



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:37 AM UTC

PDB ID : 3BXX / pdb_00003bxx
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 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:

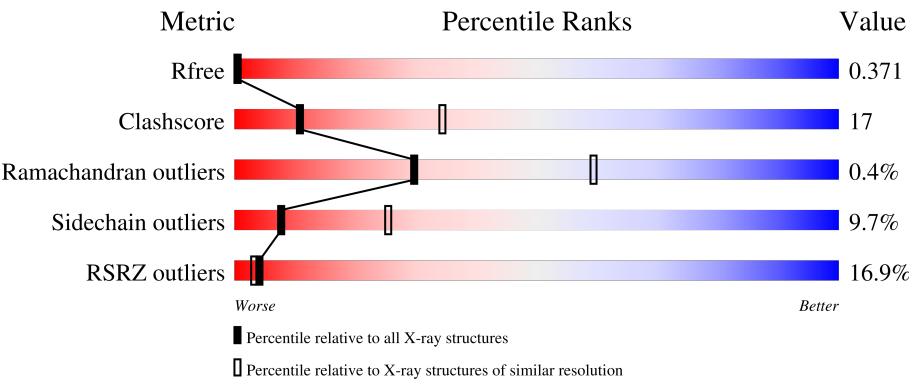
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	337	11% 63% 30% . .
1	B	337	11% 64% 28% . .
1	C	337	11% 61% 31% . .
1	D	337	19% 53% 35% 7% . .

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Mol	Chain	Length	Quality of chain
1	E	337	32% 49% 39% 7%
1	F	337	13% 59% 32% 5%

2 Entry composition ⓘ

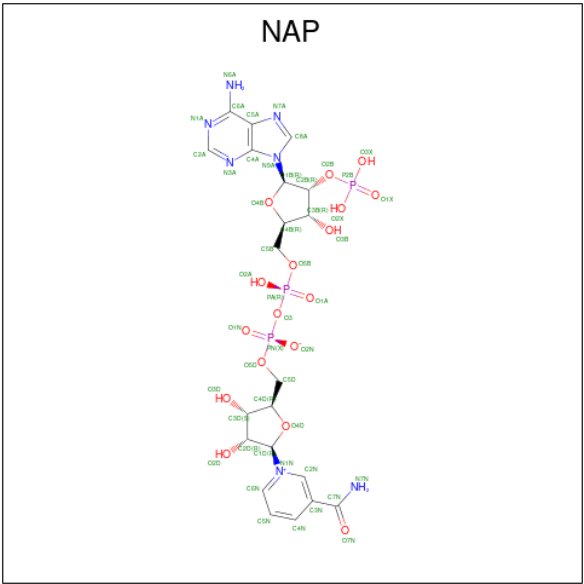
There are 4 unique types of molecules in this entry. The entry contains 15797 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

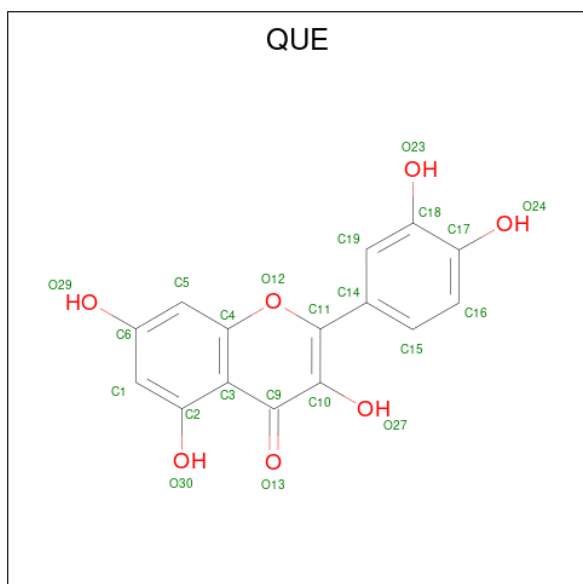
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2531	1621	417	473	20			
1	B	324	Total	C	N	O	S	0	0	0
			2531	1621	417	473	20			
1	C	324	Total	C	N	O	S	0	0	0
			2531	1621	417	473	20			
1	D	324	Total	C	N	O	S	0	0	0
			2531	1621	417	473	20			
1	E	324	Total	C	N	O	S	0	0	0
			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 (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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 (CCD ID: 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	0	0
			22	15	7		
3	D	1	Total	C	O	0	0
			22	15	7		
3	F	1	Total	C	O	0	0
			22	15	7		
3	F	1	Total	C	O	0	0
			22	15	7		

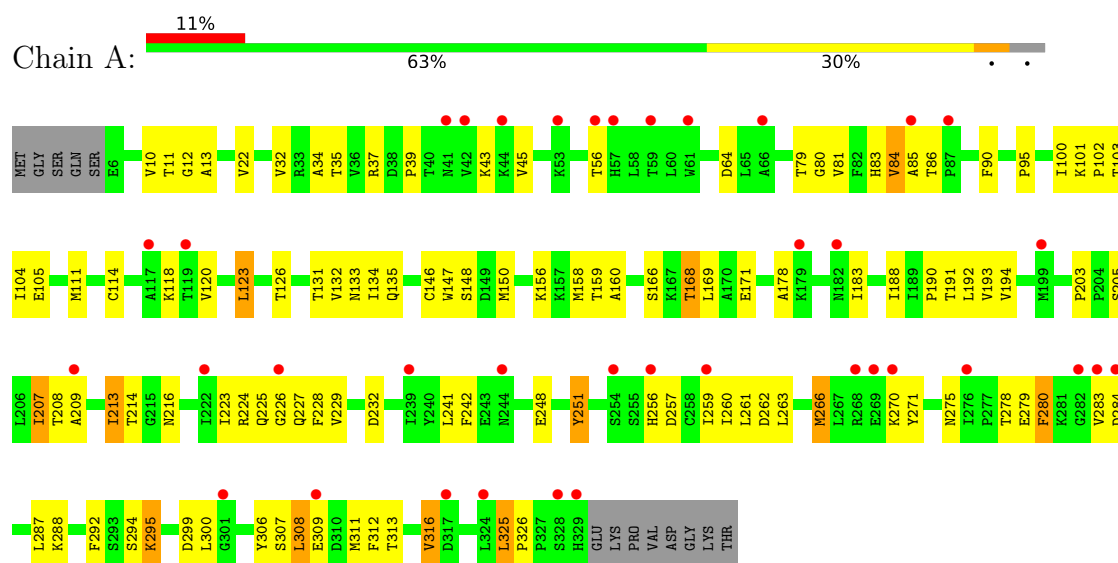
- Molecule 4 is water.

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

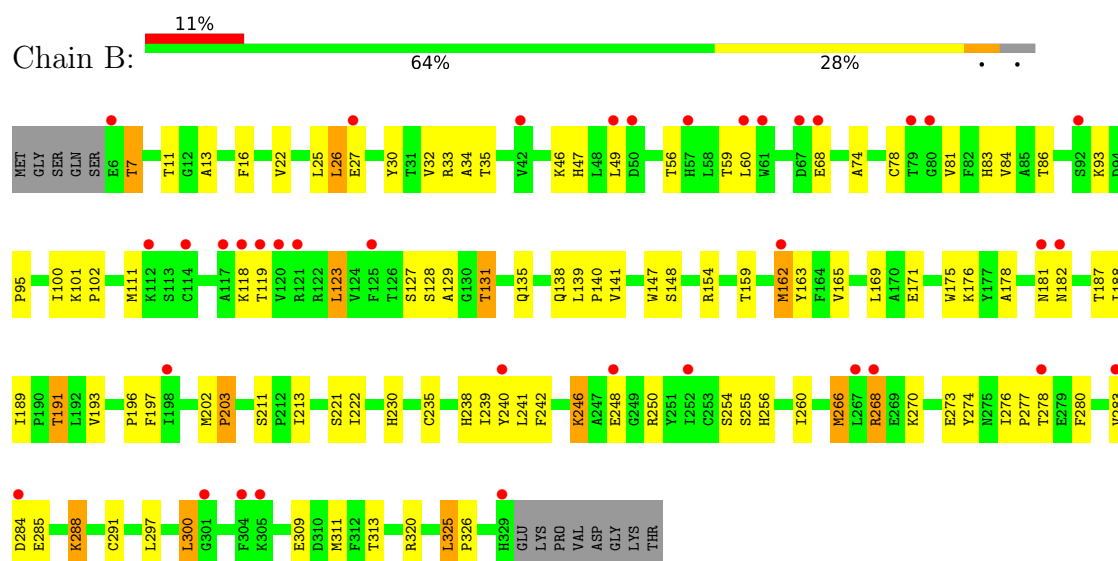
3 Residue-property plots [i](#)

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

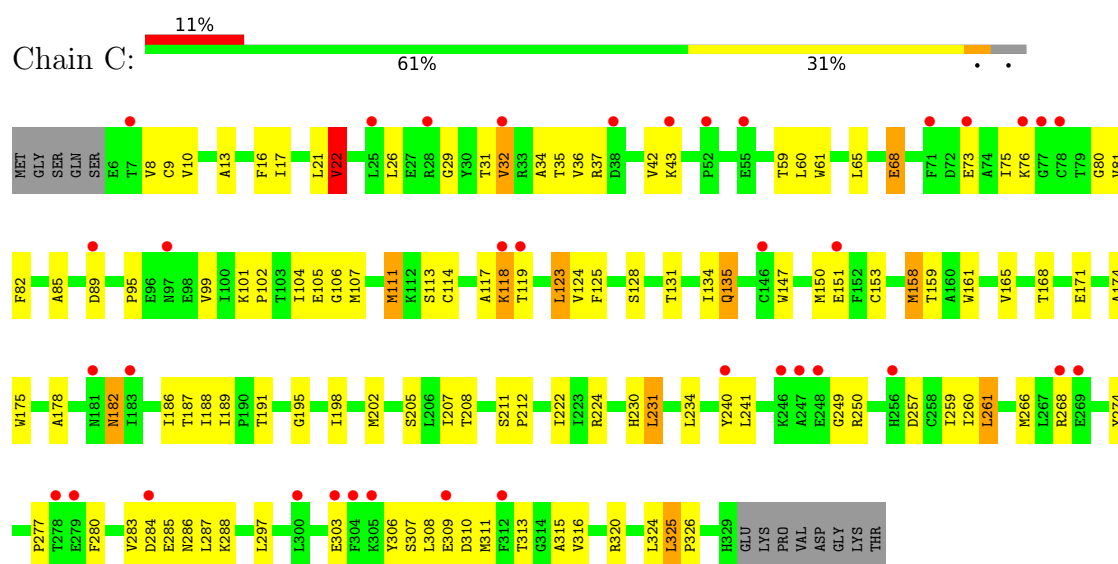
- Molecule 1: dihydroflavonol 4-reductase



- Molecule 1: dihydroflavonol 4-reductase



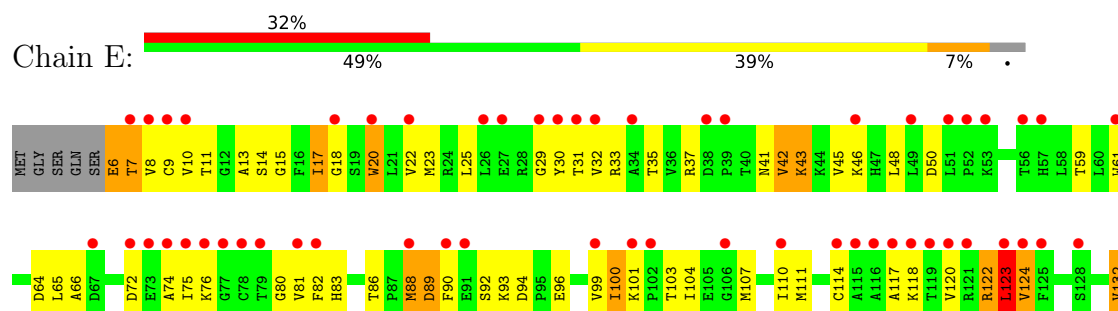
- Molecule 1: dihydroflavonol 4-reductase

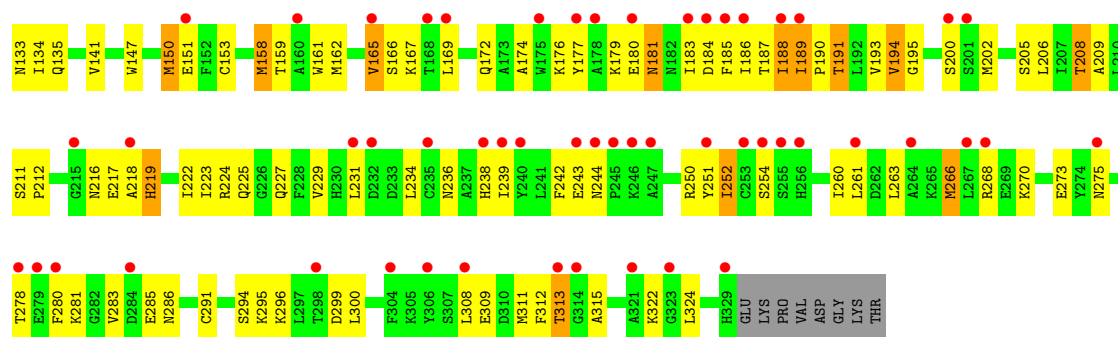


- Molecule 1: dihydroflavonol 4-reductase

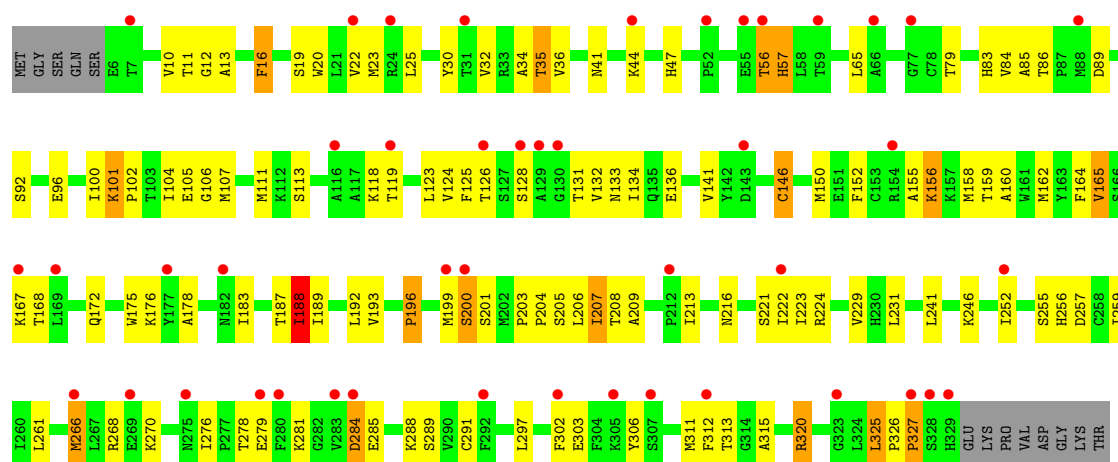


- Molecule 1: dihydroflavonol 4-reductase





● Molecule 1: dihydroflavonol 4-reductase



4 Data and refinement statistics

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 75.81 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (75.81-2.90) 100.0 (75.81-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QUE, NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.82	1/2591 (0.0%)	1.38	19/3513 (0.5%)
1	B	0.80	1/2591 (0.0%)	1.39	19/3513 (0.5%)
1	C	0.82	1/2591 (0.0%)	1.41	22/3513 (0.6%)
1	D	0.79	0/2591	1.43	20/3513 (0.6%)
1	E	0.83	1/2591 (0.0%)	1.48	24/3513 (0.7%)
1	F	0.81	0/2587	1.40	13/3508 (0.4%)
All	All	0.81	4/15542 (0.0%)	1.41	117/21073 (0.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	THR	CA-CB	5.39	1.59	1.53
1	C	134	ILE	CA-CB	5.15	1.59	1.53
1	B	131	THR	CA-CB	5.13	1.62	1.53
1	E	123	LEU	CA-C	5.08	1.58	1.52

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	32	VAL	N-CA-C	8.63	120.91	108.48
1	D	15	GLY	N-CA-C	8.36	123.46	112.25
1	B	191	THR	N-CA-C	-8.24	97.36	109.63
1	F	16	PHE	N-CA-C	7.86	120.54	111.11
1	F	172	GLN	N-CA-C	7.75	119.37	111.07
1	E	17	ILE	N-CA-C	-7.67	102.64	111.00
1	E	243	GLU	N-CA-C	7.57	120.63	111.40
1	C	119	THR	N-CA-C	-7.38	104.89	114.04
1	E	72	ASP	N-CA-C	7.36	119.99	111.02
1	D	122	ARG	N-CA-C	7.26	120.22	108.32
1	E	219	HIS	N-CA-C	7.16	121.84	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	HIS	N-CA-C	-7.10	99.03	110.32
1	B	193	VAL	CB-CA-C	7.01	118.80	111.23
1	A	208	THR	N-CA-C	6.98	120.28	111.69
1	A	226	GLY	N-CA-C	6.96	122.42	112.82
1	E	194	VAL	N-CA-C	-6.91	100.39	108.82
1	D	85	ALA	N-CA-C	6.87	119.17	110.24
1	E	15	GLY	N-CA-C	6.85	121.44	112.25
1	D	200	SER	N-CA-C	6.70	118.58	111.28
1	E	124	VAL	CB-CA-C	-6.69	102.75	111.25
1	B	203	PRO	N-CA-C	6.67	118.83	110.70
1	E	104	ILE	CB-CA-C	-6.63	103.33	112.02
1	E	88	MET	N-CA-C	-6.58	99.96	109.31
1	E	315	ALA	N-CA-C	-6.58	103.72	111.03
1	D	100	ILE	N-CA-C	6.58	116.72	110.74
1	D	191	THR	N-CA-C	-6.57	99.63	109.94
1	C	99	VAL	N-CA-C	6.53	117.19	111.90
1	D	164	PHE	N-CA-C	-6.51	101.60	111.56
1	C	99	VAL	CB-CA-C	-6.48	105.08	111.30
1	B	284	ASP	N-CA-CB	-6.47	101.13	110.45
1	F	188	ILE	CB-CA-C	-6.42	101.06	110.62
1	E	42	VAL	N-CA-C	6.39	116.56	110.42
1	B	260	ILE	N-CA-C	6.39	116.55	110.42
1	E	90	PHE	N-CA-C	6.37	118.80	111.02
1	A	203	PRO	CA-C-N	6.35	125.84	119.24
1	A	203	PRO	C-N-CA	6.35	125.84	119.24
1	C	306	TYR	N-CA-C	6.31	118.76	109.24
1	F	216	ASN	N-CA-CB	-6.26	102.11	110.57
1	C	191	THR	N-CA-C	-6.23	100.50	109.29
1	F	23	MET	N-CA-C	6.17	118.52	111.11
1	E	122	ARG	N-CA-C	6.16	118.50	108.76
1	B	93	LYS	N-CA-C	-6.11	105.85	113.55
1	F	284	ASP	N-CA-C	-6.11	100.60	110.32
1	E	133	ASN	N-CA-C	6.07	120.30	112.41
1	D	242	PHE	N-CA-C	-6.07	104.30	111.03
1	C	202	MET	CA-C-N	-6.04	114.16	120.38
1	C	202	MET	C-N-CA	-6.04	114.16	120.38
1	F	327	PRO	CB-CA-C	5.98	121.55	112.21
1	E	191	THR	N-CA-C	-5.97	99.65	109.80
1	C	36	VAL	CB-CA-C	-5.94	102.70	111.19
1	C	182	ASN	N-CA-C	5.91	123.39	110.80
1	A	103	THR	N-CA-C	-5.90	104.76	111.14
1	F	57	HIS	N-CA-C	5.90	121.26	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	99	VAL	N-CA-C	5.87	116.86	111.81
1	F	200	SER	N-CA-CB	-5.84	102.06	110.65
1	B	93	LYS	CB-CA-C	5.81	118.34	109.34
1	A	279	GLU	N-CA-C	5.80	118.92	109.06
1	B	242	PHE	N-CA-C	-5.79	106.26	113.55
1	A	316	VAL	N-CA-C	5.78	116.24	110.23
1	A	213	ILE	CB-CA-C	-5.76	104.27	112.22
1	B	68	GLU	N-CA-C	5.75	118.70	110.24
1	F	134	ILE	N-CA-C	-5.75	98.14	106.88
1	B	196	PRO	N-CA-C	-5.75	101.14	110.40
1	E	42	VAL	CB-CA-C	-5.75	104.61	111.97
1	D	247	ALA	N-CA-C	5.69	117.96	109.59
1	C	31	THR	N-CA-C	-5.68	99.64	108.90
1	E	123	LEU	N-CA-CB	-5.66	102.23	110.84
1	D	31	THR	N-CA-C	-5.61	99.14	108.34
1	B	221	SER	N-CA-C	5.60	118.16	111.71
1	D	195	GLY	CA-C-N	-5.59	112.85	119.84
1	D	195	GLY	C-N-CA	-5.59	112.85	119.84
1	B	81	VAL	CB-CA-C	-5.59	104.04	110.41
1	D	229	VAL	N-CA-C	-5.57	100.67	108.80
1	E	151	GLU	CB-CG-CD	5.53	122.00	112.60
1	C	240	TYR	N-CA-C	-5.51	104.97	110.97
1	A	228	PHE	N-CA-C	5.49	117.53	109.24
1	A	43	LYS	N-CA-C	5.49	117.97	111.33
1	E	92	SER	N-CA-C	5.46	121.16	113.56
1	D	104	ILE	N-CA-CB	5.45	117.19	110.64
1	E	20	TRP	N-CA-C	5.44	117.21	111.28
1	A	133	ASN	N-CA-C	5.44	119.44	112.26
1	A	207	ILE	CB-CA-C	-5.41	103.78	112.16
1	F	207	ILE	N-CA-CB	5.40	117.48	110.57
1	C	208	THR	N-CA-C	5.38	116.95	111.14
1	D	297	LEU	N-CA-C	-5.36	105.08	111.03
1	A	192	LEU	N-CA-C	-5.35	99.40	110.80
1	B	100	ILE	N-CA-C	-5.32	105.14	110.30
1	C	297	LEU	N-CA-C	5.32	116.76	111.07
1	B	300	LEU	CA-C-N	-5.30	117.14	123.08
1	B	300	LEU	C-N-CA	-5.30	117.14	123.08
1	A	205	SER	N-CA-C	5.28	117.79	111.71
1	F	165	VAL	CB-CA-C	-5.28	105.16	112.24
1	E	151	GLU	CB-CA-C	5.28	120.36	110.70
1	F	306	TYR	N-CA-C	5.27	118.18	109.85
1	C	22	VAL	N-CA-C	-5.22	105.44	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	PHE	N-CA-C	5.21	116.77	111.14
1	E	117	ALA	N-CA-C	5.21	119.11	112.34
1	D	246	LYS	N-CA-C	5.21	119.39	113.19
1	E	222	ILE	N-CA-C	5.20	116.55	110.62
1	D	74	ALA	N-CA-C	-5.19	104.88	111.11
1	C	231	LEU	N-CA-C	-5.18	105.33	110.97
1	B	283	VAL	CB-CA-C	5.14	118.02	110.98
1	A	275	ASN	N-CA-C	-5.13	102.31	109.96
1	D	233	ASP	N-CA-C	-5.13	105.14	111.40
1	A	280	PHE	N-CA-C	5.12	117.42	108.76
1	A	84	VAL	CB-CA-C	-5.11	106.56	111.06
1	B	49	LEU	N-CA-C	5.11	119.00	112.87
1	B	285	GLU	N-CA-CB	-5.11	102.89	110.61
1	C	42	VAL	CB-CA-C	-5.10	105.26	112.14
1	E	29	GLY	N-CA-C	5.07	122.34	115.30
1	C	324	LEU	N-CA-C	5.05	119.45	113.28
1	B	288	LYS	CB-CA-C	5.04	118.74	109.46
1	D	243	GLU	N-CA-C	5.03	117.50	111.71
1	C	257	ASP	N-CA-C	5.03	117.53	108.48
1	A	251	TYR	N-CA-C	5.02	115.62	107.23
1	C	207	ILE	N-CA-C	-5.02	105.50	110.62
1	C	261	LEU	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2531	0	2508	67	0
1	B	2531	0	2508	77	0
1	C	2531	0	2508	71	0
1	D	2531	0	2508	109	0
1	E	2531	0	2508	125	0
1	F	2527	0	2504	74	0
2	A	48	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	B	44	0	11	4	0
3	C	44	0	14	2	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	512	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 17.

