Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 05:32 am GMT

PDB ID	:	2YBT
Title	:	Crystal structure of human acidic chitinase in complex with bisdionin C
Authors	:	Sutherland, T.E.; Andersen, O.A.; Betou, M.; Eggleston, I.M.; Maizels, R.M.; van Aalten, D.; Allen, J.E.
Deposited on	:	2011-03-10
Resolution	:	2.22 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 (i) 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 (i)) were used in the production of this report:

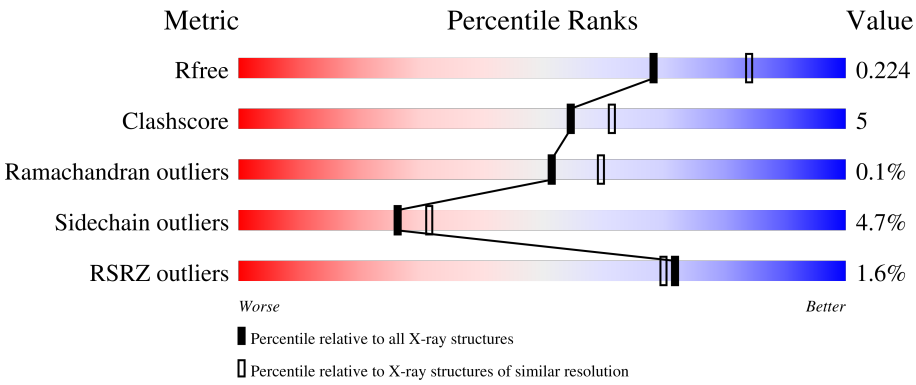
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 <=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	381	2%, 86%, 12%
1	B	381	%, 86%, 13%
1	C	381	%, 85%, 13%
1	D	381	3%, 81%, 14%
1	E	381	2%, 84%, 14%

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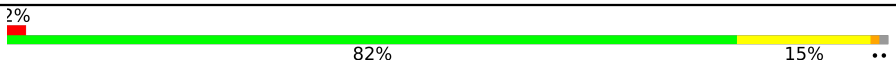
Mol	Chain	Length	Quality of chain
1	F	381	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19339 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 ACIDIC MAMMALIAN CHITINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	377	2983	1924	485	560	14	0	0	0
1	B	377	2983	1924	485	560	14	0	0	0
1	C	377	2983	1924	485	560	14	0	0	0
1	D	377	2983	1924	485	560	14	0	0	0
1	E	377	2983	1924	485	560	14	0	0	0
1	F	377	2983	1924	485	560	14	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLU	-	expression tag	UNP Q9BZP6
A	19	ALA	-	expression tag	UNP Q9BZP6
A	20	GLU	-	expression tag	UNP Q9BZP6
A	45	ASP	ASN	variant	UNP Q9BZP6
A	47	ASN	ASP	variant	UNP Q9BZP6
A	61	MET	ARG	variant	UNP Q9BZP6
B	18	GLU	-	expression tag	UNP Q9BZP6
B	19	ALA	-	expression tag	UNP Q9BZP6
B	20	GLU	-	expression tag	UNP Q9BZP6
B	45	ASP	ASN	variant	UNP Q9BZP6
B	47	ASN	ASP	variant	UNP Q9BZP6
B	61	MET	ARG	variant	UNP Q9BZP6
C	18	GLU	-	expression tag	UNP Q9BZP6
C	19	ALA	-	expression tag	UNP Q9BZP6
C	20	GLU	-	expression tag	UNP Q9BZP6
C	45	ASP	ASN	variant	UNP Q9BZP6
C	47	ASN	ASP	variant	UNP Q9BZP6

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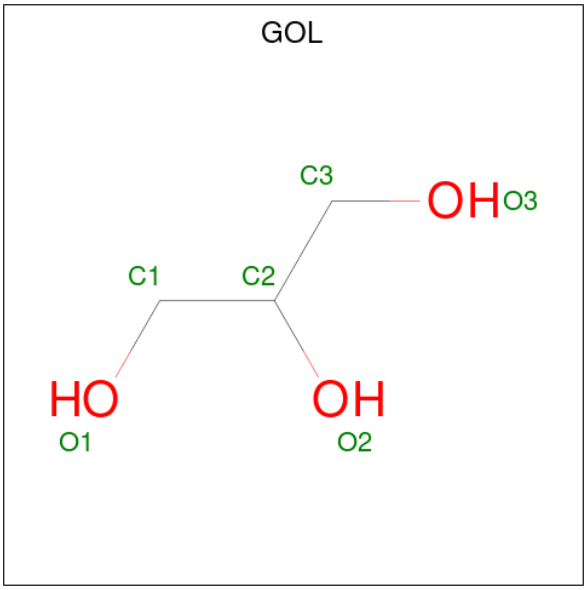
Chain	Residue	Modelled	Actual	Comment	Reference
C	61	MET	ARG	variant	UNP Q9BZP6
D	18	GLU	-	expression tag	UNP Q9BZP6
D	19	ALA	-	expression tag	UNP Q9BZP6
D	20	GLU	-	expression tag	UNP Q9BZP6
D	45	ASP	ASN	variant	UNP Q9BZP6
D	47	ASN	ASP	variant	UNP Q9BZP6
D	61	MET	ARG	variant	UNP Q9BZP6
E	18	GLU	-	expression tag	UNP Q9BZP6
E	19	ALA	-	expression tag	UNP Q9BZP6
E	20	GLU	-	expression tag	UNP Q9BZP6
E	45	ASP	ASN	variant	UNP Q9BZP6
E	47	ASN	ASP	variant	UNP Q9BZP6
E	61	MET	ARG	variant	UNP Q9BZP6
F	18	GLU	-	expression tag	UNP Q9BZP6
F	19	ALA	-	expression tag	UNP Q9BZP6
F	20	GLU	-	expression tag	UNP Q9BZP6
F	45	ASP	ASN	variant	UNP Q9BZP6
F	47	ASN	ASP	variant	UNP Q9BZP6
F	61	MET	ARG	variant	UNP Q9BZP6

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	B	1	6	3	3	0	0

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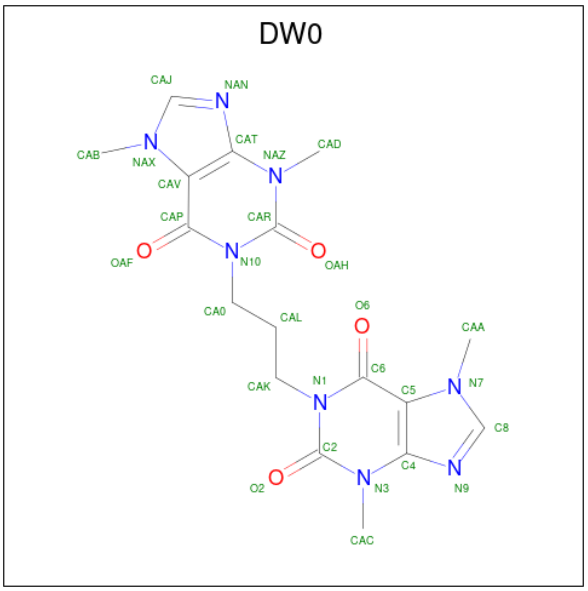
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	C	1	6	3	3		0	0
			Total	C	O			
2	D	1	6	3	3		0	0
			Total	C	O			
2	E	1	6	3	3		0	0
			Total	C	O			
2	F	1	6	3	3		0	0

- Molecule 3 is 1,1'-PROPANE-1,3-DIYLBIS(3,7-DIMETHYL-3,7-DIHYDRO-1H-PURINE-2,6-DIONE) (three-letter code: DW0) (formula: $C_{17}H_{20}N_8O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	29	17	8	4	0	0
			Total	C	N	O		
3	A	1	29	17	8	4	0	0
			Total	C	N	O		
3	B	1	29	17	8	4	0	0
			Total	C	N	O		
3	B	1	29	17	8	4	0	0
			Total	C	N	O		
3	C	1	29	17	8	4	0	0
			Total	C	N	O		
3	C	1	29	17	8	4	0	0
			Total	C	N	O		
3	D	1	29	17	8	4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	D	1	29	17	8	4	0	0
3	E	1	29	17	8	4	0	0
3	E	1	29	17	8	4	0	0
3	F	1	29	17	8	4	0	0
3	F	1	29	17	8	4	0	0

- Molecule 4 is water.

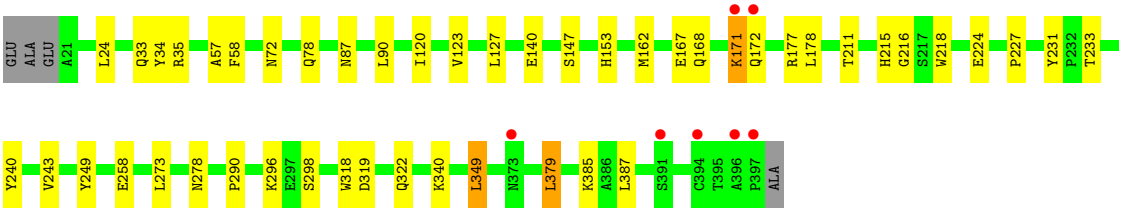
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	202	202	202	0	0
4	B	193	193	193	0	0
4	C	197	197	197	0	0
4	D	146	146	146	0	0
4	E	187	187	187	0	0
4	F	132	132	132	0	0

3 Residue-property plots (i)

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

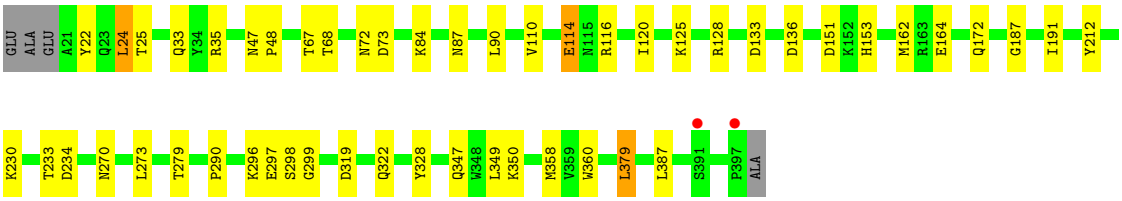
• Molecule 1: ACIDIC MAMMALIAN CHITINASE

Chain A:



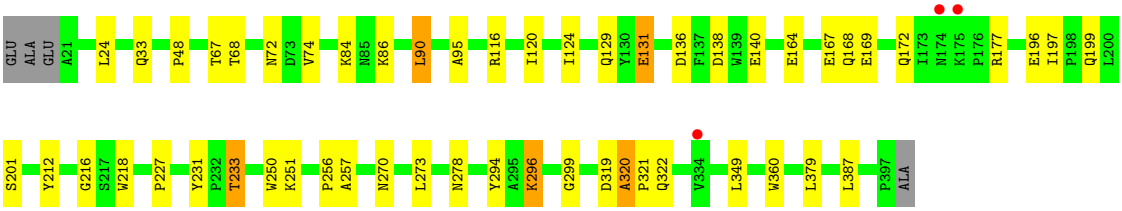
• Molecule 1: ACIDIC MAMMALIAN CHITINASE

Chain B:



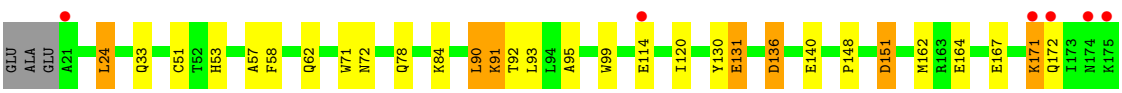
• Molecule 1: ACIDIC MAMMALIAN CHITINASE

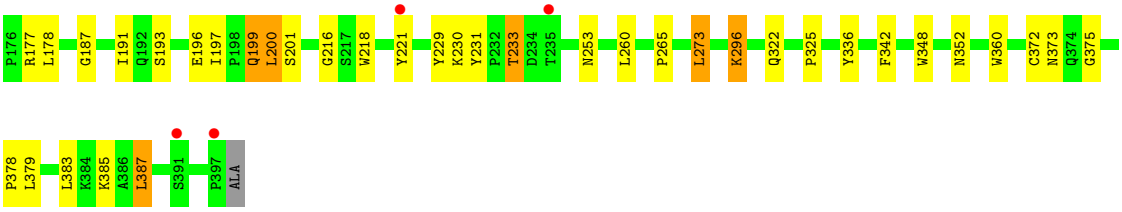
Chain C:



• Molecule 1: ACIDIC MAMMALIAN CHITINASE

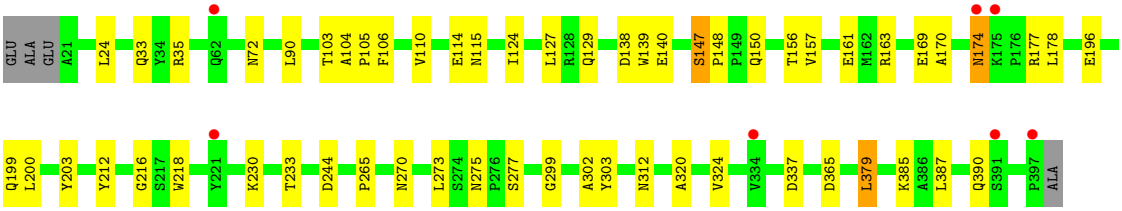
Chain D:





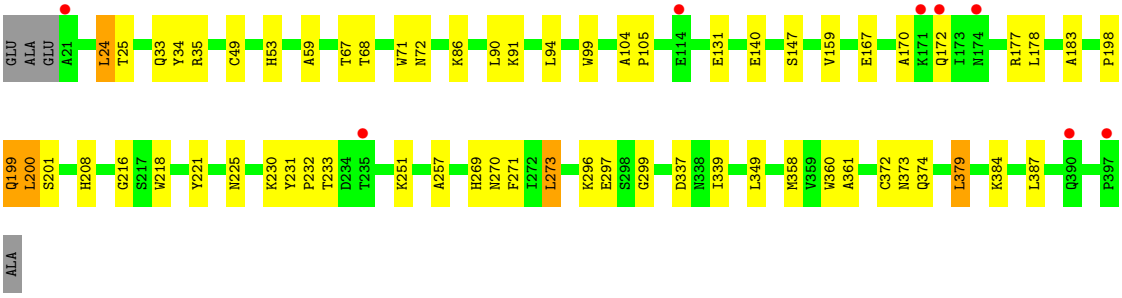
- Molecule 1: ACIDIC MAMMALIAN CHITINASE

Chain E:



- Molecule 1: ACIDIC MAMMALIAN CHITINASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	145.21Å 149.07Å 152.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.07 – 2.22 19.99 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.07-2.22) 99.2 (19.99-2.22)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.181 , 0.228 0.178 , 0.224	Depositor DCC
R_{free} test set	1631 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k 0.043 for -l,-k,-h 0.015 for k,h,-l 0.005 for k,l,h 0.005 for l,h,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19339	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, DW0

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	1.08	4/3076 (0.1%)	0.92	2/4194 (0.0%)
1	B	1.10	2/3076 (0.1%)	0.91	7/4194 (0.2%)
1	C	1.11	4/3076 (0.1%)	0.92	3/4194 (0.1%)
1	D	1.03	2/3076 (0.1%)	0.88	4/4194 (0.1%)
1	E	1.06	1/3076 (0.0%)	0.88	3/4194 (0.1%)
1	F	0.98	1/3076 (0.0%)	0.84	2/4194 (0.0%)
All	All	1.06	14/18456 (0.1%)	0.89	21/25164 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	278	ASN	CB-CG	7.91	1.69	1.51
1	D	221	TYR	CD2-CE2	6.12	1.48	1.39
1	C	320	ALA	CA-CB	6.09	1.65	1.52
1	A	278	ASN	CB-CG	6.00	1.64	1.51
1	A	258	GLU	CG-CD	5.84	1.60	1.51
1	A	298	SER	CB-OG	-5.75	1.34	1.42
1	A	249	TYR	CD2-CE2	5.60	1.47	1.39
1	B	114	GLU	CG-CD	5.56	1.60	1.51
1	B	164	GLU	CG-CD	5.53	1.60	1.51
1	E	320	ALA	CA-CB	5.52	1.64	1.52
1	C	231	TYR	CD1-CE1	5.42	1.47	1.39
1	C	164	GLU	CB-CG	5.22	1.62	1.52
1	F	297	GLU	CB-CG	-5.14	1.42	1.52
1	D	114	GLU	CG-CD	5.08	1.59	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ARG	NE-CZ-NH2	-7.41	116.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	136	ASP	CB-CG-OD1	7.07	124.66	118.30
1	D	273	LEU	CB-CG-CD1	5.79	120.85	111.00
1	A	349	LEU	CA-CB-CG	5.73	128.48	115.30
1	E	379	LEU	CB-CG-CD1	5.71	120.71	111.00
1	B	35	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	B	379	LEU	CB-CG-CD2	5.65	120.61	111.00
1	C	296	LYS	CD-CE-NZ	-5.65	98.70	111.70
1	B	24	LEU	CB-CG-CD2	5.57	120.47	111.00
1	D	273	LEU	CA-CB-CG	5.55	128.07	115.30
1	B	151	ASP	CB-CG-OD1	5.54	123.28	118.30
1	B	73	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	136	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	C	90	LEU	CA-CB-CG	5.27	127.42	115.30
1	F	24	LEU	CB-CG-CD2	5.26	119.95	111.00
1	E	35	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	151	ASP	CB-CG-OD1	5.15	122.94	118.30
1	F	35	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	E	365	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	319	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	B	234	ASP	CB-CG-OD1	5.01	122.81	118.30

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	2983	0	2828	27	0
1	B	2983	0	2828	24	0
1	C	2983	0	2828	27	0
1	D	2983	0	2828	42	0
1	E	2983	0	2828	31	0
1	F	2983	0	2828	39	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
3	A	58	0	40	4	0
3	B	58	0	40	1	0
3	C	58	0	40	3	0
3	D	58	0	40	5	0
3	E	58	0	40	3	0
3	F	58	0	40	3	0
4	A	202	0	0	1	0
4	B	193	0	0	3	0
4	C	197	0	0	3	0
4	D	146	0	0	1	0
4	E	187	0	0	2	0
4	F	132	0	0	2	0
All	All	19339	0	17256	186	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 5.

