Full wwPDB X-ray Structure Validation Report (i)

Mar 7, 2026 – 12:14 AM UTC

PDB ID	:	2YBU / pdb_00002ybu
Title	:	Crystal structure of human acidic chitinase in complex with bisdionin F
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	:	2.25 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:

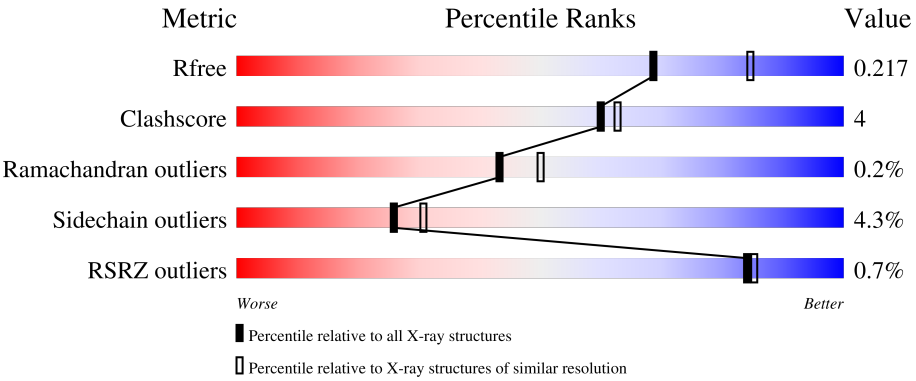
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	85% 12%
1	B	381	85% 14%
1	C	381	85% 14%
1	D	381	84% 14%
1	E	381	84% 13%

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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 19347 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
1	A	376	Total	C	N	O	S	0	0	0
			2976	1919	484	559	14			
1	B	376	Total	C	N	O	S	0	0	0
			2976	1919	484	559	14			
1	C	376	Total	C	N	O	S	0	0	0
			2976	1919	484	559	14			
1	D	376	Total	C	N	O	S	0	0	0
			2976	1919	484	559	14			
1	E	376	Total	C	N	O	S	0	0	0
			2976	1919	484	559	14			
1	F	376	Total	C	N	O	S	0	0	0
			2976	1919	484	559	14			

There are 36 discrepancies between the modelled and reference sequences:

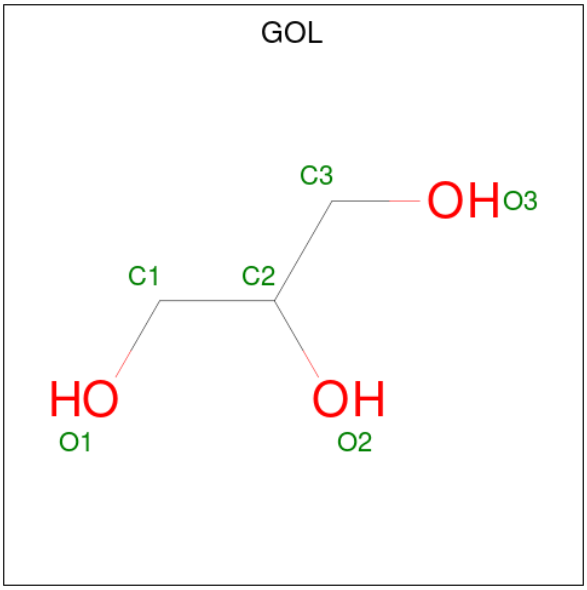
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLU	-	expression tag	UNP Q9BZP6
A	19	ALA	-	expression tag	UNP Q9BZP6
A	20	GLU	-	expression tag	UNP Q9BZP6
A	45	ASP	ASN	variant	UNP Q9BZP6
A	47	ASN	ASP	variant	UNP Q9BZP6
A	61	MET	ARG	variant	UNP Q9BZP6
B	18	GLU	-	expression tag	UNP Q9BZP6
B	19	ALA	-	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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



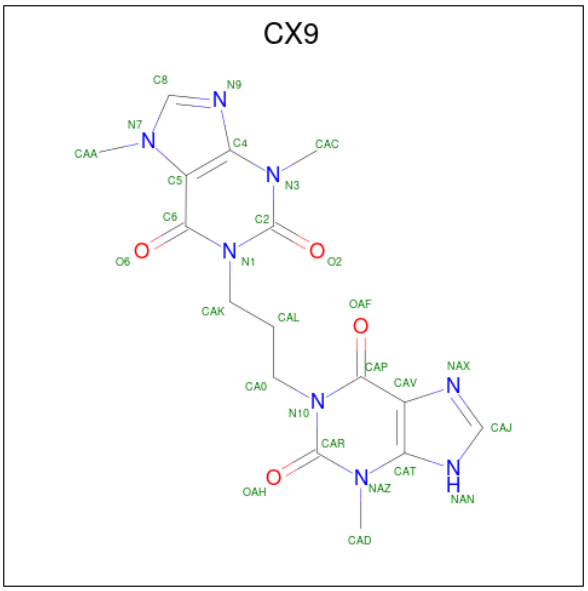
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