All (512) 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:B:95:PRO:HB3	1:B:162:MET:HE2	1.34	1.06
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:CE	2.00	0.92
1:C:111:MET:HE1	1:C:178:ALA:HB2	1.49	0.92
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:E:150:MET:HE3	1:E:150:MET:HA	1.55	0.89
1:C:158:MET:HE2	1:C:158:MET:H	1.38	0.88
1:F:10:VAL:HG11	1:F:22:VAL:HG23	1.55	0.88
1:F:111:MET:HE2	1:F:183:ILE:HD12	1.56	0.87
1:F:266:MET:HE2	1:F:266:MET:O	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:PRO:CB	1:B:162:MET:HE2	2.07	0.82
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:150:MET:HE2	1:E:165:VAL:HG22	1.62	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:F:266:MET:HE1	1:F:270:LYS:HG3	1.65	0.78
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
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:D:111:MET:HE2	1:D:183:ILE:HD12	1.67	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:C:150:MET:HE3	1:C:168:THR:HG21	1.69	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:266:MET:HE2	1:A:266:MET:O	1.89	0.72
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:E:273:GLU:N	1:E:273:GLU:OE1	2.25	0.69
1:C:325:LEU:HD22	1:C:326:PRO:HD2	1.73	0.69
1:E:89:ASP:CG	1:E:89:ASP:O	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:MET:O	1:D:266:MET:HE2	1.94	0.68
1:C:158:MET:HE2	1:C:158:MET:N	2.08	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:C:153:CYS:HA	1:C:158:MET:HE1	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:D:94:ASP:CG	1:D:97:ASN:HD22	2.04	0.64
1:E:180:GLU:C	1:E:181:ASN:HD22	2.05	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:A:111:MET:HE1	1:A:178:ALA:HB2	1.80	0.62
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
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:64:ASP:OD1	1:E:64:ASP:C	2.43	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:HG22	1:D:222:ILE:O	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:150:MET:HA	1:E:150:MET:CE	2.30	0.58
1:A:84:VAL:HG12	2:A:338:NAP:H4D	1.85	0.58
1:A:194:VAL:HG11	1:A:312:PHE:CE1	2.39	0.58
1:F:123:LEU:HD23	1:F:124:VAL:N	2.19	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
1:D:81:VAL:HB	1:D:123:LEU:HD23	1.86	0.58
1:C:13:ALA:CB	1:C:34:ALA:HB1	2.34	0.58
1:E:180:GLU:C	1:E:181:ASN:ND2	2.62	0.57
1:D:107:MET:HE3	1:D:107:MET:HA	1.85	0.57
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:99:VAL:O	1:D:103:THR:OG1	2.23	0.57
1:E:107:MET:HE2	1:E:111:MET:HG3	1.87	0.57
1:F:128:SER:OG	3:F:342:QUE:O24	2.21	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: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:13:ALA:HB1	1:E:48:LEU:HD11	1.86	0.56
1:C:307:SER:O	1:C:308:LEU:C	2.46	0.56
1:E:11:THR:HA	1:E:35:THR:OG1	2.05	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: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:B:95:PRO:HG3	1:B:162:MET:HE1	1.88	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:158:MET:H	1:C:158:MET:CE	2.15	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:B:95:PRO:CB	1:B:162:MET:HE3	2.36	0.55
1:C:158:MET:HE3	1:C:161:TRP:CB	2.37	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:D:150:MET:N	1:D:150:MET:HE2	2.23	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:E:75:ILE:O	1:E:75:ILE:HG22	2.05	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
1:F:111:MET:CE	1:F:183:ILE:HD12	2.35	0.54
1:E:188:ILE:HD12	1:E:238:HIS:NE2	2.23	0.53
2:F:338:NAP:H2N	2:F:338:NAP:O5D	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:A:266:MET:HE2	1:A:266:MET:C	2.33	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: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: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:F:126:THR:O	1:F:167:LYS:NZ	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:309:GLU:OE1	2.42	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:C:158:MET:HE3	1:C:161:TRP:HB3	1.92	0.52
1:E:150:MET:CE	1:E:165:VAL:HG22	2.38	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:D:229:VAL:C	1:D:311:MET:HE2	2.35	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:C:10:VAL:HG11	1:C:22:VAL:HG23	1.92	0.51
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:D:53:LYS:CB	4:D:360:HOH:O	2.59	0.50
1:E:14:SER:OG	2:E:338:NAP:O2X	2.20	0.50
1:E:194:VAL:HG12	1:E:195:GLY:N	2.26	0.50
1:F:101:LYS:HB3	1:F:102:PRO:HD3	1.93	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:F:65:LEU:HD21	1:F:83:HIS:CE1	2.46	0.50
1:B:274:TYR:OH	1:B:326:PRO:O	2.24	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:A:150:MET:HE3	1:A:168:THR:HG21	1.92	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:E:266:MET:HE2	1:E:266:MET:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:CD1	1:A:241:LEU:HD12	2.41	0.50
1:B:246:LYS:HB2	1:B:246:LYS:HZ2	1.77	0.50
1:C:261:LEU:HD13	1:C:283:VAL:CG1	2.41	0.50
1:D:94:ASP:CG	1:D:97:ASN:ND2	2.70	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:C:60:LEU:C	1:C:61:TRP:CD1	2.90	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:95:PRO:HD2	4:A:350:HOH:O	2.13	0.49
1:A:223:ILE:HD12	1:A:260:ILE:HG13	1.95	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:7:THR:HG22	1:E:7:THR:O	2.13	0.49
1:E:88:MET:O	1:E:99:VAL:HG22	2.12	0.49
1:E:124:VAL:HG11	1:E:188:ILE:HD11	1.95	0.49
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: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:C:128:SER:OG	3:C:342:QUE:O24	2.27	0.48
1:D:41:ASN:O	1:D:42:VAL:C	2.54	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:B:255:SER:OG	1:B:256:HIS:ND1	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:41:ASN:O	1:D:43:LYS:N	2.47	0.47
1:D:255:SER:HB3	1:D:304:PHE:CD1	2.49	0.47
1:B:46:LYS:O	1:B:47:HIS:C	2.57	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:D:266:MET:HE2	1:D:266:MET:C	2.39	0.47
1:E:268:ARG:NE	1:E:278:THR:HG22	2.30	0.47
1:F:199:MET:HE2	1:F:201:SER:O	2.15	0.47
1:E:25:LEU:O	1:E:30:TYR:HB2	2.15	0.47
1:A:224:ARG:CZ	1:A:287:LEU:HD11	2.45	0.47
1:A:270:LYS:HD3	1:A:313:THR:HG22	1.97	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:127:SER:O	2:B:338:NAP:H6N	2.15	0.47
1:F:150:MET:HE3	1:F:168:THR:HG21	1.97	0.47
1:C:165:VAL:HG12	1:C:165:VAL:O	2.13	0.47
1:C:231:LEU:O	1:C:234:LEU:HB3	2.14	0.47
1:B:119:THR:HG22	1:B:119:THR:O	2.14	0.46
1:D:219:HIS:O	1:D:220:TYR:C	2.58	0.46
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:81:VAL:HG12	2.13	0.46
1:C:81:VAL:O	1:C:123:LEU:HD23	2.15	0.46
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:F:35:THR:C	1:F:36:VAL:HG13	2.40	0.46
1:A:227:GLN:OE1	1:A:292:PHE:CE1	2.69	0.46
1:C:68:GLU:N	1:C:68:GLU:CD	2.72	0.46
1:C:195:GLY:O	1:C:315:ALA:CA	2.64	0.46
1:D:31:THR:HG23	1:D:57:HIS:CG	2.50	0.46
1:D:141:VAL:HG13	1:D:291:CYS:HB3	1.97	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:25:LEU:HD11	1:E:82:PHE:CE2	2.50	0.46
1:E:181:ASN:HD22	1:E:181:ASN:N	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LEU:HD13	1:C:283:VAL:HG12	1.96	0.46
1:E:191:THR:CG2	1:E:254:SER:HB2	2.44	0.46
1:E:194:VAL:HA	1:E:206:LEU:HD21	1.98	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:D:193:VAL:C	1:D:194:VAL:HG23	2.40	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:90:PHE:CD1	1:D:90:PHE:C	2.94	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:F:128:SER:HG	3:F:342:QUE:C17	2.29	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:158:MET:O	1:F:159:THR:C	2.59	0.45
1:A:232:ASP:OD2	1:A:306:TYR:OH	2.25	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:134:ILE:CG2	1:E:158:MET:HE2	2.46	0.45
1:E:159:THR:OG1	1:F:89:ASP:OD2	2.31	0.45
1:E:296:LYS:O	1:E:299:ASP:HB2	2.16	0.45
1:A:207:ILE:HG21	1:D:216:ASN:HD21	1.81	0.45
1:A:207:ILE:HD13	1:D:216:ASN:ND2	2.32	0.45
1:D:16:PHE:HE1	1:D:197:PHE:HB3	1.81	0.45
1:E:150:MET:HE3	1:E:153:CYS:HB2	1.97	0.45
1:B:84:VAL:HG12	1:B:84:VAL:O	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:ALA:CB	1:F:34:ALA:HB1	2.47	0.45
1:B:111:MET:HE1	1:B:178:ALA:HB2	1.98	0.45
1:B:159:THR:OG1	1:C:89:ASP:OD2	2.28	0.45
1:C:147:TRP:CH2	1:C:250:ARG:CZ	2.99	0.45
1:B:139:LEU:HD23	1:B:139:LEU:HA	1.83	0.44
1:B:162:MET:HE3	1:B:162:MET:HB3	1.73	0.44
1:E:33:ARG:NH1	1:E:61:TRP:CZ2	2.85	0.44
1:D:294:SER:O	1:D:297:LEU:N	2.50	0.44
1:E:42:VAL:O	1:E:43:LYS:C	2.59	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:E:158:MET:HB2	1:F:92:SER:O	2.17	0.44
1:B:175:TRP:O	1:B:176:LYS:C	2.60	0.44
1:D:273:GLU:OE1	1:D:273:GLU:N	2.47	0.44
1:E:217:GLU:O	1:E:218:ALA:C	2.60	0.44
1:F:11:THR:O	1:F:12:GLY:C	2.60	0.44
1:F:12:GLY:N	1:F:85:ALA:HB2	2.33	0.44
1:C:182:ASN:CG	1:C:182:ASN:O	2.60	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:E:6:GLU:HA	4:E:364:HOH:O	2.17	0.44
1:E:100:ILE:O	1:E:101:LYS:C	2.61	0.44
1:E:308:LEU:O	1:E:308:LEU:HD23	2.18	0.44
1:A:11:THR:OG1	1:A:83:HIS:HA	2.18	0.44
1:C:68:GLU:N	1:C:68:GLU:OE1	2.51	0.44
1:D:6:GLU:HA	4:D:358:HOH:O	2.17	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: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
1:E:193:VAL:HG22	1:E:229:VAL:CG1	2.48	0.43
1:C:117:ALA:O	1:C:118:LYS:HB2	2.18	0.43
1:E:20:TRP:CH2	1:E:23:MET:HE1	2.53	0.43
1:B:273:GLU:OE1	1:B:273:GLU:N	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:LEU:HD21	1:D:83:HIS:CE1	2.53	0.43
1:E:244:ASN:OD1	1:E:244:ASN:C	2.61	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:D:310:ASP:O	1:D:311:MET:C	2.61	0.43
1:E:93:LYS:N	4:E:356:HOH:O	2.51	0.43
1:A:158:MET:O	1:A:159:THR:C	2.59	0.43
1:B:246:LYS:NZ	1:B:246:LYS:CB	2.82	0.43
1:D:111:MET:CE	1:D:183:ILE:HD12	2.42	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:E:107:MET:HE3	1:E:107:MET:O	2.18	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:16:PHE:CE1	1:C:231:LEU:HD22	2.54	0.43
1:D:73:GLU:O	1:D:74:ALA:C	2.62	0.43
1:C:135:GLN:HE21	1:C:135:GLN:HB3	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: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:E:252:ILE:C	1:E:294:SER:HG	2.26	0.42
1:F:20:TRP:CH2	1:F:196:PRO:HG2	2.54	0.42
1:F:111:MET:HE1	1:F:178:ALA:HA	2.01	0.42
1:A:283:VAL:HG23	4:A:345:HOH:O	2.19	0.42
1:D:58:LEU:HD12	1:D:59:THR:N	2.34	0.42
1:D:261:LEU:HD13	1:D:283:VAL:HG12	2.00	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:98:GLU:CG	4:D:353:HOH:O	2.65	0.42
1:D:257:ASP:HB2	1:D:290:VAL:O	2.20	0.42
1:A:114:CYS:HB3	1:A:120:VAL:HG11	2.01	0.42
1:C:13:ALA:HB3	1:C:34:ALA:HB1	2.01	0.42
1:C:124:VAL:HA	1:C:186:ILE:O	2.20	0.42
1:D:32:VAL:HG12	1:D:33:ARG:N	2.34	0.42
1:D:119:THR:HG22	1:D:119:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:LEU:HD12	1:D:280:PHE:HD1	1.84	0.42
1:E:193:VAL:HG13	1:E:231:LEU:HA	2.01	0.42
1:F:105:GLU:O	1:F:106:GLY:C	2.61	0.42
1:F:175:TRP:O	1:F:176:LYS:C	2.62	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
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:A:256:HIS:CE1	1:A:307:SER:HA	2.55	0.42
1:A:266:MET:SD	1:A:308:LEU:HD23	2.59	0.42
1:C:205:SER:HB3	2:C:338:NAP:H72N	1.85	0.42
1:E:114:CYS:SG	1:E:120:VAL:HG11	2.60	0.42
1:E:295:LYS:O	1:E:296:LYS:C	2.63	0.42
1:B:128:SER:C	1:B:189:ILE:HG23	2.45	0.41
1:B:181:ASN:O	1:B:182:ASN:OD1	2.38	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:D:185:PHE:C	1:D:186:ILE:HD13	2.45	0.41
1:F:136:GLU:O	1:F:136:GLU:HG3	2.19	0.41
1:B:266:MET:C	1:B:266:MET:HE2	2.44	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:133:ASN:O	1:F:133:ASN:CG	2.61	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:C:158:MET:O	1:C:159:THR:C	2.60	0.41
1:D:127:SER:O	1:D:190:PRO:HD2	2.21	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:D:149:ASP:C	1:D:150:MET:HE2	2.46	0.41
1:E:94:ASP:OD1	1:E:96:GLU:CD	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:209:ALA:HB1	1:A:312:PHE:CZ	2.56	0.41
1:B:131:THR:O	1:B:148:SER:N	2.51	0.41
1:F:111:MET:HE1	1:F:178:ALA:CA	2.51	0.41
1:F:320:ARG:NH1	1:F:327:PRO:O	2.53	0.41
1:B:34:ALA:HB3	1:B:60:LEU:CD2	2.49	0.41
1:C:128:SER:OG	3:C:341:QUE:O27	2.28	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:A:159:THR:O	1:A:160:ALA:HB3	2.21	0.40
1:B:95:PRO:HB2	1:B:162:MET:HE3	2.00	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:B:239:ILE:O	1:B:240:TYR:C	2.63	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:230:HIS:N	1:B:311:MET:HE2	2.36	0.40
1:B:235:CYS:O	1:B:238:HIS:HB2	2.22	0.40
1:D:163:TYR:HB3	3:D:342:QUE:H19	2.03	0.40
1:D:230:HIS:CD2	1:D:311:MET:HA	2.57	0.40
1:D:270:LYS:HG2	1:D:271:TYR:CE2	2.56	0.40
1:F:25:LEU:O	1:F:30:TYR:HB2	2.21	0.40
1:F:84:VAL:O	2:F:338:NAP:H4D	2.21	0.40
1:F:128:SER:OG	3:F:342:QUE:O23	2.39	0.40
1:F:205:SER:HA	3:F:341:QUE:O29	2.21	0.40
1:F:255:SER:O	1:F:256:HIS:ND1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:THR:HA	1:A:35:THR:OG1	2.22	0.40
1:D:162:MET:HE3	1:D:162:MET:HB3	2.02	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%)	7	27
1	E	322/337 (96%)	278 (86%)	43 (13%)	1 (0%)	36	65
1	F	322/337 (96%)	292 (91%)	29 (9%)	1 (0%)	36	65
All	All	1932/2022 (96%)	1744 (90%)	181 (9%)	7 (0%)	30	59

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 ⓘ

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%)	256 (92%)	22 (8%)	11	34
1	B	278/293 (95%)	258 (93%)	20 (7%)	13	39
1	C	278/293 (95%)	256 (92%)	22 (8%)	11	34
1	D	278/293 (95%)	243 (87%)	35 (13%)	4	14
1	E	278/293 (95%)	243 (87%)	35 (13%)	4	14
1	F	277/293 (94%)	249 (90%)	28 (10%)	7	24
All	All	1667/1758 (95%)	1505 (90%)	162 (10%)	8	25

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	56	THR
1	A	79	THR
1	A	86	THR
1	A	105	GLU
1	A	118	LYS
1	A	123	LEU
1	A	135	GLN
1	A	156	LYS
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

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Mol	Chain	Res	Type
1	B	7	THR
1	B	26	LEU
1	B	27	GLU
1	B	35	THR
1	B	56	THR
1	B	59	THR
1	B	86	THR
1	B	118	LYS
1	B	123	LEU
1	B	135	GLN
1	B	162	MET
1	B	211	SER
1	B	222	ILE
1	B	246	LYS
1	B	266	MET
1	B	268	ARG
1	B	288	LYS
1	B	300	LEU
1	B	320	ARG
1	B	325	LEU
1	C	17	ILE
1	C	22	VAL
1	C	35	THR
1	C	43	LYS
1	C	68	GLU
1	C	73	GLU
1	C	76	LYS
1	C	105	GLU
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	198	ILE
1	C	222	ILE
1	C	266	MET
1	C	268	ARG
1	C	285	GLU
1	C	303	GLU
1	C	311	MET
1	C	325	LEU