All (186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:TYR:HD2	1:A:233:THR:HG22	1.26	0.97
1:A:33:GLN:HE22	1:A:72:ASN:HD21	1.20	0.90
1:E:33:GLN:HE22	1:E:72:ASN:HD21	1.27	0.82
1:C:33:GLN:HE22	1:C:72:ASN:HD21	1.30	0.77
1:C:196:GLU:HB3	1:C:199:GLN:HE21	1.49	0.76
1:A:231:TYR:CD2	1:A:233:THR:HG22	2.17	0.72
1:D:140:GLU:OE2	3:D:1399:DW0:HAAB	1.91	0.71
1:E:196:GLU:HB3	1:E:199:GLN:HE21	1.54	0.71
1:F:33:GLN:HE22	1:F:72:ASN:HD21	1.38	0.70
1:B:114:GLU:HB2	4:B:2057:HOH:O	1.91	0.69
1:F:199:GLN:H	1:F:199:GLN:HE21	1.40	0.68
1:B:33:GLN:HE22	1:B:72:ASN:HD21	1.40	0.67
1:F:273:LEU:O	4:F:2088:HOH:O	2.14	0.66
1:A:318:TRP:CH2	1:A:340:LYS:HD3	2.31	0.64
1:A:33:GLN:NE2	1:A:72:ASN:HD21	1.95	0.64
1:D:33:GLN:HE22	1:D:72:ASN:HD21	1.46	0.64
1:F:140:GLU:OE2	3:F:1399:DW0:HAAB	1.99	0.62
1:A:33:GLN:HE22	1:A:72:ASN:ND2	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:TYR:O	1:D:322:GLN:HG2	2.00	0.62
1:C:167:GLU:HG3	1:C:177:ARG:HD3	1.82	0.61
1:F:339:ILE:HD12	1:F:374:GLN:NE2	2.15	0.61
1:C:196:GLU:HB3	1:C:199:GLN:NE2	2.16	0.60
1:F:177:ARG:HG2	1:F:178:LEU:O	2.01	0.60
1:F:167:GLU:HG3	1:F:177:ARG:HD3	1.82	0.60
1:C:296:LYS:HE2	1:E:244:ASP:OD2	2.00	0.60
1:A:231:TYR:HD2	1:A:233:THR:CG2	2.08	0.60
1:D:383:LEU:O	1:D:387:LEU:HB2	2.02	0.59
1:C:116:ARG:O	1:C:120:ILE:HG13	2.03	0.58
1:D:325:PRO:HD2	1:D:336:TYR:O	2.03	0.57
1:D:196:GLU:HB3	1:D:199:GLN:NE2	2.19	0.57
1:D:148:PRO:HD2	1:D:151:ASP:OD2	2.05	0.57
1:F:198:PRO:HD2	1:F:199:GLN:NE2	2.20	0.56
1:F:33:GLN:NE2	1:F:72:ASN:HD21	2.03	0.56
1:D:253:ASN:N	1:D:253:ASN:ND2	2.55	0.55
1:E:138:ASP:OD2	3:E:1399:DW0:CAA	2.54	0.55
1:F:199:GLN:H	1:F:199:GLN:NE2	2.02	0.55
1:B:297:GLU:HG3	4:B:2154:HOH:O	2.06	0.55
1:E:216:GLY:HA3	1:E:218:TRP:CZ3	2.42	0.55
1:A:167:GLU:HG3	1:A:177:ARG:HD3	1.89	0.55
1:B:347:GLN:HE22	1:B:350:LYS:NZ	2.05	0.55
1:E:138:ASP:OD2	3:E:1399:DW0:HAA	2.07	0.55
1:F:67:THR:HG23	1:F:68:THR:O	2.08	0.54
1:E:270:ASN:OD1	1:E:299:GLY:HA2	2.07	0.54
1:E:312:ASN:HB2	4:E:2150:HOH:O	2.07	0.54
1:A:227:PRO:HB2	1:A:322:GLN:HB3	1.90	0.53
1:F:360:TRP:CD1	3:F:1399:DW0:HACB	2.44	0.53
1:D:199:GLN:NE2	1:D:199:GLN:H	2.07	0.52
1:F:216:GLY:HA3	1:F:218:TRP:CZ3	2.45	0.52
1:C:124:ILE:HG21	1:C:169:GLU:HG3	1.92	0.52
1:A:215:HIS:HB2	1:A:224:GLU:O	2.08	0.52
1:C:136:ASP:OD2	1:C:138:ASP:OD1	2.28	0.52
1:B:22:TYR:CZ	1:B:350:LYS:HG2	2.45	0.52
1:B:33:GLN:NE2	1:B:72:ASN:HD21	2.07	0.51
1:F:170:ALA:HB2	1:F:177:ARG:HA	1.93	0.51
1:B:319:ASP:OD2	1:B:322:GLN:NE2	2.38	0.51
1:D:253:ASN:N	1:D:253:ASN:HD22	2.09	0.51
1:E:170:ALA:O	1:E:174:ASN:HA	2.10	0.51
1:D:33:GLN:NE2	1:D:72:ASN:HD21	2.09	0.50
1:F:104:ALA:HB3	1:F:105:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LYS:HE3	1:B:133:ASP:OD2	2.12	0.50
1:D:187:GLY:O	1:D:191:ILE:HG13	2.11	0.50
1:D:231:TYR:HD2	1:D:233:THR:HB	1.76	0.50
1:F:216:GLY:HA3	1:F:218:TRP:CH2	2.47	0.50
1:F:198:PRO:HD2	1:F:199:GLN:HE22	1.76	0.49
1:C:33:GLN:NE2	1:C:72:ASN:HD21	2.07	0.49
1:A:211:THR:HB	1:A:243:VAL:HG22	1.95	0.49
1:F:231:TYR:CG	1:F:232:PRO:HD2	2.47	0.49
1:C:74:VAL:HG23	4:C:2031:HOH:O	2.13	0.48
1:B:187:GLY:O	1:B:191:ILE:HG13	2.13	0.48
1:E:104:ALA:HB3	1:E:105:PRO:HD3	1.94	0.48
1:E:103:THR:HG22	1:E:139:TRP:HE1	1.79	0.48
1:E:124:ILE:HG21	1:E:169:GLU:HG3	1.94	0.48
1:B:296:LYS:HE3	1:F:34:TYR:O	2.14	0.48
1:A:140:GLU:OE2	3:A:1399:DW0:HAAB	2.14	0.48
1:C:201:SER:HB3	1:C:256:PRO:HD2	1.96	0.47
1:B:360:TRP:CD1	3:B:1399:DW0:HACB	2.49	0.47
1:A:177:ARG:HG2	1:A:178:LEU:O	2.14	0.47
1:D:197:ILE:O	1:D:201:SER:OG	2.24	0.47
1:D:375:GLY:O	1:D:378:PRO:HD3	2.15	0.47
1:C:48:PRO:HG3	1:C:86:LYS:HD2	1.96	0.46
1:D:99:TRP:CZ3	3:D:1400:DW0:HA0	2.51	0.46
1:B:67:THR:HG23	1:B:68:THR:O	2.15	0.46
1:F:25:THR:O	1:F:358:MET:HA	2.16	0.46
1:D:360:TRP:CD1	3:D:1399:DW0:HACB	2.50	0.46
1:A:120:ILE:HG12	1:A:162:MET:CE	2.45	0.46
1:F:270:ASN:OD1	1:F:299:GLY:HA2	2.15	0.46
1:C:251:LYS:HD2	1:C:257:ALA:HB2	1.97	0.46
1:D:53:HIS:CD2	1:D:91:LYS:HB2	2.51	0.46
1:D:177:ARG:HG2	1:D:178:LEU:O	2.15	0.46
3:A:1400:DW0:HAA	1:D:62:GLN:NE2	2.31	0.45
1:A:319:ASP:OD2	1:A:322:GLN:NE2	2.33	0.45
1:B:87:ASN:OD1	1:B:87:ASN:C	2.54	0.45
1:F:49:CYS:O	1:F:384:LYS:HE2	2.16	0.45
1:D:84:LYS:HG2	1:D:90:LEU:HB3	1.98	0.45
1:D:24:LEU:O	1:D:51:CYS:HB3	2.16	0.45
1:C:140:GLU:OE2	3:C:1399:DW0:HAAB	2.16	0.45
1:C:216:GLY:HA3	1:C:218:TRP:CZ3	2.51	0.45
1:B:290:PRO:HA	1:F:71:TRP:CD2	2.52	0.45
1:C:233:THR:HG21	4:C:2108:HOH:O	2.15	0.44
1:F:33:GLN:HE22	1:F:72:ASN:ND2	2.09	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:TRP:O	1:D:352:ASN:ND2	2.42	0.44
1:F:91:LYS:HA	1:F:91:LYS:HD3	1.90	0.44
1:D:130:TYR:O	1:D:131:GLU:HB2	2.17	0.44
1:B:270:ASN:OD1	1:B:299:GLY:HA2	2.18	0.44
1:D:99:TRP:CZ2	3:D:1400:DW0:CAP	3.01	0.44
1:B:298:SER:OG	1:F:71:TRP:HD1	2.00	0.44
1:C:270:ASN:OD1	1:C:299:GLY:HA2	2.18	0.44
1:D:196:GLU:O	1:D:200:LEU:HB2	2.18	0.44
1:E:140:GLU:OE2	3:E:1399:DW0:HAAB	2.17	0.44
1:E:177:ARG:HG2	1:E:178:LEU:O	2.18	0.44
1:C:294:TYR:CZ	1:E:230:LYS:HD3	2.53	0.44
1:D:199:GLN:H	1:D:199:GLN:HE21	1.63	0.44
1:D:93:LEU:HD12	1:D:93:LEU:N	2.33	0.43
1:E:216:GLY:HA3	1:E:218:TRP:CH2	2.53	0.43
1:B:120:ILE:HG12	1:B:162:MET:CE	2.48	0.43
1:F:167:GLU:HG3	1:F:177:ARG:CD	2.48	0.43
1:E:106:PHE:O	1:E:110:VAL:HG22	2.19	0.43
1:F:183:ALA:HA	1:F:208:HIS:O	2.19	0.43
3:A:1400:DW0:OAF	3:A:1400:DW0:HAB	2.19	0.43
1:D:171:LYS:NZ	1:D:171:LYS:HB2	2.34	0.43
1:E:127:LEU:HD12	1:E:178:LEU:HD13	2.01	0.43
1:D:216:GLY:HA3	1:D:218:TRP:CH2	2.54	0.43
1:F:59:ALA:HB2	1:F:94:LEU:HD21	2.01	0.43
1:A:34:TYR:O	1:D:296:LYS:HE3	2.18	0.42
1:E:163:ARG:NH1	1:E:203:TYR:O	2.49	0.42
1:F:99:TRP:CZ3	3:F:1400:DW0:HA0	2.54	0.42
1:E:147:SER:HA	1:E:148:PRO:HD2	1.67	0.42
1:C:95:ALA:HA	1:C:136:ASP:O	2.18	0.42
1:F:251:LYS:HD3	1:F:257:ALA:HB2	2.01	0.42
1:B:25:THR:O	1:B:358:MET:HA	2.19	0.42
1:F:360:TRP:HA	1:F:361:ALA:HA	1.80	0.42
1:A:216:GLY:HA3	1:A:218:TRP:CH2	2.55	0.42
1:B:110:VAL:HA	1:B:116:ARG:HG2	2.01	0.42
1:E:148:PRO:HB2	1:E:150:GLN:CD	2.39	0.42
1:A:171:LYS:HB3	1:A:171:LYS:HE2	1.86	0.42
3:D:1400:DW0:OAF	3:D:1400:DW0:HAB	2.19	0.42
1:B:279:THR:HG21	1:B:328:TYR:CE2	2.54	0.42
1:F:379:LEU:HD12	1:F:379:LEU:HA	1.93	0.42
1:A:385:LYS:HB2	1:A:385:LYS:HE3	1.71	0.42
1:B:47:ASN:HA	1:B:48:PRO:HD2	1.91	0.42
1:B:153:HIS:HB3	4:B:2082:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:GLU:CB	1:C:199:GLN:HE21	2.26	0.42
1:E:33:GLN:NE2	1:E:72:ASN:HD21	2.06	0.42
1:E:33:GLN:HE22	1:E:72:ASN:ND2	2.07	0.41
1:E:157:VAL:O	1:E:161:GLU:HG3	2.20	0.41
1:E:275:ASN:OD1	1:E:277:SER:HB2	2.20	0.41
1:A:290:PRO:HA	1:D:71:TRP:CD2	2.54	0.41
1:B:33:GLN:HE22	1:B:72:ASN:ND2	2.14	0.41
1:C:129:GLN:NE2	4:C:2057:HOH:O	2.52	0.41
3:C:1400:DW0:HABB	3:C:1400:DW0:C8	2.49	0.41
1:A:123:VAL:O	1:A:127:LEU:HG	2.20	0.41
1:C:227:PRO:CB	1:C:322:GLN:HB3	2.51	0.41
1:A:57:ALA:HA	1:A:58:PHE:HA	1.89	0.41
1:C:197:ILE:HG12	1:C:250:TRP:CZ3	2.55	0.41
1:E:115:ASN:N	1:E:115:ASN:HD22	2.18	0.41
1:F:159:VAL:HG21	1:F:200:LEU:HD21	2.02	0.41
1:A:227:PRO:CB	1:A:322:GLN:HB3	2.51	0.41
1:A:379:LEU:HD12	1:A:379:LEU:HA	1.85	0.41
3:A:1400:DW0:HAA	1:D:62:GLN:HE21	1.85	0.41
1:D:372:CYS:HB2	4:D:2133:HOH:O	2.19	0.41
1:C:84:LYS:NZ	1:C:131:GLU:O	2.54	0.41
1:C:320:ALA:N	1:C:321:PRO:HD2	2.35	0.41
1:D:57:ALA:HA	1:D:58:PHE:HA	1.88	0.41
1:F:225:ASN:OD1	1:F:269:HIS:HD2	2.04	0.41
1:C:360:TRP:CD1	3:C:1399:DW0:HACB	2.56	0.41
1:D:92:THR:C	1:D:93:LEU:HD12	2.41	0.41
1:F:269:HIS:HA	1:F:299:GLY:O	2.21	0.41
1:E:196:GLU:HB3	1:E:199:GLN:NE2	2.29	0.41
1:F:271:PHE:N	1:F:271:PHE:CD1	2.89	0.41
1:D:33:GLN:HE22	1:D:72:ASN:ND2	2.17	0.40
1:D:95:ALA:HA	1:D:136:ASP:HB3	2.03	0.40
1:D:120:ILE:HG12	1:D:162:MET:CE	2.51	0.40
1:D:260:LEU:HD23	1:D:260:LEU:HA	1.97	0.40
1:B:128:ARG:HD3	1:B:128:ARG:HA	1.92	0.40
1:E:103:THR:HG22	1:E:139:TRP:NE1	2.36	0.40
1:D:167:GLU:HG3	1:D:177:ARG:HD3	2.03	0.40
1:E:302:ALA:O	1:E:303:TYR:C	2.60	0.40
1:A:87:ASN:C	1:A:87:ASN:OD1	2.59	0.40
1:A:153:HIS:HB3	4:A:2090:HOH:O	2.21	0.40
1:C:67:THR:HG23	1:C:68:THR:O	2.22	0.40
1:D:216:GLY:HA3	1:D:218:TRP:CZ3	2.56	0.40
1:A:240:TYR:N	1:A:240:TYR:CD1	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:GLN:HE21	1:E:129:GLN:HB2	1.76	0.40
1:E:390:GLN:HB2	4:E:2180:HOH:O	2.21	0.40
1:F:270:ASN:C	1:F:271:PHE:CD1	2.94	0.40
1:F:372:CYS:HB2	4:F:2119:HOH:O	2.20	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	375/381 (98%)	361 (96%)	14 (4%)	0	100	100
1	B	375/381 (98%)	366 (98%)	9 (2%)	0	100	100
1	C	375/381 (98%)	368 (98%)	7 (2%)	0	100	100
1	D	375/381 (98%)	363 (97%)	11 (3%)	1 (0%)	41	45
1	E	375/381 (98%)	365 (97%)	9 (2%)	1 (0%)	41	45
1	F	375/381 (98%)	364 (97%)	10 (3%)	1 (0%)	41	45
All	All	2250/2286 (98%)	2187 (97%)	60 (3%)	3 (0%)	51	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	174	ASN
1	F	131	GLU
1	D	131	GLU

