-5.07	117.43	123.05
2	E	338	NAP	O7N-C7N-C3N	-4.99	113.66	119.63
3	D	342	QUE	O12-C4-C5	4.98	121.94	116.11
3	C	341	QUE	O12-C4-C5	4.97	121.93	116.11
2	C	338	NAP	C3N-C7N-N7N	4.76	123.46	117.75
2	D	338	NAP	C1B-N9A-C4A	-4.76	118.28	126.64
2	C	338	NAP	O7N-C7N-N7N	-4.67	115.94	122.58
2	E	338	NAP	C2N-C3N-C4N	4.64	123.51	118.26
3	A	342	QUE	C5-C4-C3	-4.62	117.94	123.05
3	F	342	QUE	C15-C14-C11	4.57	126.67	120.29
3	C	342	QUE	C5-C4-C3	-4.50	118.06	123.05
3	F	342	QUE	C9-C3-C2	4.46	129.49	121.85
3	F	341	QUE	C5-C4-C3	-4.40	118.18	123.05
3	F	341	QUE	C19-C18-C17	-4.33	116.04	119.86
3	C	342	QUE	O12-C4-C5	4.32	121.17	116.11
3	C	342	QUE	C16-C17-C18	-4.23	115.02	119.67
3	F	342	QUE	O12-C4-C5	4.22	121.05	116.11
3	C	341	QUE	C5-C4-C3	-4.10	118.51	123.05
2	E	338	NAP	C1B-N9A-C4A	-4.10	119.44	126.64
3	D	341	QUE	O12-C4-C5	4.07	120.88	116.11
3	A	342	QUE	C14-C19-C18	4.01	123.87	120.68
2	F	338	NAP	C3N-C2N-N1N	-3.98	116.53	120.43
3	B	342	QUE	O23-C18-C19	3.96	130.07	119.46
2	E	338	NAP	C4N-C3N-C7N	-3.95	110.47	121.04
3	D	342	QUE	C5-C4-C3	-3.93	118.70	123.05
3	D	342	QUE	C14-C19-C18	3.89	123.78	120.68
3	B	342	QUE	C9-C3-C2	3.87	128.49	121.85
3	A	342	QUE	O12-C4-C5	3.84	120.60	116.11
2	E	338	NAP	O2X-P2B-O1X	3.80	125.56	110.68
3	D	341	QUE	C19-C14-C11	3.78	125.56	120.29
3	F	341	QUE	C1-C2-C3	-3.77	116.24	120.61
3	C	342	QUE	O24-C17-C16	3.76	129.56	119.33
2	F	338	NAP	C3N-C7N-N7N	3.74	122.24	117.75
3	D	342	QUE	C19-C18-C17	-3.66	116.63	119.86
2	E	338	NAP	C2N-N1N-C1D	3.65	127.27	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	338	NAP	O5B-C5B-C4B	-3.64	96.47	108.99
3	B	342	QUE	O12-C4-C5	3.63	120.36	116.11
2	E	338	NAP	O2X-P2B-O2B	-3.63	89.74	105.99
2	B	338	NAP	O5D-PN-O1N	3.61	123.18	109.07
3	F	342	QUE	O24-C17-C16	3.61	129.14	119.33
3	F	341	QUE	O12-C4-C5	3.58	120.30	116.11
2	E	338	NAP	C5N-C4N-C3N	-3.48	116.22	120.34
2	A	338	NAP	O7N-C7N-C3N	-3.47	115.47	119.63
2	D	338	NAP	O2X-P2B-O1X	3.44	124.13	110.68
3	F	342	QUE	C19-C14-C11	-3.41	115.53	120.29
3	D	342	QUE	O23-C18-C19	3.36	128.47	119.46
2	E	338	NAP	O4D-C1D-C2D	-3.31	102.09	106.93
3	C	342	QUE	C14-C19-C18	3.30	123.31	120.68
2	C	338	NAP	C5A-C6A-N6A	-3.26	115.39	120.35
2	A	338	NAP	N3A-C2A-N1A	-3.19	123.69	128.68
2	C	338	NAP	C1B-N9A-C4A	-3.17	121.07	126.64
3	C	341	QUE	C9-C3-C2	3.17	127.28	121.85
2	E	338	NAP	O2B-C2B-C1B	-3.12	98.87	110.10
3	B	341	QUE	C16-C17-C18	-3.07	116.29	119.67
2	F	338	NAP	C2N-C3N-C4N	3.06	121.72	118.26
2	F	338	NAP	O5D-PN-O1N	3.04	120.93	109.07
3	F	341	QUE	C15-C14-C11	-3.03	116.07	120.29
2	F	338	NAP	O5D-C5D-C4D	2.99	119.27	108.99
2	D	338	NAP	C5A-C6A-N6A	2.95	124.83	120.35
2	D	338	NAP	C6N-N1N-C2N	-2.90	119.33	121.97
2	C	338	NAP	O4B-C1B-C2B	2.87	111.57	106.59
2	D	338	NAP	C2N-C3N-C4N	2.85	121.49	118.26
3	F	342	QUE	C5-C4-C3	-2.82	119.93	123.05
3	B	341	QUE	C10-C9-C3	-2.81	117.44	121.38
2	F	338	NAP	O5B-PA-O1A	2.79	119.98	109.07
3	D	341	QUE	C19-C18-C17	-2.79	117.40	119.86
3	D	342	QUE	C9-C3-C2	2.76	126.57	121.85
2	F	338	NAP	C4N-C3N-C7N	-2.75	113.68	121.04
3	A	342	QUE	C19-C18-C17	-2.73	117.45	119.86
2	E	338	NAP	C6N-N1N-C2N	-2.73	119.48	121.97
2	E	338	NAP	O3X-P2B-O2B	2.71	118.14	105.99
3	F	341	QUE	C5-C6-C1	2.70	123.12	120.94
2	A	338	NAP	C3N-C7N-N7N	2.69	120.97	117.75
3	A	342	QUE	O24-C17-C16	2.68	126.62	119.33
3	D	341	QUE	C10-C9-C3	-2.65	117.67	121.38
3	F	342	QUE	O29-C6-C1	2.59	126.59	119.84
2	A	338	NAP	O2D-C2D-C3D	2.59	120.21	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	338	NAP	O2B-C2B-C3B	-2.59	102.30	111.68
3	D	342	QUE	C5-C6-C1	2.59	123.03	120.94
2	C	338	NAP	O2B-C2B-C3B	-2.58	102.34	111.68
3	F	341	QUE	C2-C1-C6	2.57	122.03	119.70
2	F	338	NAP	C2N-N1N-C1D	2.52	124.75	119.14
3	B	342	QUE	C6-C5-C4	2.49	123.92	120.42
3	B	342	QUE	O23-C18-C17	-2.46	111.89	118.45
3	A	342	QUE	C9-C3-C2	2.45	126.05	121.85
2	A	338	NAP	C3D-C2D-C1D	-2.41	97.35	100.98
2	F	338	NAP	O2A-PA-O1A	2.41	124.14	112.24
3	F	342	QUE	O29-C6-C5	-2.40	114.08	120.98
2	E	338	NAP	C3N-C2N-N1N	-2.40	118.09	120.43
2	E	338	NAP	O3D-C3D-C4D	-2.39	104.12	111.05
2	D	338	NAP	C5B-C4B-C3B	-2.38	106.25	115.18
2	A	338	NAP	C3B-C2B-C1B	2.37	107.35	102.89
3	F	341	QUE	C19-C14-C11	2.37	123.60	120.29
3	D	341	QUE	C15-C14-C19	2.36	121.50	118.16
3	C	342	QUE	C15-C16-C17	2.36	122.93	120.50
3	F	342	QUE	O24-C17-C18	-2.33	112.25	118.45
3	A	342	QUE	C6-C5-C4	2.32	123.68	120.42
3	C	341	QUE	C6-C5-C4	2.32	123.68	120.42
2	B	338	NAP	O4D-C1D-C2D	-2.32	103.54	106.93
2	C	338	NAP	O3B-C3B-C4B	2.31	117.72	111.05
2	E	338	NAP	O4B-C4B-C3B	2.31	109.68	105.11
2	F	338	NAP	O7N-C7N-C3N	-2.31	116.87	119.63
2	D	338	NAP	C3N-C7N-N7N	2.29	120.49	117.75
3	F	341	QUE	O24-C17-C18	2.27	124.50	118.45
2	C	338	NAP	N6A-C6A-N1A	2.27	123.28	118.57
2	F	338	NAP	N3A-C2A-N1A	-2.26	125.15	128.68
3	C	341	QUE	C2-C1-C6	2.26	121.74	119.70
3	A	342	QUE	C10-C9-C3	-2.25	118.23	121.38
3	D	342	QUE	O24-C17-C16	2.24	125.42	119.33
2	F	338	NAP	O2D-C2D-C1D	2.24	119.12	110.85
2	E	338	NAP	C3B-C2B-C1B	2.23	107.08	102.89
3	C	341	QUE	C5-C6-C1	-2.21	119.15	120.94
2	E	338	NAP	O2A-PA-O5B	2.19	117.92	107.75
2	B	338	NAP	C3N-C7N-N7N	2.18	120.37	117.75
2	D	338	NAP	O4B-C4B-C5B	2.18	116.53	109.37
3	C	342	QUE	C9-C3-C2	2.17	125.56	121.85
2	C	338	NAP	C3N-C2N-N1N	-2.16	118.32	120.43
3	C	341	QUE	C15-C14-C11	2.15	123.29	120.29
2	C	338	NAP	C2N-C3N-C4N	2.14	120.68	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	338	NAP	O7N-C7N-C3N	-2.14	117.08	119.63
2	E	338	NAP	O4D-C4D-C3D	-2.11	100.94	105.11
2	C	338	NAP	N3A-C2A-N1A	-2.09	125.41	128.68
2	C	338	NAP	O5B-PA-O1A	2.09	117.22	109.07
2	D	338	NAP	O7N-C7N-N7N	-2.08	119.62	122.58
2	F	338	NAP	C3B-C2B-C1B	2.08	106.80	102.89
3	B	342	QUE	C19-C18-C17	-2.07	118.03	119.86
3	C	341	QUE	C14-C19-C18	2.07	122.33	120.68
2	E	338	NAP	C2N-C3N-C7N	2.07	125.47	119.46
2	D	338	NAP	C4A-C5A-N7A	-2.06	107.25	109.40
3	F	342	QUE	C6-C5-C4	2.06	123.31	120.42
2	D	338	NAP	C4N-C3N-C7N	-2.05	115.54	121.04
3	F	342	QUE	O12-C4-C3	-2.05	119.02	121.03
3	D	341	QUE	C9-C3-C2	2.05	125.36	121.85
3	B	342	QUE	O12-C4-C3	2.04	123.05	121.03
2	D	338	NAP	C3B-C2B-C1B	2.03	106.71	102.89
2	D	338	NAP	C2D-C3D-C4D	2.03	106.59	102.64
3	B	342	QUE	O24-C17-C16	2.02	124.82	119.33
2	A	338	NAP	N6A-C6A-N1A	2.01	122.75	118.57
2	D	338	NAP	C2N-N1N-C1D	2.00	123.59	119.14

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	342	QUE	C10-C11-C14-C15
3	C	342	QUE	C10-C11-C14-C15
2	F	338	NAP	C2B-O2B-P2B-O3X
2	F	338	NAP	O4D-C1D-N1N-C2N
2	C	338	NAP	C5D-O5D-PN-O2N
2	E	338	NAP	C5D-O5D-PN-O2N
2	E	338	NAP	O4D-C1D-N1N-C2N
2	E	338	NAP	O4D-C1D-N1N-C6N
2	E	338	NAP	C2D-C1D-N1N-C2N
2	E	338	NAP	C2D-C1D-N1N-C6N
2	B	338	NAP	C2B-O2B-P2B-O3X
3	F	342	QUE	C10-C11-C14-C15
3	F	342	QUE	C10-C11-C14-C19
2	A	338	NAP	C2B-O2B-P2B-O3X
2	A	338	NAP	O4D-C1D-N1N-C2N
3	D	342	QUE	C10-C11-C14-C19
3	D	341	QUE	O12-C11-C14-C15

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Mol	Chain	Res	Type	Atoms
3	D	341	QUE	O12-C11-C14-C19
2	F	338	NAP	O4D-C4D-C5D-O5D
2	E	338	NAP	C4N-C3N-C7N-N7N
3	C	342	QUE	C10-C11-C14-C19
2	E	338	NAP	C4N-C3N-C7N-O7N
3	C	341	QUE	O12-C11-C14-C15
3	C	341	QUE	O12-C11-C14-C19
3	F	341	QUE	O12-C11-C14-C15
3	F	341	QUE	O12-C11-C14-C19
2	F	338	NAP	C3D-C4D-C5D-O5D
3	B	341	QUE	O12-C11-C14-C15
3	B	341	QUE	O12-C11-C14-C19
3	D	342	QUE	C10-C11-C14-C15
2	E	338	NAP	C2N-C3N-C7N-O7N
2	F	338	NAP	PN-O3-PA-O1A
3	B	342	QUE	C10-C11-C14-C15
3	B	342	QUE	C10-C11-C14-C19
3	A	342	QUE	C10-C11-C14-C19
2	E	338	NAP	C2N-C3N-C7N-N7N
2	B	338	NAP	O4B-C4B-C5B-O5B
2	D	338	NAP	C2B-O2B-P2B-O3X
2	E	338	NAP	C5D-O5D-PN-O3
2	B	338	NAP	C2B-O2B-P2B-O2X
2	D	338	NAP	PN-O3-PA-O2A
2	B	338	NAP	PN-O3-PA-O2A
2	B	338	NAP	O4D-C4D-C5D-O5D
2	D	338	NAP	PN-O3-PA-O1A
2	F	338	NAP	PN-O3-PA-O2A
2	C	338	NAP	PN-O3-PA-O2A
2	E	338	NAP	C2B-O2B-P2B-O2X
2	A	338	NAP	C2B-O2B-P2B-O2X
2	D	338	NAP	O4B-C4B-C5B-O5B
2	C	338	NAP	O4B-C4B-C5B-O5B
2	E	338	NAP	O4B-C4B-C5B-O5B
2	A	338	NAP	O4B-C4B-C5B-O5B
2	C	338	NAP	PN-O3-PA-O1A
2	B	338	NAP	PN-O3-PA-O1A
2	C	338	NAP	C5D-O5D-PN-O1N
2	E	338	NAP	C5D-O5D-PN-O1N
2	F	338	NAP	O4B-C4B-C5B-O5B
3	B	342	QUE	O12-C11-C14-C15

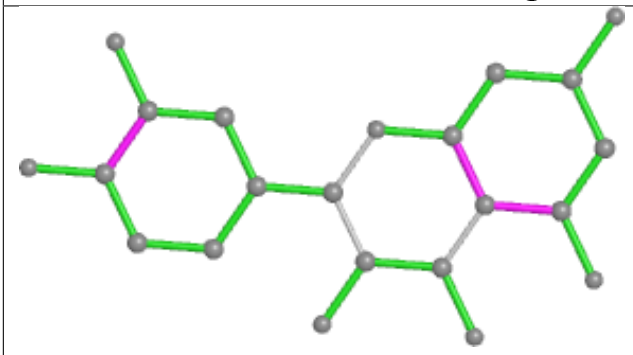
There are no ring outliers.