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Mol	Chain	Res	Type
1	D	8	VAL
1	D	31	THR
1	D	43	LYS
1	D	45	VAL
1	D	73	GLU
1	D	76	LYS
1	D	78	CYS
1	D	79	THR
1	D	86	THR
1	D	92	SER
1	D	98	GLU
1	D	99	VAL
1	D	103	THR
1	D	110	ILE
1	D	118	LYS
1	D	123	LEU
1	D	135	GLN
1	D	141	VAL
1	D	143	ASP
1	D	151	GLU
1	D	156	LYS
1	D	183	ILE
1	D	186	ILE
1	D	188	ILE
1	D	198	ILE
1	D	200	SER
1	D	201	SER
1	D	229	VAL
1	D	266	MET
1	D	279	GLU
1	D	285	GLU
1	D	298	THR
1	D	305	LYS
1	D	308	LEU
1	D	311	MET
1	E	6	GLU
1	E	7	THR
1	E	43	LYS
1	E	59	THR
1	E	76	LYS
1	E	86	THR
1	E	89	ASP

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Mol	Chain	Res	Type
1	E	100	ILE
1	E	118	LYS
1	E	123	LEU
1	E	132	VAL
1	E	135	GLN
1	E	150	MET
1	E	158	MET
1	E	162	MET
1	E	176	LYS
1	E	177	TYR
1	E	179	LYS
1	E	181	ASN
1	E	183	ILE
1	E	188	ILE
1	E	189	ILE
1	E	200	SER
1	E	202	MET
1	E	208	THR
1	E	223	ILE
1	E	252	ILE
1	E	261	LEU
1	E	266	MET
1	E	270	LYS
1	E	281	LYS
1	E	285	GLU
1	E	286	ASN
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	146	CYS
1	F	156	LYS
1	F	162	MET
1	F	188	ILE
1	F	200	SER
1	F	221	SER

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Mol	Chain	Res	Type
1	F	222	ILE
1	F	246	LYS
1	F	252	ILE
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	320	ARG
1	F	325	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	HIS
1	A	181	ASN
1	A	216	ASN
1	B	97	ASN
1	B	133	ASN
1	B	236	ASN
1	C	135	GLN
1	C	137	HIS
1	C	181	ASN
1	C	236	ASN
1	C	244	ASN
1	D	97	ASN
1	D	138	GLN
1	D	172	GLN
1	D	216	ASN
1	D	219	HIS
1	D	236	ASN
1	D	329	HIS
1	E	47	HIS
1	E	181	ASN
1	E	236	ASN
1	F	41	ASN
1	F	57	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
2	NAP	A	338	-	50,52,52	1.79	7 (14%)	71,80,80	1.55	15 (21%)
3	QUE	C	342	-	24,24,24	3.22	4 (16%)	36,36,36	2.96	19 (52%)
2	NAP	B	338	-	50,52,52	1.78	6 (12%)	71,80,80	1.67	12 (16%)
3	QUE	F	341	-	24,24,24	3.33	4 (16%)	36,36,36	2.69	16 (44%)
2	NAP	E	338	-	50,52,52	1.66	6 (12%)	71,80,80	2.63	32 (45%)
2	NAP	D	338	-	50,52,52	1.59	5 (10%)	71,80,80	2.06	26 (36%)
3	QUE	F	342	-	24,24,24	3.26	5 (20%)	36,36,36	2.95	17 (47%)
2	NAP	F	338	-	50,52,52	1.69	5 (10%)	71,80,80	1.87	20 (28%)
2	NAP	C	338	-	50,52,52	1.66	6 (12%)	71,80,80	1.86	20 (28%)
3	QUE	D	341	-	24,24,24	3.33	4 (16%)	36,36,36	2.16	11 (30%)
3	QUE	A	342	-	24,24,24	3.40	5 (20%)	36,36,36	2.78	16 (44%)
3	QUE	B	342	-	24,24,24	3.12	4 (16%)	36,36,36	2.84	18 (50%)
3	QUE	C	341	-	24,24,24	3.27	5 (20%)	36,36,36	2.65	14 (38%)
3	QUE	B	341	-	24,24,24	2.54	5 (20%)	36,36,36	1.95	12 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	QUE	D	342	-	24,24,24	3.55	5 (20%)	36,36,36	2.58	15 (41%)

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
2	NAP	A	338	-	-	3/35/67/67	0/5/5/5
3	QUE	C	342	-	-	0/4/4/4	0/3/3/3
2	NAP	B	338	-	-	6/35/67/67	0/5/5/5
3	QUE	F	341	-	-	4/4/4/4	0/3/3/3
2	NAP	E	338	-	-	10/35/67/67	0/5/5/5
2	NAP	D	338	-	-	5/35/67/67	0/5/5/5
3	QUE	F	342	-	-	0/4/4/4	0/3/3/3
2	NAP	F	338	-	-	7/35/67/67	0/5/5/5
2	NAP	C	338	-	-	3/35/67/67	0/5/5/5
3	QUE	D	341	-	-	4/4/4/4	0/3/3/3
3	QUE	A	342	-	-	0/4/4/4	0/3/3/3
3	QUE	B	342	-	-	0/4/4/4	0/3/3/3
3	QUE	C	341	-	-	4/4/4/4	0/3/3/3
3	QUE	B	341	-	-	4/4/4/4	0/3/3/3
3	QUE	D	342	-	-	0/4/4/4	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	341	QUE	C10-C11	13.95	1.50	1.36
3	A	342	QUE	C10-C11	13.86	1.49	1.36
3	D	342	QUE	C10-C11	13.81	1.49	1.36
3	F	342	QUE	C10-C11	13.37	1.49	1.36
3	D	341	QUE	C10-C11	13.09	1.49	1.36
3	C	342	QUE	C10-C11	12.89	1.49	1.36
3	F	341	QUE	C10-C11	12.57	1.48	1.36
3	B	342	QUE	C10-C11	12.43	1.48	1.36
3	B	341	QUE	C10-C11	9.83	1.46	1.36
2	B	338	NAP	O7N-C7N	9.39	1.41	1.24
2	A	338	NAP	O7N-C7N	9.28	1.41	1.24
2	F	338	NAP	O7N-C7N	9.12	1.41	1.24
2	D	338	NAP	O7N-C7N	8.66	1.40	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	338	NAP	O7N-C7N	8.47	1.39	1.24
2	C	338	NAP	O7N-C7N	7.62	1.38	1.24
3	D	342	QUE	C3-C2	6.64	1.52	1.41
3	F	341	QUE	C3-C2	6.12	1.51	1.41
3	B	342	QUE	C3-C2	6.03	1.51	1.41
3	C	342	QUE	C3-C2	5.97	1.50	1.41
3	D	341	QUE	C3-C2	5.65	1.50	1.41
3	D	342	QUE	C3-C4	5.65	1.50	1.40
3	F	341	QUE	C18-C17	5.37	1.49	1.40
3	F	341	QUE	C3-C4	5.28	1.50	1.40
3	D	341	QUE	C18-C17	5.20	1.48	1.40
3	F	342	QUE	C3-C2	5.18	1.49	1.41
3	D	341	QUE	C3-C4	5.05	1.49	1.40
3	A	342	QUE	C3-C2	4.97	1.49	1.41
3	B	341	QUE	C18-C17	4.50	1.47	1.40
3	B	342	QUE	C3-C4	4.48	1.48	1.40
3	C	341	QUE	C3-C2	4.43	1.48	1.41
3	A	342	QUE	C18-C17	4.42	1.47	1.40
3	A	342	QUE	C3-C4	4.37	1.48	1.40
3	B	342	QUE	C18-C17	4.36	1.47	1.40
3	F	342	QUE	C18-C17	4.28	1.47	1.40
3	C	341	QUE	C18-C17	4.17	1.47	1.40
3	D	342	QUE	C18-C17	4.11	1.47	1.40
3	C	342	QUE	C18-C17	3.84	1.46	1.40
3	B	341	QUE	C3-C2	3.78	1.47	1.41
3	C	342	QUE	C3-C4	3.62	1.47	1.40
3	B	341	QUE	C3-C4	3.56	1.47	1.40
3	C	341	QUE	C3-C4	3.46	1.46	1.40
2	A	338	NAP	C2A-N1A	3.46	1.40	1.33
3	F	342	QUE	C3-C4	3.45	1.46	1.40
2	C	338	NAP	C2A-N3A	3.36	1.39	1.33
2	F	338	NAP	C2A-N1A	3.30	1.39	1.33
2	A	338	NAP	C2A-N3A	3.30	1.39	1.33
2	F	338	NAP	C2N-N1N	3.20	1.38	1.35
2	C	338	NAP	C2A-N1A	3.10	1.39	1.33
2	E	338	NAP	C2N-N1N	2.99	1.38	1.35
2	B	338	NAP	PA-O3	2.81	1.62	1.59
2	C	338	NAP	C5A-N7A	-2.79	1.34	1.39
2	E	338	NAP	C2A-N3A	2.77	1.38	1.33
3	C	341	QUE	C14-C11	2.75	1.51	1.47
2	E	338	NAP	C2A-N1A	2.73	1.38	1.33
2	B	338	NAP	C2A-N1A	2.68	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	338	NAP	C8A-N7A	2.63	1.36	1.31
2	B	338	NAP	C2A-N3A	2.55	1.38	1.33
3	A	342	QUE	C14-C11	2.52	1.51	1.47
2	E	338	NAP	C8A-N7A	2.46	1.36	1.31
3	F	342	QUE	C14-C11	2.46	1.51	1.47
2	D	338	NAP	C2A-N1A	2.44	1.38	1.33
2	C	338	NAP	P2B-O2B	2.44	1.63	1.59
2	E	338	NAP	PA-O3	2.40	1.62	1.59
2	D	338	NAP	C2N-N1N	2.37	1.37	1.35
2	F	338	NAP	C2A-N3A	2.37	1.38	1.33
2	D	338	NAP	C2A-N3A	2.33	1.38	1.33
2	D	338	NAP	C8A-N7A	2.25	1.36	1.31
3	D	342	QUE	C14-C11	2.23	1.50	1.47
2	A	338	NAP	C8A-N7A	2.21	1.35	1.31
2	A	338	NAP	PN-O3	2.20	1.61	1.59
2	B	338	NAP	O4B-C4B	-2.18	1.40	1.45
3	B	341	QUE	O12-C11	-2.14	1.35	1.37
2	F	338	NAP	C5A-N7A	-2.13	1.35	1.39
2	C	338	NAP	C3B-C2B	-2.07	1.48	1.53
2	A	338	NAP	PA-O3	2.04	1.61	1.59
2	A	338	NAP	O4D-C4D	-2.03	1.40	1.45

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	338	NAP	C4D-O4D-C1D	8.52	117.72	109.92
3	A	342	QUE	O12-C11-C14	7.47	121.34	110.87
3	B	342	QUE	O27-C10-C11	7.07	128.05	120.74
2	D	338	NAP	N3A-C2A-N1A	-7.05	117.91	128.58
3	F	342	QUE	C4-O12-C11	6.98	131.36	120.67
2	E	338	NAP	N3A-C2A-N1A	-6.90	118.14	128.58
3	C	341	QUE	O12-C11-C14	6.84	120.45	110.87
3	C	342	QUE	C15-C14-C11	6.82	130.74	120.71
3	F	341	QUE	C14-C11-C10	-6.81	117.72	128.44
3	F	341	QUE	O12-C11-C14	6.72	120.28	110.87
3	F	342	QUE	O12-C11-C10	-6.56	113.97	120.19
3	D	342	QUE	O27-C10-C11	6.55	127.51	120.74
3	A	342	QUE	C15-C14-C11	6.41	130.14	120.71
3	C	342	QUE	C19-C14-C11	-6.38	111.64	120.65
3	F	341	QUE	C11-C10-C9	-6.34	116.99	121.52
2	F	338	NAP	O3-PA-O1A	-6.17	92.14	110.70
3	B	342	QUE	C4-C3-C9	-6.16	112.59	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	338	NAP	N3A-C2A-N1A	-6.05	119.43	128.58
3	C	341	QUE	C4-O12-C11	5.87	129.66	120.67
3	A	342	QUE	C19-C14-C11	-5.60	112.75	120.65
3	F	342	QUE	C2-C3-C9	5.44	129.49	121.45
3	B	341	QUE	O12-C4-C5	5.42	123.51	115.83
2	E	338	NAP	C3N-C7N-N7N	5.30	124.26	117.74
3	D	341	QUE	C15-C14-C11	-5.29	112.93	120.71
3	C	341	QUE	O12-C11-C10	-5.28	115.19	120.19
3	C	342	QUE	C11-C10-C9	-4.98	117.96	121.52
2	E	338	NAP	O7N-C7N-C3N	-4.85	113.66	119.60
3	B	342	QUE	C2-C3-C9	4.76	128.49	121.45
3	C	342	QUE	O12-C11-C14	4.72	117.49	110.87
3	F	342	QUE	C11-C10-C9	-4.71	118.16	121.52
3	B	342	QUE	O12-C11-C14	4.66	117.40	110.87
2	C	338	NAP	C3N-C7N-N7N	4.65	123.46	117.74
2	C	338	NAP	O7N-C7N-N7N	-4.62	115.94	122.62
3	A	342	QUE	C14-C11-C10	-4.59	121.21	128.44
2	E	338	NAP	C2N-C3N-C4N	4.52	123.51	118.26
2	B	338	NAP	C4A-N9A-C1B	-4.51	116.08	126.63
3	C	342	QUE	C4-O12-C11	4.48	127.54	120.67
3	B	342	QUE	C3-C9-C10	4.45	123.19	116.88
2	D	338	NAP	N9A-C8A-N7A	-4.44	107.64	113.94
3	F	342	QUE	C4-C3-C9	-4.44	114.68	120.03
3	D	341	QUE	C11-C10-C9	-4.37	118.40	121.52
3	D	342	QUE	O12-C11-C14	4.37	117.00	110.87
3	C	342	QUE	C16-C17-C18	-4.35	115.02	119.66
3	A	342	QUE	C14-C19-C18	4.34	123.87	120.09
3	B	341	QUE	O12-C11-C14	4.33	116.94	110.87
3	D	341	QUE	C14-C11-C10	-4.32	121.64	128.44
3	D	342	QUE	O12-C4-C5	4.31	121.94	115.83
3	C	341	QUE	O12-C4-C5	4.30	121.93	115.83
3	D	342	QUE	C4-O12-C11	4.28	127.22	120.67
3	D	342	QUE	C14-C19-C18	4.23	123.78	120.09
2	E	338	NAP	C5N-C4N-C3N	-4.22	116.22	120.36
3	B	342	QUE	C11-C10-C9	-4.19	118.53	121.52
3	F	342	QUE	C3-C9-C10	4.18	122.80	116.88
3	F	341	QUE	C1-C2-C3	-4.18	116.24	120.92
3	F	341	QUE	C19-C18-C17	-4.16	116.04	119.89
2	E	338	NAP	O4B-C1B-N9A	4.14	116.04	108.09
2	E	338	NAP	O2X-P2B-O2B	-4.13	89.74	105.85
3	D	341	QUE	O12-C11-C14	4.11	116.63	110.87
3	F	342	QUE	C15-C14-C11	4.05	126.67	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	341	QUE	C11-C10-C9	-4.04	118.64	121.52
2	F	338	NAP	O3-PN-O1N	-4.04	98.55	110.70
2	B	338	NAP	C1B-N9A-C8A	3.98	135.93	127.09
3	C	341	QUE	C2-C3-C9	3.94	127.28	121.45
3	B	342	QUE	O23-C18-C19	3.93	130.07	119.45
2	E	338	NAP	C4N-C3N-C7N	-3.89	110.47	121.06
3	C	342	QUE	O24-C17-C16	3.80	129.56	119.36
2	E	338	NAP	O2X-P2B-O1X	3.78	125.56	110.83
3	D	342	QUE	C11-C10-C9	-3.78	118.82	121.52
3	C	342	QUE	O12-C4-C5	3.76	121.17	115.83
2	A	338	NAP	C5A-C4A-N3A	-3.73	121.58	126.72
2	E	338	NAP	C2A-N3A-C4A	3.70	120.87	111.83
2	E	338	NAP	C2N-N1N-C1D	3.69	127.27	119.13
3	C	342	QUE	C14-C19-C18	3.69	123.31	120.09
3	F	342	QUE	O12-C4-C5	3.68	121.05	115.83
2	C	338	NAP	O5B-C5B-C4B	-3.68	96.47	108.99
2	F	338	NAP	C3N-C7N-N7N	3.65	122.24	117.74
3	F	342	QUE	O24-C17-C16	3.64	129.14	119.36
2	E	338	NAP	N9A-C8A-N7A	-3.64	108.78	113.94
3	F	342	QUE	C19-C14-C11	-3.63	115.53	120.65
2	F	338	NAP	O2A-PA-O3	3.62	117.05	107.27
2	B	338	NAP	O5D-PN-O1N	3.59	123.18	108.94
2	D	338	NAP	C4A-N9A-C1B	-3.57	118.28	126.63
3	D	341	QUE	O12-C4-C5	3.56	120.88	115.83
2	D	338	NAP	C2A-N3A-C4A	3.54	120.49	111.83
2	B	338	NAP	O3-PN-O1N	-3.54	100.05	110.70
3	D	342	QUE	C19-C18-C17	-3.52	116.63	119.89
3	A	342	QUE	O12-C11-C10	-3.52	116.85	120.19
2	D	338	NAP	C5A-N7A-C8A	3.52	108.98	103.45
2	E	338	NAP	C5A-C4A-N3A	-3.49	121.91	126.72
3	D	341	QUE	C19-C14-C11	3.47	125.56	120.65
3	C	342	QUE	C4-C3-C9	-3.47	115.84	120.03
3	D	342	QUE	C2-C3-C9	3.46	126.57	121.45
2	F	338	NAP	C6N-N1N-C1D	-3.46	112.93	119.73
2	F	338	NAP	N9A-C8A-N7A	-3.45	109.04	113.94
3	C	342	QUE	O12-C11-C10	-3.43	116.94	120.19
2	D	338	NAP	O2X-P2B-O1X	3.41	124.13	110.83
3	A	342	QUE	C4-O12-C11	3.41	125.89	120.67
2	D	338	NAP	O2N-PN-O3	3.40	116.46	107.27
2	E	338	NAP	C6N-N1N-C1D	-3.38	113.09	119.73
3	C	342	QUE	O13-C9-C3	-3.38	115.94	122.06
2	A	338	NAP	O7N-C7N-C3N	-3.37	115.47	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	342	QUE	O12-C4-C5	3.37	120.60	115.83
3	D	342	QUE	O23-C18-C19	3.34	128.47	119.45
3	C	341	QUE	C4-C3-C9	-3.26	116.09	120.03
2	A	338	NAP	N3A-C2A-N1A	-3.23	123.69	128.58
2	C	338	NAP	C5A-C4A-N3A	-3.20	122.31	126.72
3	B	342	QUE	O12-C4-C5	3.19	120.36	115.83
2	C	338	NAP	C5A-C6A-N6A	-3.19	115.39	123.29
2	E	338	NAP	O2B-C2B-C1B	-3.18	98.87	110.05
3	B	342	QUE	O12-C11-C10	-3.18	117.18	120.19
2	A	338	NAP	C6A-C5A-C4A	3.17	121.51	117.18
2	E	338	NAP	O3X-P2B-O2B	3.16	118.14	105.85
3	F	341	QUE	C15-C14-C11	-3.15	116.07	120.71
3	F	341	QUE	O12-C4-C5	3.15	120.30	115.83
3	B	341	QUE	C16-C17-C18	-3.15	116.29	119.66
3	D	341	QUE	O27-C10-C9	3.14	122.67	116.89
3	B	342	QUE	C4-C5-C6	3.13	123.92	118.98
3	B	342	QUE	C4-O12-C11	3.13	125.46	120.67
3	A	342	QUE	C2-C3-C9	3.11	126.05	121.45
2	E	338	NAP	C4A-N9A-C1B	-3.07	119.44	126.63
3	D	342	QUE	C4-C3-C9	-3.07	116.33	120.03
3	A	342	QUE	O27-C10-C11	3.06	123.91	120.74
3	B	341	QUE	C4-O12-C11	3.05	125.34	120.67
2	F	338	NAP	O5D-PN-O1N	3.03	120.93	108.94
3	F	342	QUE	O12-C11-C14	3.02	115.10	110.87
2	F	338	NAP	O5D-C5D-C4D	3.02	119.27	108.99
2	D	338	NAP	C4D-O4D-C1D	3.01	112.68	109.92
2	D	338	NAP	C6N-N1N-C2N	-2.99	119.33	121.88
3	D	342	QUE	O13-C9-C10	-2.99	113.54	119.61
3	A	342	QUE	C4-C5-C6	2.98	123.68	118.98
3	C	341	QUE	C4-C5-C6	2.98	123.68	118.98
3	B	342	QUE	C5-C4-C3	-2.98	116.60	121.79
2	F	338	NAP	C2N-C3N-C4N	2.98	121.72	118.26
2	C	338	NAP	N9A-C8A-N7A	-2.96	109.74	113.94
3	C	341	QUE	O13-C9-C3	-2.96	116.71	122.06
2	C	338	NAP	O3-PN-O1N	2.92	119.49	110.70
2	D	338	NAP	C4A-C5A-N7A	-2.91	107.25	110.58
2	F	338	NAP	C5A-N7A-C8A	2.91	108.02	103.45
2	C	338	NAP	O4B-C1B-C2B	2.89	111.57	106.59
2	E	338	NAP	O3-PN-O1N	-2.88	102.03	110.70
3	C	342	QUE	C3-C9-C10	2.87	120.95	116.88
2	A	338	NAP	O3-PN-O1N	-2.87	102.07	110.70
3	B	341	QUE	C5-C4-C3	-2.85	116.83	121.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	338	NAP	N3A-C4A-N9A	2.84	131.99	127.17
3	D	342	QUE	O12-C11-C10	-2.83	117.51	120.19
2	E	338	NAP	C6N-N1N-C2N	-2.81	119.48	121.88
3	C	341	QUE	C3-C9-C10	2.81	120.86	116.88
3	B	341	QUE	C14-C11-C10	-2.81	124.02	128.44
2	F	338	NAP	O5B-PA-O1A	2.79	119.98	108.94
3	C	342	QUE	C2-C3-C9	2.78	125.56	121.45
2	D	338	NAP	C2N-C3N-C4N	2.78	121.49	118.26
3	C	341	QUE	C16-C15-C14	2.76	123.74	120.80
2	E	338	NAP	C5A-N7A-C8A	2.75	107.77	103.45
3	F	342	QUE	C4-C5-C6	2.75	123.31	118.98
2	D	338	NAP	C1B-N9A-C8A	2.74	133.17	127.09
3	B	342	QUE	O13-C9-C10	-2.74	114.05	119.61
3	D	342	QUE	C3-C9-C10	2.73	120.75	116.88
3	B	341	QUE	O27-C10-C9	2.73	121.92	116.89
2	B	338	NAP	N9A-C8A-N7A	-2.73	110.07	113.94
2	F	338	NAP	C4N-C3N-C7N	-2.71	113.68	121.06
3	A	342	QUE	O24-C17-C16	2.70	126.62	119.36
3	D	341	QUE	C19-C18-C17	-2.69	117.40	119.89
2	B	338	NAP	O2N-PN-O3	2.69	114.54	107.27
2	E	338	NAP	N3A-C4A-N9A	2.67	131.70	127.17
2	D	338	NAP	C4A-N9A-C8A	2.66	108.53	105.74
3	D	341	QUE	C2-C3-C9	2.64	125.36	121.45
3	A	342	QUE	C19-C18-C17	-2.64	117.45	119.89
2	A	338	NAP	C3N-C7N-N7N	2.63	120.97	117.74
3	F	341	QUE	C2-C3-C4	2.62	119.91	117.41
2	A	338	NAP	O2D-C2D-C3D	2.62	120.21	111.82
2	B	338	NAP	O2B-C2B-C3B	-2.61	102.30	111.68
2	F	338	NAP	C6A-C5A-C4A	2.61	120.74	117.18
2	C	338	NAP	O2B-C2B-C3B	-2.60	102.34	111.68
3	C	341	QUE	C14-C11-C10	-2.60	124.36	128.44
3	A	342	QUE	C4-C3-C9	-2.59	116.91	120.03
3	F	342	QUE	O13-C9-C3	-2.58	117.38	122.06
3	F	342	QUE	O29-C6-C1	2.57	126.59	119.85
3	C	341	QUE	C14-C19-C18	2.57	122.33	120.09
3	F	341	QUE	O27-C10-C9	2.57	121.61	116.89
3	C	342	QUE	C4-C5-C6	2.56	123.01	118.98
3	F	341	QUE	C2-C1-C6	2.55	122.03	119.67
2	A	338	NAP	O2A-PA-O3	-2.55	100.39	107.27
3	D	341	QUE	C4-C5-C6	2.55	123.00	118.98
2	F	338	NAP	C2N-N1N-C1D	2.54	124.75	119.13
2	D	338	NAP	O4B-C1B-N9A	2.54	112.97	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	338	NAP	O2A-PA-O1A	2.51	124.14	112.44
3	B	341	QUE	O27-C10-C11	-2.51	118.15	120.74
3	D	341	QUE	C5-C4-C3	-2.50	117.43	121.79
2	C	338	NAP	C4D-O4D-C1D	-2.50	107.64	109.92
2	C	338	NAP	O3-PA-O1A	-2.49	103.21	110.70
2	D	338	NAP	C5B-C4B-C3B	-2.49	106.25	115.21
2	D	338	NAP	C6A-C5A-N7A	2.49	136.89	132.09
2	F	338	NAP	C2B-C1B-N9A	2.48	117.84	113.75
3	B	342	QUE	O23-C18-C17	-2.45	111.89	118.42
3	C	342	QUE	C15-C16-C17	2.43	122.93	120.50
2	E	338	NAP	O3D-C3D-C4D	-2.42	104.12	111.08
3	C	342	QUE	O27-C10-C9	2.42	121.34	116.89
3	F	341	QUE	C14-C19-C18	2.41	122.19	120.09
2	E	338	NAP	C1B-N9A-C8A	2.41	132.44	127.09
2	F	338	NAP	C5A-C4A-N3A	-2.39	123.43	126.72
2	C	338	NAP	C4A-N9A-C1B	-2.38	121.07	126.63
2	D	338	NAP	O3-PN-O1N	-2.38	103.56	110.70
2	A	338	NAP	C3B-C2B-C1B	2.37	107.35	102.81
3	B	341	QUE	O13-C9-C10	2.35	124.39	119.61
2	A	338	NAP	C2B-C1B-N9A	2.32	117.57	113.75
3	F	342	QUE	O24-C17-C18	-2.31	112.25	118.42
2	C	338	NAP	O3B-C3B-C4B	2.31	117.72	111.08
3	F	341	QUE	C4-C3-C9	-2.30	117.26	120.03
2	E	338	NAP	O2N-PN-O3	2.29	113.47	107.27
2	E	338	NAP	O2A-PA-O5B	2.29	117.92	107.57
2	E	338	NAP	O4B-C4B-C3B	2.28	109.68	105.15
3	F	341	QUE	O24-C17-C18	2.28	124.50	118.42
2	B	338	NAP	C2A-N3A-C4A	2.27	117.38	111.83
3	B	341	QUE	C4-C5-C6	2.27	122.56	118.98
2	F	338	NAP	N3A-C2A-N1A	-2.27	125.15	128.58
3	D	342	QUE	O24-C17-C16	2.26	125.42	119.36
2	D	338	NAP	O4B-C4B-C5B	2.25	116.53	109.33
3	C	341	QUE	C2-C1-C6	2.24	121.74	119.67
2	D	338	NAP	C3N-C7N-N7N	2.24	120.49	117.74
2	E	338	NAP	C3B-C2B-C1B	2.23	107.08	102.81
2	F	338	NAP	O7N-C7N-C3N	-2.23	116.87	119.60
2	E	338	NAP	C4A-N9A-C8A	2.23	108.08	105.74
3	B	341	QUE	C11-C10-C9	-2.22	119.93	121.52
3	C	342	QUE	C1-C2-C3	-2.22	118.43	120.92
2	D	338	NAP	C5A-C4A-N3A	-2.22	123.66	126.72
3	F	342	QUE	O12-C4-C3	-2.21	119.02	121.19
3	A	342	QUE	C5-C4-C3	-2.21	117.94	121.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	342	QUE	C15-C14-C19	-2.21	116.69	119.25
3	F	342	QUE	O29-C6-C5	-2.21	114.08	119.85
2	C	338	NAP	N6A-C6A-N1A	2.20	123.28	118.38
3	B	342	QUE	C1-C2-C3	-2.19	118.46	120.92
2	A	338	NAP	C5A-N7A-C8A	2.15	106.83	103.45
3	B	341	QUE	O13-C9-C3	-2.15	118.17	122.06
2	C	338	NAP	C5A-N7A-C8A	2.15	106.83	103.45
2	A	338	NAP	C2A-N3A-C4A	2.14	117.06	111.83
3	C	342	QUE	C5-C4-C3	-2.14	118.06	121.79
2	B	338	NAP	C3N-C7N-N7N	2.13	120.37	117.74
2	B	338	NAP	C4A-N9A-C8A	2.13	107.98	105.74
2	E	338	NAP	O2B-P2B-O1X	-2.13	101.75	109.33
2	E	338	NAP	O4D-C4D-C3D	-2.12	100.94	105.15
2	C	338	NAP	N3A-C2A-N1A	-2.10	125.41	128.58
2	C	338	NAP	O5B-PA-O1A	2.09	117.22	108.94
2	C	338	NAP	C2N-C3N-C4N	2.09	120.68	118.26
3	F	341	QUE	C19-C14-C11	2.08	123.60	120.65
2	F	338	NAP	C3B-C2B-C1B	2.08	106.80	102.81
2	E	338	NAP	C2N-C3N-C7N	2.08	125.47	119.46
2	D	338	NAP	O7N-C7N-N7N	-2.08	119.62	122.62
3	F	341	QUE	C5-C4-C3	-2.07	118.18	121.79
2	C	338	NAP	C4A-N9A-C8A	2.07	107.91	105.74
3	B	342	QUE	O30-C2-C3	2.07	124.98	121.14
2	D	338	NAP	C2A-N1A-C6A	2.07	122.13	118.73
2	B	338	NAP	O7N-C7N-C3N	-2.06	117.08	119.60
2	D	338	NAP	C2D-C3D-C4D	2.06	106.59	102.61
3	F	341	QUE	C3-C9-C10	2.06	119.80	116.88
2	A	338	NAP	C5A-C4A-N9A	2.04	108.04	105.81
2	D	338	NAP	C3B-C2B-C1B	2.04	106.71	102.81
3	B	342	QUE	O24-C17-C16	2.03	124.82	119.36
2	A	338	NAP	N9A-C8A-N7A	-2.03	111.05	113.94
2	D	338	NAP	C4N-C3N-C7N	-2.03	115.54	121.06
2	A	338	NAP	C4D-O4D-C1D	-2.02	108.07	109.92
2	D	338	NAP	C2N-N1N-C1D	2.02	123.59	119.13
3	D	342	QUE	O13-C9-C3	2.01	125.71	122.06
3	B	342	QUE	C19-C18-C17	-2.01	118.03	119.89