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	312/314 (99%)	300 (96%)	12 (4%)	33	41
1	B	312/314 (99%)	301 (96%)	11 (4%)	36	44
1	C	312/314 (99%)	301 (96%)	11 (4%)	36	44
1	D	312/314 (99%)	292 (94%)	20 (6%)	17	18
1	E	312/314 (99%)	297 (95%)	15 (5%)	25	30
1	F	312/314 (99%)	293 (94%)	19 (6%)	18	20
All	All	1872/1884 (99%)	1784 (95%)	88 (5%)	26	31

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	78	GLN
1	A	90	LEU
1	A	147	SER
1	A	168	GLN
1	A	171	LYS
1	A	172	GLN
1	A	273	LEU
1	A	296	LYS
1	A	349	LEU
1	A	379	LEU
1	A	387	LEU
1	B	24	LEU
1	B	90	LEU
1	B	125	LYS
1	B	172	GLN
1	B	212	TYR
1	B	230	LYS
1	B	233	THR
1	B	273	LEU
1	B	349	LEU
1	B	379	LEU
1	B	387	LEU
1	C	24	LEU
1	C	90	LEU
1	C	131	GLU

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Mol	Chain	Res	Type
1	C	168	GLN
1	C	172	GLN
1	C	212	TYR
1	C	233	THR
1	C	273	LEU
1	C	349	LEU
1	C	379	LEU
1	C	387	LEU
1	D	24	LEU
1	D	78	GLN
1	D	90	LEU
1	D	91	LYS
1	D	164	GLU
1	D	171	LYS
1	D	172	GLN
1	D	193	SER
1	D	199	GLN
1	D	200	LEU
1	D	230	LYS
1	D	233	THR
1	D	265	PRO
1	D	273	LEU
1	D	296	LYS
1	D	342	PHE
1	D	373	ASN
1	D	379	LEU
1	D	385	LYS
1	D	387	LEU
1	E	24	LEU
1	E	90	LEU
1	E	114	GLU
1	E	147	SER
1	E	156	THR
1	E	200	LEU
1	E	212	TYR
1	E	233	THR
1	E	265	PRO
1	E	273	LEU
1	E	324	VAL
1	E	337	ASP
1	E	379	LEU
1	E	385	LYS

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Mol	Chain	Res	Type
1	E	387	LEU
1	F	24	LEU
1	F	53	HIS
1	F	86	LYS
1	F	90	LEU
1	F	147	SER
1	F	172	GLN
1	F	199	GLN
1	F	200	LEU
1	F	201	SER
1	F	221	TYR
1	F	230	LYS
1	F	233	THR
1	F	273	LEU
1	F	296	LYS
1	F	337	ASP
1	F	349	LEU
1	F	373	ASN
1	F	379	LEU
1	F	387	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	ASN
1	A	85	ASN
1	A	115	ASN
1	A	129	GLN
1	A	168	GLN
1	A	192	GLN
1	A	199	GLN
1	A	312	ASN
1	A	347	GLN
1	B	33	GLN
1	B	62	GLN
1	B	64	ASN
1	B	85	ASN
1	B	100	ASN
1	B	115	ASN
1	B	129	GLN
1	B	160	GLN

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Mol	Chain	Res	Type
1	B	172	GLN
1	B	192	GLN
1	B	312	ASN
1	B	347	GLN
1	C	33	GLN
1	C	62	GLN
1	C	64	ASN
1	C	78	GLN
1	C	100	ASN
1	C	115	ASN
1	C	117	GLN
1	C	129	GLN
1	C	199	GLN
1	D	33	GLN
1	D	62	GLN
1	D	64	ASN
1	D	100	ASN
1	D	115	ASN
1	D	129	GLN
1	D	192	GLN
1	D	199	GLN
1	D	202	GLN
1	D	347	GLN
1	D	373	ASN
1	E	33	GLN
1	E	64	ASN
1	E	78	GLN
1	E	85	ASN
1	E	100	ASN
1	E	115	ASN
1	E	129	GLN
1	E	160	GLN
1	E	192	GLN
1	E	199	GLN
1	F	33	GLN
1	F	64	ASN
1	F	100	ASN
1	F	115	ASN
1	F	129	GLN
1	F	160	GLN
1	F	168	GLN
1	F	192	GLN

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Mol	Chain	Res	Type
1	F	199	GLN
1	F	347	GLN
1	F	373	ASN
1	F	390	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

18 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	GOL	D	1398	-	5,5,5	0.43	0	5,5,5	0.84	0
3	DW0	F	1400	-	26,32,32	2.31	9 (34%)	27,49,49	3.53	15 (55%)
2	GOL	C	1398	-	5,5,5	0.35	0	5,5,5	1.08	0
2	GOL	A	1398	-	5,5,5	0.50	0	5,5,5	1.30	0
2	GOL	F	1398	-	5,5,5	0.46	0	5,5,5	0.39	0
3	DW0	B	1399	-	26,32,32	2.34	8 (30%)	27,49,49	3.00	8 (29%)
3	DW0	E	1399	-	26,32,32	2.10	8 (30%)	27,49,49	3.42	15 (55%)
3	DW0	B	1400	-	26,32,32	1.95	8 (30%)	27,49,49	3.42	13 (48%)
3	DW0	D	1400	-	26,32,32	2.50	13 (50%)	27,49,49	3.64	16 (59%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DW0	A	1399	-	26,32,32	2.06	8 (30%)	27,49,49	2.90	10 (37%)
3	DW0	C	1399	-	26,32,32	1.86	7 (26%)	27,49,49	3.14	14 (51%)
3	DW0	C	1400	-	26,32,32	2.00	9 (34%)	27,49,49	3.53	16 (59%)
3	DW0	A	1400	-	26,32,32	1.94	8 (30%)	27,49,49	3.22	15 (55%)
2	GOL	B	1398	-	5,5,5	0.42	0	5,5,5	0.99	0
2	GOL	E	1398	-	5,5,5	0.59	0	5,5,5	1.18	1 (20%)
3	DW0	D	1399	-	26,32,32	1.89	7 (26%)	27,49,49	2.44	12 (44%)
3	DW0	F	1399	-	26,32,32	1.86	7 (26%)	27,49,49	3.05	12 (44%)
3	DW0	E	1400	-	26,32,32	1.95	8 (30%)	27,49,49	3.47	16 (59%)

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	GOL	D	1398	-	-	2/4/4/4	-
3	DW0	F	1400	-	-	3/6/6/6	0/4/4/4
2	GOL	C	1398	-	-	4/4/4/4	-
2	GOL	A	1398	-	-	2/4/4/4	-
2	GOL	F	1398	-	-	2/4/4/4	-
3	DW0	B	1399	-	-	0/6/6/6	0/4/4/4
3	DW0	E	1399	-	-	0/6/6/6	0/4/4/4
3	DW0	B	1400	-	-	2/6/6/6	0/4/4/4
3	DW0	D	1400	-	-	5/6/6/6	0/4/4/4
3	DW0	A	1399	-	-	0/6/6/6	0/4/4/4
3	DW0	C	1399	-	-	0/6/6/6	0/4/4/4
3	DW0	C	1400	-	-	1/6/6/6	0/4/4/4
3	DW0	A	1400	-	-	3/6/6/6	0/4/4/4
2	GOL	B	1398	-	-	4/4/4/4	-
2	GOL	E	1398	-	-	4/4/4/4	-
3	DW0	D	1399	-	-	2/6/6/6	0/4/4/4
3	DW0	F	1399	-	-	0/6/6/6	0/4/4/4
3	DW0	E	1400	-	-	0/6/6/6	0/4/4/4

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1400	DW0	CAR-NAZ	6.86	1.46	1.38
3	D	1400	DW0	CAR-NAZ	6.42	1.45	1.38
3	B	1399	DW0	CAR-NAZ	6.22	1.45	1.38
3	A	1399	DW0	C4-N3	6.22	1.46	1.38
3	E	1399	DW0	CAR-NAZ	5.56	1.44	1.38
3	B	1399	DW0	C4-N3	5.49	1.45	1.38
3	B	1400	DW0	CAR-NAZ	5.18	1.44	1.38
3	D	1399	DW0	C4-N3	4.50	1.44	1.38
3	F	1399	DW0	C4-N3	4.40	1.43	1.38
3	B	1399	DW0	C2-N3	4.30	1.43	1.38
3	E	1400	DW0	C2-N3	4.30	1.43	1.38
3	C	1399	DW0	CAR-NAZ	4.28	1.43	1.38
3	A	1400	DW0	CAR-NAZ	4.00	1.42	1.38
3	E	1400	DW0	CAR-NAZ	4.00	1.42	1.38
3	D	1400	DW0	C2-N3	3.99	1.42	1.38
3	E	1399	DW0	C2-N3	3.97	1.42	1.38
3	C	1400	DW0	C2-N3	3.95	1.42	1.38
3	C	1399	DW0	C4-N3	3.94	1.43	1.38
3	A	1400	DW0	C2-N3	3.85	1.42	1.38
3	F	1400	DW0	CAR-N10	3.85	1.45	1.38
3	C	1399	DW0	C2-N3	3.82	1.42	1.38
3	E	1400	DW0	CAA-N7	3.82	1.56	1.47
3	F	1399	DW0	CAR-NAZ	3.71	1.42	1.38
3	D	1400	DW0	CAC-N3	3.61	1.52	1.46
3	E	1399	DW0	C2-N1	3.61	1.45	1.38
3	B	1399	DW0	CAA-N7	3.60	1.55	1.47
3	D	1399	DW0	CAT-NAZ	3.56	1.42	1.38
3	C	1400	DW0	CAR-NAZ	3.55	1.42	1.38
3	D	1400	DW0	C5-C6	-3.47	1.38	1.46
3	A	1400	DW0	C5-C6	-3.41	1.39	1.46
3	C	1400	DW0	C6-N1	3.37	1.46	1.40
3	A	1400	DW0	CAT-NAZ	3.36	1.42	1.38
3	C	1400	DW0	CAB-NAX	3.36	1.55	1.47
3	B	1400	DW0	C5-C6	-3.32	1.39	1.46
3	E	1399	DW0	CAV-CAP	-3.24	1.39	1.46
3	D	1400	DW0	CA0-N10	3.23	1.54	1.47
3	F	1400	DW0	C2-N1	3.22	1.44	1.38
3	D	1399	DW0	CAR-N10	3.16	1.44	1.38
3	E	1399	DW0	CAD-NAZ	3.13	1.51	1.46
3	C	1400	DW0	C2-N1	3.12	1.44	1.38
3	A	1399	DW0	CAA-N7	3.12	1.54	1.47
3	D	1399	DW0	CAP-N10	3.11	1.46	1.40
3	E	1400	DW0	CAR-N10	3.02	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1400	DW0	C5-C6	-3.01	1.39	1.46
3	A	1399	DW0	CAD-NAZ	2.98	1.51	1.46
3	D	1400	DW0	C2-N1	2.97	1.44	1.38
3	E	1400	DW0	CAC-N3	2.95	1.51	1.46
3	F	1400	DW0	C2-N3	2.93	1.41	1.38
3	F	1400	DW0	CAD-NAZ	2.88	1.51	1.46
3	D	1400	DW0	CAP-N10	2.87	1.45	1.40
3	F	1399	DW0	C6-N1	2.86	1.45	1.40
3	F	1400	DW0	CAT-NAZ	2.86	1.42	1.38
3	D	1400	DW0	CAA-N7	2.80	1.54	1.47
3	D	1400	DW0	CAR-N10	2.79	1.43	1.38
3	C	1400	DW0	CAV-CAP	-2.78	1.40	1.46
3	A	1399	DW0	C5-C6	-2.76	1.40	1.46
3	A	1399	DW0	O2-C2	2.73	1.27	1.22
3	F	1399	DW0	CAD-NAZ	2.67	1.51	1.46
3	B	1400	DW0	CAT-NAZ	2.67	1.41	1.38
3	B	1400	DW0	CAP-N10	2.66	1.45	1.40
3	A	1400	DW0	CAR-N10	2.64	1.43	1.38
3	C	1399	DW0	CAC-N3	2.61	1.51	1.46
3	B	1400	DW0	CAV-CAP	-2.58	1.40	1.46
3	D	1400	DW0	CAD-NAZ	2.56	1.51	1.46
3	D	1399	DW0	OAF-CAP	2.55	1.27	1.22
3	B	1399	DW0	CAC-N3	2.55	1.51	1.46
3	B	1399	DW0	CAD-NAZ	2.54	1.51	1.46
3	D	1400	DW0	CAV-CAP	-2.54	1.40	1.46
3	B	1400	DW0	CAC-N3	2.52	1.50	1.46
3	A	1399	DW0	CAC-N3	2.52	1.50	1.46
3	F	1399	DW0	C2-N1	2.51	1.43	1.38
3	B	1400	DW0	CAA-N7	2.50	1.53	1.47
3	B	1400	DW0	CAR-N10	2.48	1.43	1.38
3	E	1399	DW0	C4-N3	2.46	1.41	1.38
3	D	1399	DW0	CAD-NAZ	2.44	1.50	1.46
3	E	1399	DW0	CAR-N10	2.44	1.43	1.38
3	E	1400	DW0	CAD-NAZ	2.41	1.50	1.46
3	C	1399	DW0	CAV-CAP	-2.41	1.41	1.46
3	F	1400	DW0	CAC-N3	2.41	1.50	1.46
3	F	1399	DW0	CAR-N10	2.40	1.43	1.38
3	F	1400	DW0	C5-C6	-2.40	1.41	1.46
3	D	1400	DW0	CAB-NAX	2.39	1.53	1.47
3	F	1399	DW0	OAF-CAP	2.38	1.27	1.22
3	C	1399	DW0	CAA-N7	2.37	1.53	1.47
3	C	1400	DW0	CAC-N3	2.37	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1399	DW0	CAB-NAX	2.35	1.52	1.47
3	E	1399	DW0	C5-C6	-2.34	1.41	1.46
3	A	1399	DW0	CAV-CAP	-2.31	1.41	1.46
3	A	1400	DW0	CAV-CAP	-2.30	1.41	1.46
3	F	1400	DW0	CA0-N10	2.26	1.52	1.47
3	A	1400	DW0	CAP-N10	2.25	1.44	1.40
3	E	1400	DW0	CAV-CAP	-2.23	1.41	1.46
3	B	1399	DW0	CAP-N10	2.22	1.44	1.40
3	A	1399	DW0	CAR-N10	2.21	1.42	1.38
3	D	1400	DW0	CAT-NAZ	2.18	1.41	1.38
3	C	1400	DW0	CAR-N10	2.07	1.42	1.38
3	C	1400	DW0	C5-C6	-2.05	1.41	1.46
3	D	1399	DW0	CAR-NAZ	2.03	1.40	1.38
3	A	1400	DW0	CAK-N1	2.02	1.51	1.47
3	C	1399	DW0	CAK-N1	2.00	1.51	1.47