11 monomers are involved in 29 short contacts:

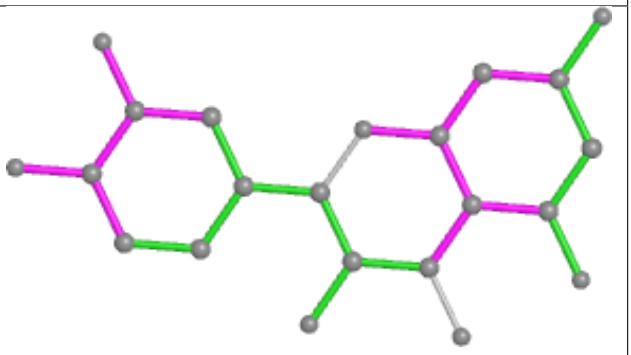
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	342	QUE	3	0
2	D	338	NAP	3	0
2	F	338	NAP	2	0
2	C	338	NAP	5	0
3	F	341	QUE	1	0
2	E	338	NAP	6	0
2	B	338	NAP	1	0
3	F	342	QUE	4	0
2	A	338	NAP	1	0
3	B	341	QUE	1	0
3	D	342	QUE	2	0

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 then 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.

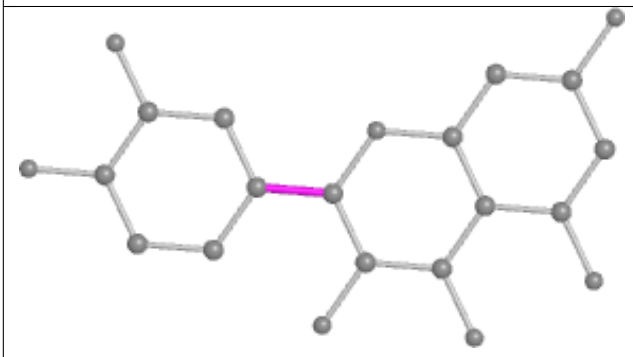
Ligand QUE B 342



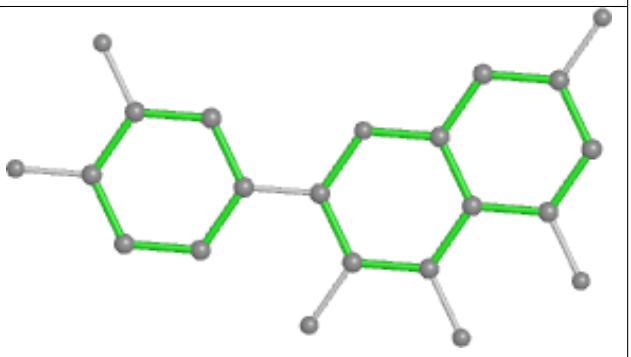
Bond lengths



Bond angles

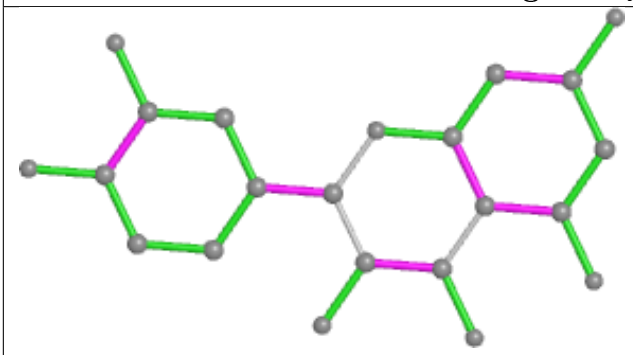


Torsions

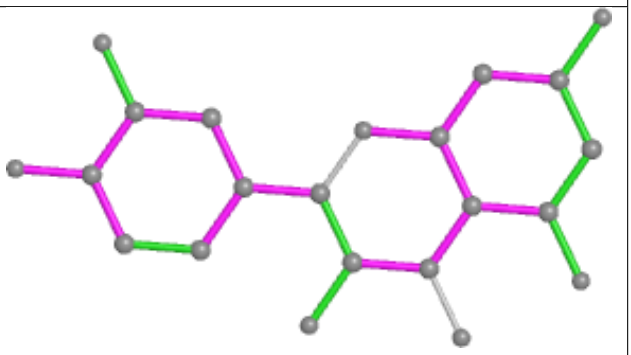


Rings

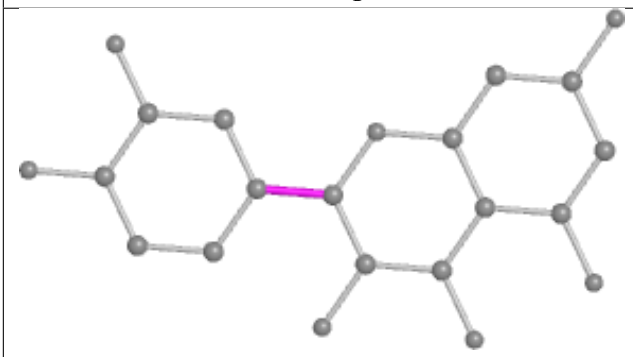
Ligand QUE A 342



Bond lengths



Bond angles



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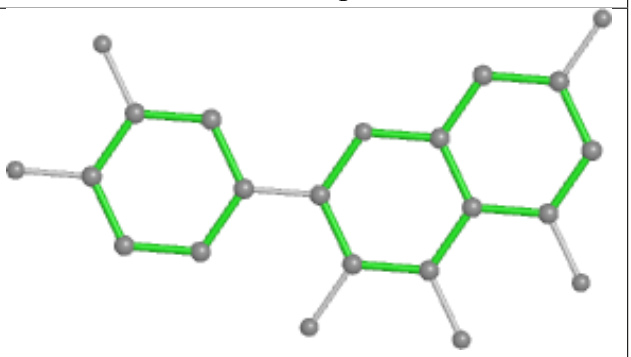
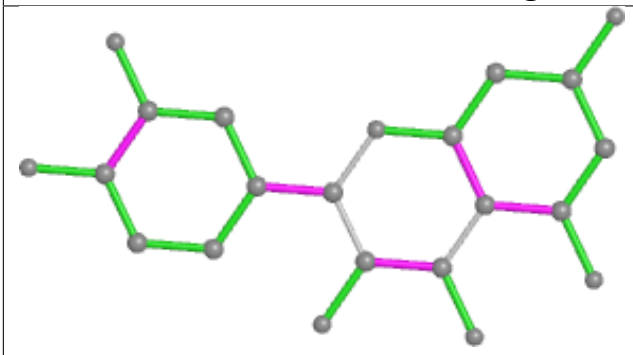


Rings

Ligand QUE C 342



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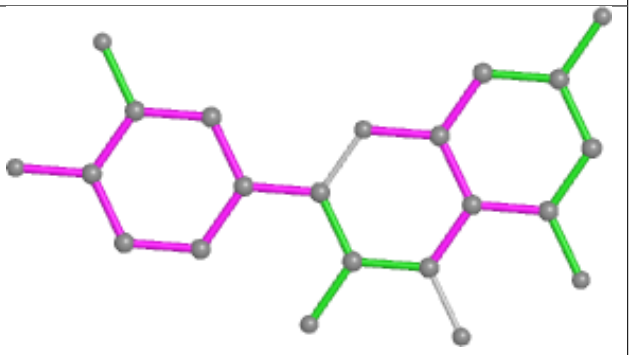
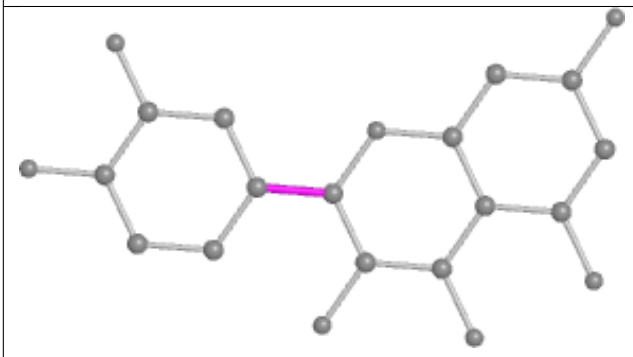
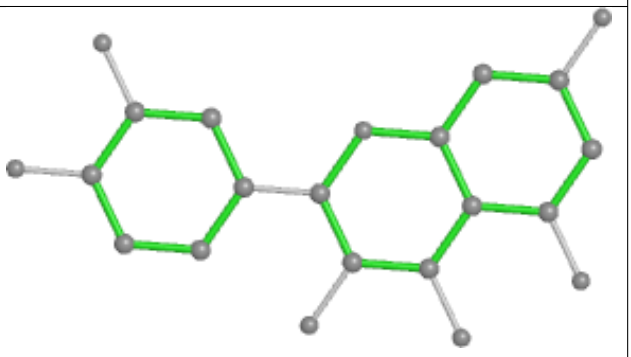


Bond angles

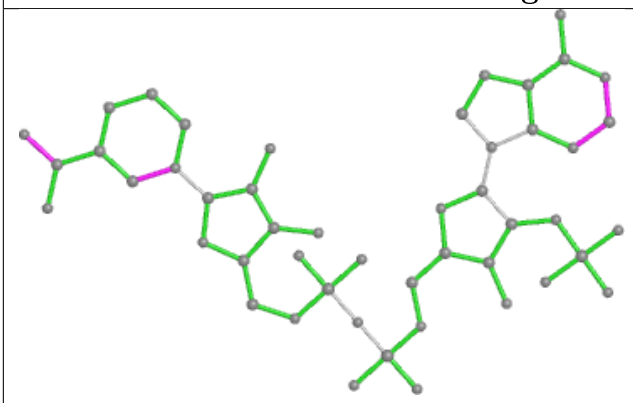


Torsions



Rings

Ligand NAP D 338



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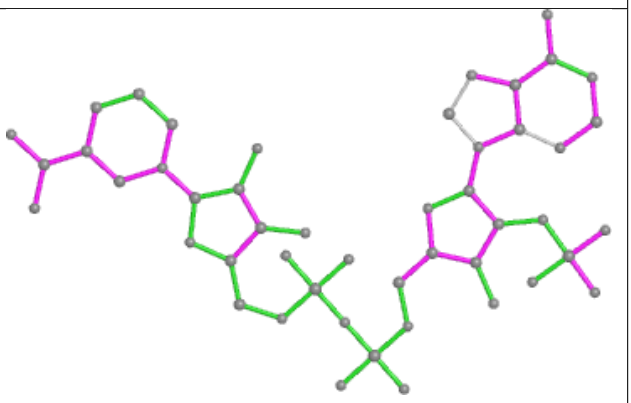
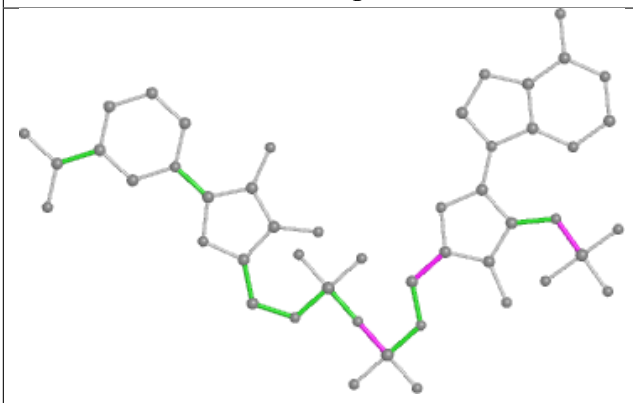
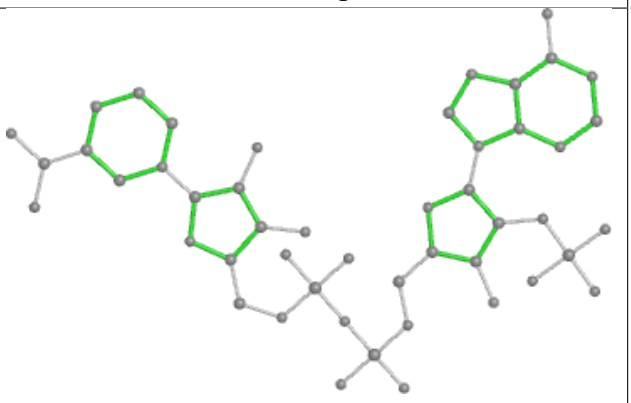