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	338	NAP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	C	338	NAP	C5D-O5D-PN-O2N
2	E	338	NAP	C5D-O5D-PN-O3
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	F	338	NAP	O4D-C1D-N1N-C2N
3	D	341	QUE	C10-C11-C14-C15
3	D	341	QUE	C10-C11-C14-C19
2	F	338	NAP	O4D-C4D-C5D-O5D
3	C	341	QUE	C10-C11-C14-C15
3	F	341	QUE	C10-C11-C14-C15
3	F	341	QUE	C10-C11-C14-C19
2	E	338	NAP	C4N-C3N-C7N-N7N
2	E	338	NAP	C4N-C3N-C7N-O7N
3	C	341	QUE	C10-C11-C14-C19
3	D	341	QUE	O12-C11-C14-C15
2	F	338	NAP	C3D-C4D-C5D-O5D
3	B	341	QUE	C10-C11-C14-C15
3	B	341	QUE	C10-C11-C14-C19
3	D	341	QUE	O12-C11-C14-C19
2	E	338	NAP	C2N-C3N-C7N-O7N
2	F	338	NAP	PN-O3-PA-O1A
2	E	338	NAP	C2N-C3N-C7N-N7N
2	B	338	NAP	PN-O3-PA-O2A
2	D	338	NAP	PN-O3-PA-O2A
3	C	341	QUE	O12-C11-C14-C15
3	F	341	QUE	O12-C11-C14-C15
2	B	338	NAP	O4D-C4D-C5D-O5D
2	C	338	NAP	PN-O3-PA-O2A
2	D	338	NAP	PN-O3-PA-O1A
2	F	338	NAP	PN-O3-PA-O2A
2	A	338	NAP	C2B-O2B-P2B-O3X
2	B	338	NAP	C2B-O2B-P2B-O3X
2	F	338	NAP	C2B-O2B-P2B-O3X
3	F	341	QUE	O12-C11-C14-C19
3	C	341	QUE	O12-C11-C14-C19
2	B	338	NAP	O4B-C4B-C5B-O5B
2	A	338	NAP	O4D-C1D-N1N-C6N
2	D	338	NAP	O4D-C1D-N1N-C2N
2	D	338	NAP	O4D-C1D-N1N-C6N

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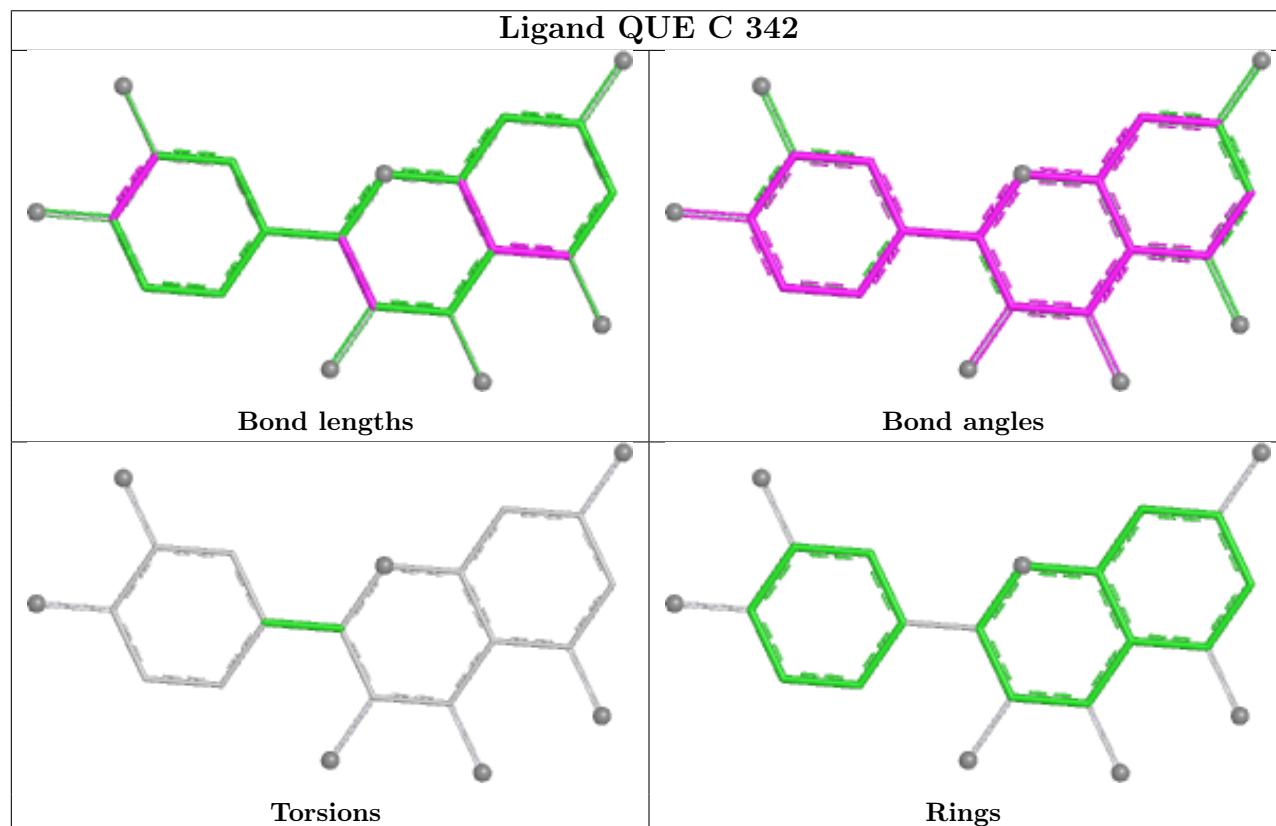
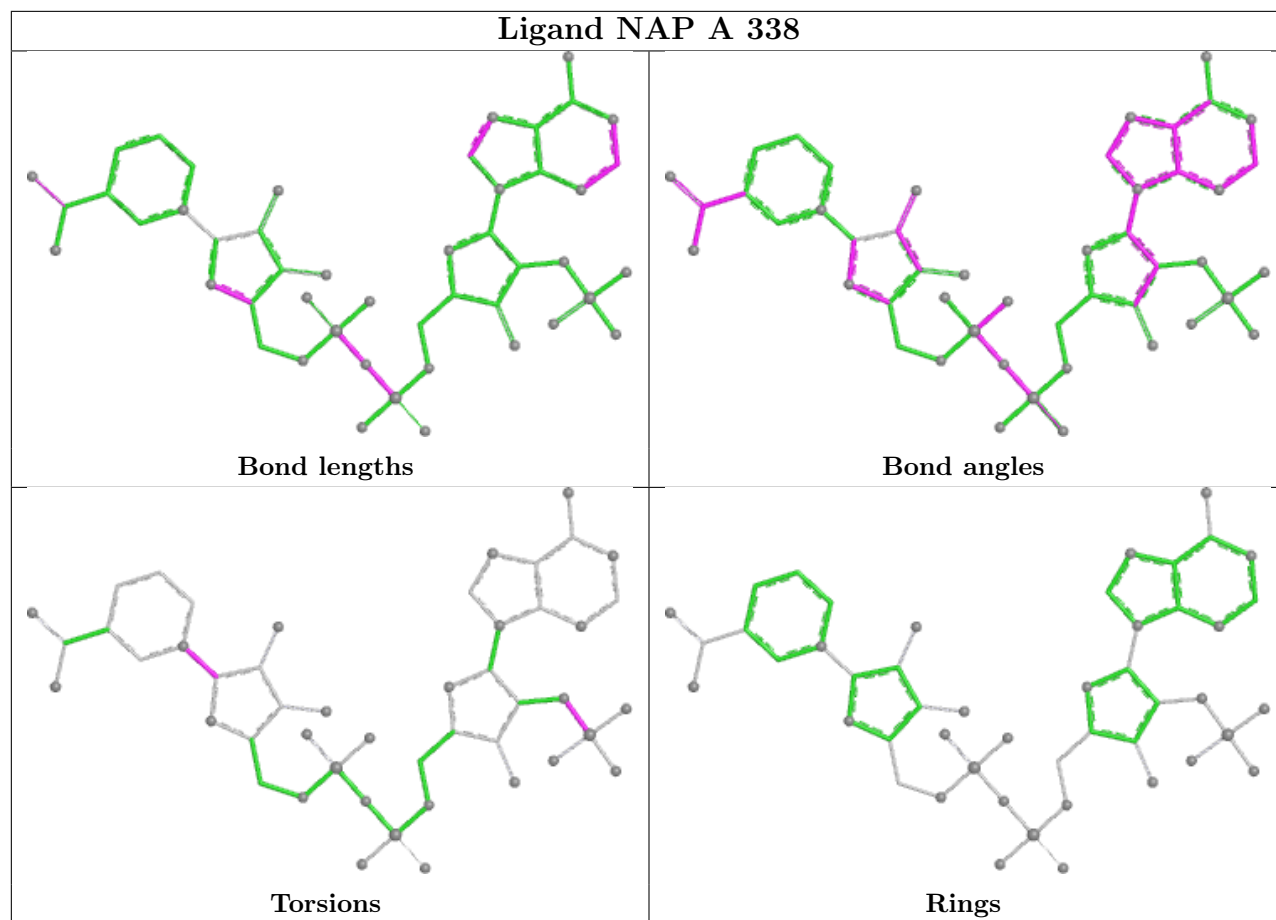
Mol	Chain	Res	Type	Atoms
2	F	338	NAP	O4D-C1D-N1N-C6N
3	B	341	QUE	O12-C11-C14-C15
2	B	338	NAP	PN-O3-PA-O1A
2	C	338	NAP	PN-O3-PA-O1A
2	B	338	NAP	C2B-O2B-P2B-O2X
2	D	338	NAP	C2B-O2B-P2B-O3X
3	B	341	QUE	O12-C11-C14-C19

There are no ring outliers.