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1399	DW0	C5-C6-N1	10.33	122.04	113.58
3	B	1399	DW0	C5-C6-N1	9.73	121.56	113.58
3	F	1400	DW0	CAV-CAP-N10	9.35	121.25	113.58
3	D	1400	DW0	CAV-CAP-N10	9.28	121.19	113.58
3	B	1400	DW0	CAV-CAP-N10	9.13	121.06	113.58
3	C	1399	DW0	C5-C6-N1	8.83	120.81	113.58
3	F	1399	DW0	C5-C6-N1	8.24	120.33	113.58
3	A	1399	DW0	C5-C6-N1	7.89	120.05	113.58
3	A	1399	DW0	OAH-CAR-NAZ	-7.88	115.22	122.08
3	C	1400	DW0	CAV-CAP-N10	7.83	119.99	113.58
3	D	1399	DW0	C5-C6-N1	7.65	119.84	113.58
3	A	1400	DW0	CAV-CAP-N10	7.41	119.65	113.58
3	E	1400	DW0	CAV-CAP-N10	7.29	119.55	113.58
3	A	1400	DW0	C5-C6-N1	7.29	119.55	113.58
3	B	1400	DW0	CAC-N3-C2	7.26	125.01	117.35
3	F	1399	DW0	O2-C2-N3	-7.18	115.83	122.08
3	C	1400	DW0	CAC-N3-C2	7.01	124.75	117.35
3	E	1400	DW0	C5-C6-N1	7.00	119.32	113.58
3	D	1400	DW0	C5-C6-N1	6.93	119.26	113.58
3	D	1400	DW0	CAC-N3-C2	6.90	124.63	117.35
3	F	1400	DW0	C5-C6-N1	6.70	119.06	113.58
3	C	1400	DW0	C5-C6-N1	6.55	118.95	113.58
3	E	1400	DW0	CAC-N3-C2	6.50	124.20	117.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1399	DW0	CAD-NAZ-CAR	6.39	124.09	117.35
3	C	1399	DW0	CAD-NAZ-CAR	6.35	124.04	117.35
3	E	1400	DW0	OAH-CAR-NAZ	-6.28	116.61	122.08
3	F	1399	DW0	CAD-NAZ-CAR	6.07	123.75	117.35
3	E	1399	DW0	CAV-CAP-N10	6.04	118.53	113.58
3	C	1400	DW0	CAD-NAZ-CAR	5.71	123.37	117.35
3	B	1400	DW0	C5-C6-N1	5.56	118.13	113.58
3	B	1399	DW0	O6-C6-N1	-5.55	112.27	120.13
3	A	1400	DW0	CAC-N3-C2	5.52	123.18	117.35
3	F	1400	DW0	CAD-NAZ-CAR	5.52	123.17	117.35
3	D	1399	DW0	OAH-CAR-NAZ	-5.45	117.34	122.08
3	C	1399	DW0	CAV-CAP-N10	5.43	118.03	113.58
3	E	1400	DW0	CAD-NAZ-CAR	5.28	122.92	117.35
3	B	1399	DW0	CAV-CAP-N10	5.18	117.82	113.58
3	D	1400	DW0	OAF-CAP-CAV	-5.16	116.83	125.33
3	F	1400	DW0	O2-C2-N3	-5.09	117.65	122.08
3	D	1400	DW0	CA0-N10-CAR	5.03	125.20	117.67
3	F	1400	DW0	CAC-N3-C2	4.86	122.47	117.35
3	B	1399	DW0	CAD-NAZ-CAR	4.84	122.46	117.35
3	C	1400	DW0	CAC-N3-C4	-4.82	115.63	120.13
3	B	1399	DW0	CAT-NAZ-CAR	-4.74	117.67	122.20
3	E	1399	DW0	CAT-NAZ-CAR	-4.69	117.71	122.20
3	B	1400	DW0	CA0-N10-CAR	4.61	124.58	117.67
3	C	1399	DW0	O6-C6-N1	-4.59	113.62	120.13
3	A	1400	DW0	OAH-CAR-NAZ	-4.51	118.15	122.08
3	B	1400	DW0	C4-N3-C2	-4.51	117.89	122.20
3	D	1400	DW0	CAD-NAZ-CAR	4.42	122.01	117.35
3	F	1400	DW0	CA0-N10-CAR	4.38	124.23	117.67
3	A	1399	DW0	CAT-NAZ-CAR	-4.31	118.08	122.20
3	B	1400	DW0	OAH-CAR-NAZ	-4.29	118.35	122.08
3	A	1400	DW0	O6-C6-C5	-4.23	118.37	125.33
3	C	1399	DW0	CAT-NAZ-CAR	-4.15	118.23	122.20
3	F	1399	DW0	CAT-NAZ-CAR	-4.09	118.29	122.20
3	E	1399	DW0	CAK-N1-C2	4.05	123.74	117.67
3	C	1400	DW0	OAH-CAR-NAZ	-4.04	118.56	122.08
3	D	1400	DW0	C4-N3-C2	-4.04	118.34	122.20
3	F	1400	DW0	CAK-N1-C2	4.03	123.71	117.67
3	E	1400	DW0	CA0-N10-CAR	3.99	123.65	117.67
3	E	1399	DW0	O6-C6-N1	-3.98	114.48	120.13
3	C	1400	DW0	OAF-CAP-CAV	-3.98	118.79	125.33
3	D	1400	DW0	OAH-CAR-NAZ	-3.97	118.62	122.08
3	F	1400	DW0	C4-N3-C2	-3.87	118.50	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1400	DW0	OAH-CAR-NAZ	-3.82	118.75	122.08
3	B	1400	DW0	O2-C2-N3	-3.81	118.76	122.08
3	A	1399	DW0	CAV-CAP-N10	3.76	116.66	113.58
3	B	1400	DW0	OAF-CAP-CAV	-3.73	119.19	125.33
3	A	1400	DW0	OAF-CAP-CAV	-3.73	119.19	125.33
3	B	1400	DW0	CAK-N1-C2	3.71	123.23	117.67
3	C	1400	DW0	O2-C2-N3	-3.68	118.88	122.08
3	C	1400	DW0	CAT-NAZ-CAR	-3.67	118.69	122.20
3	E	1400	DW0	C4-N3-C2	-3.62	118.74	122.20
3	F	1400	DW0	OAF-CAP-CAV	-3.62	119.38	125.33
3	F	1400	DW0	N1-C2-N3	3.56	121.79	116.75
3	A	1399	DW0	N10-CAR-NAZ	3.52	121.73	116.75
3	E	1400	DW0	CAT-NAZ-CAR	-3.50	118.85	122.20
3	E	1400	DW0	N10-CAR-NAZ	3.50	121.70	116.75
3	E	1399	DW0	OAF-CAP-CAV	-3.45	119.66	125.33
3	F	1400	DW0	CAD-NAZ-CAT	-3.38	116.97	120.13
3	A	1399	DW0	CAC-N3-C4	3.38	123.29	120.13
3	D	1400	DW0	O6-C6-C5	-3.37	119.78	125.33
3	C	1400	DW0	CA0-N10-CAR	3.35	122.68	117.67
3	F	1399	DW0	CA0-N10-CAP	3.33	122.31	117.58
3	B	1400	DW0	CAC-N3-C4	-3.32	117.02	120.13
3	D	1400	DW0	CAC-N3-C4	-3.32	117.03	120.13
3	D	1399	DW0	CAT-NAZ-CAR	-3.30	119.05	122.20
3	E	1400	DW0	CAC-N3-C4	-3.28	117.06	120.13
3	B	1400	DW0	N1-C2-N3	3.28	121.39	116.75
3	E	1400	DW0	N1-C2-N3	3.27	121.38	116.75
3	E	1400	DW0	O2-C2-N1	-3.27	117.45	121.99
3	A	1400	DW0	N10-CAR-NAZ	3.26	121.36	116.75
3	A	1400	DW0	CA0-N10-CAR	3.25	122.53	117.67
3	A	1400	DW0	C4-N3-C2	-3.22	119.12	122.20
3	A	1399	DW0	CAK-CAL-CA0	-3.15	102.33	112.86
3	C	1399	DW0	OAH-CAR-N10	-3.08	117.71	121.99
3	E	1399	DW0	CA0-N10-CAP	3.08	121.95	117.58
3	C	1399	DW0	O2-C2-N1	-3.07	117.72	121.99
3	A	1400	DW0	CAD-NAZ-CAR	3.06	120.57	117.35
3	A	1400	DW0	O2-C2-N1	-3.06	117.74	121.99
3	C	1399	DW0	N10-CAR-NAZ	3.03	121.04	116.75
3	D	1399	DW0	O2-C2-N3	-3.02	119.45	122.08
3	C	1399	DW0	N1-C2-N3	2.94	120.91	116.75
3	C	1400	DW0	N10-CAR-NAZ	2.92	120.88	116.75
3	D	1400	DW0	CAL-CA0-N10	2.90	119.10	112.39
3	C	1399	DW0	C4-N3-C2	-2.89	119.43	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1400	DW0	CAK-N1-C2	2.89	122.00	117.67
3	D	1400	DW0	CAK-N1-C2	2.83	121.91	117.67
3	E	1399	DW0	N10-CAR-NAZ	2.82	120.74	116.75
3	C	1400	DW0	N1-C2-N3	2.82	120.74	116.75
3	A	1400	DW0	N1-C2-N3	2.82	120.73	116.75
3	E	1399	DW0	CAC-N3-C2	2.80	120.30	117.35
3	B	1399	DW0	N10-CAR-NAZ	2.80	120.71	116.75
3	A	1400	DW0	CAT-NAZ-CAR	-2.79	119.53	122.20
3	A	1399	DW0	CAD-NAZ-CAT	2.78	122.73	120.13
3	F	1399	DW0	OAH-CAR-N10	-2.77	118.14	121.99
3	B	1400	DW0	CAD-NAZ-CAR	2.75	120.25	117.35
3	B	1399	DW0	CAK-CAL-CA0	-2.74	103.69	112.86
3	C	1400	DW0	C4-N3-C2	-2.73	119.59	122.20
3	C	1400	DW0	O6-C6-C5	-2.71	120.87	125.33
3	D	1400	DW0	CAD-NAZ-CAT	-2.69	117.62	120.13
3	D	1399	DW0	CAK-CAL-CA0	-2.67	103.92	112.86
3	B	1399	DW0	OAH-CAR-N10	-2.66	118.30	121.99
3	A	1400	DW0	CAC-N3-C4	-2.60	117.70	120.13
3	E	1399	DW0	O2-C2-N3	-2.60	119.82	122.08
3	F	1399	DW0	N10-CAR-NAZ	2.57	120.39	116.75
3	C	1399	DW0	CAD-NAZ-CAT	-2.57	117.73	120.13
3	F	1399	DW0	CAV-CAP-N10	2.55	115.67	113.58
3	D	1400	DW0	N10-CAR-NAZ	2.55	120.36	116.75
3	E	1399	DW0	OAH-CAR-NAZ	-2.54	119.87	122.08
3	E	1399	DW0	C4-N3-C2	-2.53	119.78	122.20
3	E	1400	DW0	CAK-N1-C2	2.47	121.38	117.67
3	F	1400	DW0	CAT-NAZ-CAR	-2.45	119.86	122.20
3	A	1399	DW0	CA0-N10-CAR	2.39	121.26	117.67
3	F	1400	DW0	O6-C6-C5	-2.39	121.40	125.33
3	C	1399	DW0	CA0-N10-CAP	2.38	120.96	117.58
3	E	1400	DW0	O6-C6-C5	-2.37	121.44	125.33
3	C	1400	DW0	CAD-NAZ-CAT	-2.37	117.92	120.13
3	F	1399	DW0	CAC-N3-C4	2.36	122.34	120.13
3	F	1399	DW0	CAD-NAZ-CAT	-2.32	117.96	120.13
3	D	1399	DW0	O6-C6-N1	-2.27	116.91	120.13
3	F	1399	DW0	O6-C6-N1	-2.26	116.93	120.13
3	D	1399	DW0	N10-CAR-NAZ	2.24	119.92	116.75
3	C	1399	DW0	CAK-N1-C2	2.24	121.02	117.67
3	E	1400	DW0	OAF-CAP-CAV	-2.23	121.66	125.33
3	D	1400	DW0	CAL-CAK-N1	-2.21	107.27	112.39
2	E	1398	GOL	C3-C2-C1	-2.18	103.24	111.70
3	D	1399	DW0	C4-N3-C2	-2.16	120.14	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1400	DW0	O2-C2-N3	-2.14	120.22	122.08
3	B	1400	DW0	O6-C6-C5	-2.12	121.84	125.33
3	E	1399	DW0	N1-C2-N3	2.10	119.72	116.75
3	D	1399	DW0	CAC-N3-C4	2.10	122.10	120.13
3	E	1399	DW0	CAD-NAZ-CAT	-2.10	118.17	120.13
3	D	1399	DW0	CAD-NAZ-CAR	2.09	119.56	117.35
3	C	1399	DW0	CAK-CAL-CA0	-2.08	105.90	112.86
3	F	1399	DW0	N1-C2-N3	2.08	119.69	116.75
3	D	1399	DW0	CAV-CAP-N10	2.04	115.25	113.58
3	F	1400	DW0	N10-CAR-NAZ	2.04	119.64	116.75
3	A	1400	DW0	CAK-N1-C6	2.04	120.47	117.58
3	D	1399	DW0	CAK-N1-C6	2.04	120.47	117.58
3	E	1400	DW0	CAD-NAZ-CAT	-2.03	118.23	120.13
3	A	1399	DW0	C4-N3-C2	-2.03	120.26	122.20

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1398	GOL	O1-C1-C2-C3
2	C	1398	GOL	O1-C1-C2-C3
2	C	1398	GOL	C1-C2-C3-O3
2	C	1398	GOL	O2-C2-C3-O3
2	D	1398	GOL	C1-C2-C3-O3
2	E	1398	GOL	C1-C2-C3-O3
2	F	1398	GOL	C1-C2-C3-O3
2	F	1398	GOL	O2-C2-C3-O3
3	A	1400	DW0	CAL-CA0-N10-CAP
3	D	1400	DW0	CAL-CA0-N10-CAP
3	D	1400	DW0	CAL-CA0-N10-CAR
2	A	1398	GOL	C1-C2-C3-O3
2	B	1398	GOL	C1-C2-C3-O3
2	B	1398	GOL	O1-C1-C2-O2
2	C	1398	GOL	O1-C1-C2-O2
2	D	1398	GOL	O2-C2-C3-O3
2	E	1398	GOL	O2-C2-C3-O3
3	B	1400	DW0	CAL-CAK-N1-C6
3	A	1400	DW0	CAL-CA0-N10-CAR
3	D	1399	DW0	CAL-CA0-N10-CAP
2	A	1398	GOL	O2-C2-C3-O3
3	B	1400	DW0	CAL-CAK-N1-C2
3	F	1400	DW0	CAL-CA0-N10-CAP

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Mol	Chain	Res	Type	Atoms
2	B	1398	GOL	O2-C2-C3-O3
3	D	1400	DW0	N1-CAK-CAL-CA0
3	D	1400	DW0	N10-CA0-CAL-CAK
3	C	1400	DW0	CAL-CAK-N1-C6
3	A	1400	DW0	N10-CA0-CAL-CAK
3	D	1399	DW0	CAL-CA0-N10-CAR
2	E	1398	GOL	O1-C1-C2-C3
3	F	1400	DW0	N1-CAK-CAL-CA0
2	E	1398	GOL	O1-C1-C2-O2
3	D	1400	DW0	CAL-CAK-N1-C6
3	F	1400	DW0	CAL-CAK-N1-C6