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

- Molecule 3 is 3,7-DIMETHYL-1-[3-(3-METHYL-2,6-DIOXO-9H-PURIN-1-YL)PROPYL]PURINE-2,6-DIONE (CCD ID: CX9) (formula: $C_{16}H_{18}N_8O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 28 16 8 4	0	0
3	A	1	Total C N O 28 16 8 4	0	0
3	B	1	Total C N O 28 16 8 4	0	0
3	B	1	Total C N O 28 16 8 4	0	0
3	C	1	Total C N O 28 16 8 4	0	0
3	C	1	Total C N O 28 16 8 4	0	0
3	D	1	Total C N O 28 16 8 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			28	16	8	4		
3	E	1	Total	C	N	O	0	0
			28	16	8	4		
3	E	1	Total	C	N	O	0	0
			28	16	8	4		
3	F	1	Total	C	N	O	0	0
			28	16	8	4		
3	F	1	Total	C	N	O	0	0
			28	16	8	4		

- Molecule 4 is water.

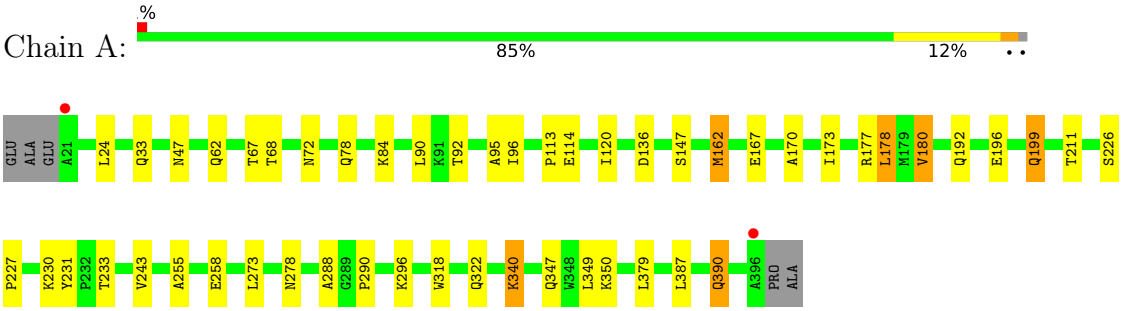
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	213	Total	O	0	0
			213	213		
4	B	220	Total	O	0	0
			220	220		
4	C	199	Total	O	0	0
			199	199		
4	D	171	Total	O	0	0
			171	171		
4	E	193	Total	O	0	0
			193	193		
4	F	123	Total	O	0	0
			123	123		

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.

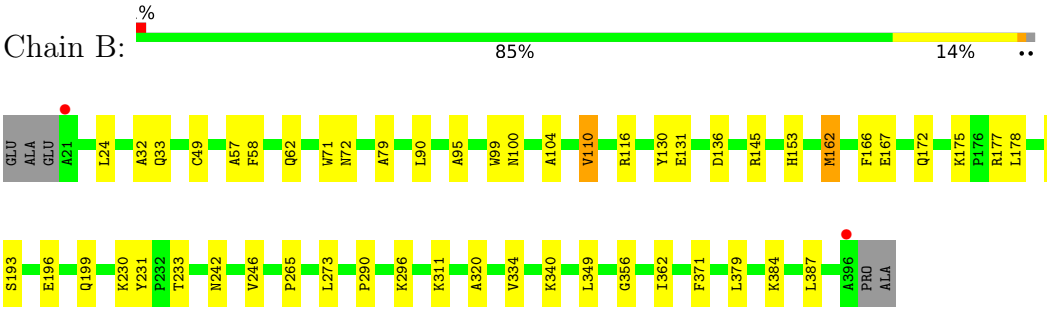
• Molecule 1: ACIDIC MAMMALIAN CHITINASE

Chain A:



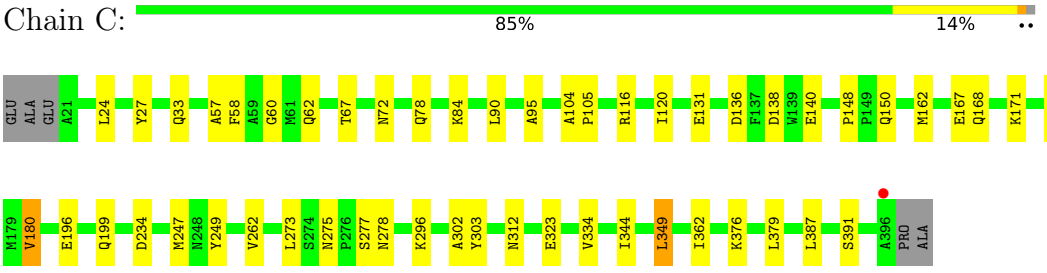
• Molecule 1: ACIDIC MAMMALIAN CHITINASE

Chain B:



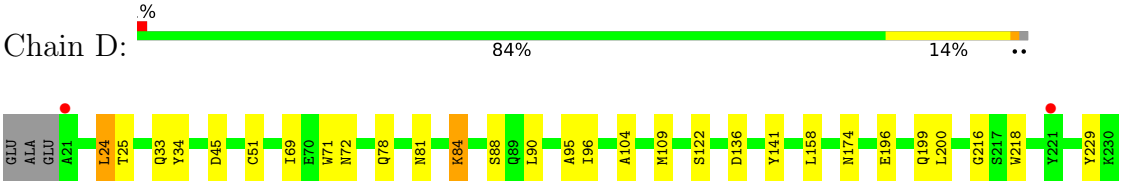
• Molecule 1: ACIDIC MAMMALIAN CHITINASE

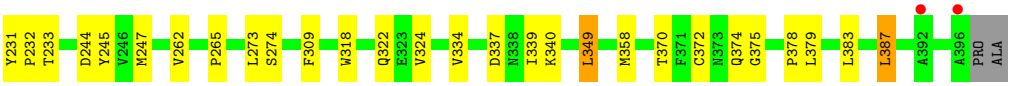
Chain C:



• Molecule 1: ACIDIC MAMMALIAN CHITINASE

Chain D:



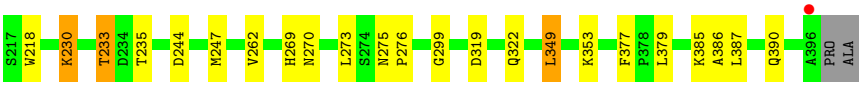


• Molecule 1: ACIDIC MAMMALIAN CHITINASE

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	144.78Å 149.19Å 151.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.25 19.97 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.97-2.25) 99.4 (19.97-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.42 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.173 , 0.219 0.171 , 0.217	Depositor DCC
R_{free} test set	1544 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k 0.049 for -l,-k,-h 0.016 for k,h,-l 0.006 for k,l,h 0.006 for l,h,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19347	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CX9