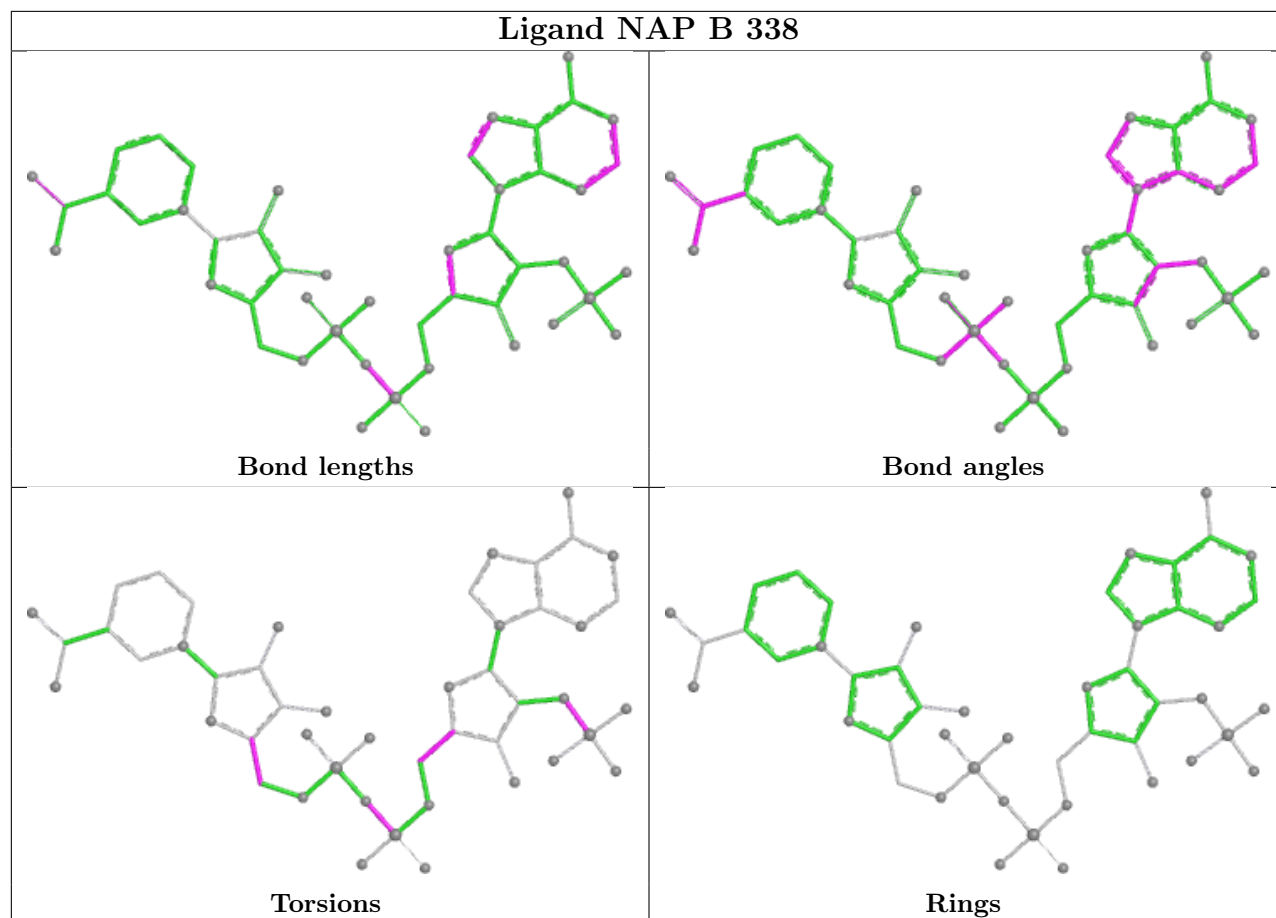
13 monomers are involved in 31 short contacts:

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

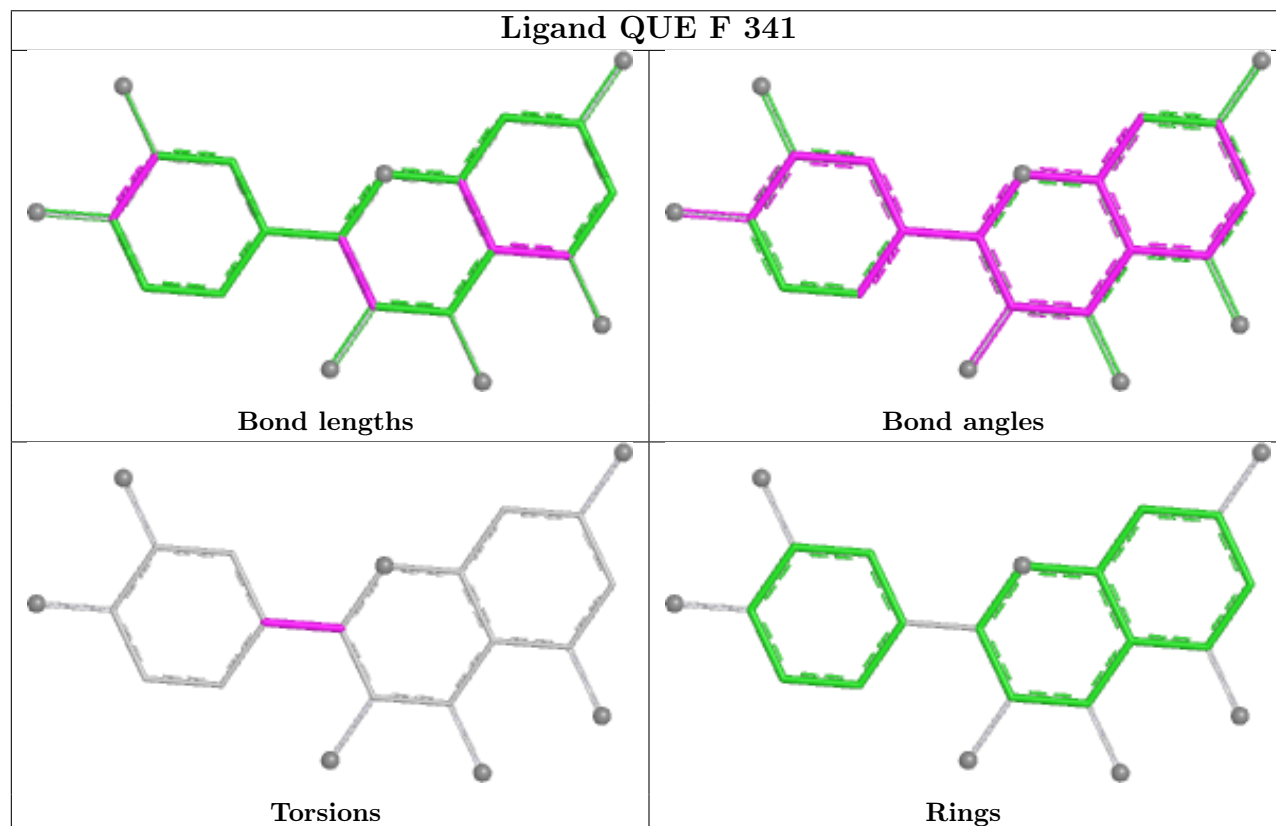
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

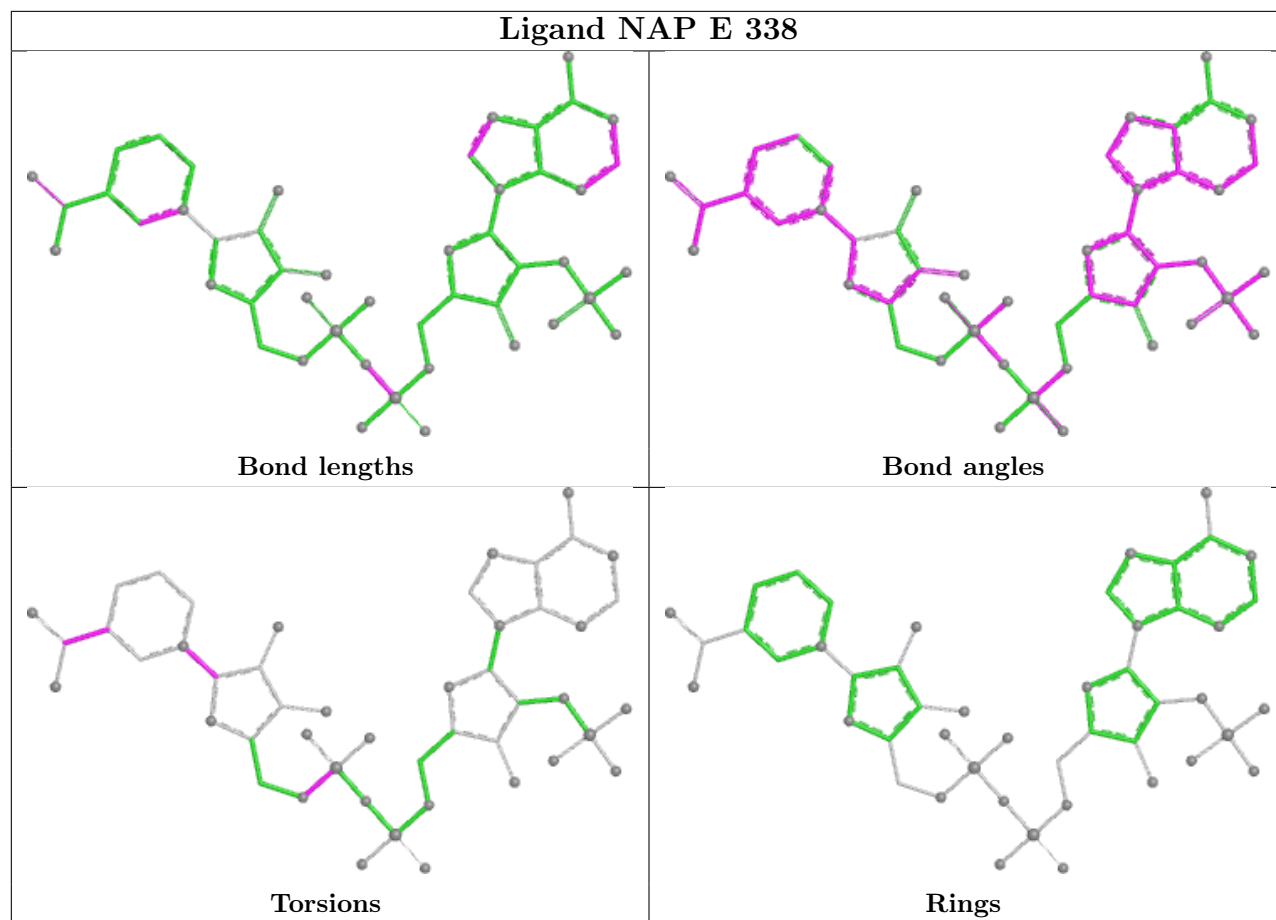


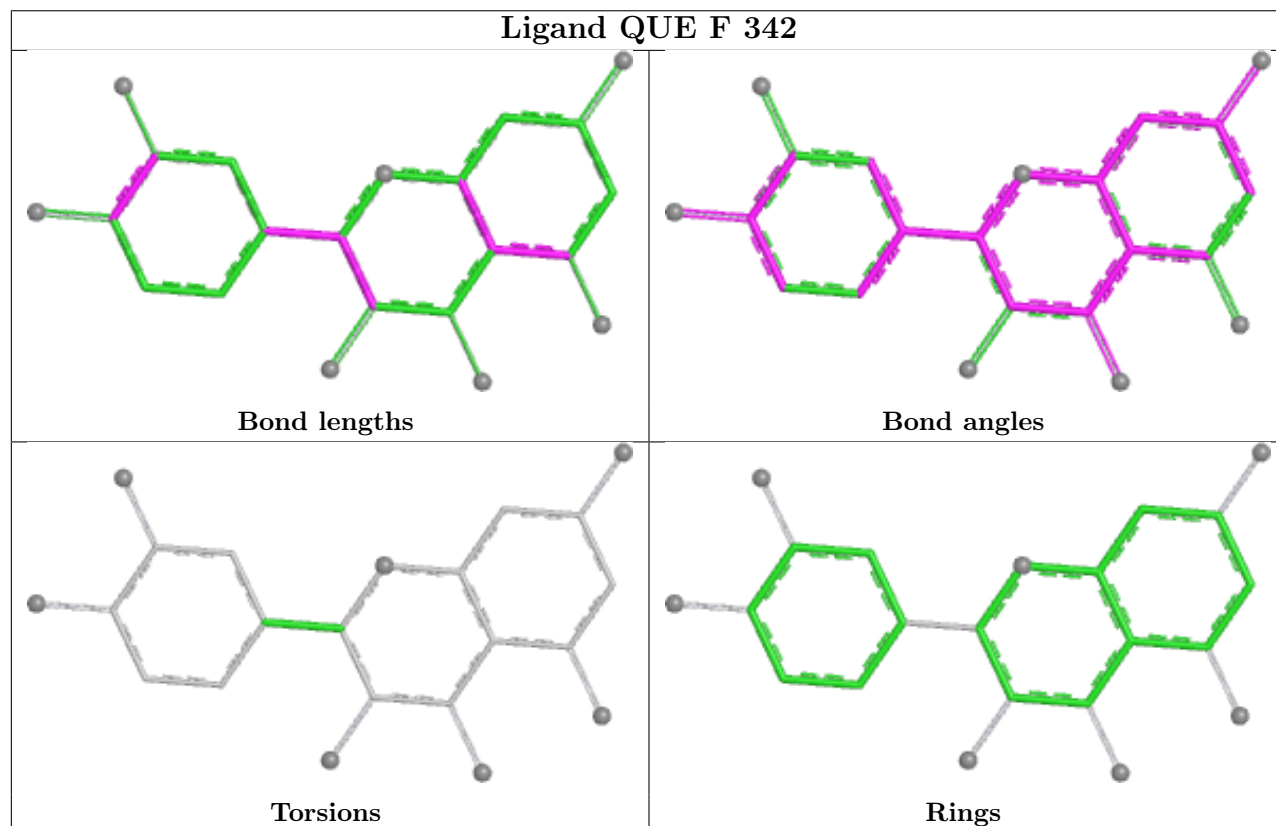
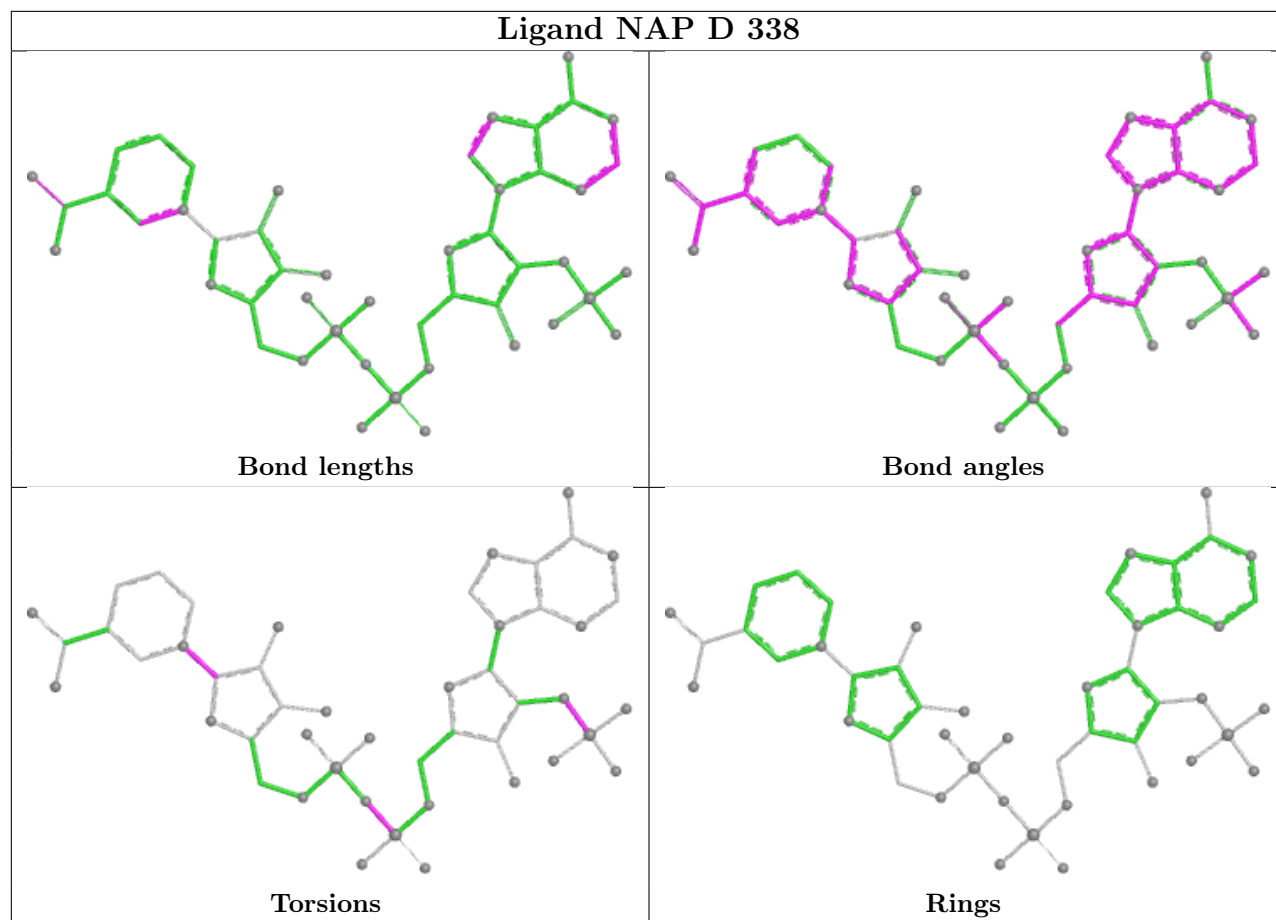
Ligand NAP B 338