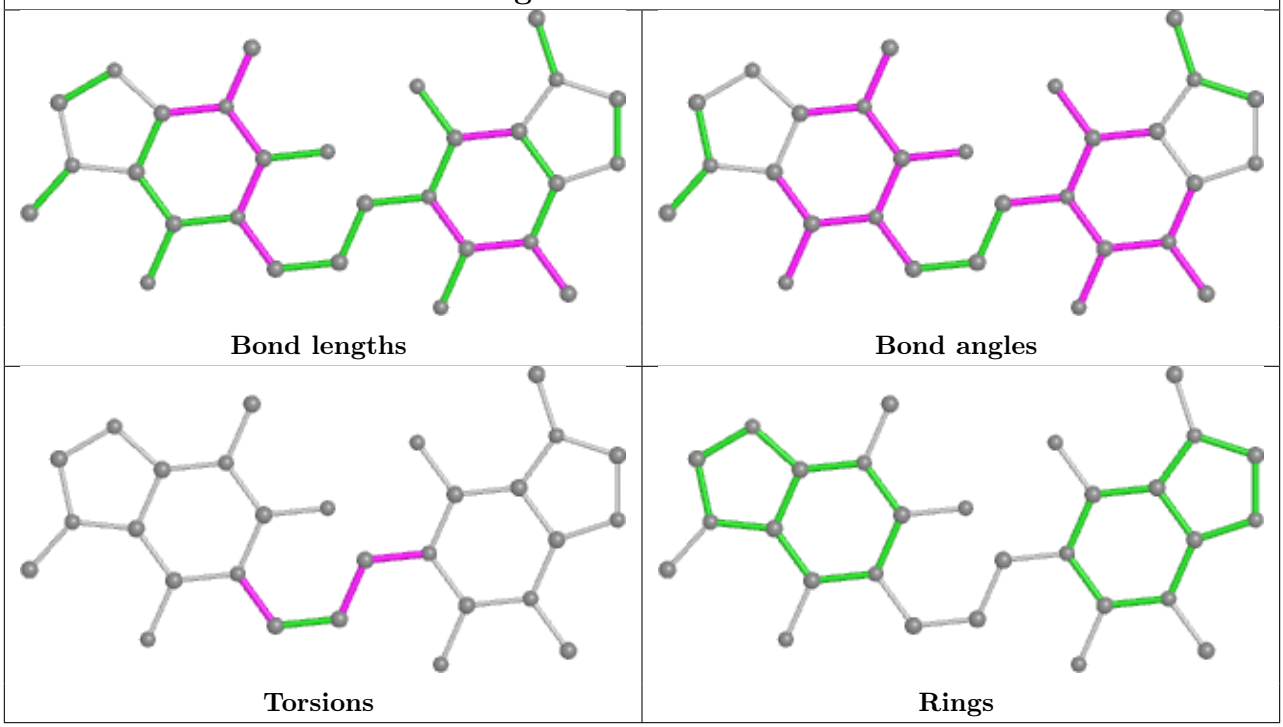
There are no ring outliers.

10 monomers are involved in 19 short contacts:

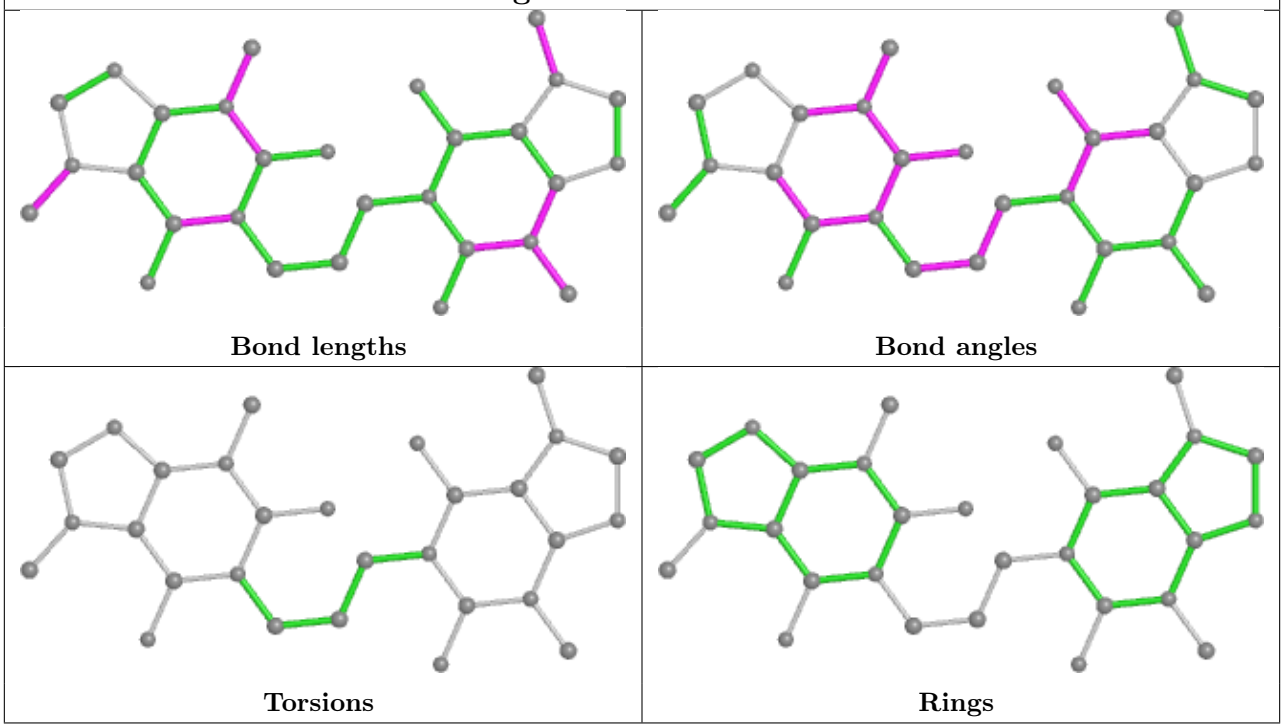
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1400	DW0	1	0
3	B	1399	DW0	1	0
3	E	1399	DW0	3	0
3	D	1400	DW0	3	0
3	A	1399	DW0	1	0
3	C	1399	DW0	2	0
3	C	1400	DW0	1	0
3	A	1400	DW0	3	0
3	D	1399	DW0	2	0
3	F	1399	DW0	2	0

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.