Bond angles

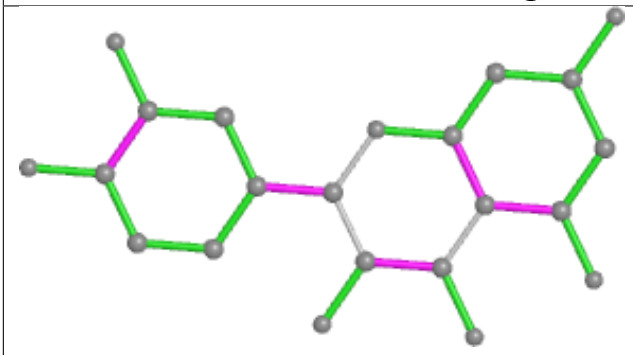


Torsions

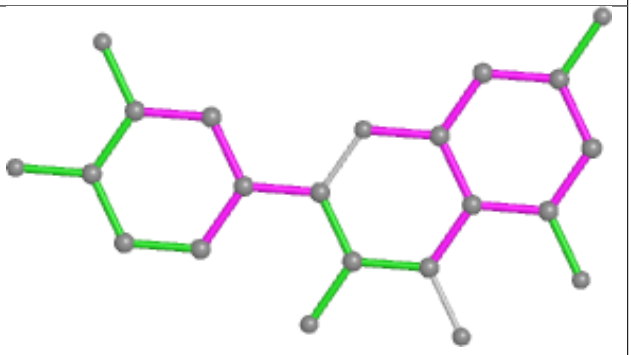


Rings

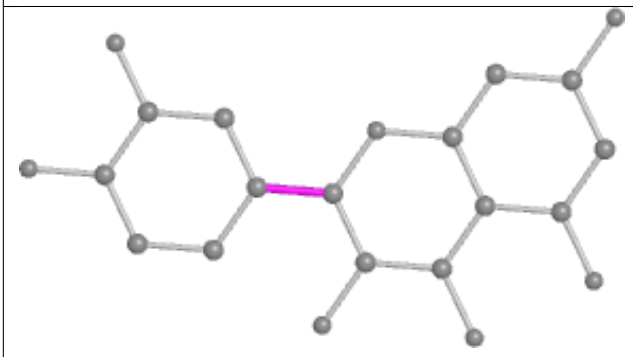
Ligand QUE C 341



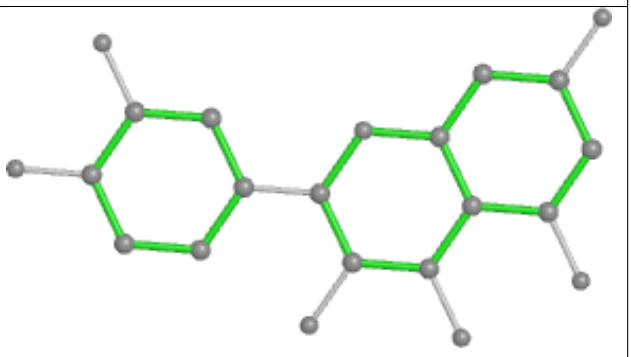
Bond lengths



Bond angles

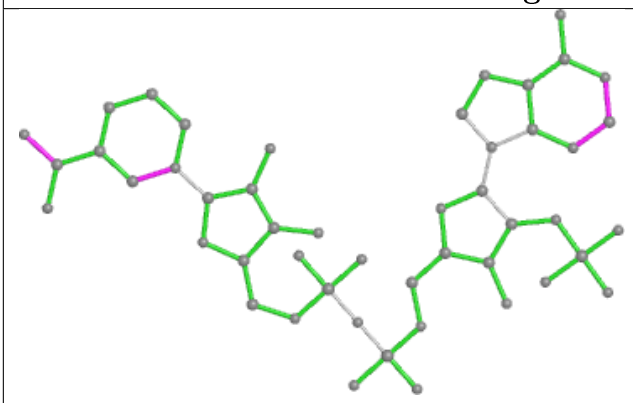


Torsions



Rings

Ligand NAP F 338



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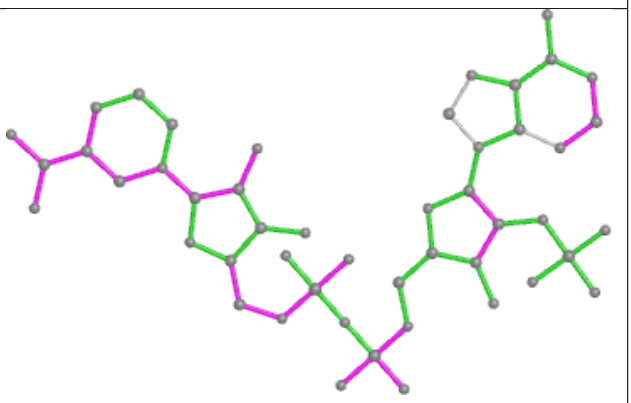
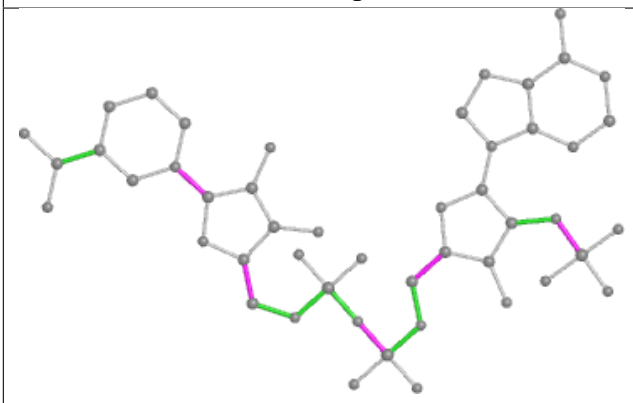


Bond angles



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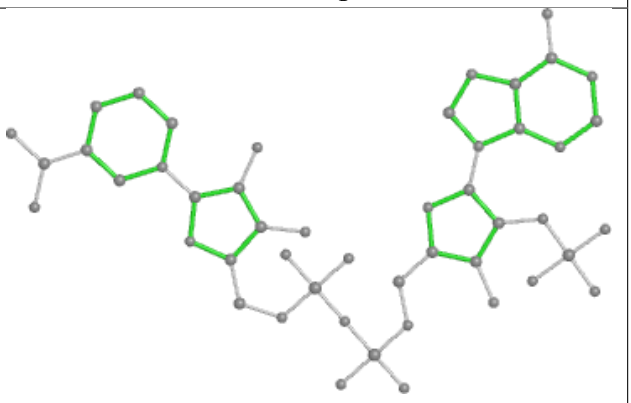
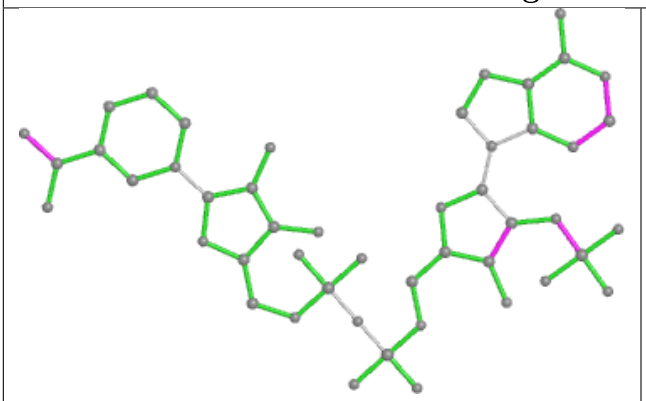


Rings

Ligand NAP C 338



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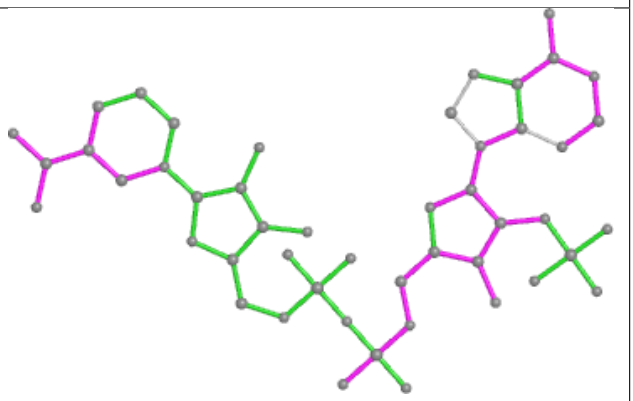
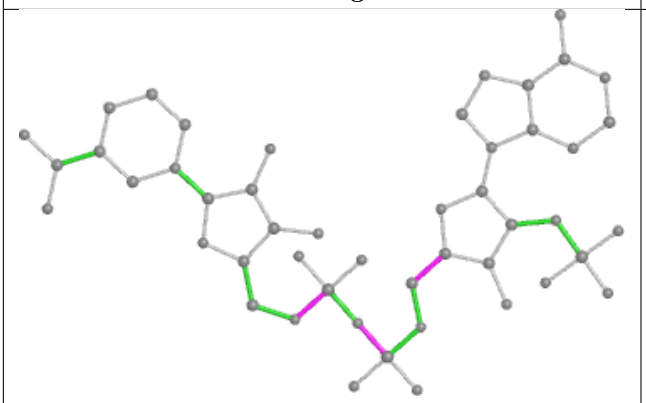


Bond angles



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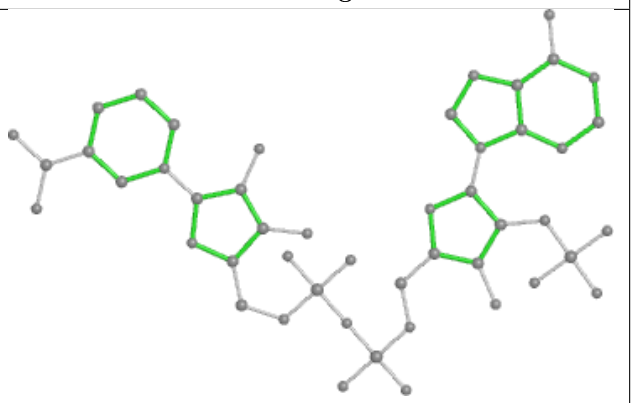
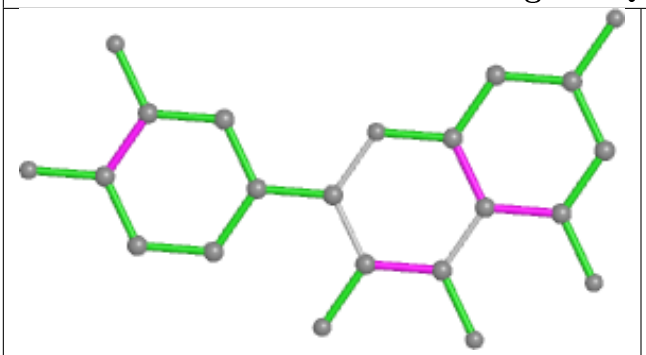
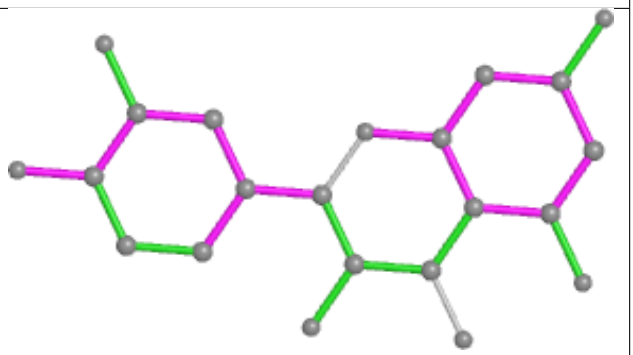