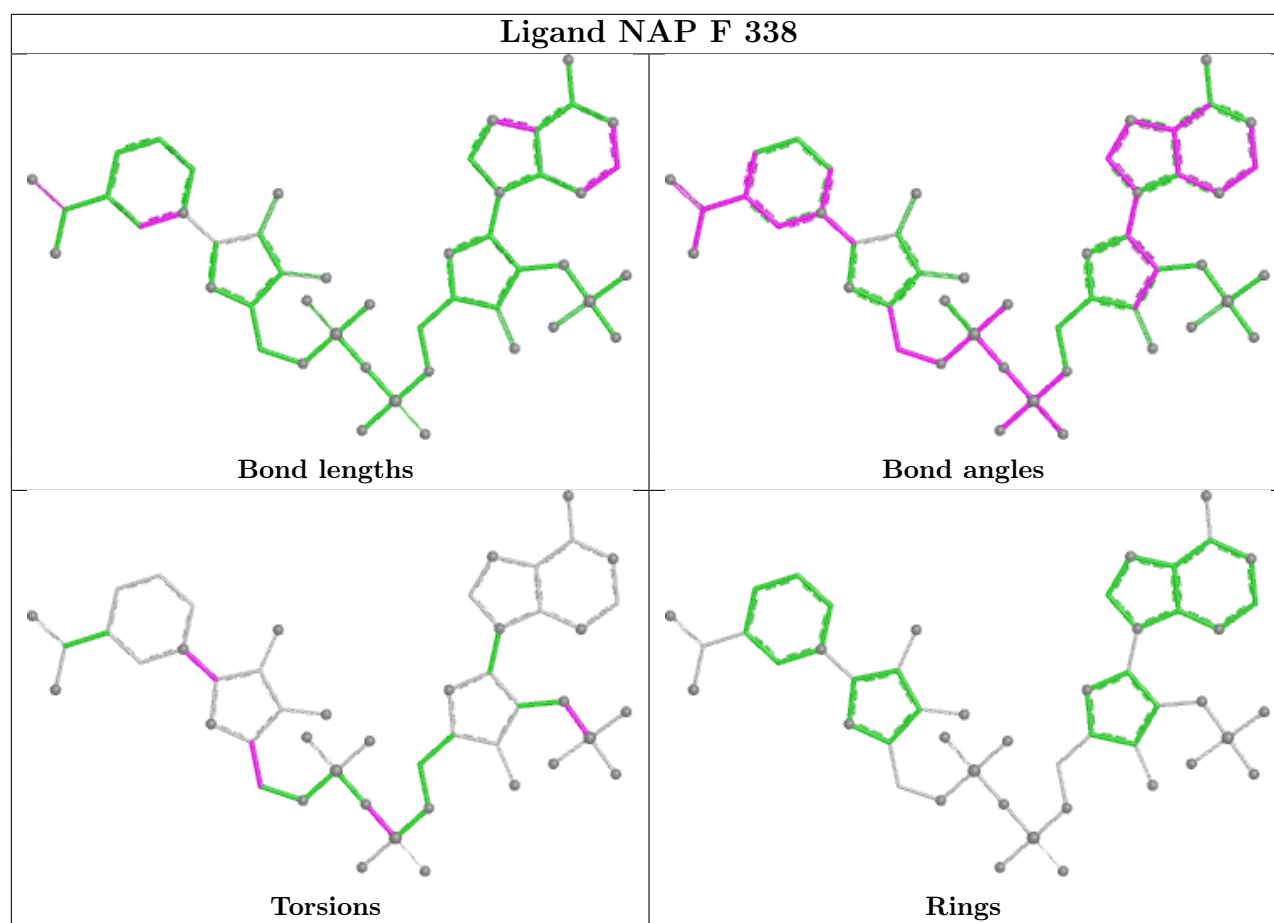


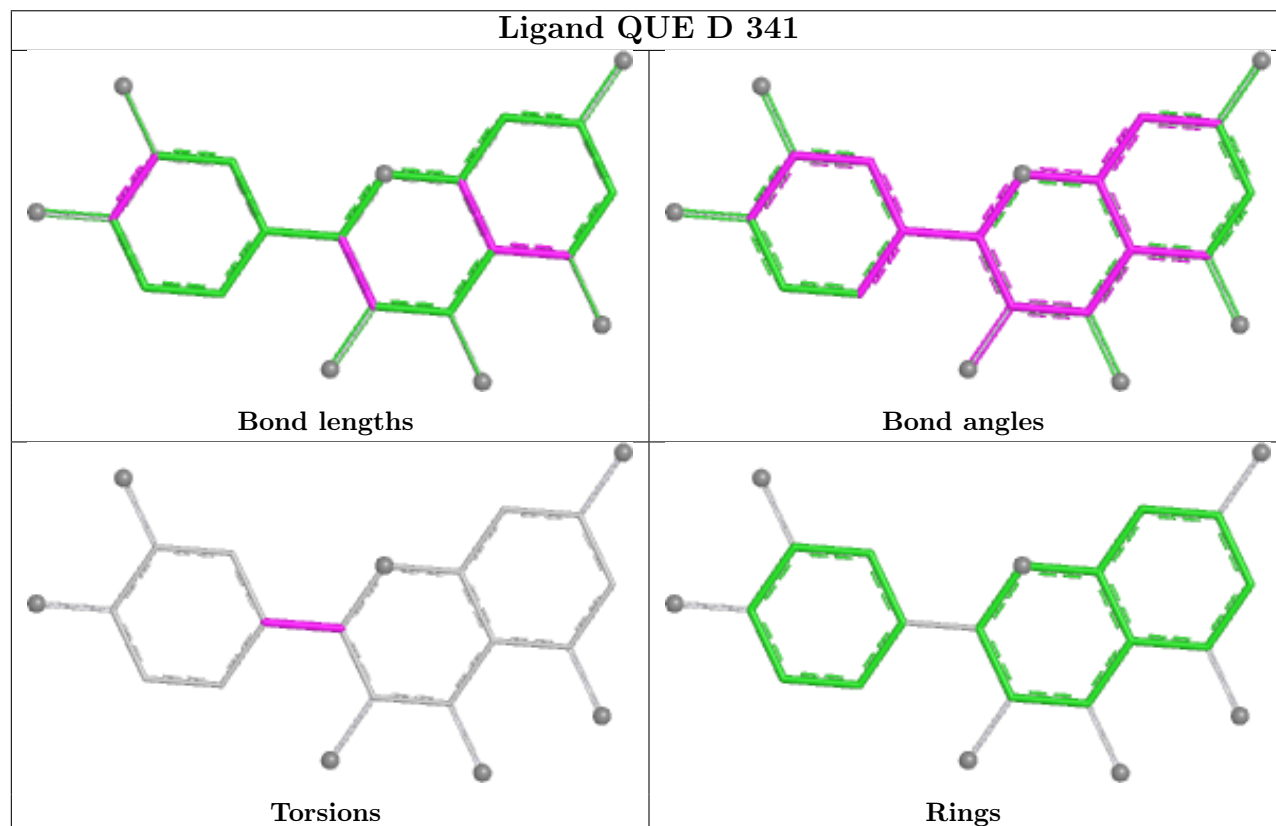
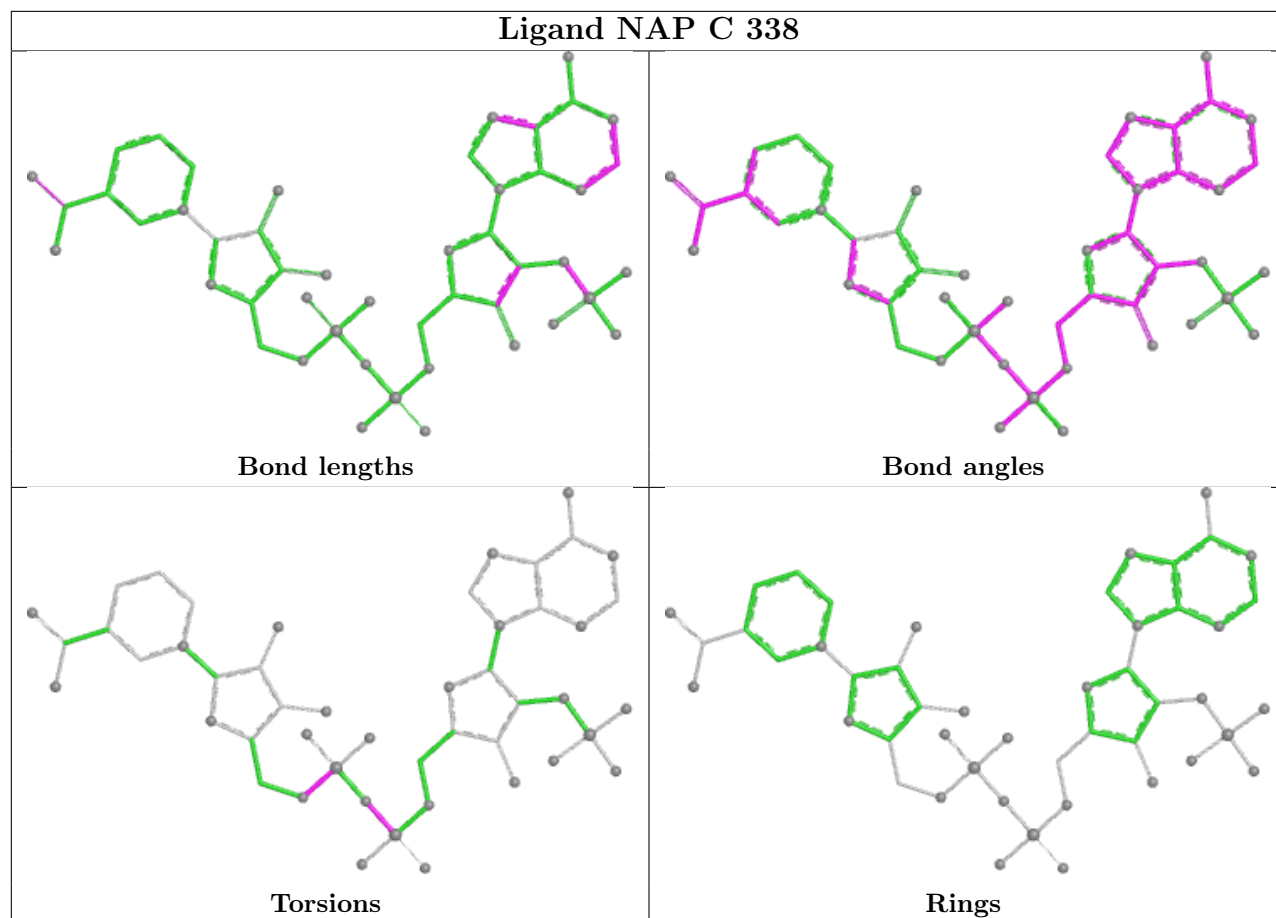
Ligand QUE F 341

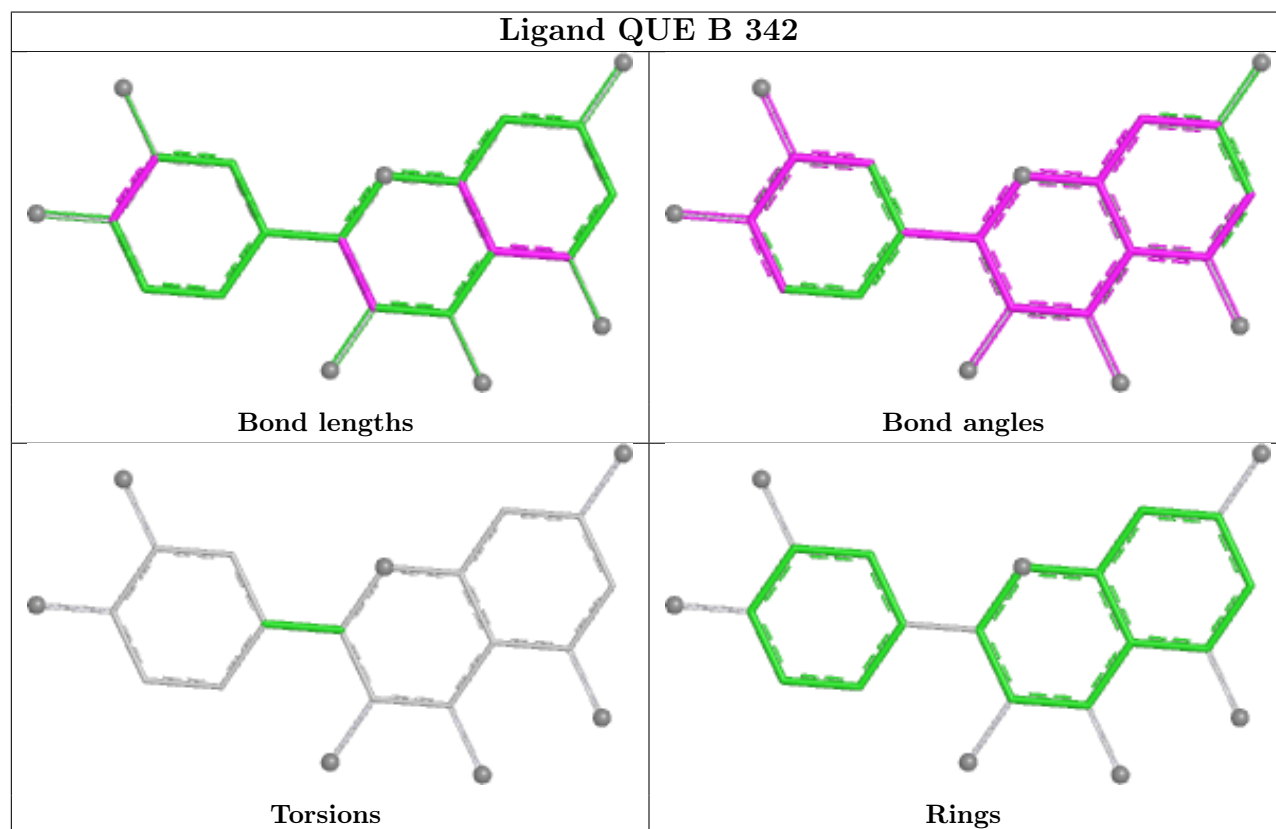
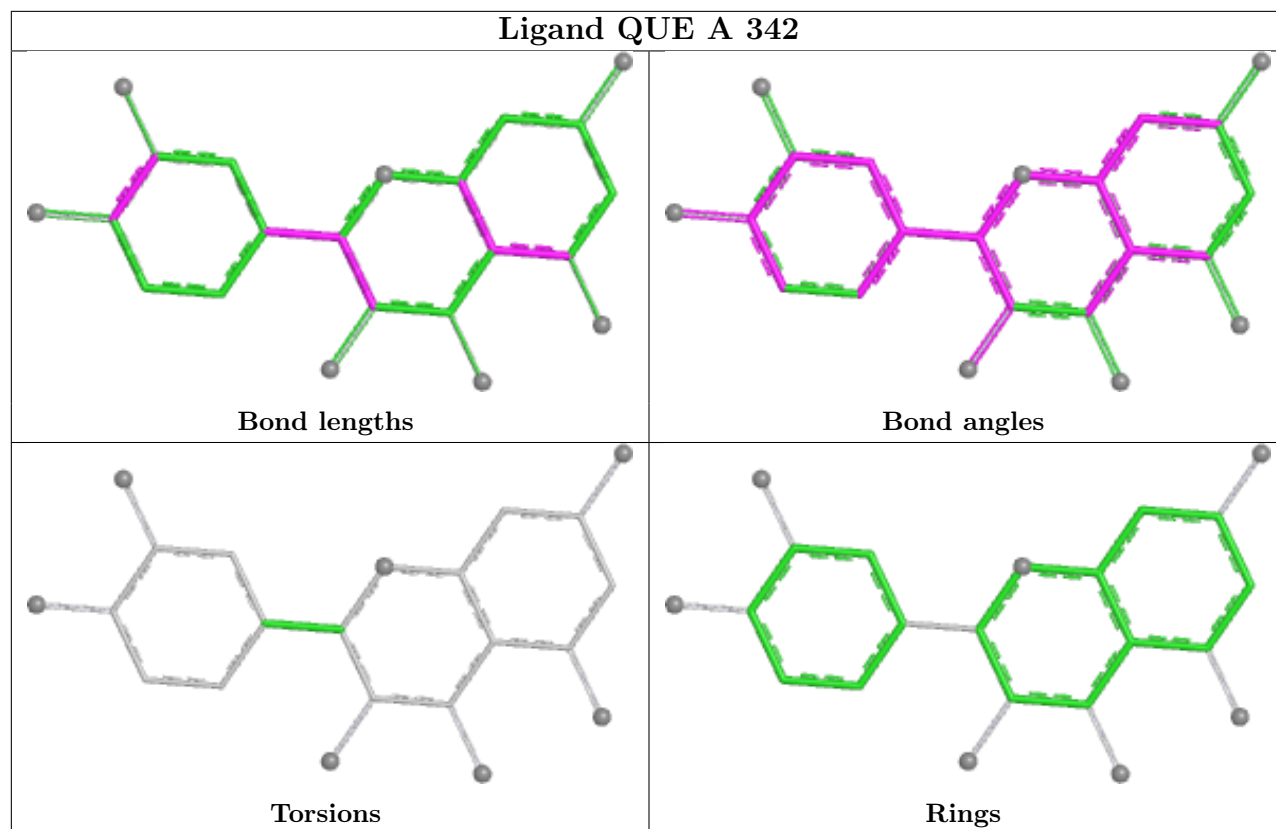




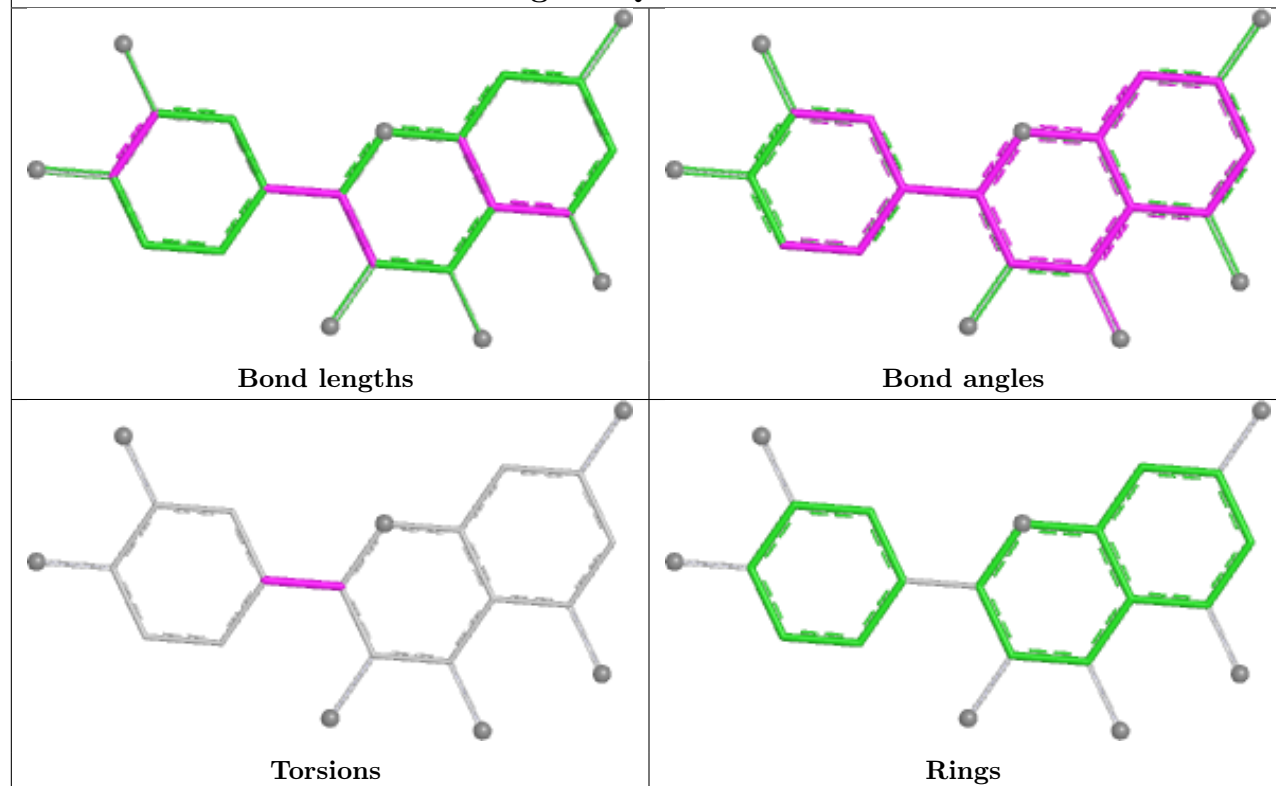




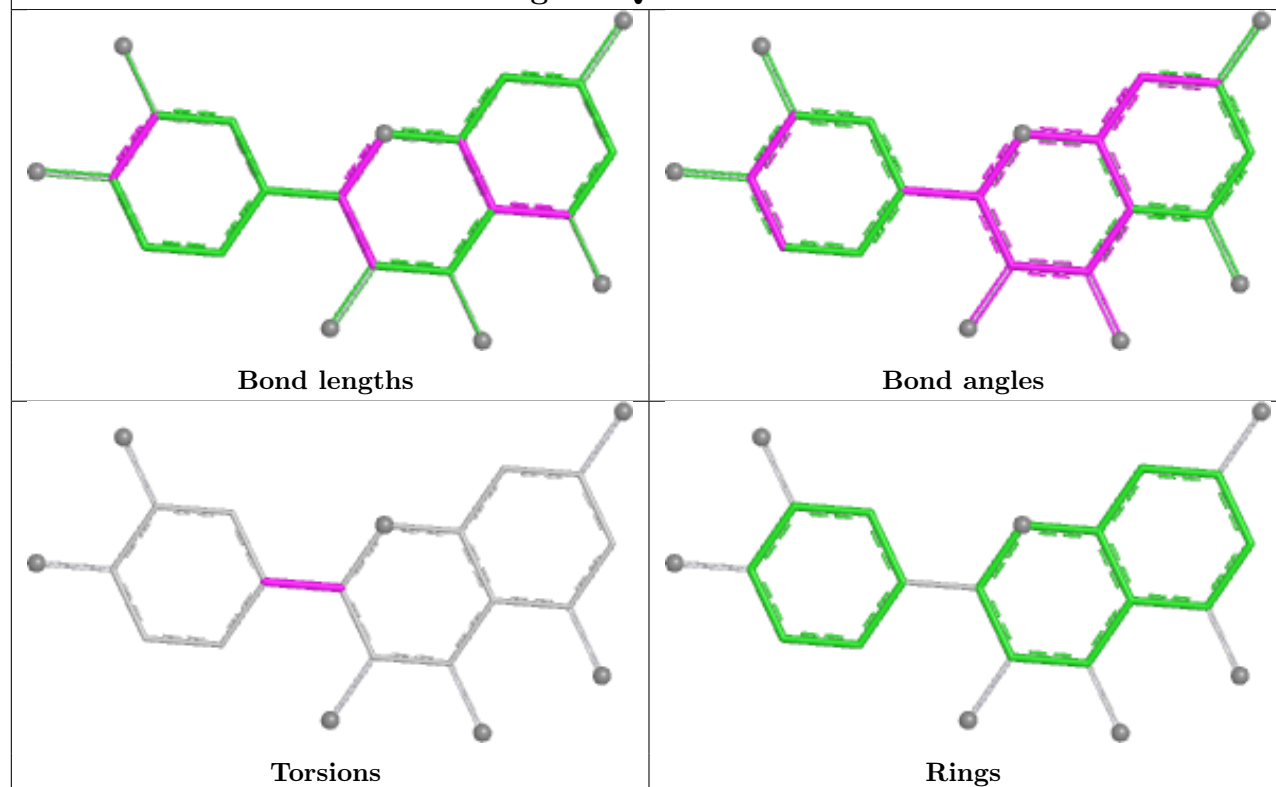


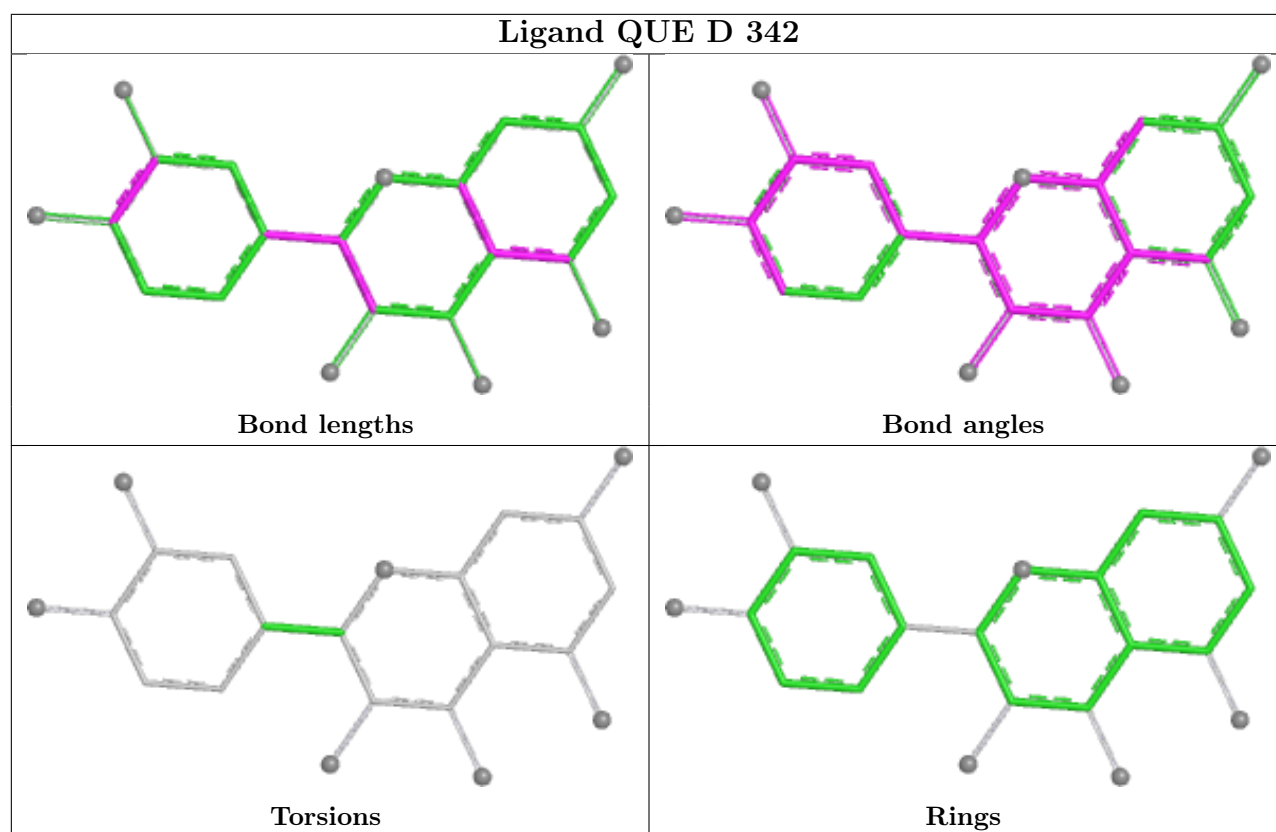


Ligand QUE C 341



Ligand QUE B 341





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	324/337 (96%)	1.15	37 (11%) 10 8	14, 28, 41, 46	0
1	B	324/337 (96%)	0.93	37 (11%) 10 8	4, 20, 38, 43	0
1	C	324/337 (96%)	0.99	37 (11%) 10 8	4, 19, 38, 42	0
1	D	324/337 (96%)	1.35	64 (19%) 3 2	13, 28, 42, 47	0
1	E	324/337 (96%)	1.61	108 (33%) 1 1	13, 29, 43, 48	0
1	F	324/337 (96%)	1.18	45 (13%) 6 5	12, 28, 42, 46	0
All	All	1944/2022 (96%)	1.20	328 (16%) 4 3	4, 26, 41, 48	0