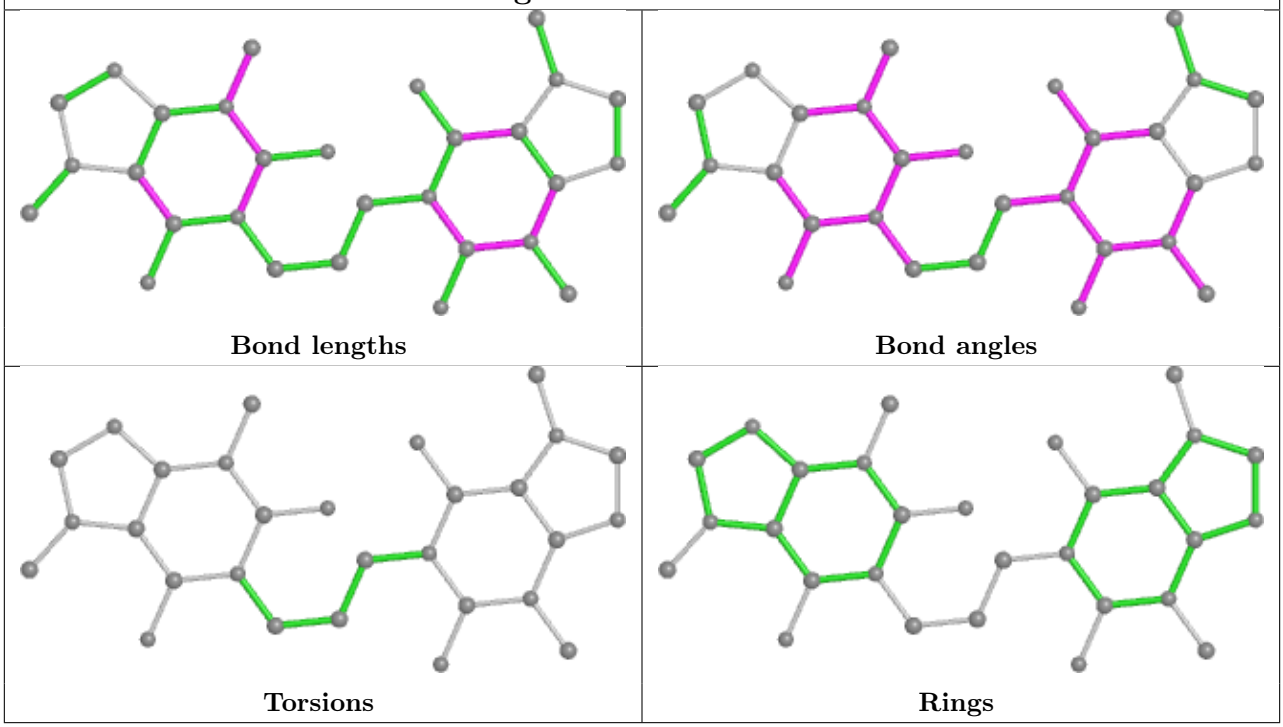
Ligand DW0 F 1400



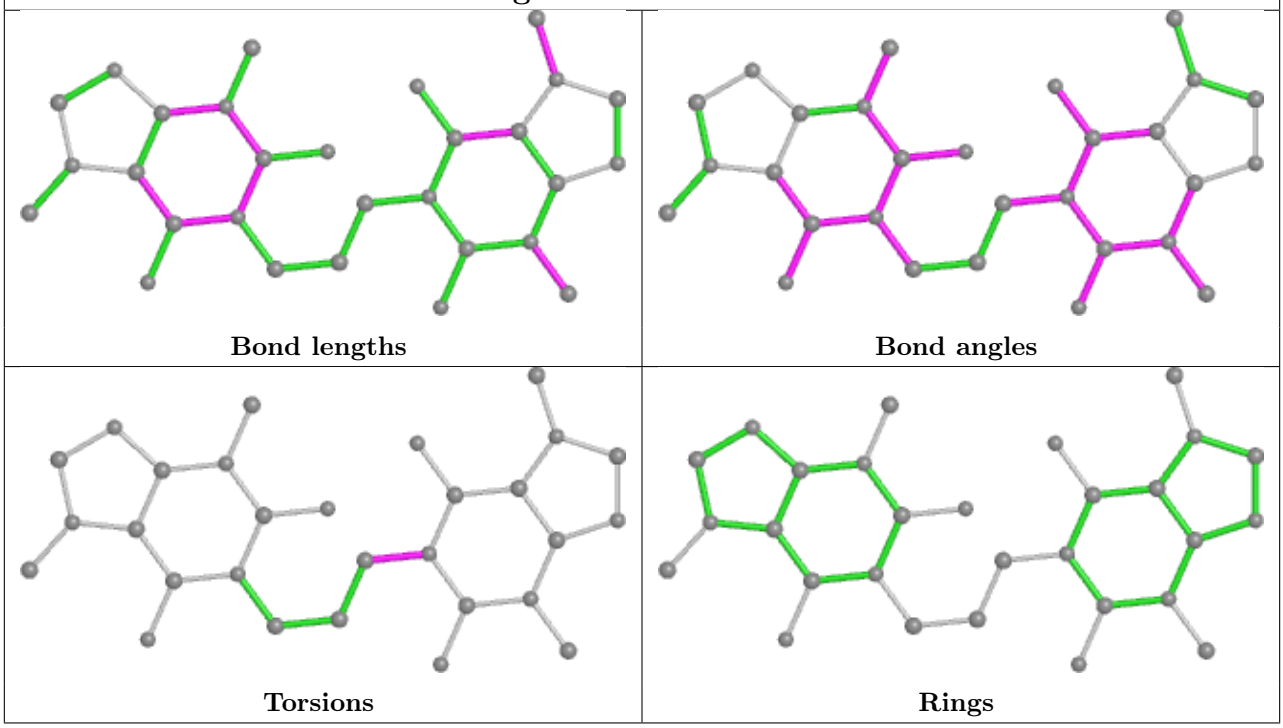
Ligand DW0 B 1399



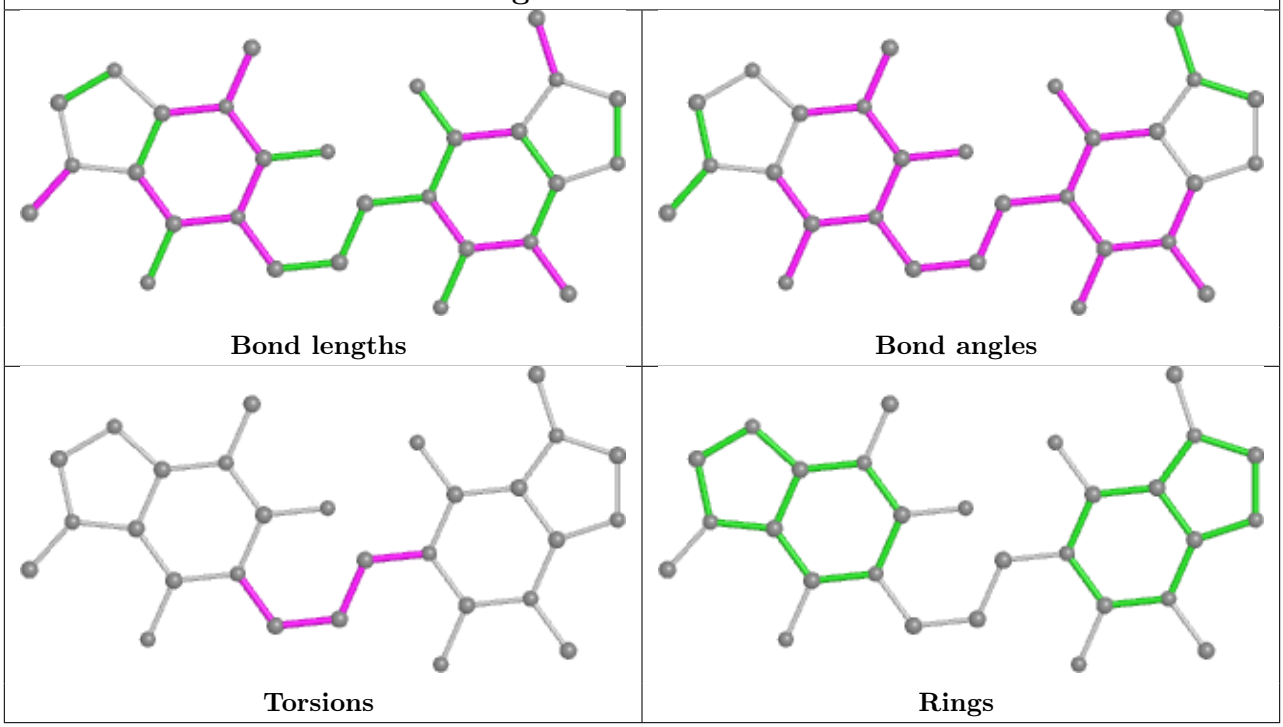
Ligand DW0 E 1399



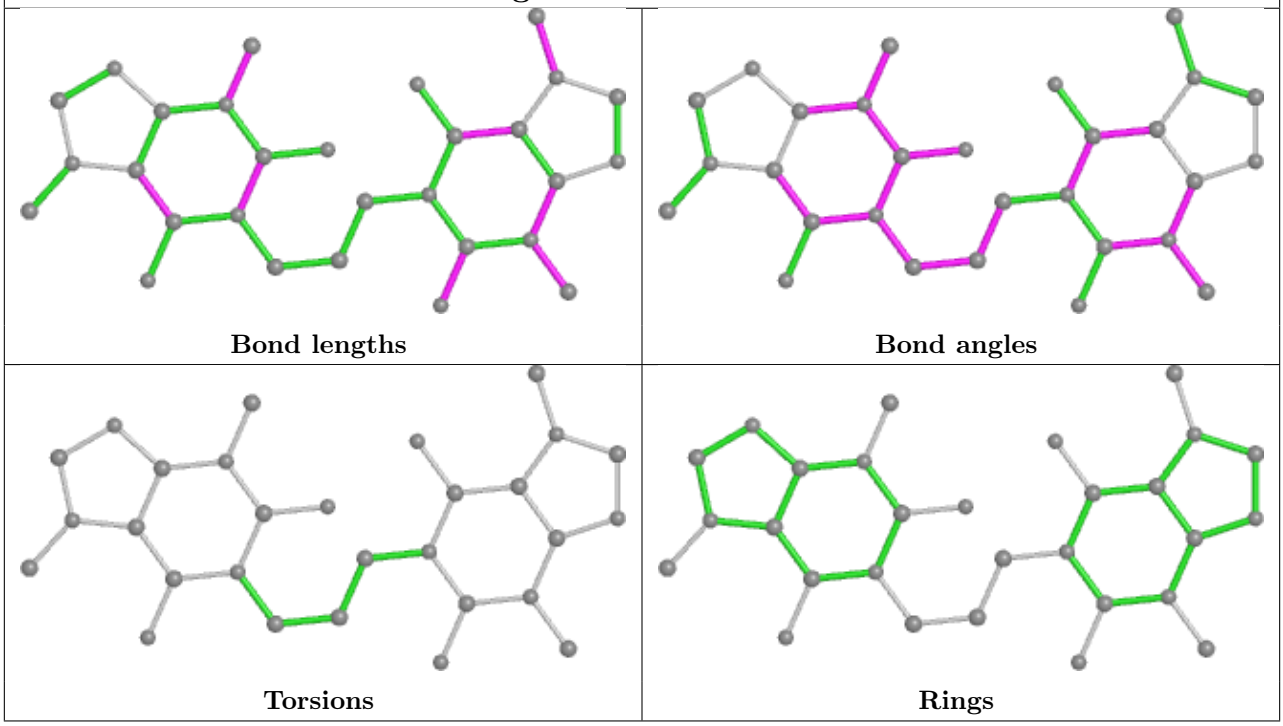
Ligand DW0 B 1400



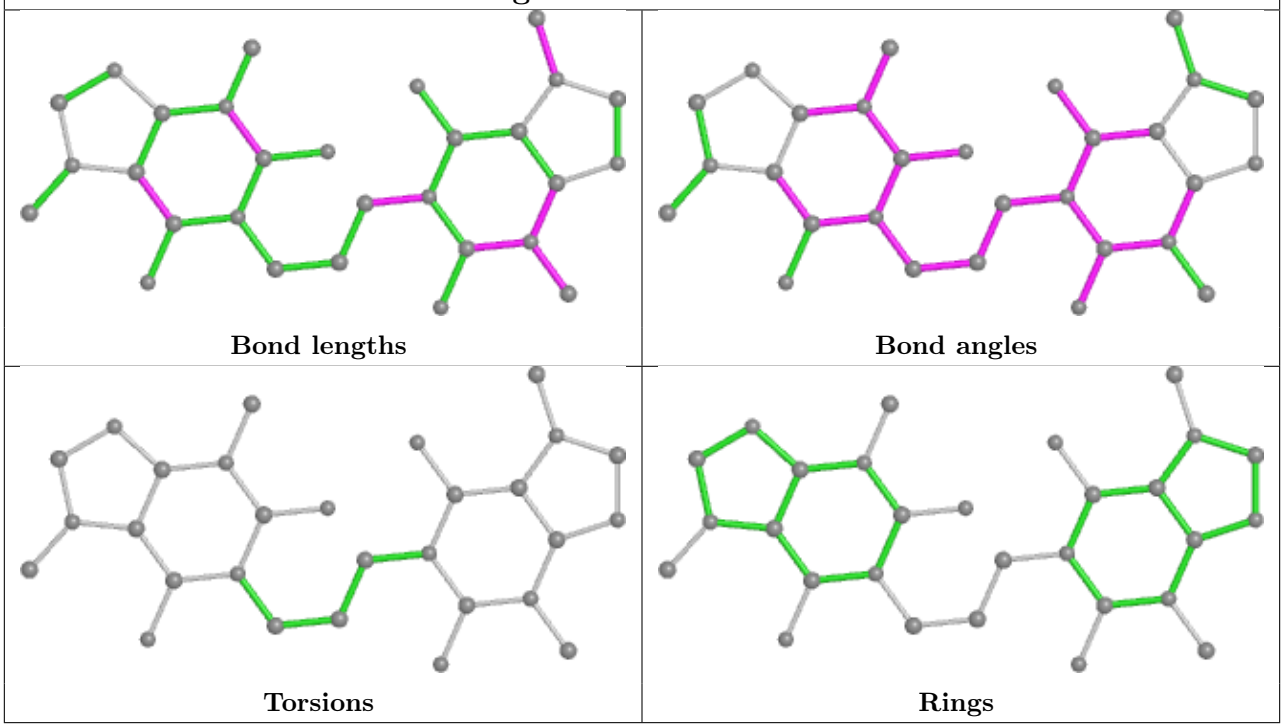
Ligand DW0 D 1400



Ligand DW0 A 1399



Ligand DW0 C 1399



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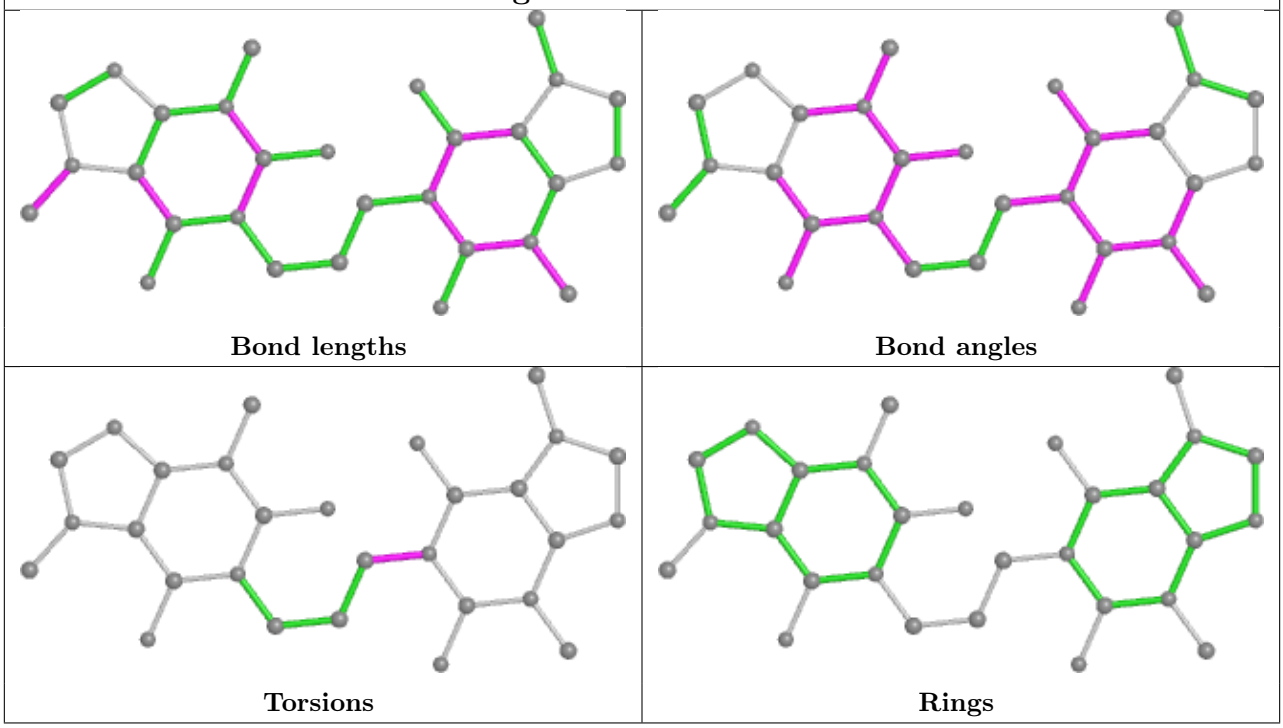

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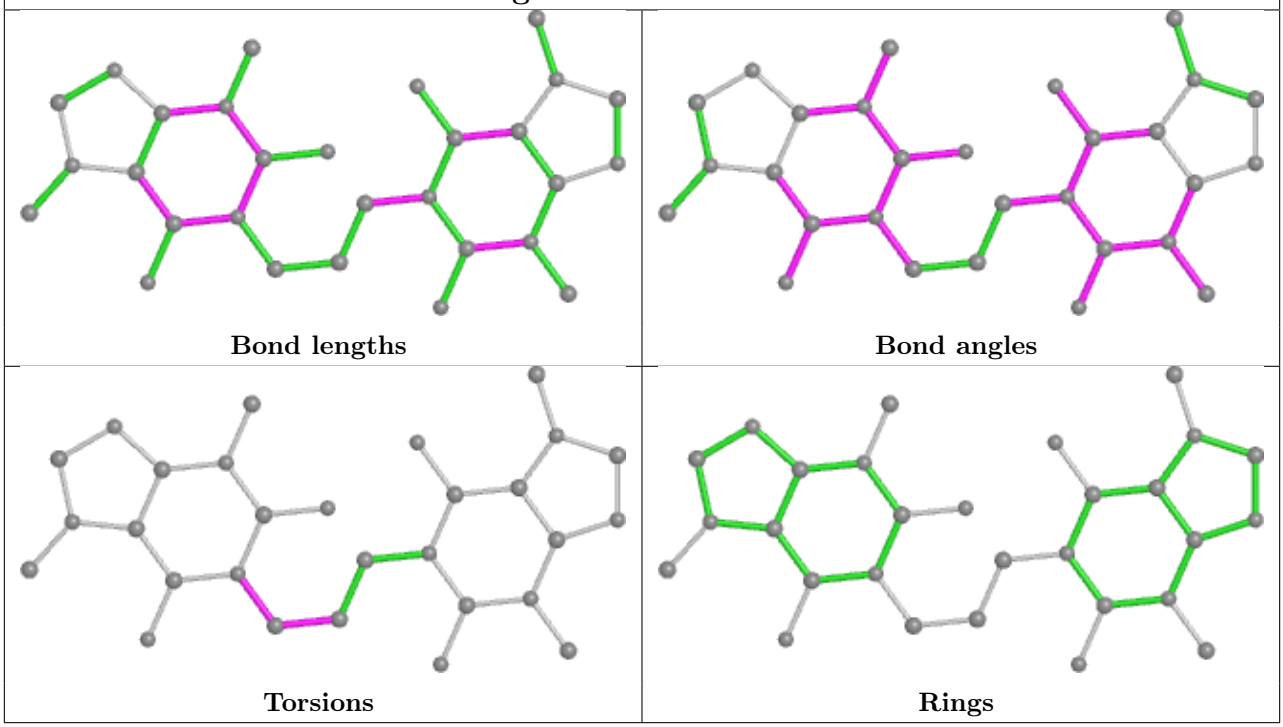
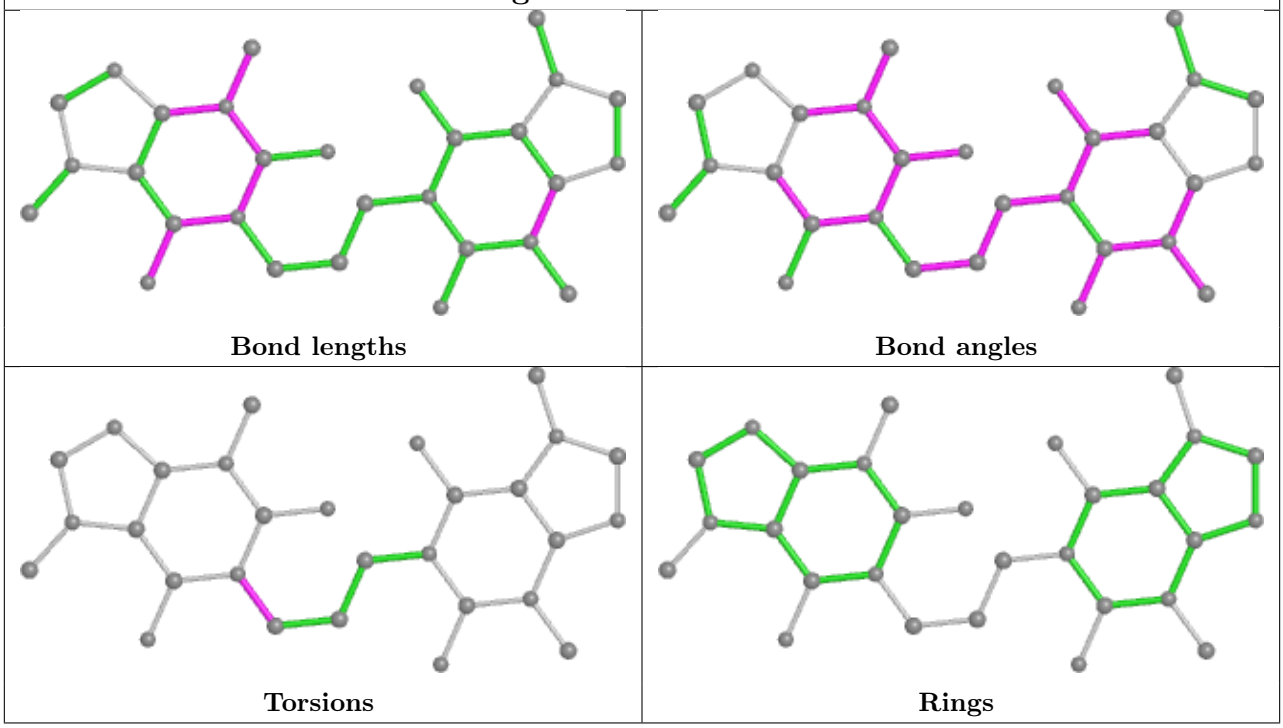
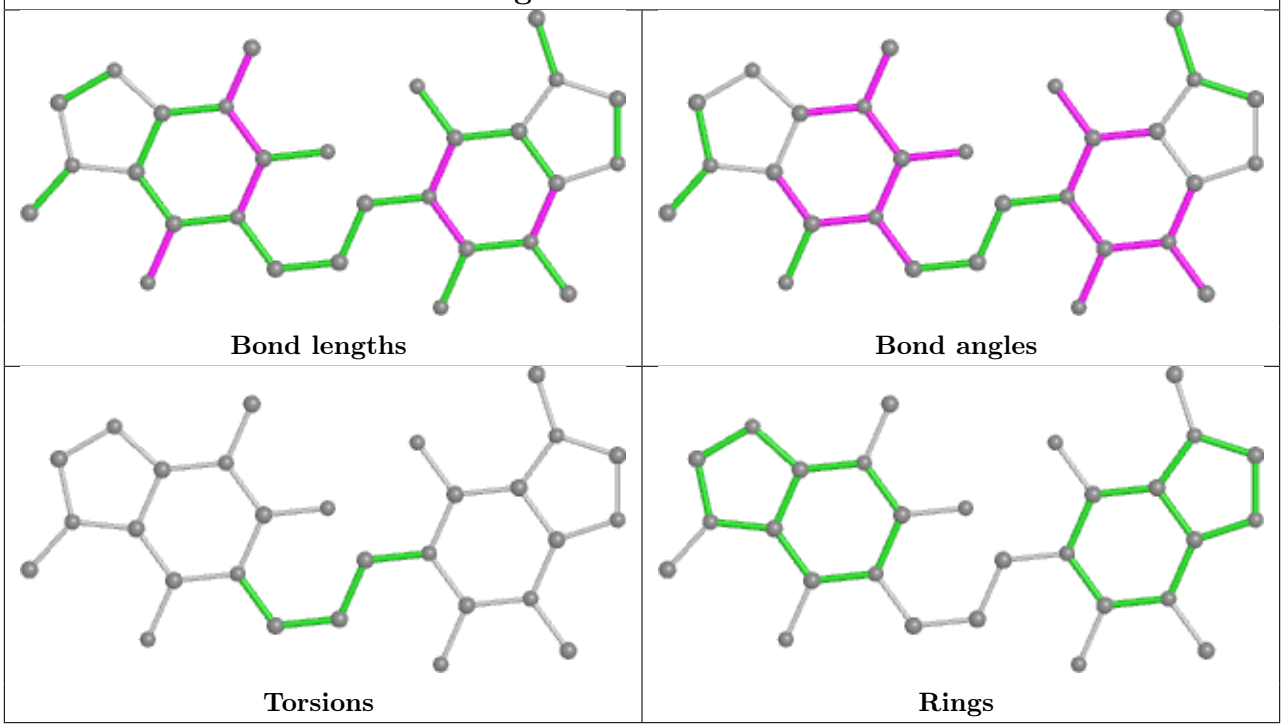