Rings

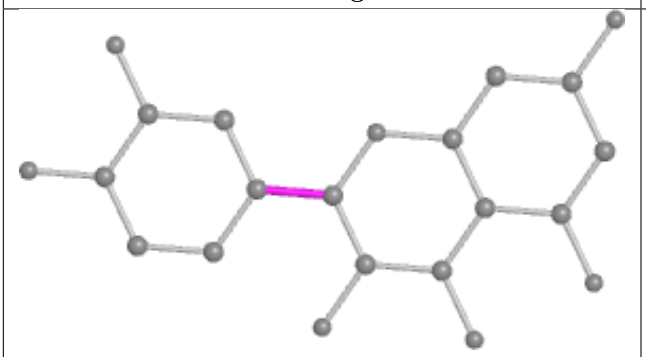
Ligand QUE F 341



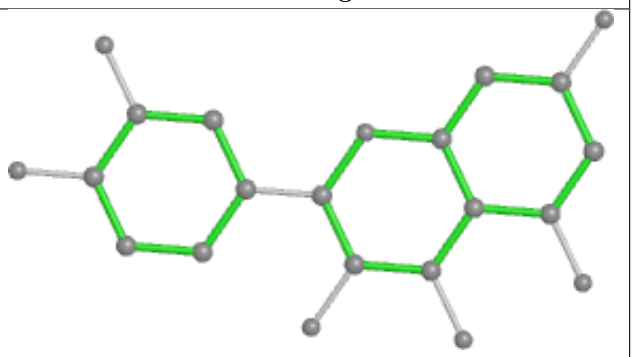
Bond lengths



Bond angles

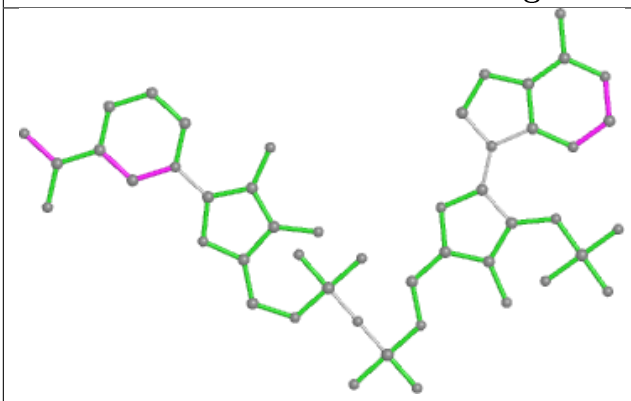


Torsions

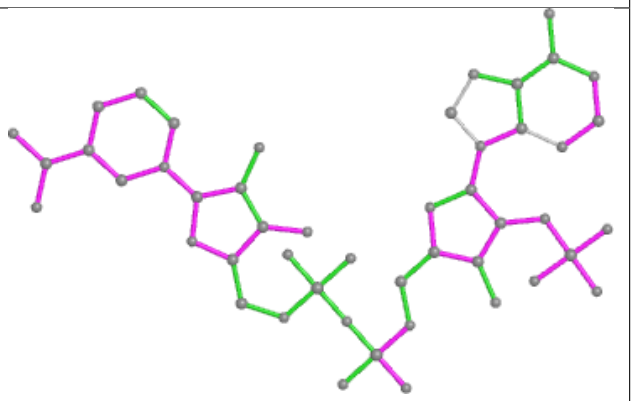


Rings

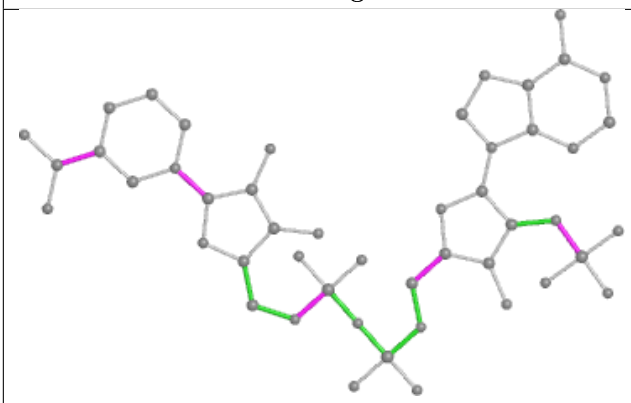
Ligand NAP E 338



Bond lengths



Bond angles



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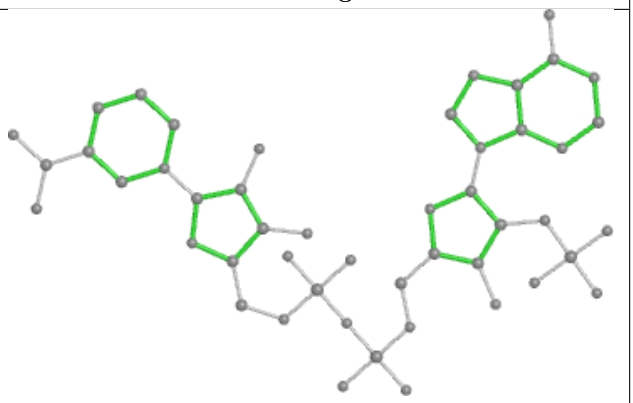
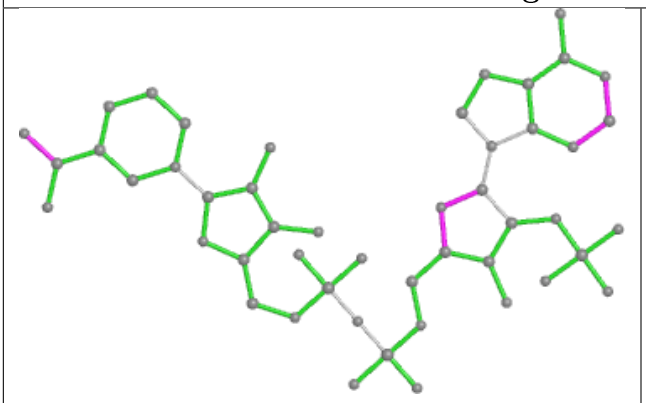


Rings

Ligand NAP B 338



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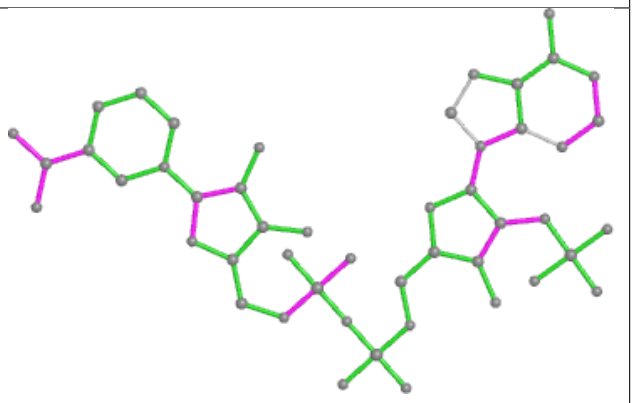
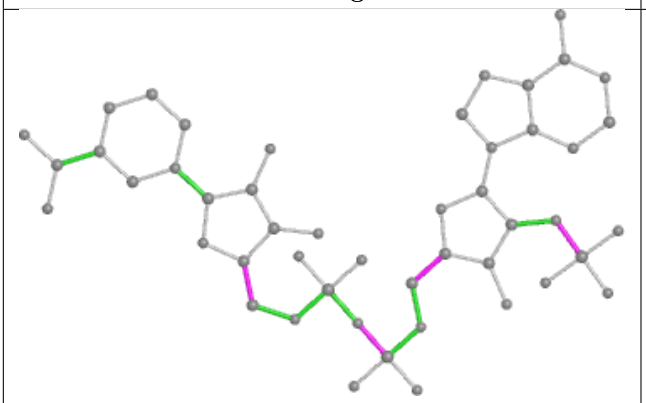


Bond angles



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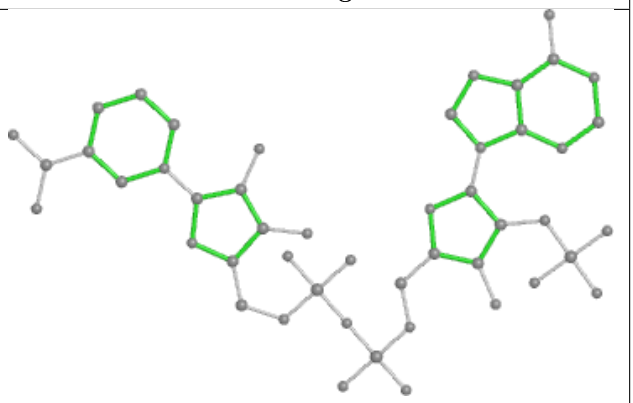
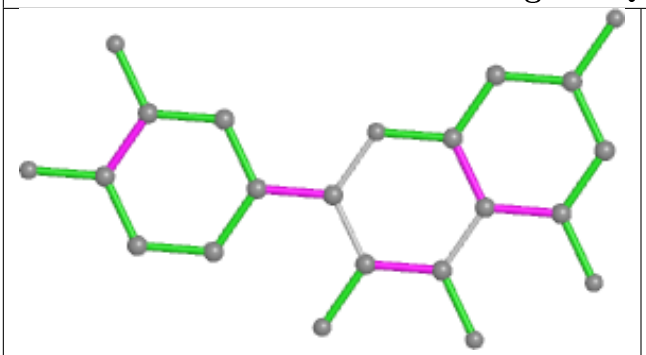
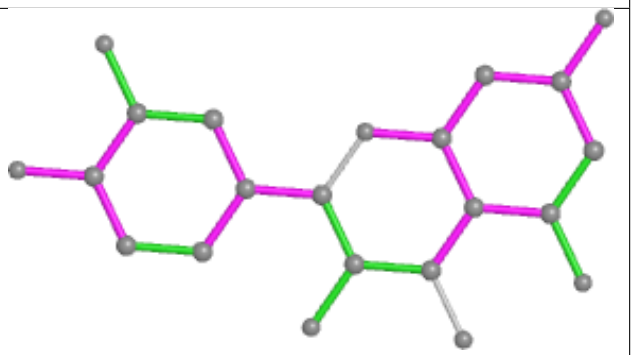