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	77	GLY	6.0
1	D	201	SER	5.5
1	D	88	MET	5.1
1	E	88	MET	4.9
1	A	182	ASN	4.6
1	D	6	GLU	4.4
1	E	119	THR	4.2
1	D	275	ASN	4.2
1	D	54	ALA	4.2
1	E	184	ASP	4.1
1	E	20	TRP	4.1
1	C	279	GLU	4.1
1	F	55	GLU	4.0
1	B	182	ASN	3.9
1	F	199	MET	3.9
1	C	119	THR	3.8
1	C	32	VAL	3.8
1	D	279	GLU	3.8
1	B	268	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	115	ALA	3.8
1	E	32	VAL	3.7
1	D	278	THR	3.7
1	C	118	LYS	3.7
1	B	118	LYS	3.6
1	E	120	VAL	3.6
1	D	7	THR	3.6
1	E	52	PRO	3.6
1	A	309	GLU	3.5
1	E	275	ASN	3.5
1	A	301	GLY	3.5
1	F	279	GLU	3.5
1	E	73	GLU	3.4
1	D	66	ALA	3.4
1	C	151	GLU	3.4
1	D	242	PHE	3.4
1	E	77	GLY	3.3
1	E	123	LEU	3.3
1	F	126	THR	3.3
1	B	6	GLU	3.3
1	E	218	ALA	3.2
1	D	300	LEU	3.2
1	B	284	ASP	3.2
1	F	284	ASP	3.2
1	C	97	ASN	3.2
1	E	306	TYR	3.1
1	B	121	ARG	3.1
1	D	31	THR	3.1
1	E	160	ALA	3.1
1	B	252	ILE	3.1
1	F	327	PRO	3.1
1	B	112	LYS	3.1
1	E	117	ALA	3.1
1	E	308	LEU	3.1
1	A	256	HIS	3.1
1	E	329	HIS	3.1
1	C	269	GLU	3.1
1	D	116	ALA	3.0
1	C	240	TYR	3.0
1	E	255	SER	3.0
1	E	178	ALA	3.0
1	E	183	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	244	ASN	3.0
1	D	26	LEU	3.0
1	C	146	CYS	3.0
1	E	264	ALA	3.0
1	E	124	VAL	3.0
1	E	121	ARG	3.0
1	A	328	SER	3.0
1	E	31	THR	3.0
1	B	301	GLY	2.9
1	E	51	LEU	2.9
1	C	38	ASP	2.9
1	F	280	PHE	2.9
1	E	238	HIS	2.9
1	E	75	ILE	2.9
1	A	42	VAL	2.9
1	E	168	THR	2.9
1	A	199	MET	2.9
1	A	317	ASP	2.9
1	E	278	THR	2.9
1	F	329	HIS	2.9
1	E	114	CYS	2.9
1	C	300	LEU	2.9
1	C	73	GLU	2.9
1	E	321	ALA	2.9
1	B	119	THR	2.9
1	A	329	HIS	2.8
1	D	230	HIS	2.8
1	A	270	LYS	2.8
1	E	177	TYR	2.8
1	B	304	PHE	2.8
1	E	7	THR	2.8
1	E	201	SER	2.8
1	E	118	LYS	2.8
1	F	200	SER	2.8
1	E	53	LYS	2.8
1	D	79	THR	2.8
1	D	307	SER	2.8
1	E	200	SER	2.8
1	F	88	MET	2.7
1	F	182	ASN	2.7
1	D	19	SER	2.7
1	D	272	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	119	THR	2.7
1	D	198	ILE	2.7
1	F	292	PHE	2.7
1	F	312	PHE	2.7
1	B	42	VAL	2.7
1	B	125	PHE	2.6
1	D	118	LYS	2.6
1	D	246	LYS	2.6
1	D	236	ASN	2.6
1	C	55	GLU	2.6
1	C	248	GLU	2.6
1	D	50	ASP	2.6
1	F	129	ALA	2.6
1	D	256	HIS	2.6
1	E	9	CYS	2.6
1	E	313	THR	2.6
1	E	232	ASP	2.6
1	A	254	SER	2.6
1	B	57	HIS	2.6
1	A	282	GLY	2.6
1	E	76	LYS	2.6
1	E	78	CYS	2.6
1	E	26	LEU	2.6
1	A	239	ILE	2.6
1	B	68	GLU	2.6
1	E	151	GLU	2.6
1	D	200	SER	2.6
1	C	52	PRO	2.6
1	D	251	TYR	2.6
1	E	251	TYR	2.6
1	D	120	VAL	2.6
1	E	235	CYS	2.6
1	F	252	ILE	2.6
1	D	203	PRO	2.5
1	E	10	VAL	2.5
1	F	177	TYR	2.5
1	A	119	THR	2.5
1	C	304	PHE	2.5
1	D	298	THR	2.5
1	E	280	PHE	2.5
1	D	264	ALA	2.5
1	E	169	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	61	TRP	2.5
1	E	27	GLU	2.5
1	E	125	PHE	2.5
1	F	269	GLU	2.5
1	A	41	ASN	2.5
1	D	9	CYS	2.5
1	E	267	LEU	2.5
1	D	77	GLY	2.5
1	E	18	GLY	2.5
1	B	248	GLU	2.5
1	E	30	TYR	2.5
1	F	305	LYS	2.5
1	A	259	ILE	2.4
1	B	120	VAL	2.4
1	B	283	VAL	2.4
1	E	106	GLY	2.4
1	F	283	VAL	2.4
1	E	91	GLU	2.4
1	F	119	THR	2.4
1	D	51	LEU	2.4
1	E	253	CYS	2.4
1	E	239	ILE	2.4
1	A	53	LYS	2.4
1	A	117	ALA	2.4
1	C	278	THR	2.4
1	C	78	CYS	2.4
1	B	80	GLY	2.4
1	E	82	PHE	2.4
1	E	128	SER	2.4
1	E	180	GLU	2.4
1	F	307	SER	2.4
1	F	328	SER	2.4
1	E	188	ILE	2.4
1	E	102	PRO	2.4
1	E	165	VAL	2.4
1	C	305	LYS	2.4
1	E	61	TRP	2.4
1	C	7	THR	2.4
1	B	60	LEU	2.4
1	E	256	HIS	2.4
1	C	246	LYS	2.3
1	D	76	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	121	ARG	2.3
1	E	29	GLY	2.3
1	E	314	GLY	2.3
1	B	49	LEU	2.3
1	B	329	HIS	2.3
1	F	31	THR	2.3
1	A	276	ILE	2.3
1	C	43	LYS	2.3
1	E	323	GLY	2.3
1	F	275	ASN	2.3
1	E	185	PHE	2.3
1	E	284	ASP	2.3
1	E	247	ALA	2.3
1	E	56	THR	2.3
1	A	268	ARG	2.3
1	E	99	VAL	2.3
1	F	130	GLY	2.3
1	F	302	PHE	2.3
1	A	66	ALA	2.3
1	A	284	ASP	2.3
1	F	143	ASP	2.3
1	D	241	LEU	2.3
1	D	57	HIS	2.3
1	D	239	ILE	2.3
1	E	57	HIS	2.3
1	B	278	THR	2.3
1	F	56	THR	2.3
1	C	28	ARG	2.3
1	C	303	GLU	2.3
1	D	74	ALA	2.3
1	E	116	ALA	2.3
1	A	44	LYS	2.3
1	D	44	LYS	2.3
1	D	112	LYS	2.3
1	E	189	ILE	2.3
1	A	56	THR	2.3
1	F	7	THR	2.3
1	E	245	PRO	2.3
1	A	209	ALA	2.2
1	A	244	ASN	2.2
1	E	49	LEU	2.2
1	B	50	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	72	ASP	2.2
1	A	222	ILE	2.2
1	F	222	ILE	2.2
1	F	59	THR	2.2
1	B	117	ALA	2.2
1	D	98	GLU	2.2
1	B	181	ASN	2.2
1	C	76	LYS	2.2
1	C	181	ASN	2.2
1	E	46	LYS	2.2
1	C	284	ASP	2.2
1	E	22	VAL	2.2
1	E	81	VAL	2.2
1	F	52	PRO	2.2
1	B	240	TYR	2.2
1	E	254	SER	2.2
1	B	162	MET	2.2
1	D	218	ALA	2.2
1	E	110	ILE	2.2
1	F	24	ARG	2.2
1	E	67	ASP	2.2
1	E	39	PRO	2.2
1	F	212	PRO	2.2
1	D	78	CYS	2.2
1	D	266	MET	2.2
1	E	240	TYR	2.2
1	F	77	GLY	2.2
1	F	323	GLY	2.2
1	C	247	ALA	2.2
1	E	279	GLU	2.2
1	E	186	ILE	2.2
1	A	87	PRO	2.2
1	B	67	ASP	2.2
1	E	79	THR	2.2
1	A	61	TRP	2.2
1	A	226	GLY	2.2
1	D	93	LYS	2.2
1	D	274	TYR	2.2
1	B	92	SER	2.2
1	C	312	PHE	2.2
1	B	267	LEU	2.2
1	D	254	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	169	LEU	2.2
1	A	85	ALA	2.2
1	C	268	ARG	2.1
1	A	283	VAL	2.1
1	F	22	VAL	2.1
1	E	246	LYS	2.1
1	E	231	LEU	2.1
1	F	128	SER	2.1
1	A	269	GLU	2.1
1	A	179	LYS	2.1
1	B	305	LYS	2.1
1	A	324	LEU	2.1
1	E	90	PHE	2.1
1	E	268	ARG	2.1
1	F	66	ALA	2.1
1	B	114	CYS	2.1
1	D	91	GLU	2.1
1	C	256	HIS	2.1
1	E	8	VAL	2.1
1	F	167	LYS	2.1
1	C	25	LEU	2.1
1	E	215	GLY	2.1
1	E	261	LEU	2.1
1	B	79	THR	2.1
1	C	89	ASP	2.1
1	D	280	PHE	2.1
1	E	38	ASP	2.1
1	E	298	THR	2.1
1	E	304	PHE	2.1
1	D	306	TYR	2.1
1	E	243	GLU	2.1
1	A	57	HIS	2.1
1	D	238	HIS	2.1
1	E	101	LYS	2.1
1	D	18	GLY	2.1
1	D	106	GLY	2.1
1	D	168	THR	2.1
1	B	61	TRP	2.1
1	B	198	ILE	2.1
1	D	160	ALA	2.1
1	E	175	TRP	2.1
1	D	255	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	71	PHE	2.0
1	F	154	ARG	2.0
1	C	183	ILE	2.0
1	E	34	ALA	2.0
1	F	116	ALA	2.0
1	D	281	LYS	2.0
1	F	44	LYS	2.0
1	D	324	LEU	2.0
1	A	59	THR	2.0
1	D	115	ALA	2.0
1	E	74	ALA	2.0
1	B	27	GLU	2.0
1	C	309	GLU	2.0
1	F	266	MET	2.0
1	D	8	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

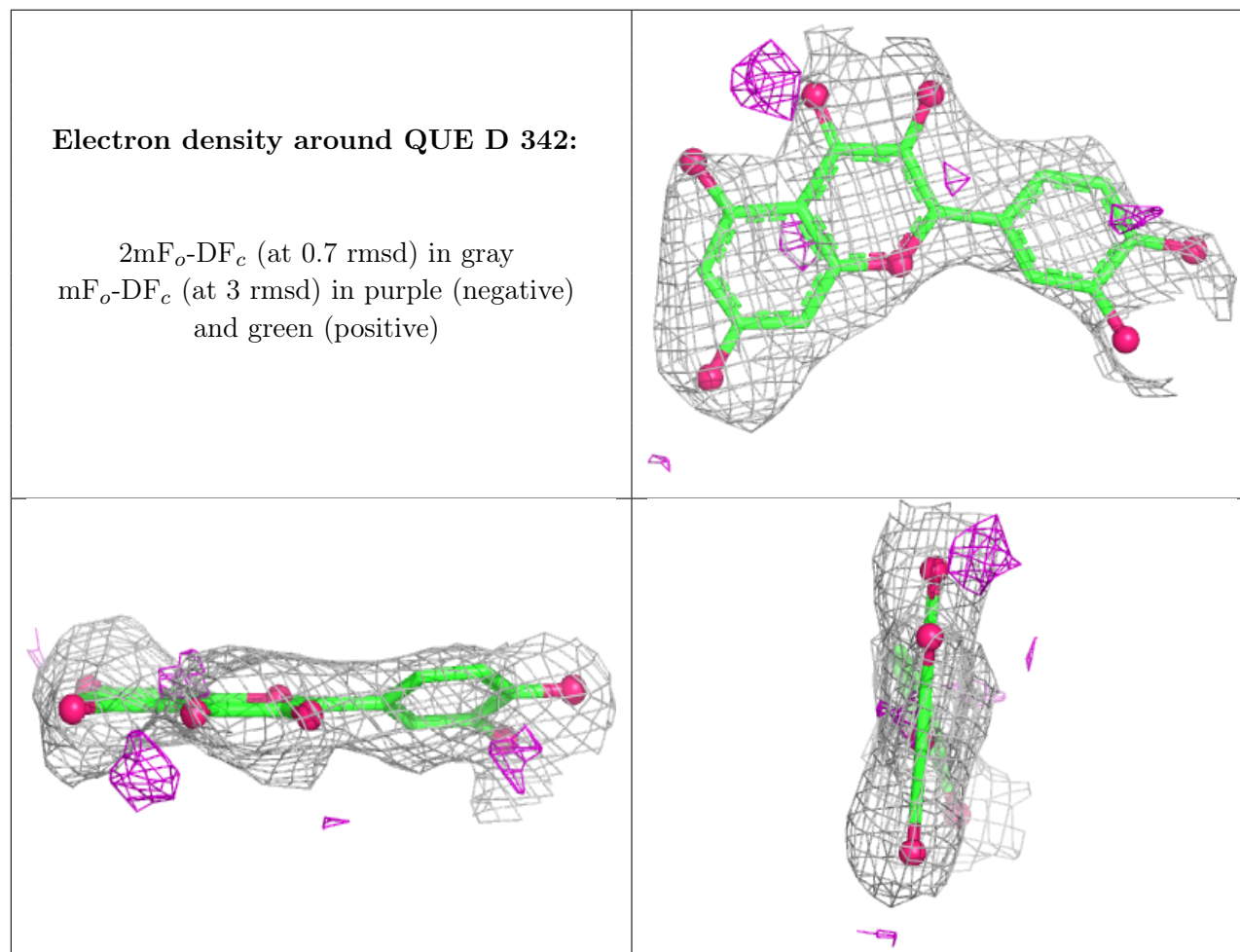
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	QUE	D	342	22/22	0.81	0.17	24,24,25,25	0
3	QUE	F	342	22/22	0.81	0.16	22,23,23,24	0
3	QUE	F	341	22/22	0.85	0.15	18,19,20,21	0
3	QUE	A	342	22/22	0.85	0.14	18,19,20,20	0
3	QUE	D	341	22/22	0.86	0.14	24,25,26,26	0
3	QUE	C	342	22/22	0.88	0.14	10,12,13,13	0
2	NAP	A	338	48/48	0.89	0.14	17,20,26,27	0
3	QUE	B	342	22/22	0.90	0.12	11,11,12,13	0

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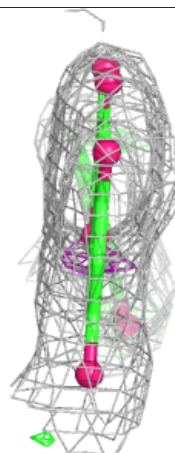
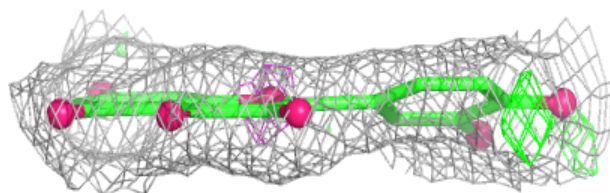
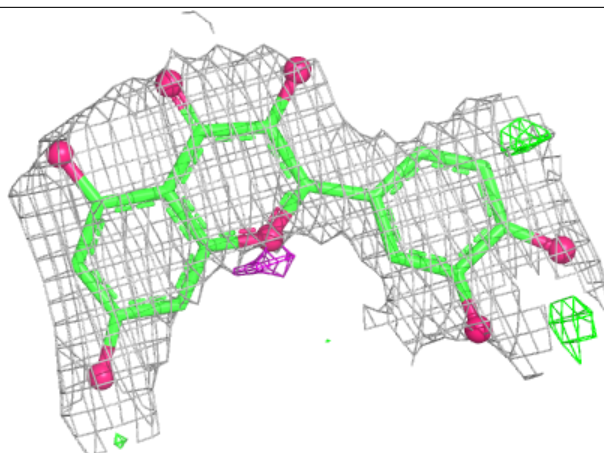
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	F	338	48/48	0.90	0.12	14,18,21,22	0
2	NAP	E	338	48/48	0.92	0.11	14,17,21,21	0
3	QUE	B	341	22/22	0.92	0.13	11,11,12,12	0
2	NAP	D	338	48/48	0.93	0.11	11,18,21,22	0
3	QUE	C	341	22/22	0.95	0.09	8,9,10,10	0
2	NAP	B	338	48/48	0.96	0.09	4,6,13,14	0
2	NAP	C	338	48/48	0.97	0.08	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.