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	1.34	5/3068 (0.2%)	1.17	7/4182 (0.2%)
1	B	1.38	10/3068 (0.3%)	1.15	6/4182 (0.1%)
1	C	1.32	3/3068 (0.1%)	1.16	2/4182 (0.0%)
1	D	1.25	2/3068 (0.1%)	1.16	12/4182 (0.3%)
1	E	1.27	4/3068 (0.1%)	1.18	8/4182 (0.2%)
1	F	1.11	2/3068 (0.1%)	1.10	9/4182 (0.2%)
All	All	1.28	26/18408 (0.1%)	1.15	44/25092 (0.2%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	377	PHE	C-O	-7.28	1.20	1.23
1	B	320	ALA	CA-CB	7.25	1.63	1.53
1	C	278	ASN	CB-CG	6.90	1.69	1.52
1	B	104	ALA	CA-CB	6.66	1.61	1.53
1	B	334	VAL	C-O	6.63	1.30	1.24
1	A	178	LEU	N-CA	6.12	1.53	1.46
1	F	57	ALA	CA-CB	-6.00	1.45	1.53
1	C	334	VAL	CA-CB	5.92	1.63	1.54
1	B	362	ILE	CA-CB	-5.89	1.46	1.54
1	A	278	ASN	CB-CG	5.74	1.66	1.52
1	B	265	PRO	CA-C	5.66	1.58	1.52
1	A	288	ALA	CA-CB	5.55	1.62	1.53
1	A	258	GLU	CG-CD	5.34	1.65	1.52
1	D	69	ILE	N-CA	5.28	1.51	1.46
1	A	199	GLN	CG-CD	5.27	1.65	1.52
1	B	145	ARG	C-O	5.26	1.30	1.23
1	B	32	ALA	CA-CB	-5.25	1.44	1.53
1	E	386	ALA	CA-CB	-5.24	1.44	1.53
1	C	234	ASP	CA-C	5.20	1.59	1.52
1	D	274	SER	N-CA	5.17	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	110	VAL	CA-CB	5.17	1.60	1.54
1	E	197	ILE	N-CA	-5.16	1.40	1.46
1	F	308	THR	C-O	-5.15	1.18	1.24
1	B	79	ALA	CA-CB	5.15	1.61	1.53
1	B	320	ALA	C-O	-5.08	1.19	1.24
1	B	110	VAL	CA-CB	5.03	1.60	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	45	ASP	N-CA-C	-8.64	102.75	113.38
1	E	180	VAL	CB-CA-C	-7.76	99.05	110.62
1	F	147	SER	CA-C-N	7.20	127.79	120.38
1	F	147	SER	C-N-CA	7.20	127.79	120.38
1	C	180	VAL	CB-CA-C	-7.16	99.48	110.50
1	F	255	ALA	CA-C-N	6.79	127.16	119.83
1	F	255	ALA	C-N-CA	6.79	127.16	119.83
1	C	174	ASN	N-CA-C	6.71	120.67	111.54
1	E	233	THR	N-CA-C	6.63	120.63	112.54
1	D	334	VAL	CA-C-N	-6.60	116.59	122.73
1	D	334	VAL	C-N-CA	-6.60	116.59	122.73
1	D	141	TYR	CA-C-N	-6.47	113.09	119.76
1	D	141	TYR	C-N-CA	-6.47	113.09	119.76
1	A	147	SER	CA-C-N	6.32	126.89	120.38
1	A	147	SER	C-N-CA	6.32	126.89	120.38
1	D	104	ALA	CA-C-N	-5.76	113.09	119.19
1	D	104	ALA	C-N-CA	-5.76	113.09	119.19
1	F	180	VAL	CB-CA-C	-5.73	102.14	110.63
1	F	104	ALA	CA-C-N	-5.71	113.00	119.28
1	F	104	ALA	C-N-CA	-5.71	113.00	119.28
1	D	309	PHE	N-CA-C	-5.55	105.31	111.36
1	D	324	VAL	CA-C-N	-5.53	114.88	120.85
1	D	324	VAL	C-N-CA	-5.53	114.88	120.85
1	B	356	GLY	N-CA-C	5.51	117.43	110.38
1	E	230	LYS	CD-CE-NZ	-5.47	94.39	111.90
1	F	238	ASN	N-CA-C	5.43	118.70	111.75
1	D	88	SER	N-CA-C	-5.38	106.55	113.23
1	B	79	ALA	N-CA-C	-5.37	105.51	111.36
1	E	120	ILE	N-CA-C	5.25	115.47	110.42
1	B	175	LYS	CA-C-N	-5.24	115.18	120.21
1	B	175	LYS	C-N-CA	-5.24	115.18	120.21
1	E	52	THR	N-CA-C	-5.21	107.08	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	104	ALA	CA-C-N	-5.14	113.74	119.19
1	B	104	ALA	C-N-CA	-5.14	113.74	119.19
1	F	195	TYR	N-CA-C	5.13	117.81	109.24
1	A	180	VAL	CB-CA-C	-5.10	103.53	110.77
1	A	255	ALA	CA-C-N	-5.10	114.55	119.90
1	A	255	ALA	C-N-CA	-5.10	114.55	119.90
1	E	233	THR	N-CA-CB	-5.08	101.97	110.39
1	E	72	ASN	N-CA-C	5.05	118.75	112.59
1	A	226	SER	CA-C-N	-5.04	114.76	119.85
1	A	226	SER	C-N-CA	-5.04	114.76	119.85
1	E	183	ALA	N-CA-C	-5.03	101.05	109.24
1	D	370	THR	N-CA-C	5.00	119.09	112.89