Rings

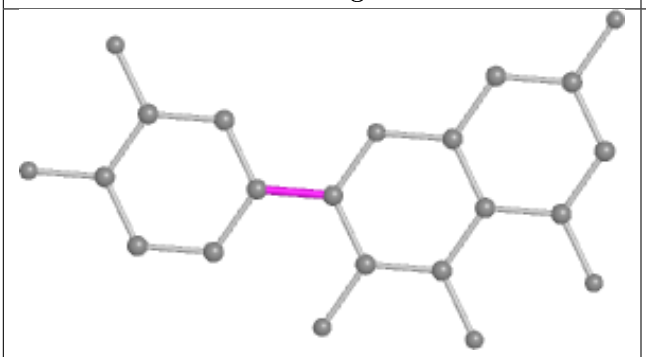
Ligand QUE F 342



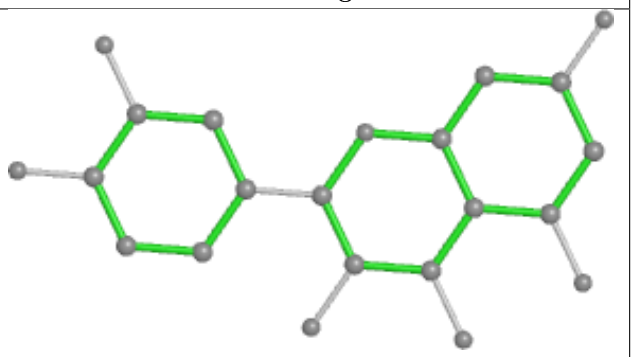
Bond lengths



Bond angles

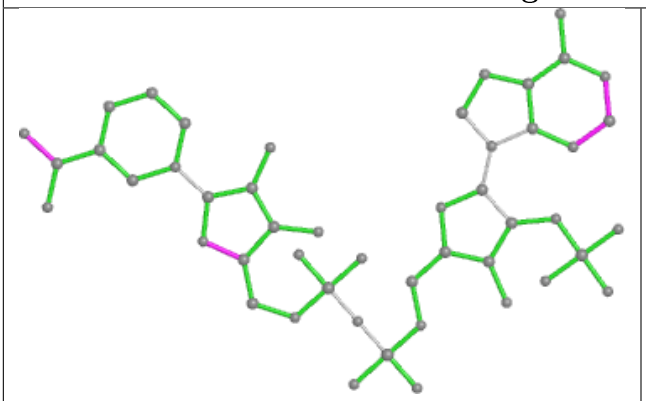


Torsions

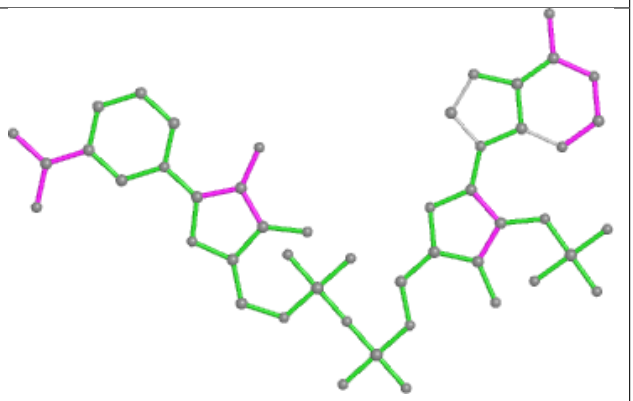


Rings

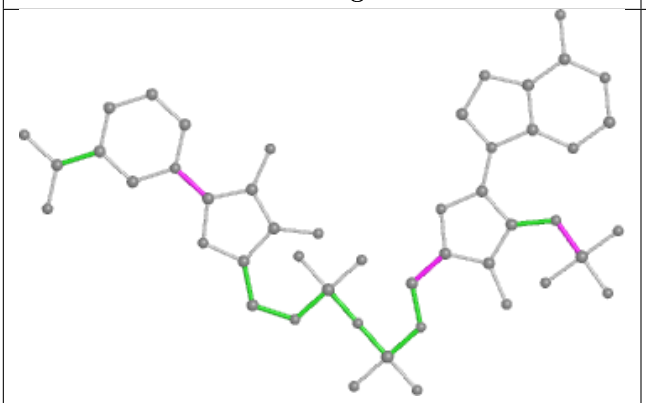
Ligand NAP A 338



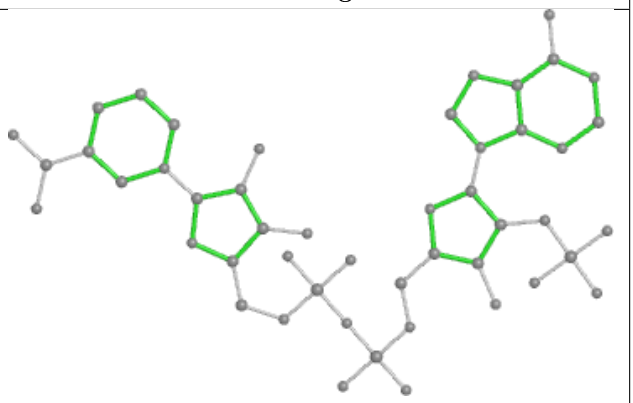
Bond lengths



Bond angles

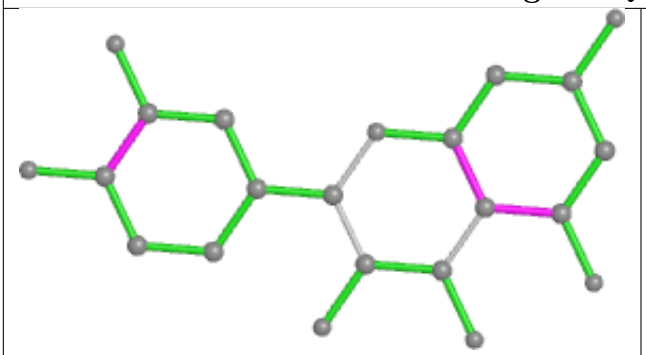


Torsions

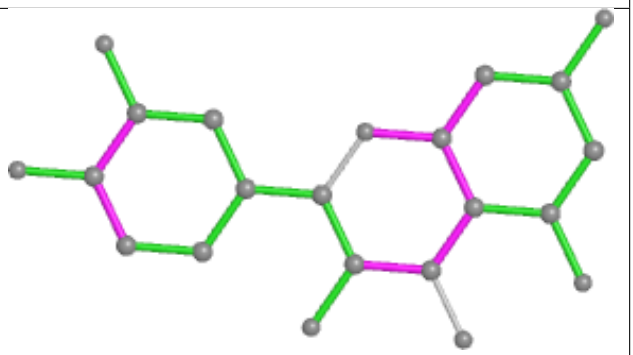


Rings

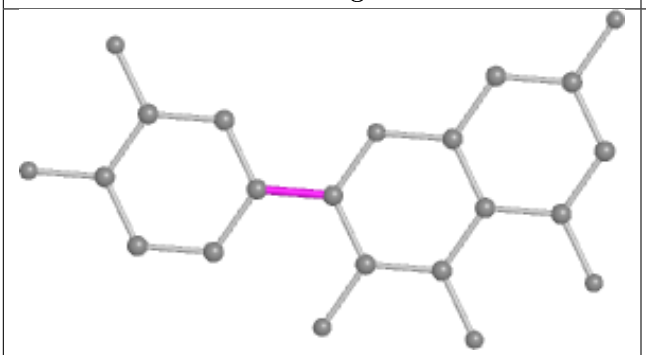
Ligand QUE B 341



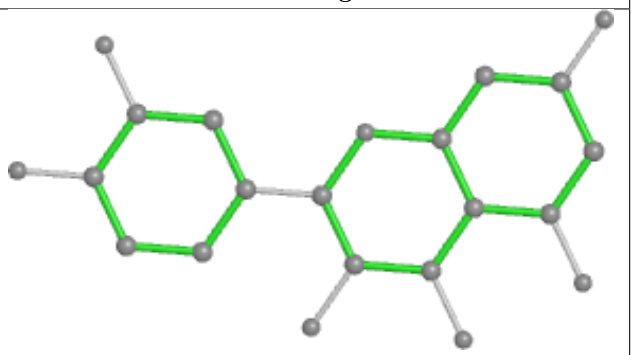
Bond lengths



Bond angles

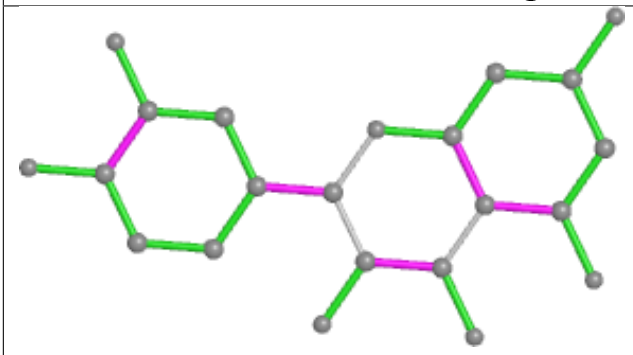


Torsions

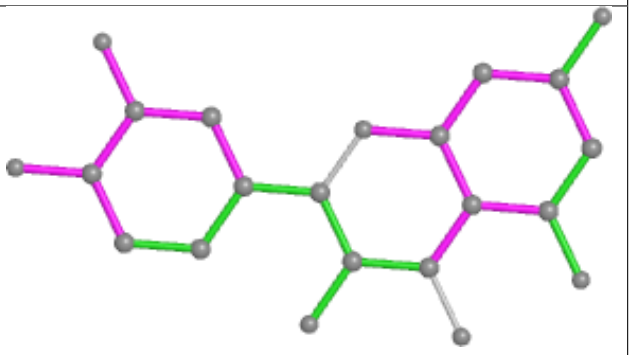


Rings

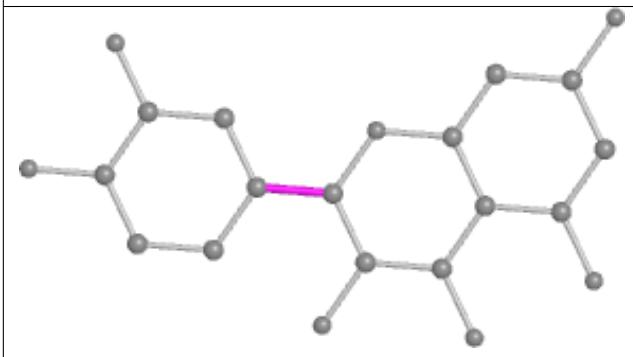
Ligand QUE D 342



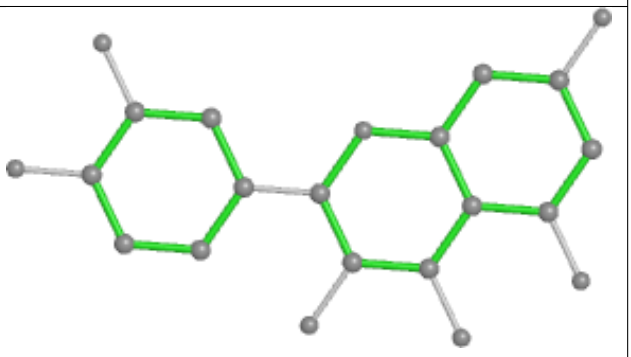
Bond lengths



Bond angles

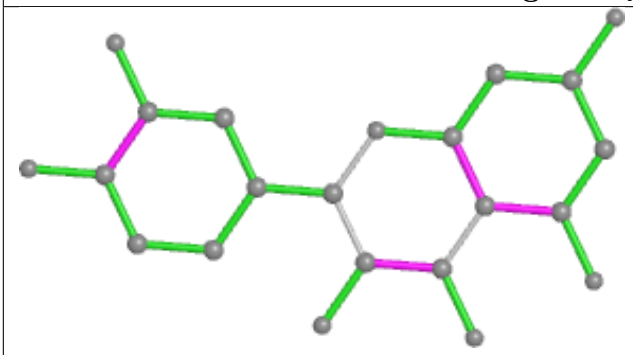


Torsions

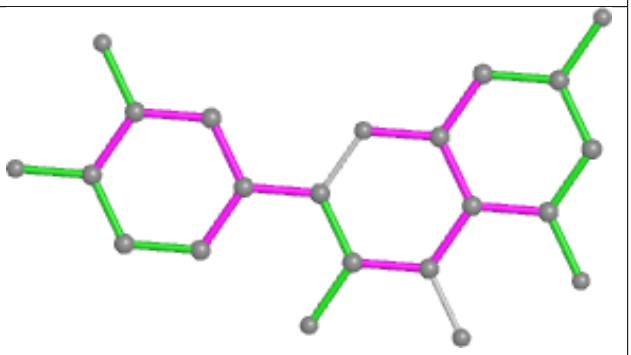


Rings

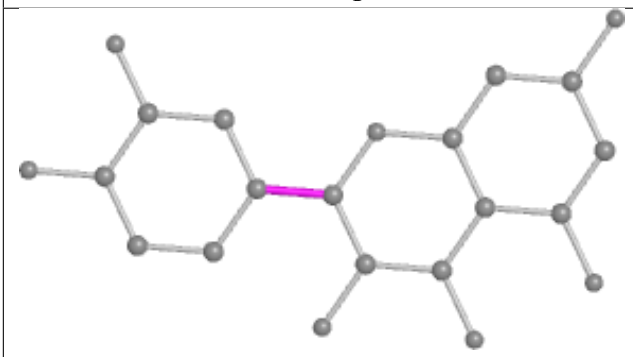
Ligand QUE D 341



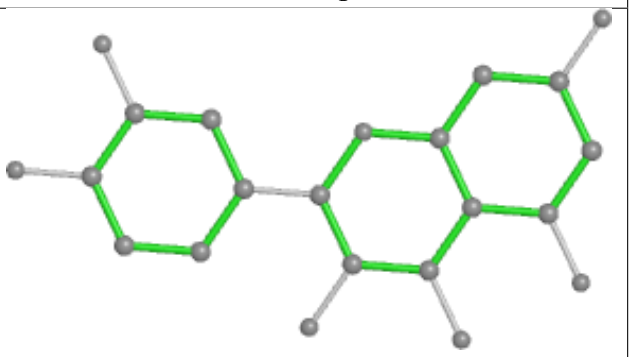
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	324/337 (96%)	0.46	11 (3%) 45 40	14, 28, 41, 46	0
1	B	324/337 (96%)	0.19	1 (0%) 94 94	4, 20, 38, 43	0
1	C	324/337 (96%)	0.18	2 (0%) 89 89	4, 19, 38, 42	0
1	D	324/337 (96%)	0.89	33 (10%) 6 5	13, 28, 42, 47	0
1	E	324/337 (96%)	0.97	40 (12%) 4 3	13, 29, 43, 48	0
1	F	324/337 (96%)	0.37	8 (2%) 57 55	12, 28, 42, 46	0
All	All	1944/2022 (96%)	0.51	95 (4%) 29 26	4, 26, 41, 48	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	ASN	4.7
1	D	120	VAL	4.5
1	D	278	THR	4.5
1	D	230	HIS	4.4
1	E	20	TRP	4.4
1	E	308	LEU	4.1
1	D	266	MET	3.8
1	E	278	THR	3.7
1	E	119	THR	3.7
1	D	88	MET	3.5
1	E	266	MET	3.5
1	E	184	ASP	3.5
1	E	329	HIS	3.4
1	D	121	ARG	3.4
1	F	55	GLU	3.3
1	D	251	TYR	3.3
1	E	201	SER	3.2
1	D	201	SER	3.2
1	E	253	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	78	CYS	3.2
1	E	52	PRO	3.1
1	E	189	ILE	3.1
1	D	79	THR	3.1
1	A	87	PRO	3.0
1	E	141	VAL	3.0
1	D	119	THR	3.0
1	E	313	THR	2.9
1	D	75	ILE	2.9
1	D	188	ILE	2.9
1	D	6	GLU	2.9
1	E	230	HIS	2.9
1	D	303	GLU	2.8
1	D	203	PRO	2.8
1	F	323	GLY	2.8
1	D	242	PHE	2.8
1	D	204	PRO	2.8
1	D	7	THR	2.8
1	D	57	HIS	2.7
1	F	129	ALA	2.7
1	D	160	ALA	2.7
1	E	160	ALA	2.7
1	E	238	HIS	2.7
1	D	19	SER	2.6
1	B	6	GLU	2.6
1	A	317	ASP	2.6
1	D	72	ASP	2.6
1	D	200	SER	2.6
1	E	34	ALA	2.6
1	E	306	TYR	2.6
1	A	183	ILE	2.6
1	E	255	SER	2.6
1	E	113	SER	2.5
1	E	267	LEU	2.5
1	F	182	ASN	2.5
1	E	327	PRO	2.5
1	E	88	MET	2.5
1	D	63	ALA	2.4
1	E	247	ALA	2.4
1	E	268	ARG	2.4
1	C	77	GLY	2.4
1	E	51	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	204	PRO	2.4
1	E	242	PHE	2.4
1	D	24	ARG	2.4
1	A	297	LEU	2.3
1	A	41	ASN	2.3
1	E	123	LEU	2.3
1	D	238	HIS	2.3
1	A	45	VAL	2.2
1	E	234	LEU	2.2
1	D	180	GLU	2.2
1	A	328	SER	2.2
1	E	31	THR	2.2
1	C	32	VAL	2.2
1	E	121	ARG	2.2
1	F	199	MET	2.2
1	A	168	THR	2.2
1	E	57	HIS	2.2
1	F	327	PRO	2.2
1	E	9	CYS	2.2
1	E	30	TYR	2.2
1	E	45	VAL	2.2
1	D	306	TYR	2.2
1	D	174	ALA	2.1
1	D	184	ASP	2.1
1	E	32	VAL	2.1
1	E	245	PRO	2.1
1	D	30	TYR	2.1
1	E	120	VAL	2.1
1	F	126	THR	2.0
1	D	326	PRO	2.0
1	A	282	GLY	2.0
1	A	40	THR	2.0
1	D	80	GLY	2.0
1	F	269	GLU	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 carbohydrates in this entry.