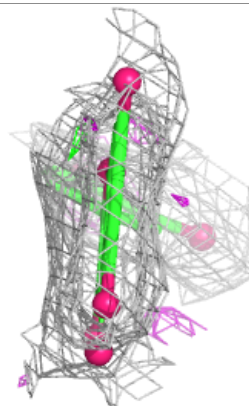
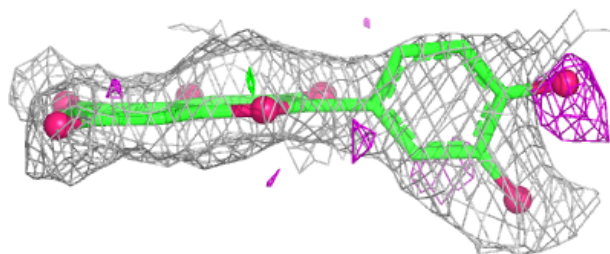
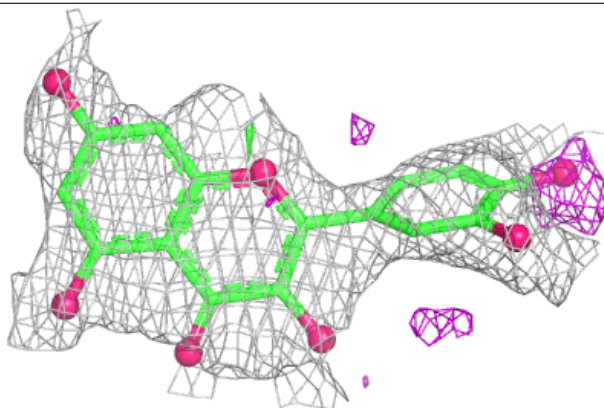


Electron density around QUE F 342:

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

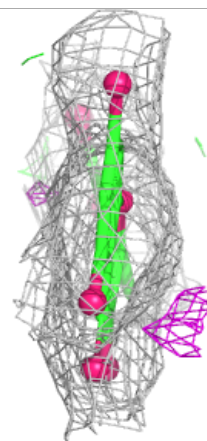
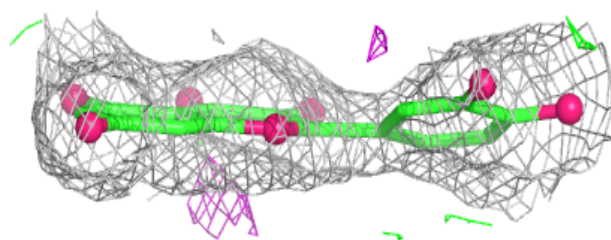
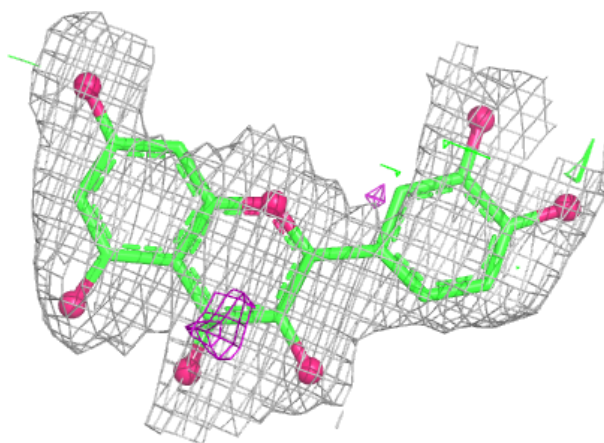
**Electron density around QUE F 341:**

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



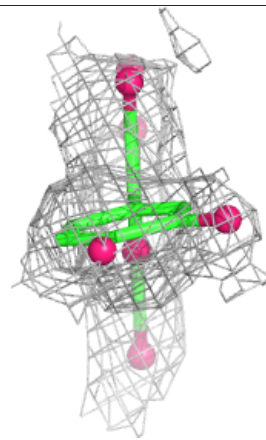
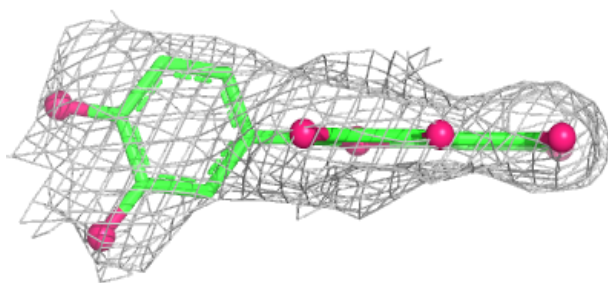
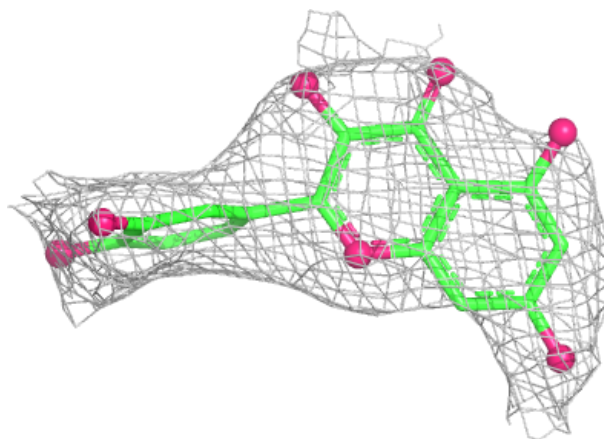
Electron density around QUE A 342:

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



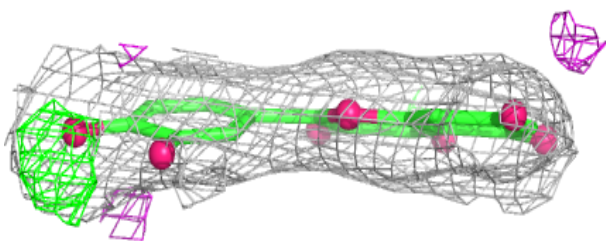
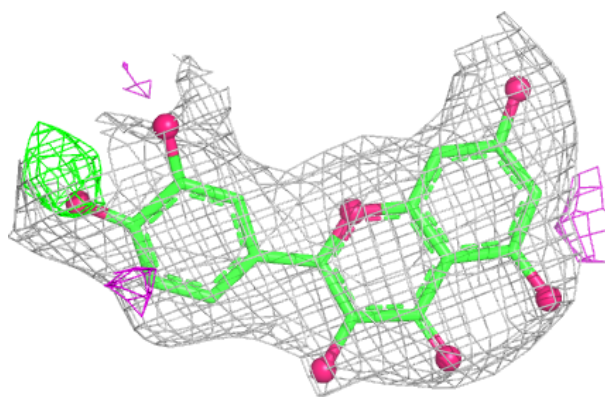
Electron density around QUE D 341:

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



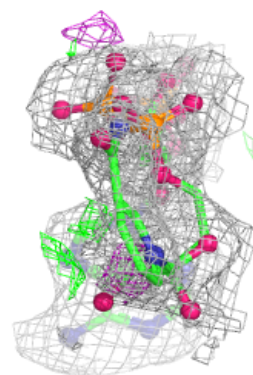
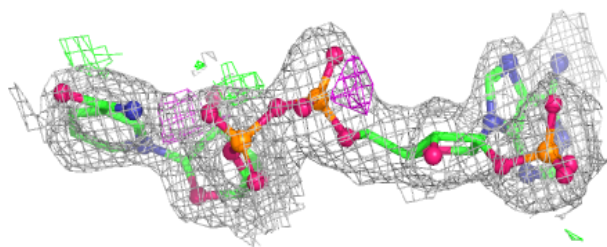
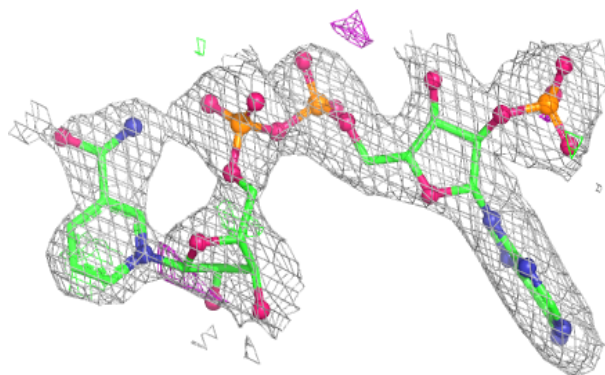
Electron density around QUE C 342:

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



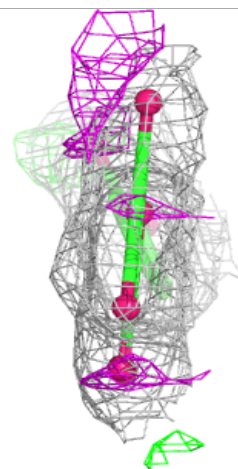
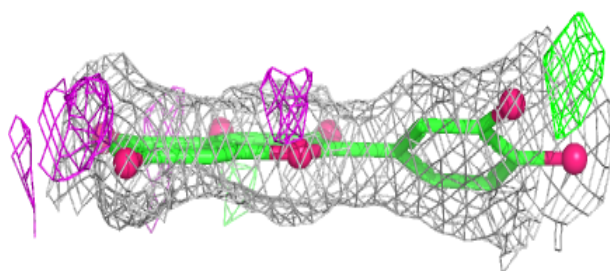
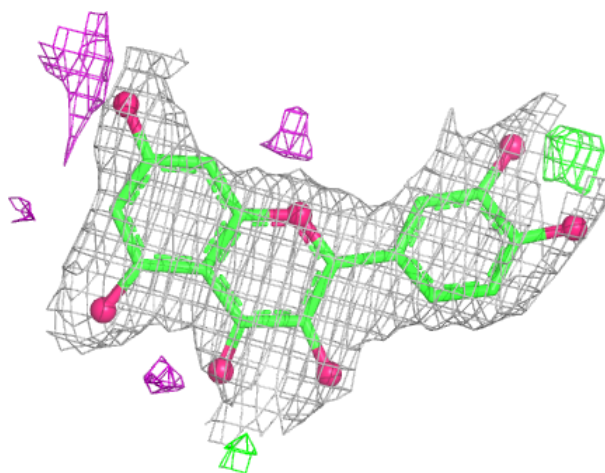
Electron density around NAP A 338:

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



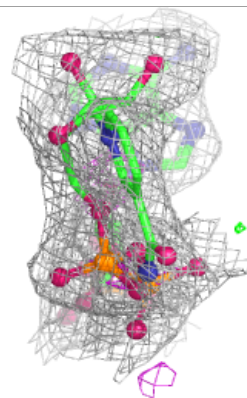
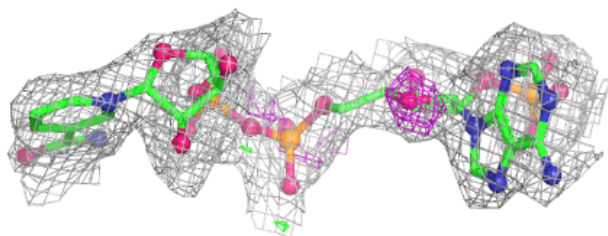
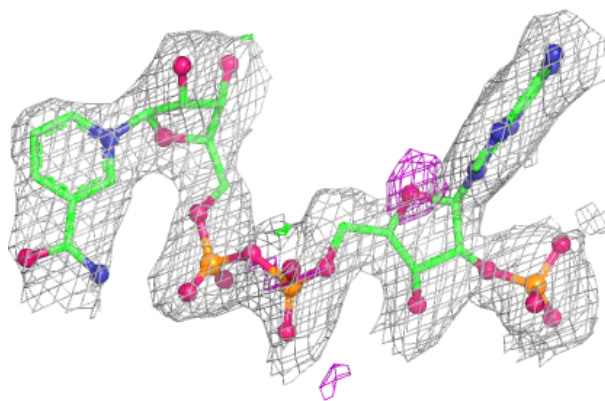
Electron density around QUE B 342:

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

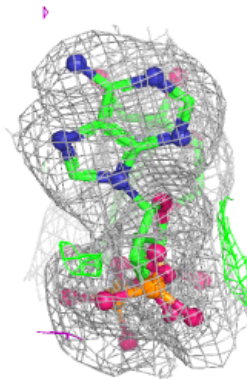
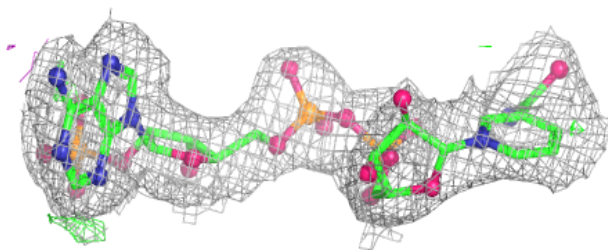
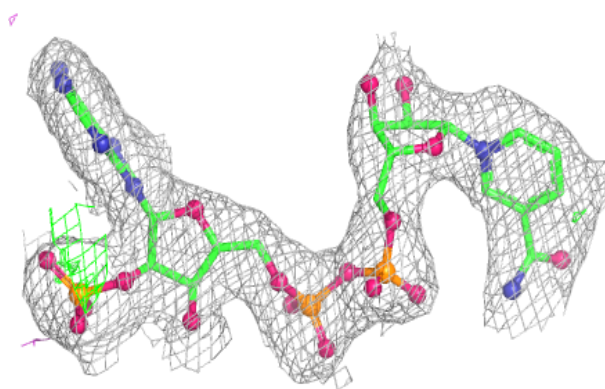


Electron density around NAP F 338:

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

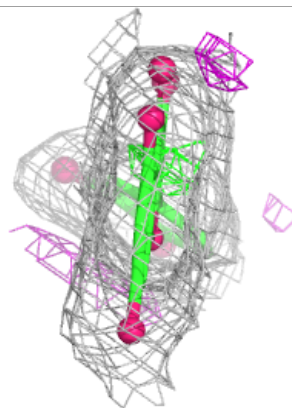
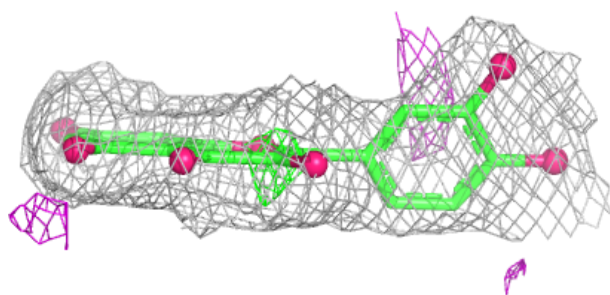
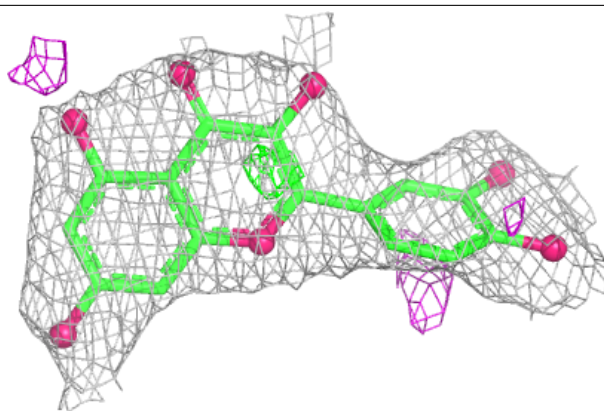
**Electron density around NAP E 338:**

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

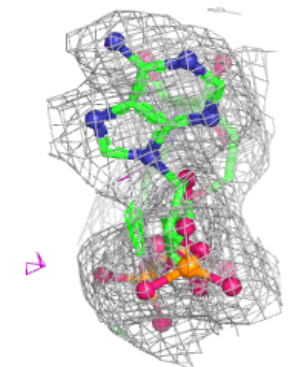
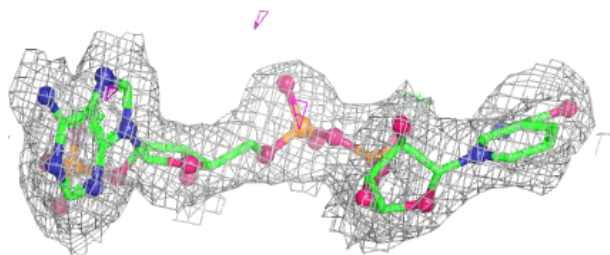
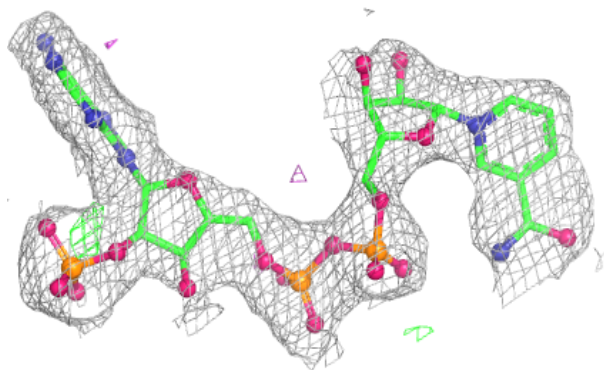


Electron density around QUE B 341:

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

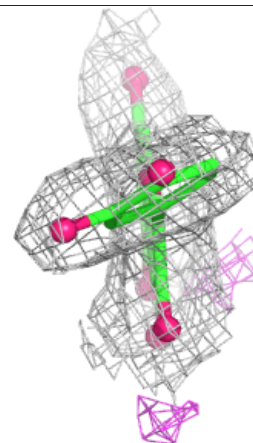
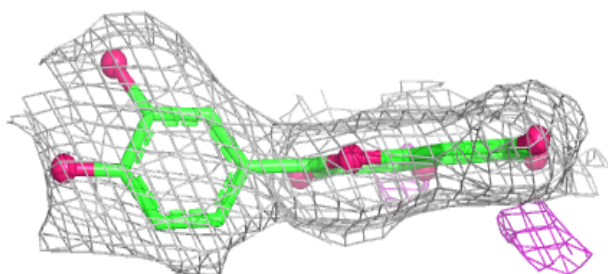
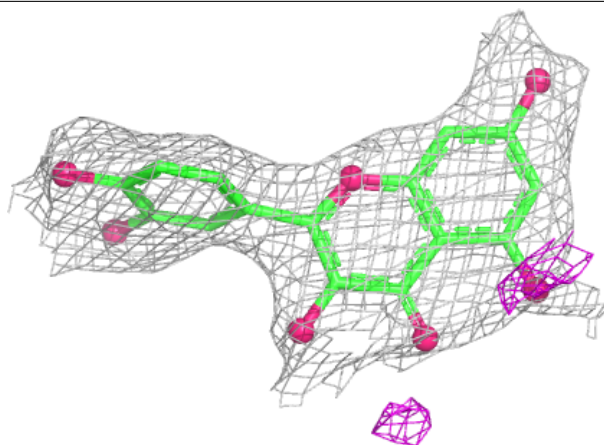
**Electron density around NAP D 338:**

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

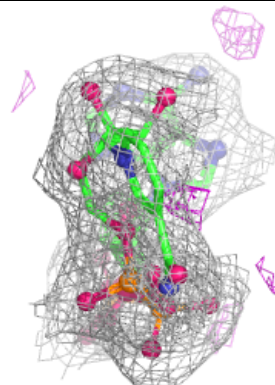
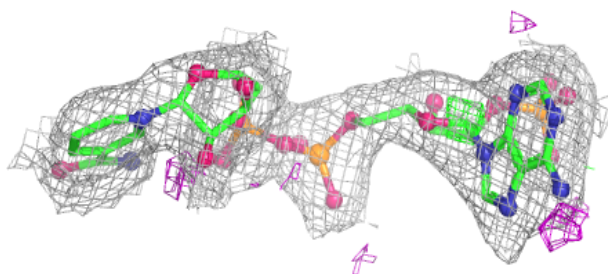
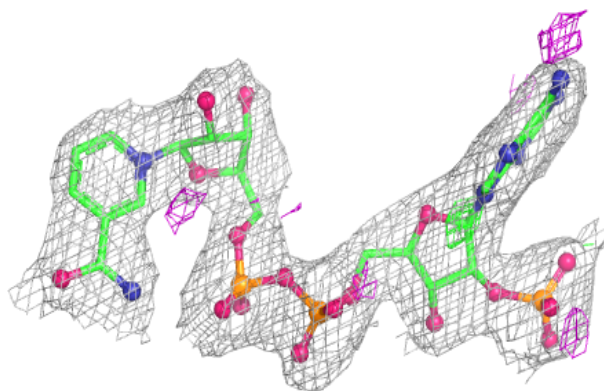


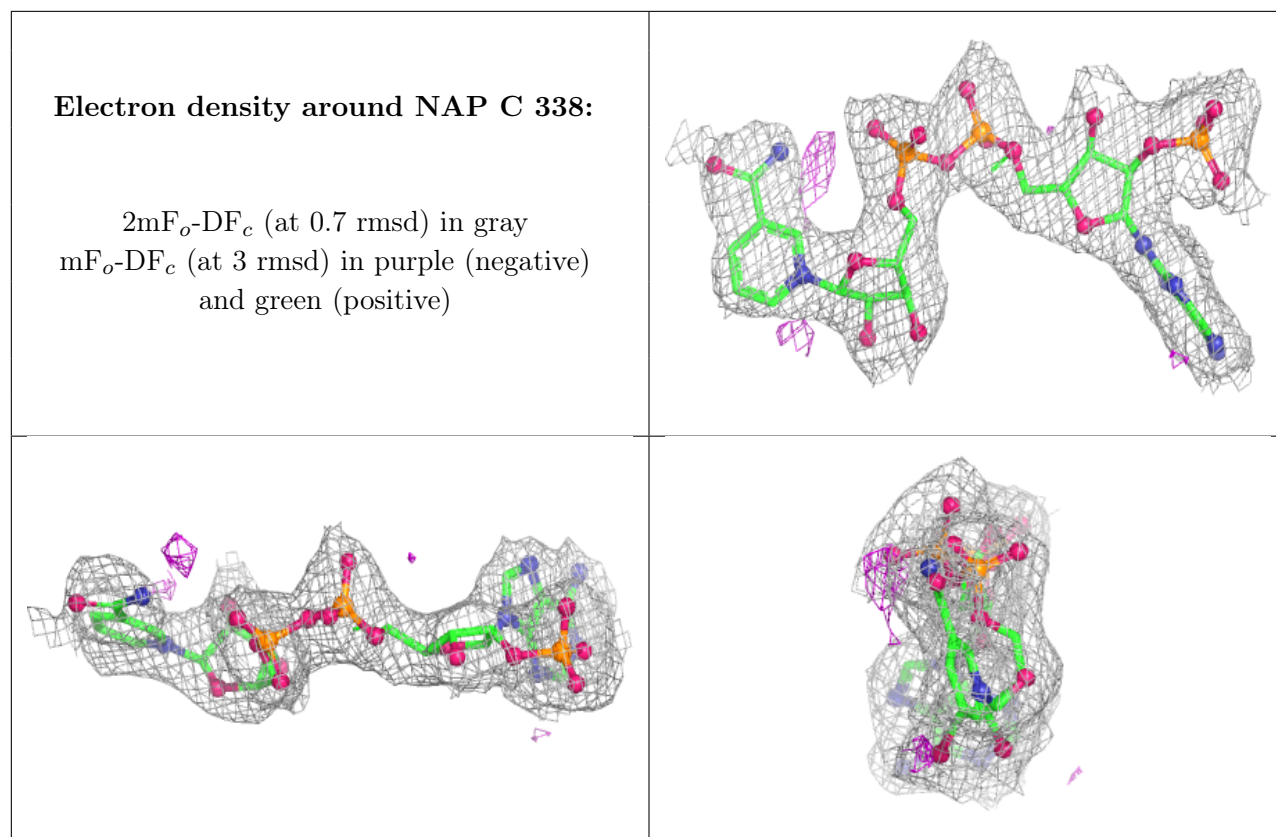
Electron density around QUE C 341:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.