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	2976	0	2821	23	0
1	B	2976	0	2821	26	0
1	C	2976	0	2821	29	0
1	D	2976	0	2821	25	0
1	E	2976	0	2821	28	0
1	F	2976	0	2821	24	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
3	A	56	0	36	2	0
3	B	56	0	36	1	0
3	C	56	0	36	0	0
3	D	56	0	36	2	0
3	E	56	0	36	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	56	0	36	1	0
4	A	213	0	0	1	0
4	B	220	0	0	2	0
4	C	199	0	0	2	0
4	D	171	0	0	2	0
4	E	193	0	0	1	0
4	F	123	0	0	0	0
All	All	19347	0	17190	151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (151) 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:196:GLU:HB3	1:B:199:GLN:HE21	1.40	0.86
1:C:33:GLN:HE22	1:C:72:ASN:HD21	1.22	0.84
1:C:196:GLU:HB3	1:C:199:GLN:HE21	1.42	0.84
1:A:231:TYR:HD2	1:A:233:THR:HG22	1.43	0.84
3:E:1399:CX9:OAF	3:E:1399:CX9:HAL	1.78	0.83
1:B:231:TYR:HD2	1:B:233:THR:HG22	1.41	0.82
1:E:196:GLU:HB3	1:E:199:GLN:HE21	1.46	0.81
1:E:61:MET:HE2	1:E:119:PHE:CE1	2.17	0.79
1:B:33:GLN:HE22	1:B:72:ASN:HD21	1.29	0.78
1:D:196:GLU:HB3	1:D:199:GLN:HE21	1.47	0.77
1:A:120:ILE:HG12	1:A:162:MET:HE3	1.69	0.74
1:F:339:ILE:HD12	1:F:374:GLN:NE2	2.02	0.73
1:A:318:TRP:CH2	1:A:340:LYS:HD2	2.25	0.71
1:A:33:GLN:HE22	1:A:72:ASN:HD21	1.39	0.71
1:E:33:GLN:HE22	1:E:72:ASN:HD21	1.37	0.69
1:C:323:GLU:OE1	4:C:2163:HOH:O	2.10	0.69
1:F:167:GLU:HG3	1:F:177:ARG:HD3	1.73	0.68
1:D:339:ILE:HD12	1:D:374:GLN:NE2	2.08	0.67
1:E:61:MET:HE2	1:E:119:PHE:CD1	2.28	0.67
1:F:33:GLN:HE22	1:F:72:ASN:HD21	1.43	0.63
1:B:231:TYR:CD2	1:B:233:THR:HG22	2.30	0.63
1:A:113:PRO:HG2	1:A:114:GLU:OE2	1.99	0.62
1:A:390:GLN:HB2	4:A:2211:HOH:O	2.01	0.60
1:B:162:MET:HE2	1:B:166:PHE:CE1	2.36	0.60
1:A:296:LYS:HD3	1:D:34:TYR:HB3	1.84	0.59
1:B:33:GLN:NE2	1:B:72:ASN:HD21	1.97	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:GLN:HE22	1:D:72:ASN:HD21	1.49	0.58
1:F:33:GLN:NE2	1:F:72:ASN:HD21	2.02	0.58
1:E:127:LEU:HD12	1:E:178:LEU:HD13	1.86	0.58
1:B:153:HIS:HB3	4:B:2096:HOH:O	2.04	0.56
1:C:296:LYS:HE2	1:E:244:ASP:CG	2.31	0.55
1:A:196:GLU:HB3	1:A:199:GLN:HE21	1.72	0.55
1:C:148:PRO:HB2	1:C:150:GLN:OE1	2.08	0.54
1:E:115:ASN:N	1:E:115:ASN:HD22	2.05	0.54
1:F:225:ASN:OD1	1:F:269:HIS:HD2	1.92	0.53
1:D:231:TYR:CG	1:D:232:PRO:HD2	2.44	0.52
1:C:247:MET:HE2	1:C:262:VAL:HG22	1.91	0.52
1:B:371:PHE:CE2	1:C:376:LYS:HD3	2.44	0.52
1:C:120:ILE:HG12	1:C:162:MET:HE3	1.90	0.52
1:A:167:GLU:HG3	1:A:177:ARG:HD3	1.90	0.52
1:E:196:GLU:HB3	1:E:199:GLN:NE2	2.20	0.52