6.4 Ligands (i)

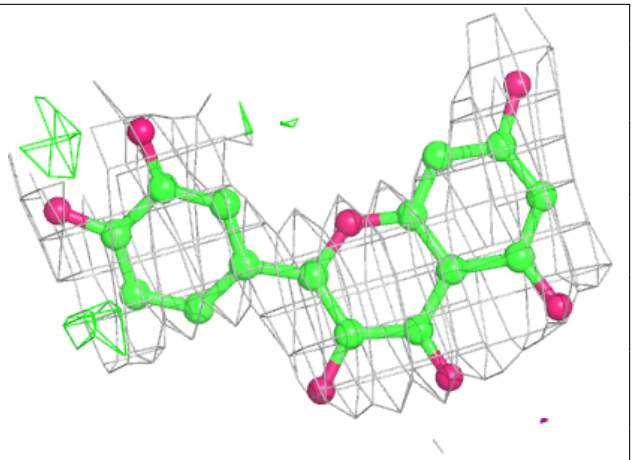
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

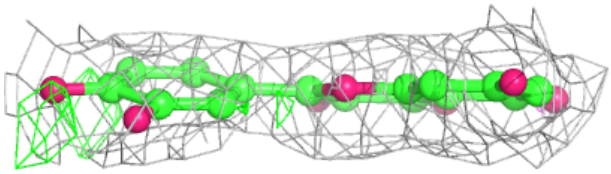
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	QUE	F	342	22/22	0.84	0.26	22,23,23,24	0
3	QUE	D	342	22/22	0.85	0.31	24,24,25,25	0
3	QUE	F	341	22/22	0.88	0.34	18,19,20,21	0
3	QUE	C	342	22/22	0.89	0.24	10,12,13,13	0
3	QUE	A	342	22/22	0.89	0.21	18,19,20,20	0
3	QUE	D	341	22/22	0.90	0.32	24,25,26,26	0
2	NAP	A	338	48/48	0.92	0.22	17,20,26,27	0
3	QUE	B	342	22/22	0.93	0.23	11,11,12,13	0
2	NAP	E	338	48/48	0.93	0.19	14,17,21,21	0
2	NAP	F	338	48/48	0.93	0.20	14,18,21,22	0
2	NAP	D	338	48/48	0.94	0.20	11,18,21,22	0
3	QUE	B	341	22/22	0.94	0.23	11,11,12,12	0
3	QUE	C	341	22/22	0.95	0.26	8,9,10,10	0
2	NAP	B	338	48/48	0.96	0.17	4,6,13,14	0
2	NAP	C	338	48/48	0.97	0.17	4,4,9,10	0

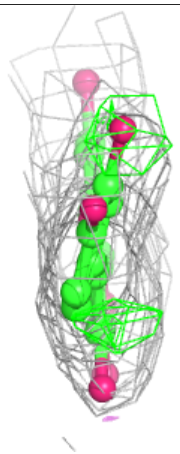
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QUE F 342:

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

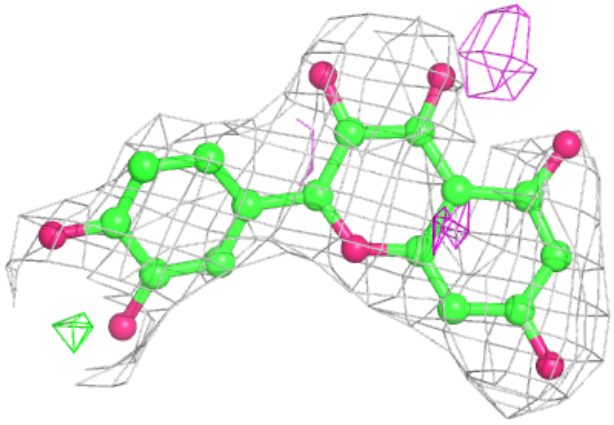


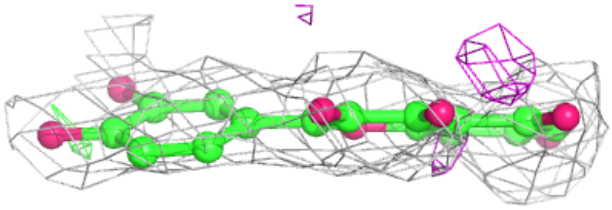




Electron density around QUE D 342:

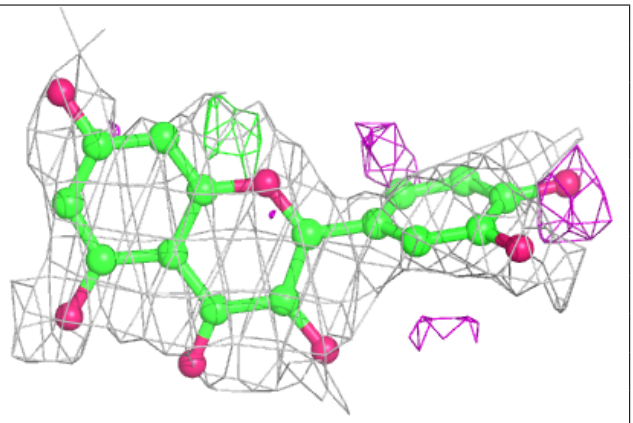
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

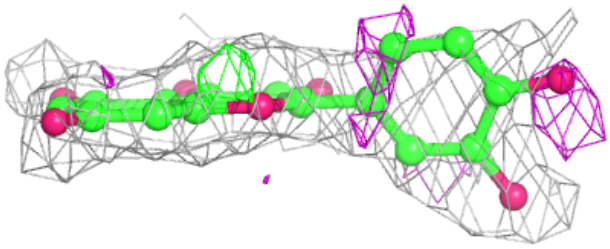


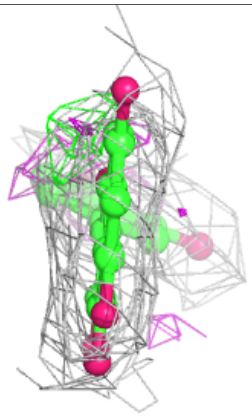


Electron density around QUE F 341:

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

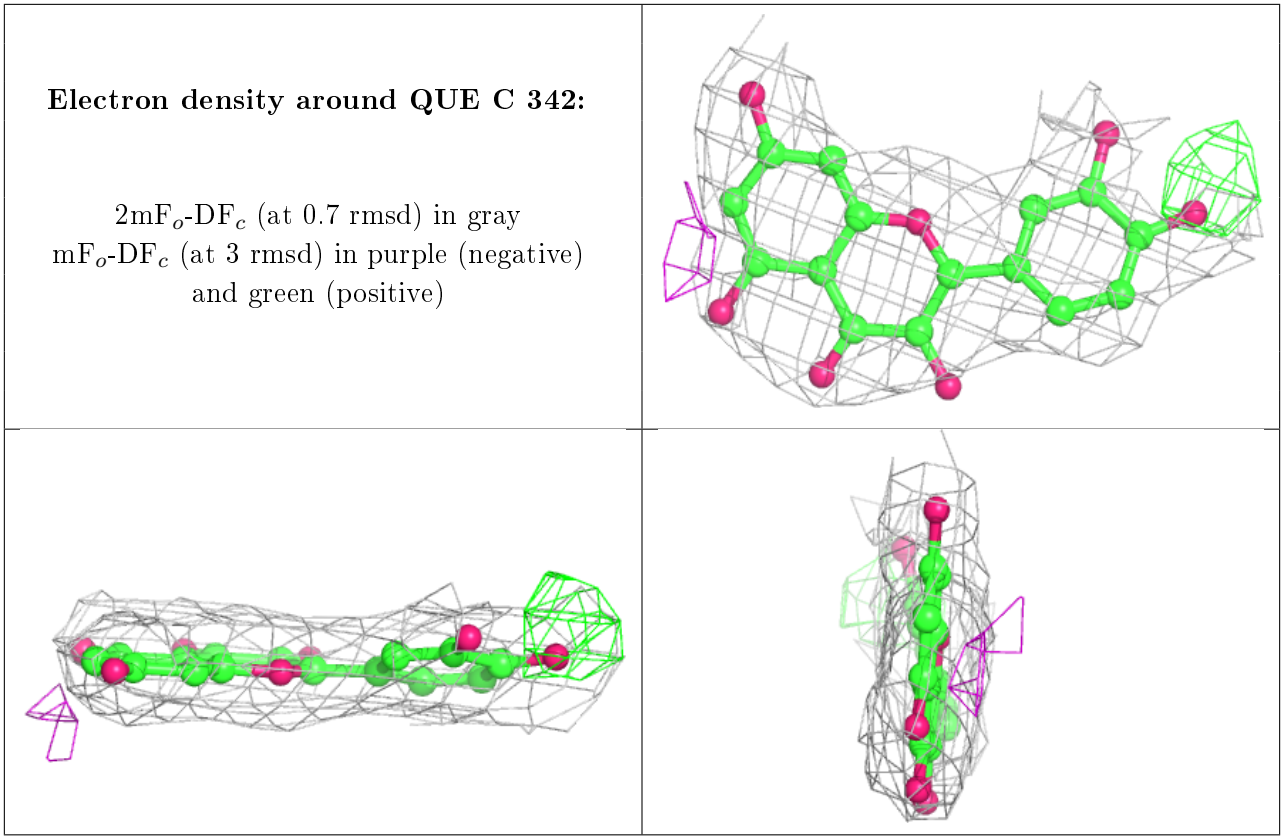






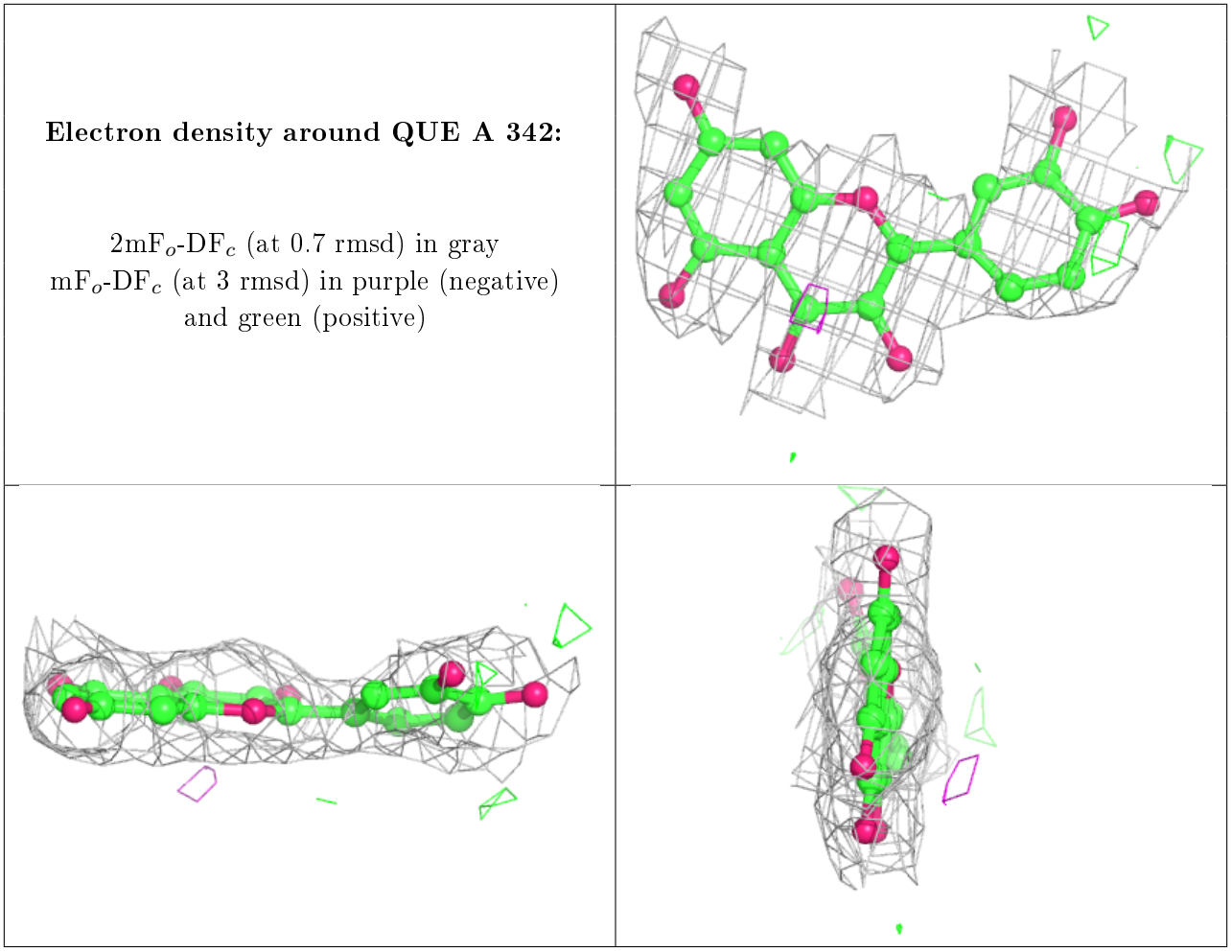
Electron density around QUE C 342:

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



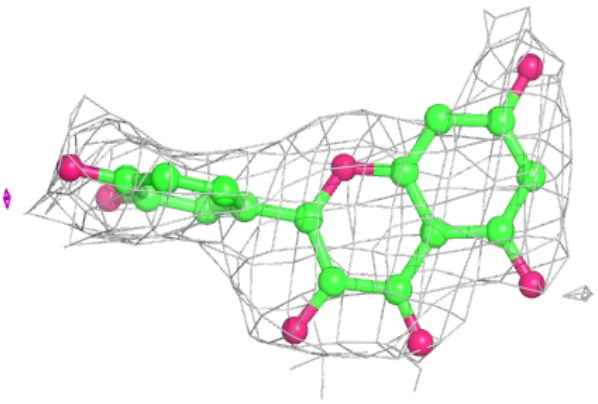
Electron density around QUE A 342:

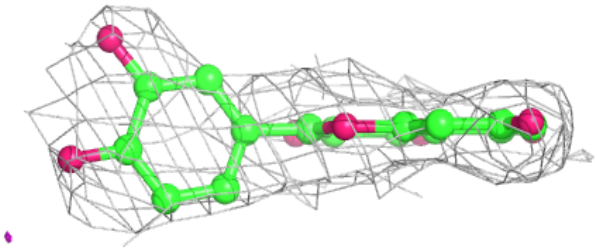
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

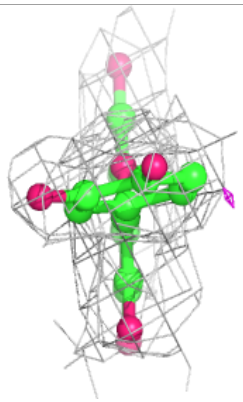


Electron density around QUE D 341:

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

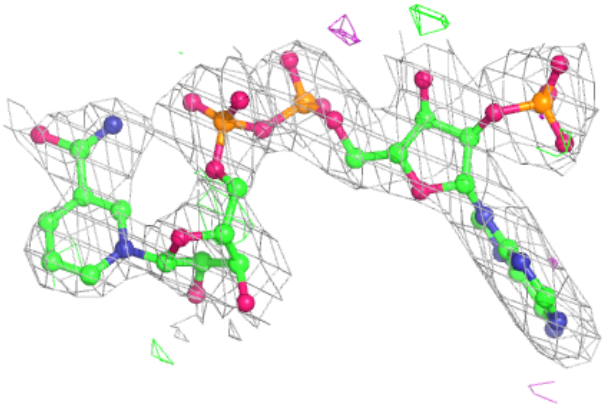


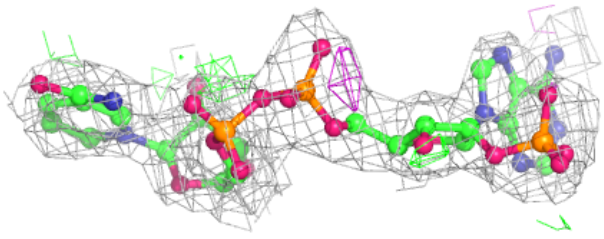


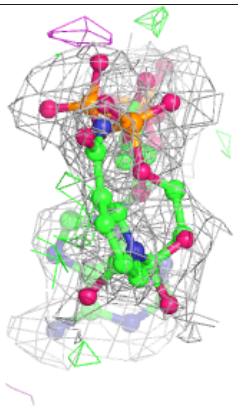


Electron density around NAP A 338:

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

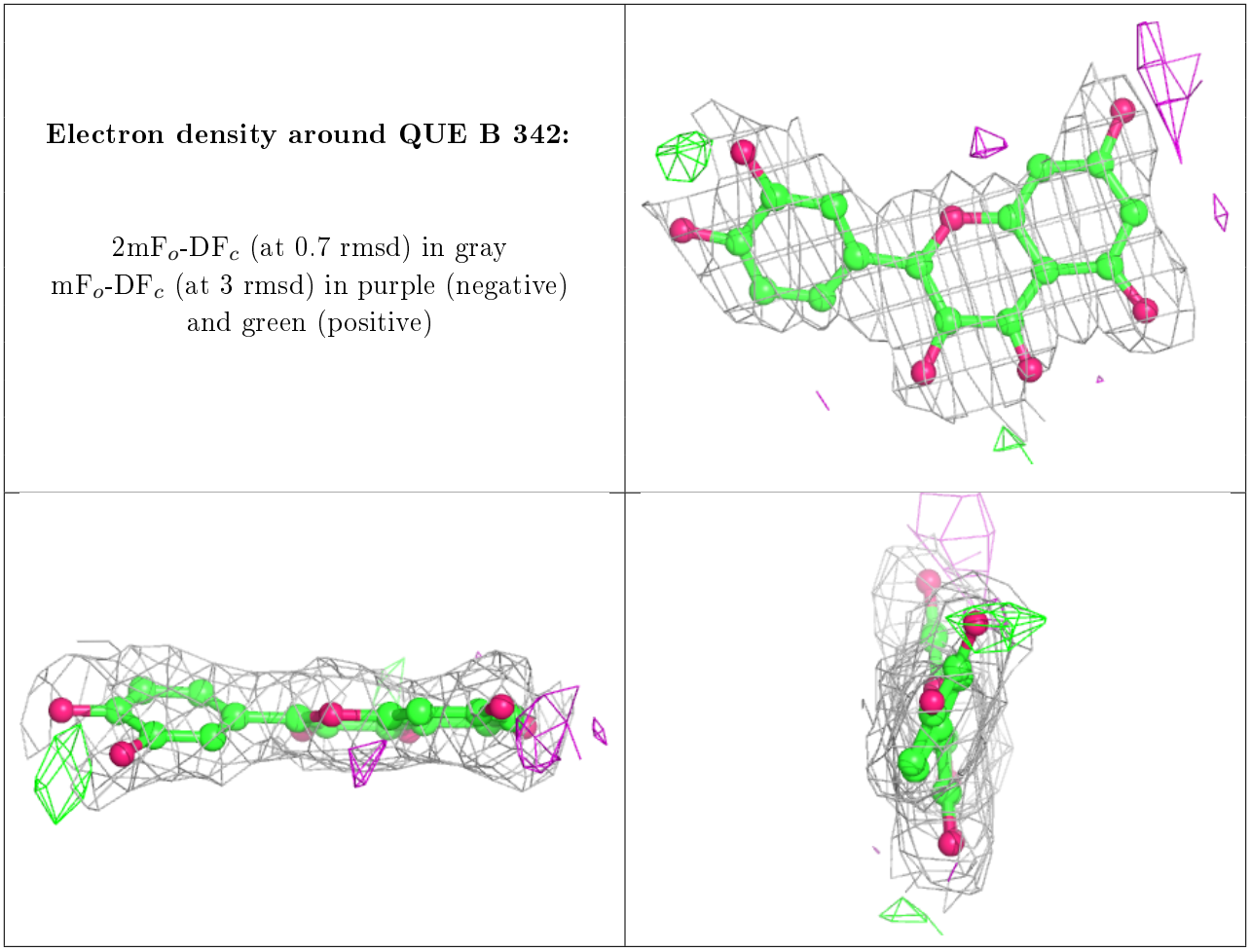






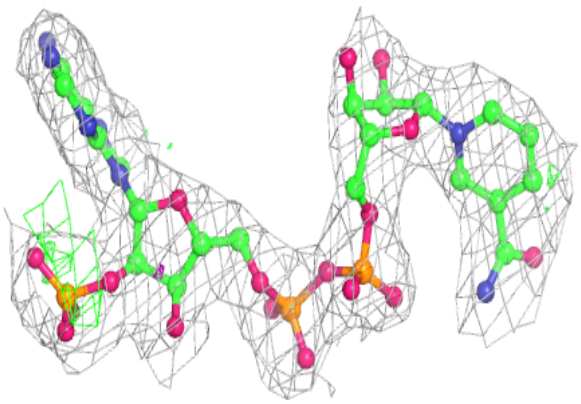
Electron density around QUE B 342:

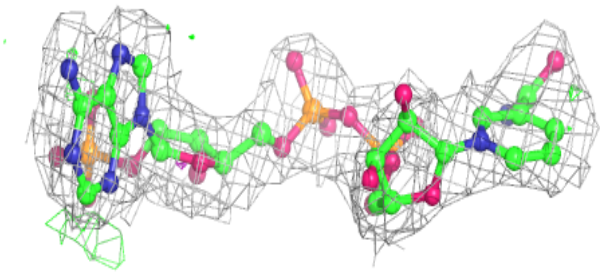
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

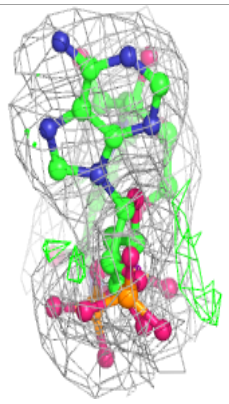


Electron density around NAP E 338:

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

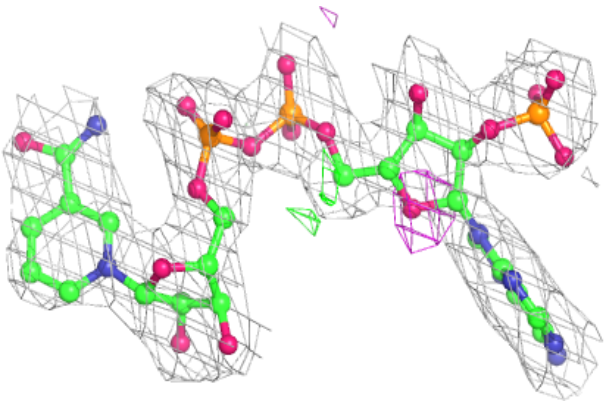


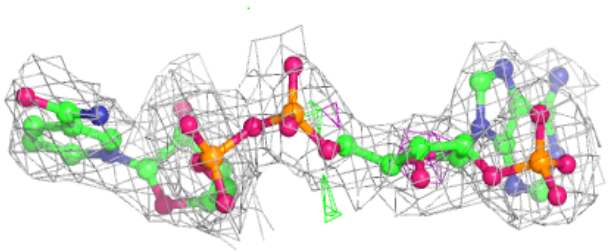


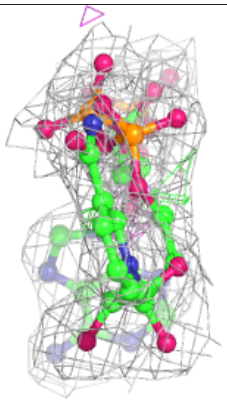


Electron density around NAP F 338:

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

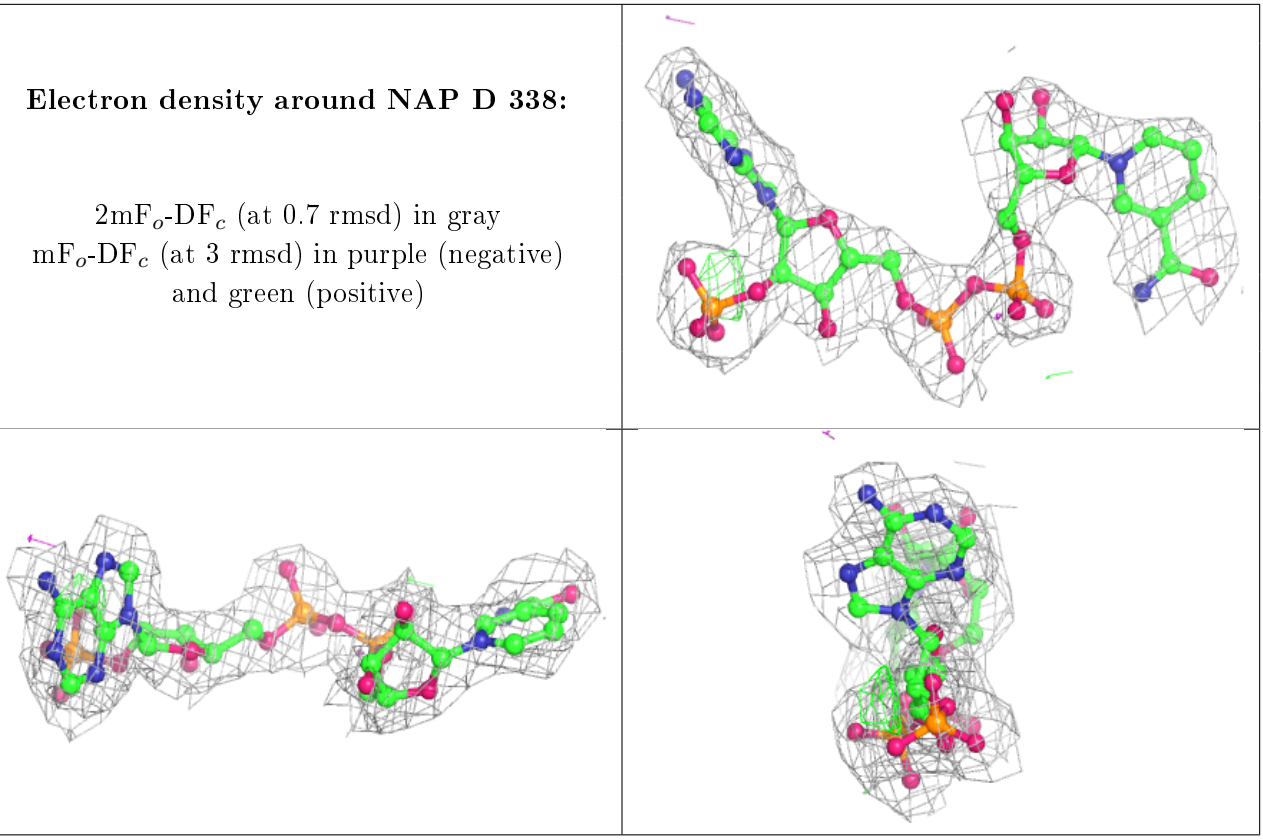






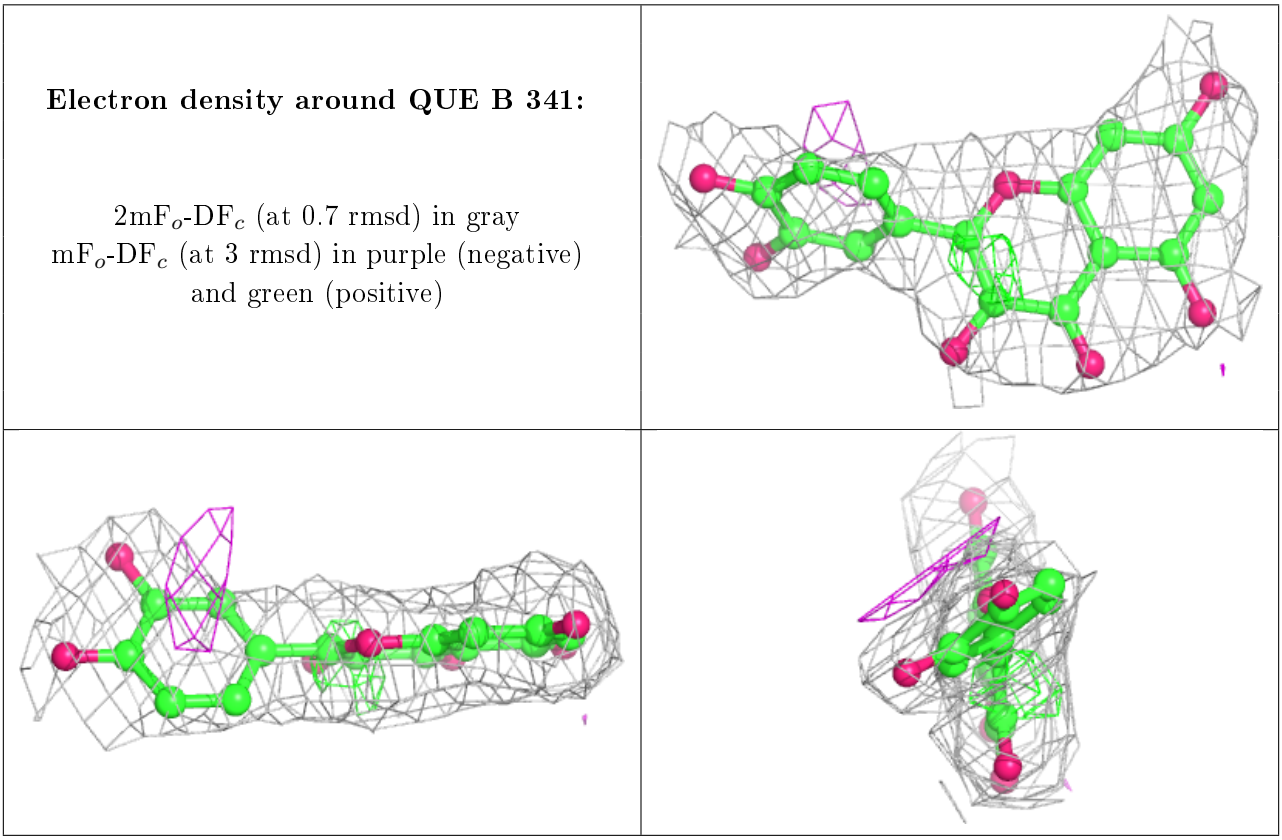
Electron density around NAP D 338:

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



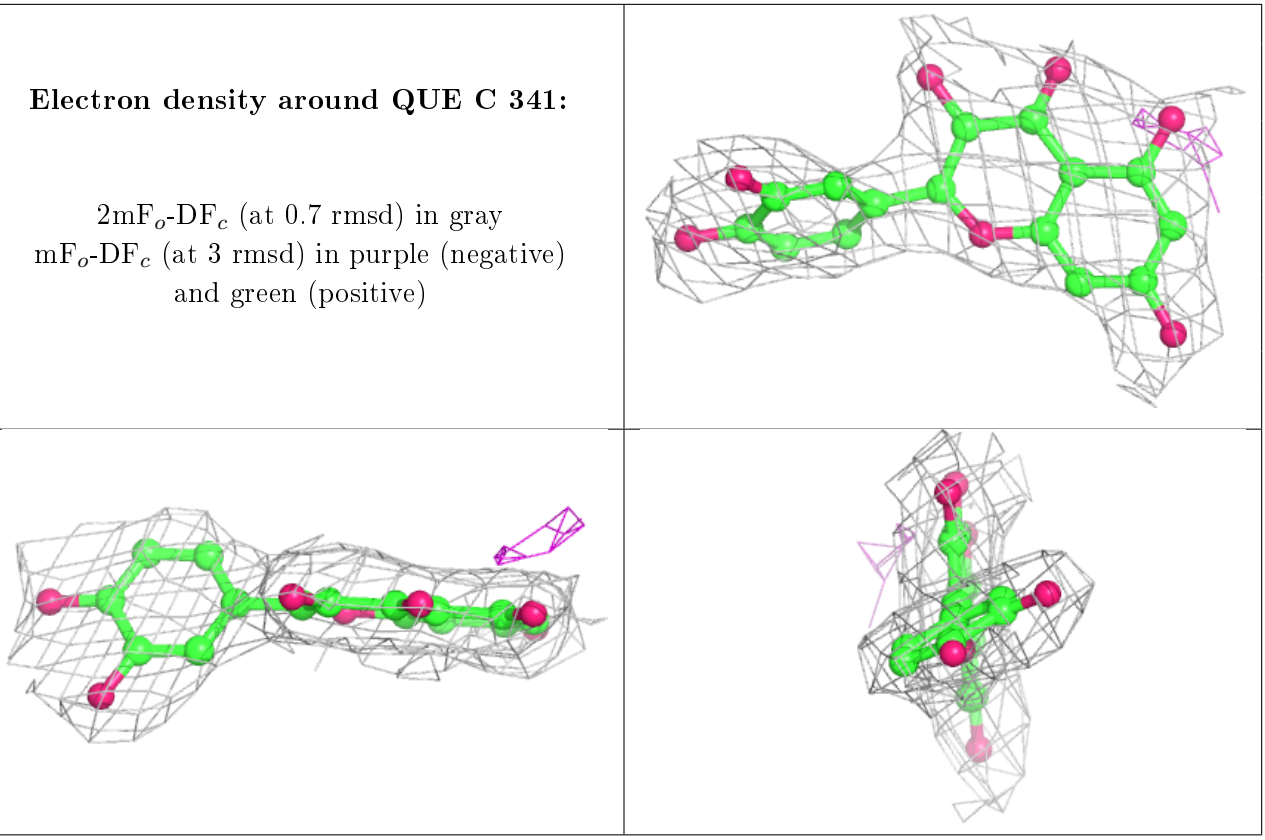
Electron density around QUE B 341:

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



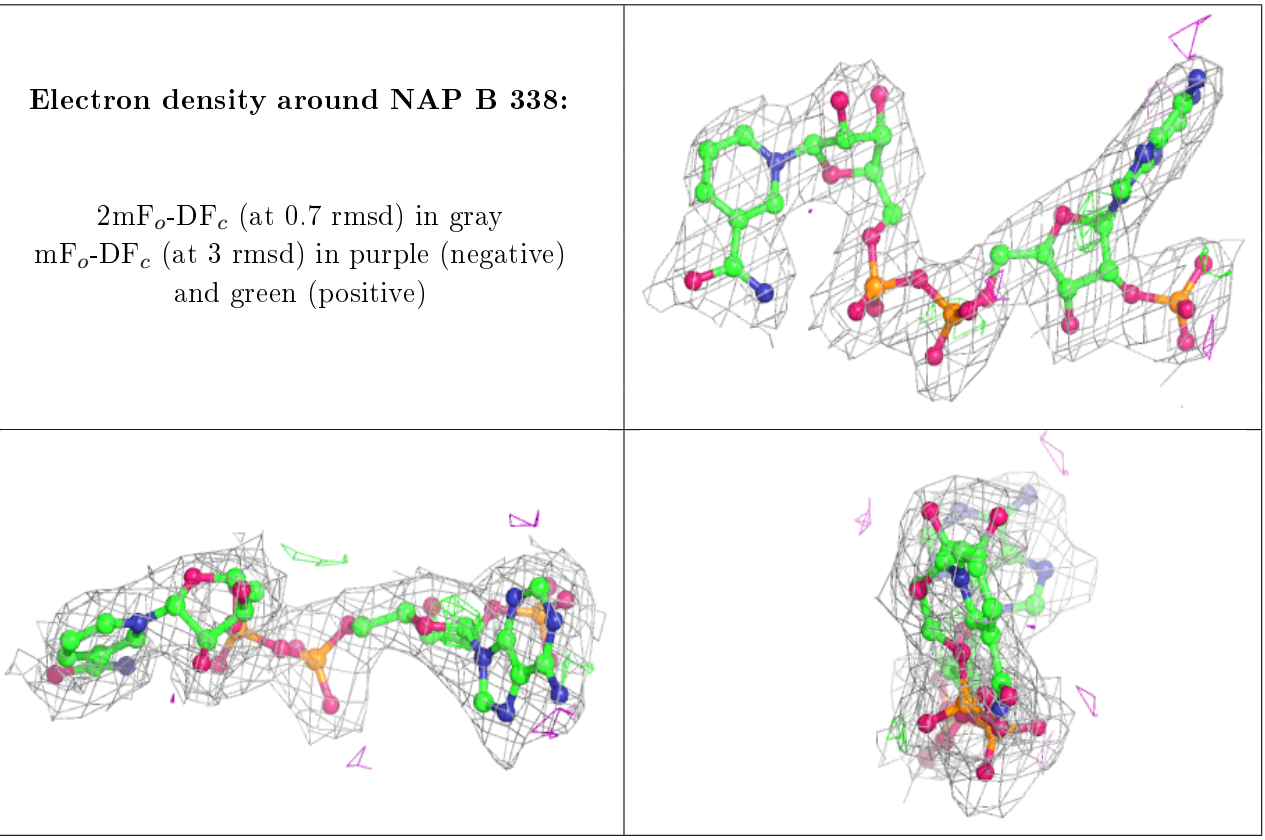
Electron density around QUE C 341:

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



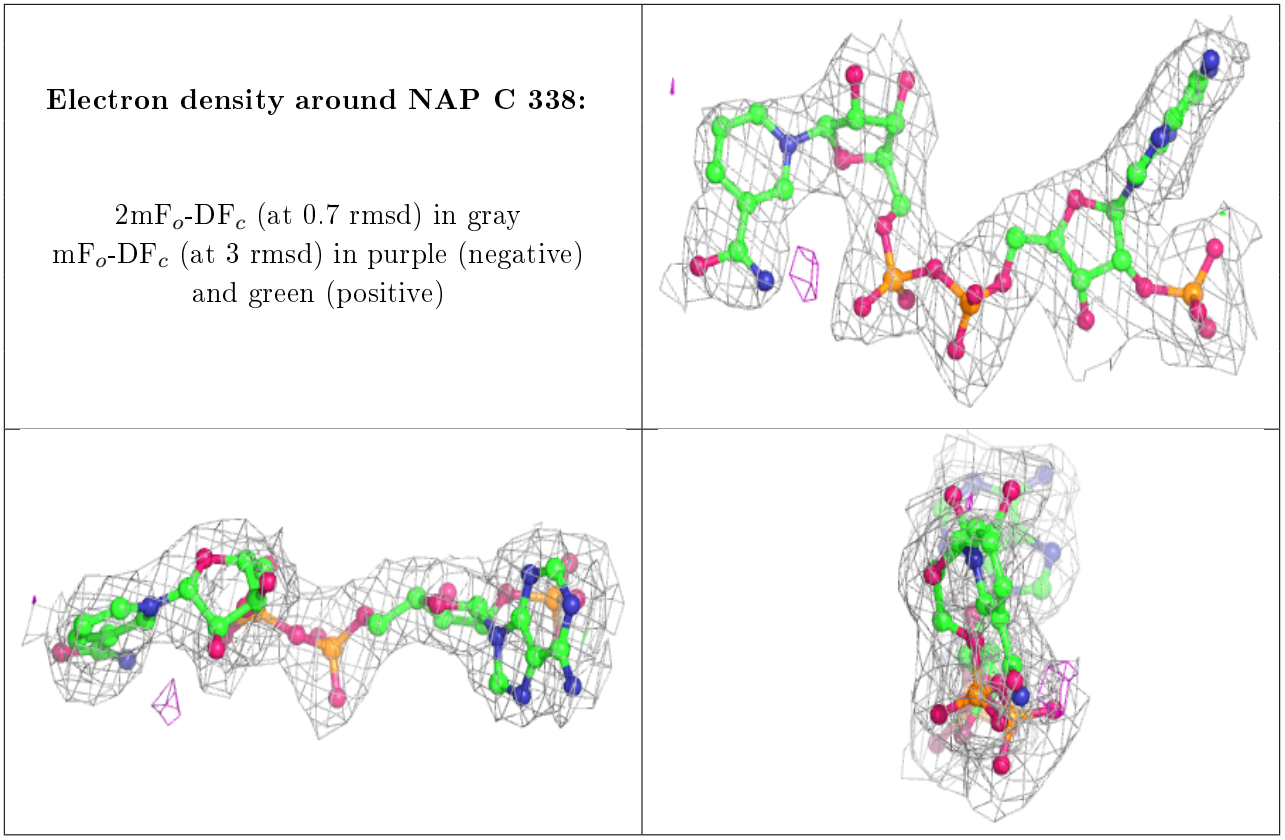
Electron density around NAP B 338:

$2mF_o$-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 338:

$2mF_o$-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.