Ligand DW0 D 1399



Ligand DW0 F 1399



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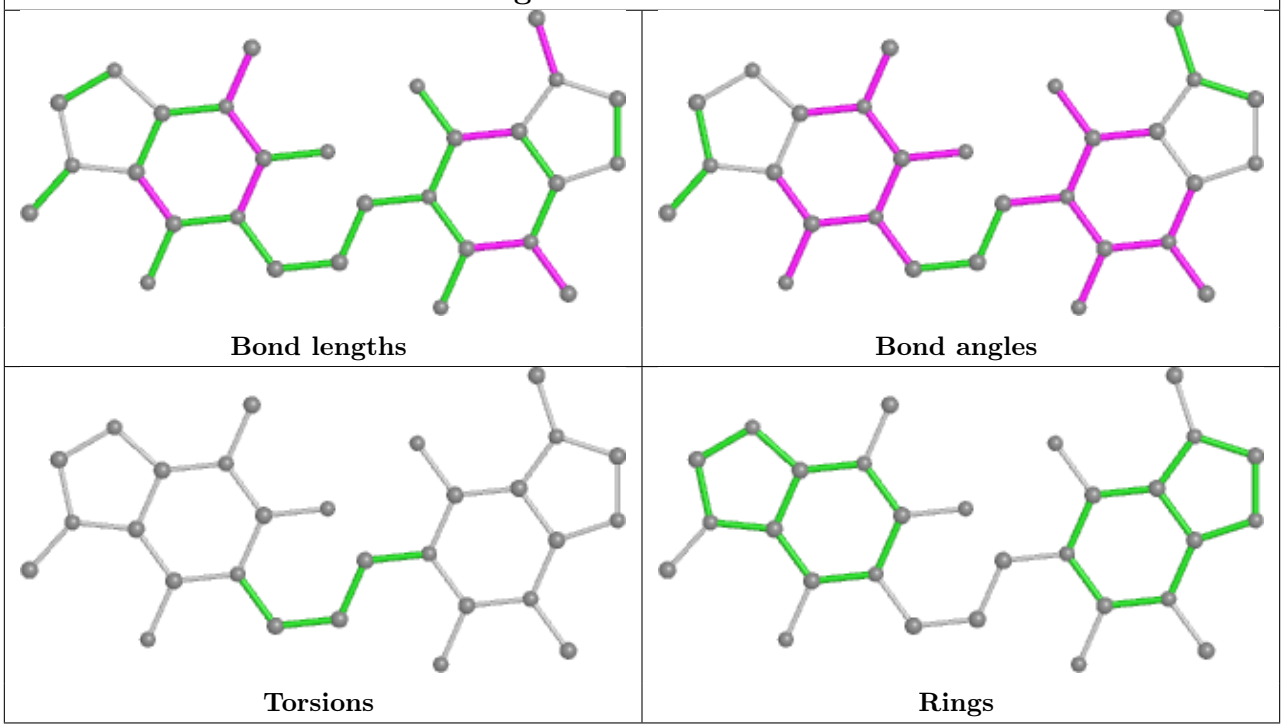

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	377/381 (98%)	-0.52	7 (1%)	66	65	16, 25, 44, 63	0
1	B	377/381 (98%)	-0.56	2 (0%)	91	90	17, 26, 42, 63	0
1	C	377/381 (98%)	-0.52	3 (0%)	86	85	15, 27, 45, 66	0
1	D	377/381 (98%)	-0.35	10 (2%)	54	52	17, 34, 59, 75	0
1	E	377/381 (98%)	-0.46	7 (1%)	66	65	15, 28, 49, 70	0
1	F	377/381 (98%)	-0.28	8 (2%)	63	61	19, 37, 61, 73	0
All	All	2262/2286 (98%)	-0.45	37 (1%)	72	70	15, 29, 52, 75	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	397	PRO	5.5
1	D	174	ASN	4.5
1	A	391	SER	4.1
1	B	397	PRO	4.1
1	B	391	SER	3.6
1	E	391	SER	3.4
1	F	390	GLN	2.9
1	C	174	ASN	2.8
1	D	221	TYR	2.8
1	A	397	PRO	2.8
1	F	171	LYS	2.8
1	A	373	ASN	2.8
1	F	114	GLU	2.7
1	F	174	ASN	2.7
1	A	396	ALA	2.7
1	F	235	THR	2.7
1	D	21	ALA	2.7
1	E	174	ASN	2.7
1	A	172	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	235	THR	2.6
1	D	171	LYS	2.6
1	A	171	LYS	2.5
1	F	397	PRO	2.4
1	F	21	ALA	2.4
1	D	172	GLN	2.4
1	E	175	LYS	2.3
1	A	394	CYS	2.3
1	C	175	LYS	2.3
1	E	397	PRO	2.3
1	D	175	LYS	2.2
1	F	172	GLN	2.2
1	C	334	VAL	2.1
1	E	334	VAL	2.1
1	D	114	GLU	2.1
1	E	221	TYR	2.1
1	E	62	GLN	2.1
1	D	391	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DW0	F	1400	29/29	0.82	0.22	51,55,58,59	29
3	DW0	A	1400	29/29	0.83	0.21	41,50,59,59	29
3	DW0	C	1400	29/29	0.84	0.19	30,41,49,49	29
3	DW0	E	1400	29/29	0.86	0.16	33,42,48,50	29
3	DW0	B	1400	29/29	0.87	0.20	41,45,49,50	29

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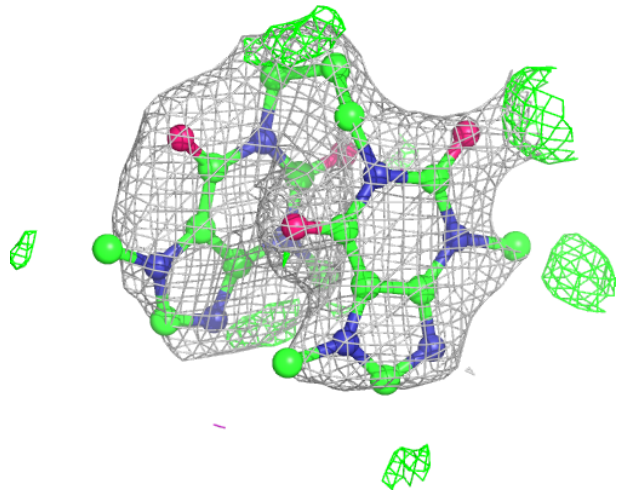
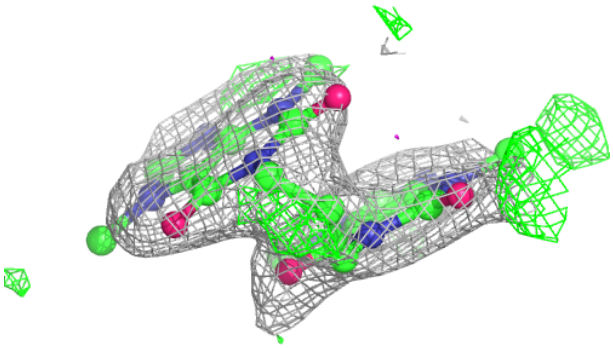
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	C	1398	6/6	0.88	0.16	39,49,56,63	0
3	DW0	D	1400	29/29	0.88	0.18	42,45,50,51	29
2	GOL	E	1398	6/6	0.90	0.14	29,41,47,49	0
3	DW0	F	1399	29/29	0.91	0.13	44,48,52,54	0
3	DW0	B	1399	29/29	0.92	0.13	29,38,48,49	0
3	DW0	D	1399	29/29	0.92	0.13	38,44,49,51	0
3	DW0	E	1399	29/29	0.93	0.11	29,36,49,51	0
3	DW0	C	1399	29/29	0.93	0.12	28,39,56,57	0
2	GOL	D	1398	6/6	0.94	0.13	28,35,42,47	0
3	DW0	A	1399	29/29	0.95	0.11	25,34,38,45	0
2	GOL	A	1398	6/6	0.95	0.09	26,34,40,47	0
2	GOL	F	1398	6/6	0.96	0.10	36,43,46,50	0
2	GOL	B	1398	6/6	0.97	0.10	34,41,45,46	0

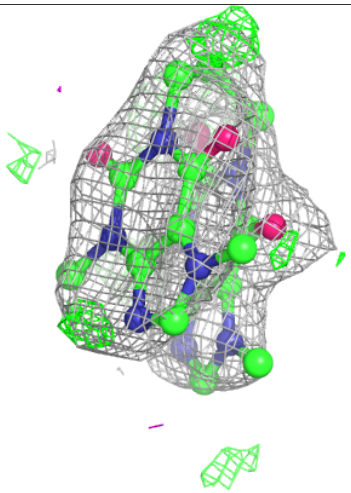
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DW0 F 1400:

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

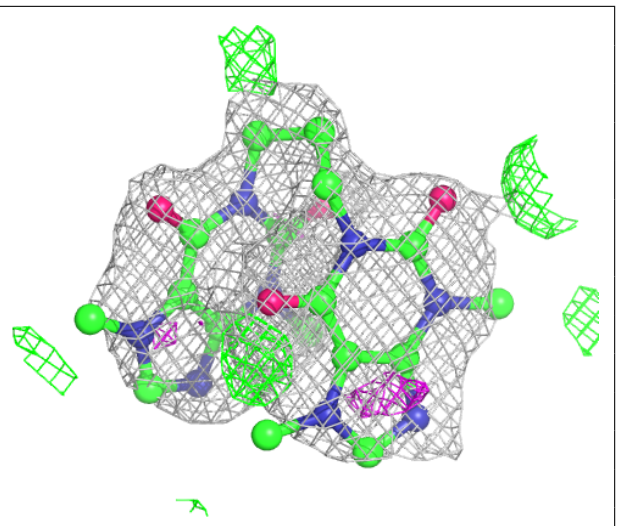


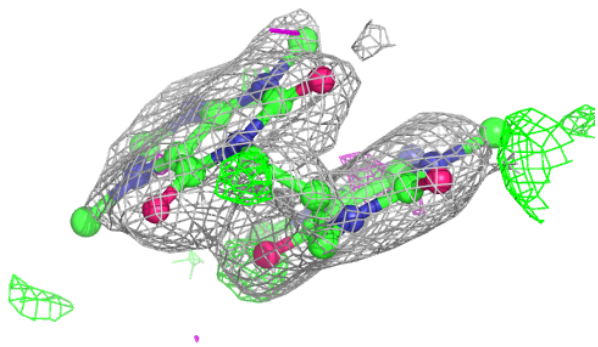


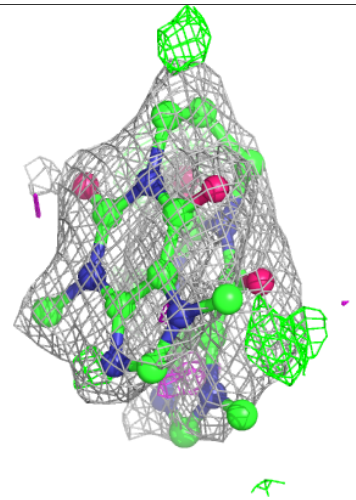


Electron density around DW0 A 1400:

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

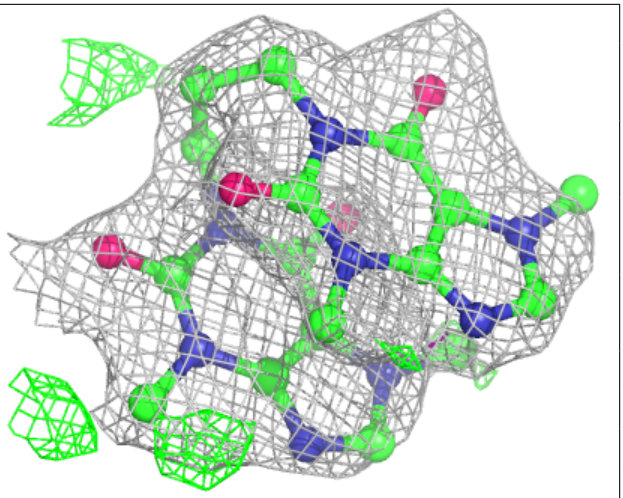


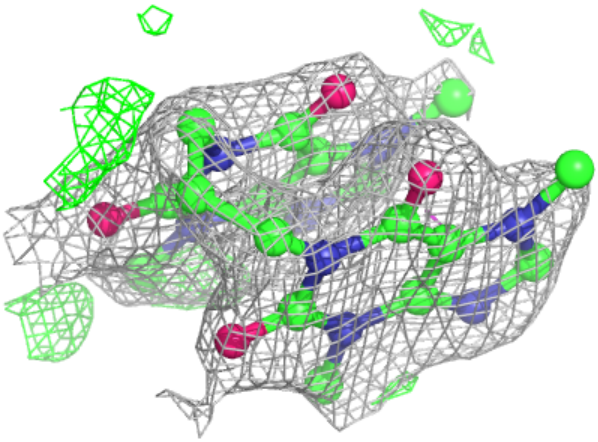


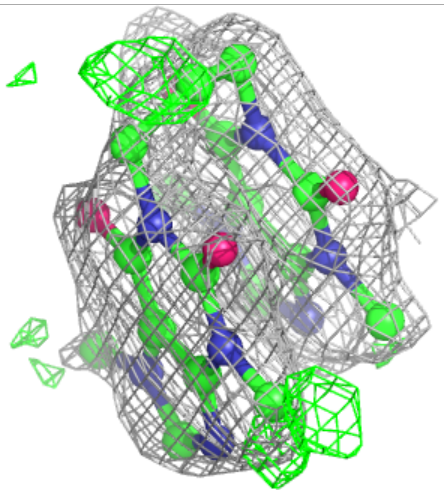


Electron density around DW0 C 1400:

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

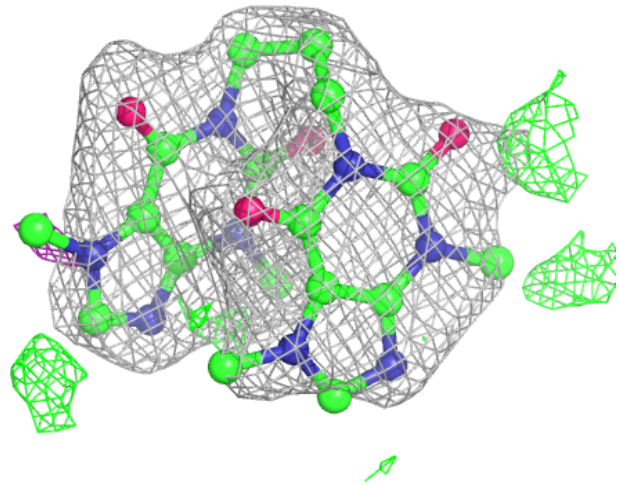


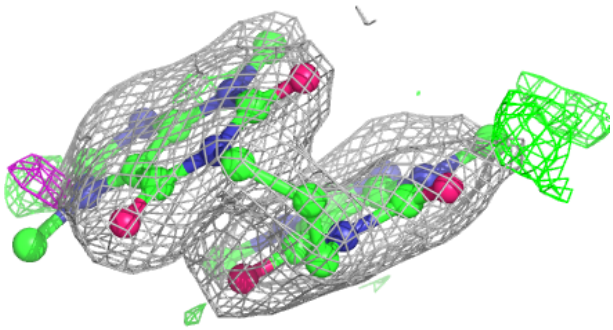


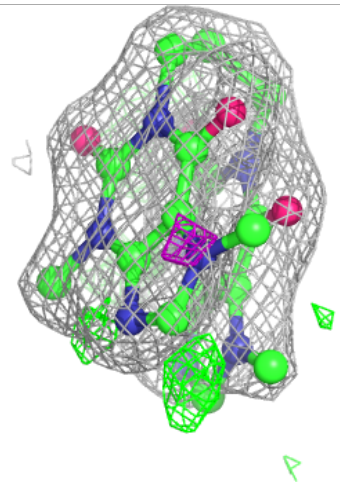


Electron density around DW0 E 1400:

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

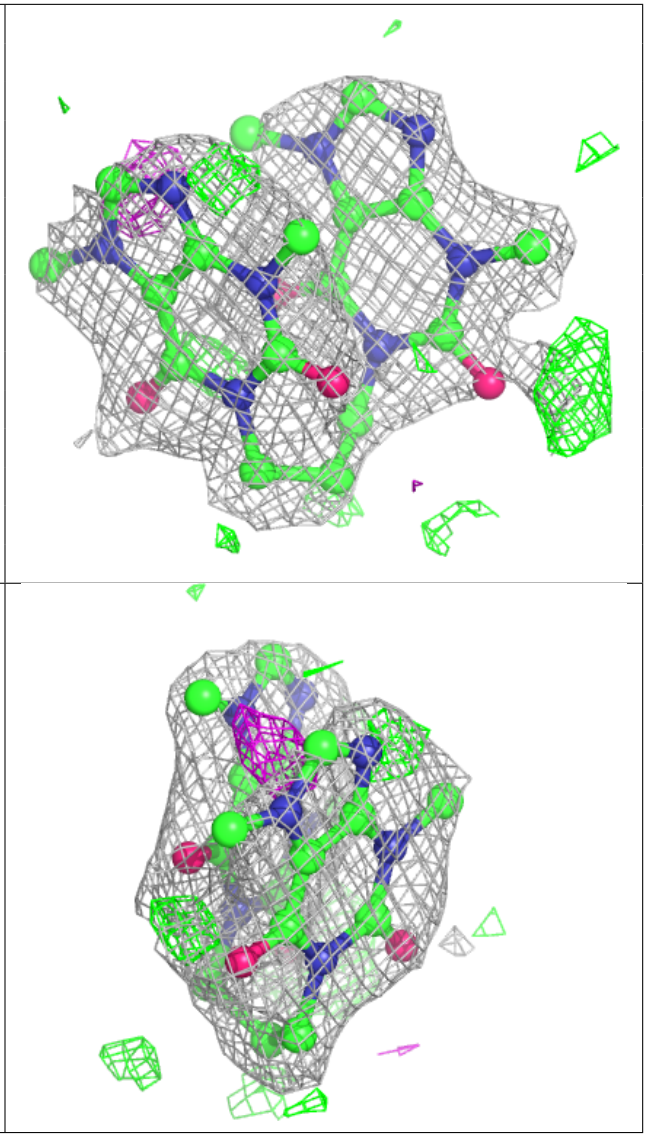






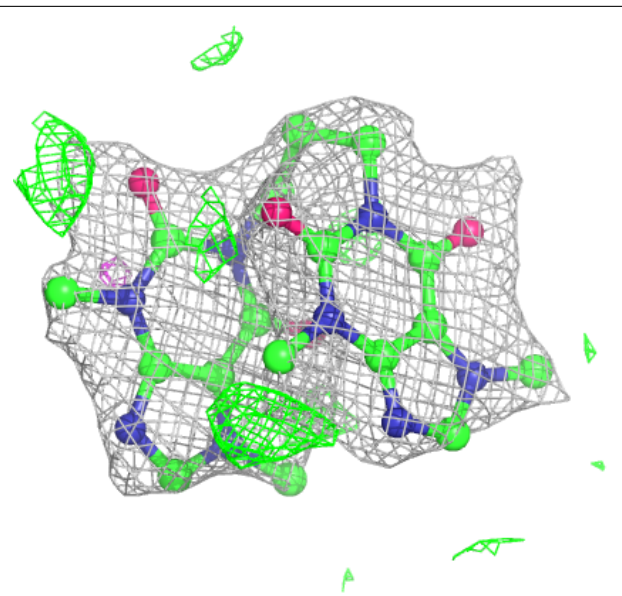
Electron density around DW0 B 1400:

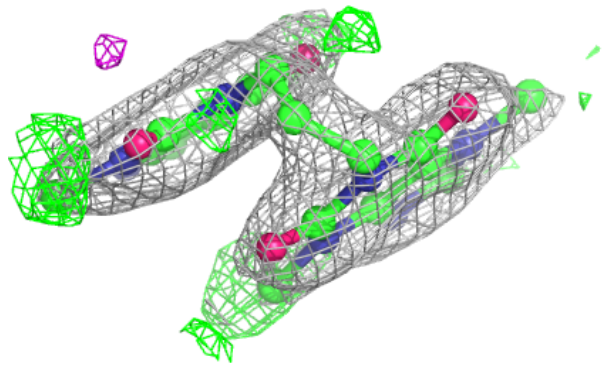
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

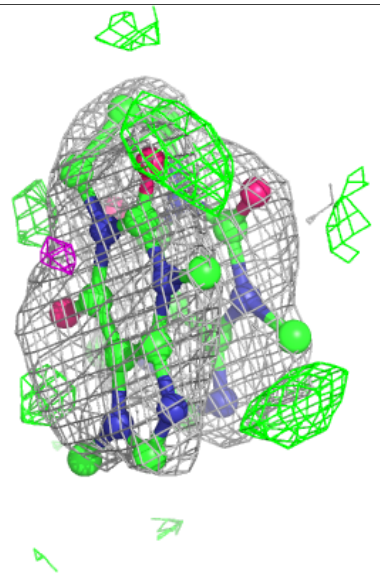


Electron density around DW0 D 1400:

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

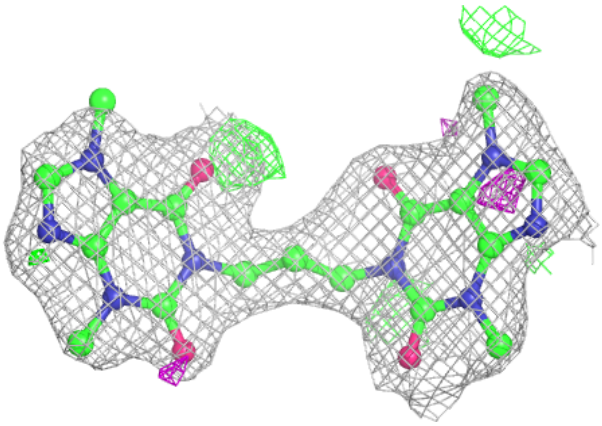


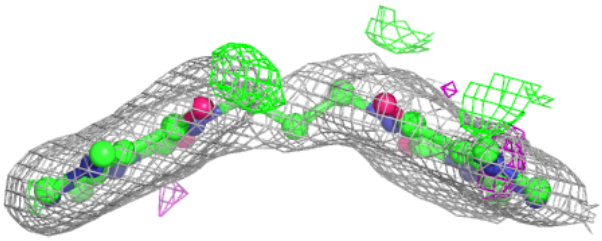


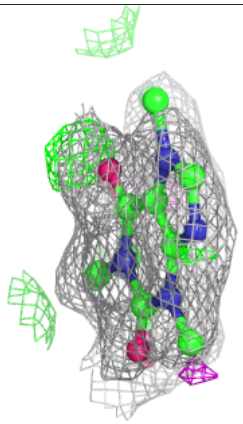


Electron density around DW0 F 1399:

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

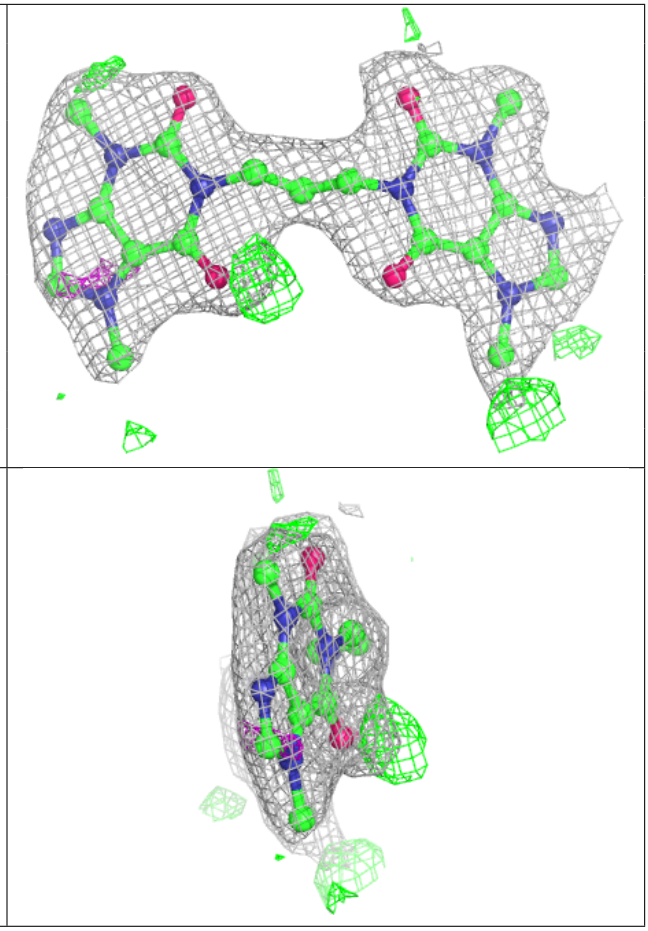






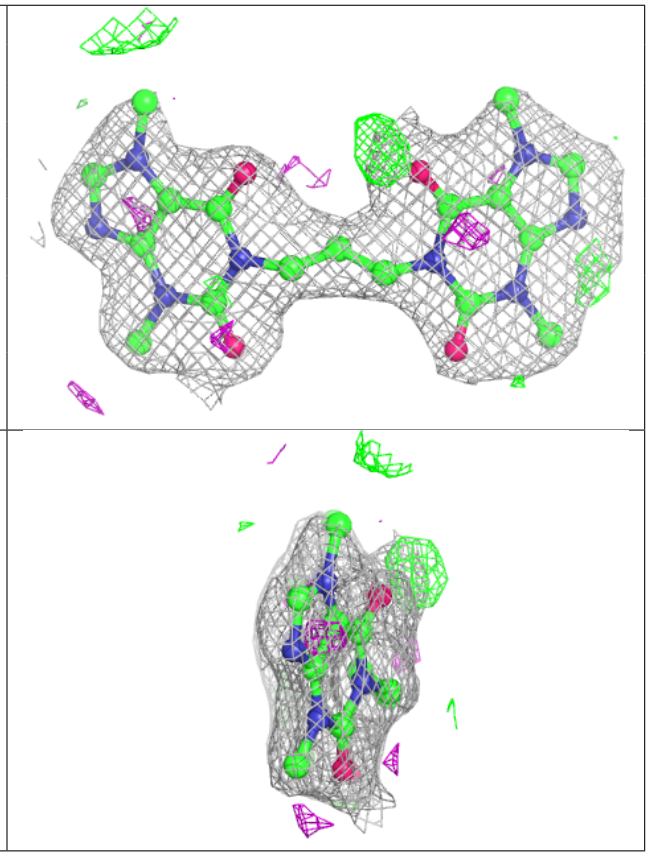
Electron density around DW0 B 1399:

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



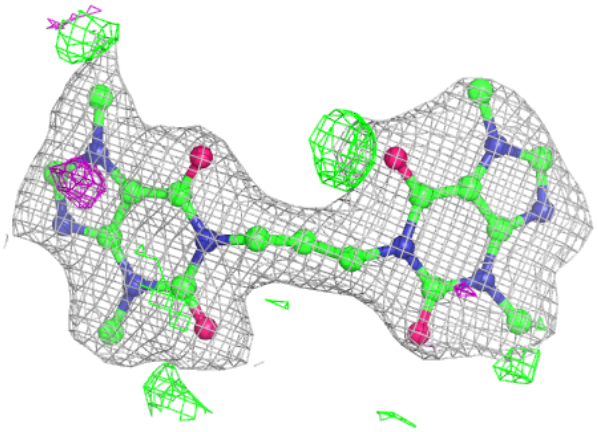
Electron density around DW0 D 1399:

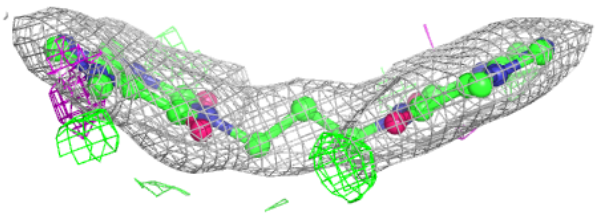
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

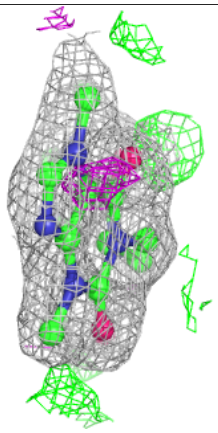


Electron density around DW0 E 1399:

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

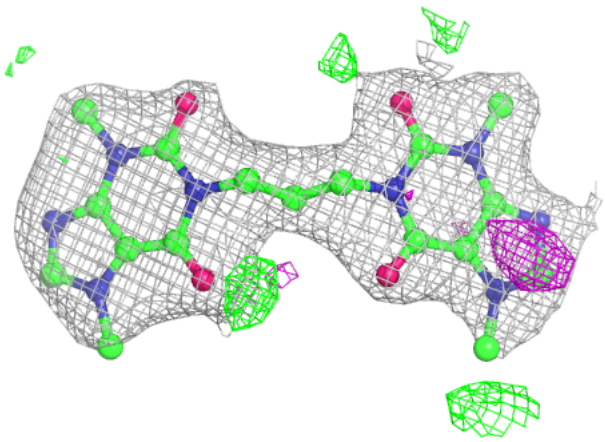


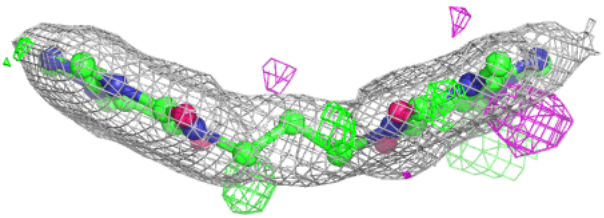


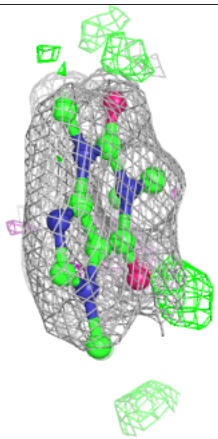


Electron density around DW0 C 1399:

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

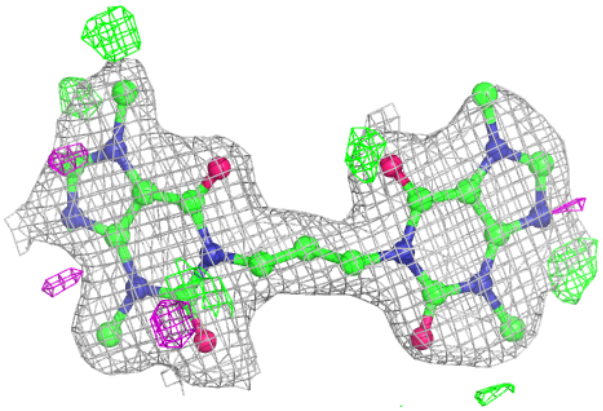


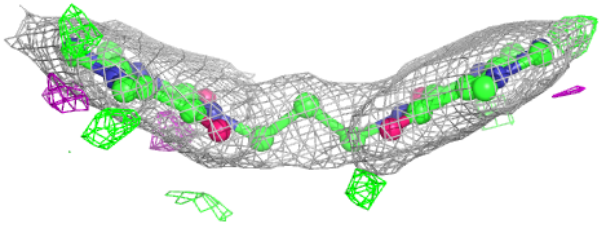


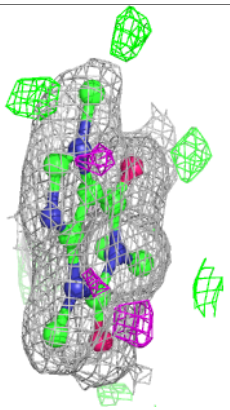


Electron density around DW0 A 1399:

$2mF_o$-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.