1:B:296:LYS:HD3	1:F:34:TYR:HB3	1.91	0.51
1:C:391:SER:HB2	4:C:2196:HOH:O	2.09	0.51
1:B:340:LYS:HE3	4:B:2204:HOH:O	2.08	0.51
1:C:312:ASN:HD21	1:E:235:THR:HB	1.76	0.51
1:F:347:GLN:NE2	1:F:347:GLN:HA	2.25	0.51
1:E:319:ASP:OD2	1:E:322:GLN:NE2	2.35	0.51
1:A:33:GLN:NE2	1:A:72:ASN:HD21	2.07	0.50
1:B:167:GLU:HG3	1:B:177:ARG:HD3	1.94	0.49
1:E:177:ARG:HG2	1:E:178:LEU:O	2.12	0.49
1:D:372:CYS:HB2	4:D:2159:HOH:O	2.11	0.49
1:E:172:GLN:O	1:E:173:ILE:HG23	2.13	0.49
1:E:216:GLY:HA3	1:E:218:TRP:CZ3	2.48	0.49
1:A:170:ALA:HB2	1:A:177:ARG:HA	1.95	0.48
1:B:196:GLU:HB3	1:B:199:GLN:NE2	2.21	0.48
1:C:275:ASN:OD1	1:C:277:SER:HB2	2.14	0.48
1:D:24:LEU:O	1:D:51:CYS:HB3	2.13	0.48
1:D:33:GLN:NE2	1:D:72:ASN:HD21	2.12	0.47
1:F:33:GLN:HE22	1:F:72:ASN:ND2	2.12	0.47
1:D:229:TYR:O	1:D:322:GLN:HG2	2.14	0.47
1:E:116:ARG:HE	1:E:161:GLU:CD	2.23	0.47
1:C:344:ILE:HG13	1:F:38:LEU:HD21	1.95	0.47
1:D:196:GLU:HB3	1:D:199:GLN:NE2	2.23	0.47
1:F:225:ASN:OD1	1:F:269:HIS:CD2	2.68	0.47
1:A:290:PRO:HA	1:D:71:TRP:CD2	2.49	0.47
1:A:33:GLN:HE22	1:A:72:ASN:ND2	2.10	0.47
1:B:110:VAL:HA	1:B:116:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:HIS:HA	1:E:299:GLY:O	2.15	0.47
1:E:247:MET:HE2	1:E:262:VAL:HG22	1.97	0.47
1:F:216:GLY:HA3	1:F:218:TRP:CZ3	2.49	0.47
3:A:1399:CX9:CAP	3:A:1399:CX9:C6	2.93	0.47
1:B:130:TYR:O	1:B:131:GLU:HB2	2.14	0.47
3:F:1399:CX9:CAP	3:F:1399:CX9:C6	2.92	0.46
1:D:383:LEU:O	1:D:387:LEU:HB2	2.15	0.46
1:A:84:LYS:HD2	1:A:92:THR:HG23	1.97	0.46
1:B:95:ALA:HA	1:B:136:ASP:O	2.15	0.46
1:C:95:ALA:HA	1:C:136:ASP:O	2.15	0.46
1:D:216:GLY:HA3	1:D:218:TRP:CH2	2.51	0.46
1:D:231:TYR:CD1	1:D:232:PRO:HD2	2.50	0.46
1:D:375:GLY:O	1:D:378:PRO:HD3	2.16	0.46
3:D:1399:CX9:O6	3:D:1399:CX9:HAL	2.15	0.46
1:A:211:THR:HB	1:A:243:VAL:HG22	1.97	0.45
1:D:122:SER:HB2	4:D:2023:HOH:O	2.15	0.45
1:E:157:VAL:O	1:E:161:GLU:HG3	2.16	0.45
1:A:192:GLN:NE2	1:B:193:SER:HB3	2.32	0.45
1:B:49:CYS:O	1:B:384:LYS:HE2	2.16	0.45
1:E:54:LEU:HB3	1:E:80:PHE:CZ	2.52	0.45
1:D:95:ALA:HA	1:D:136:ASP:O	2.17	0.45
1:F:95:ALA:HA	1:F:136:ASP:O	2.16	0.44
1:C:167:GLU:HG3	1:C:177:ARG:HD3	1.98	0.44
1:E:349:LEU:C	1:E:349:LEU:HD12	2.42	0.44
1:F:187:GLY:O	1:F:191:ILE:HG13	2.18	0.44
1:B:187:GLY:O	1:B:191:ILE:HG13	2.18	0.44
1:B:71:TRP:CD2	1:F:290:PRO:HA	2.53	0.44
1:D:318:TRP:CH2	1:D:340:LYS:HD2	2.52	0.44
1:C:60:GLY:C	1:C:67:THR:HG22	2.43	0.44
1:A:347:GLN:HE22	1:A:350:LYS:NZ	2.16	0.43
1:E:270:ASN:OD1	1:E:299:GLY:HA2	2.18	0.43
1:C:104:ALA:HB3	1:C:105:PRO:HD3	1.99	0.43
1:E:275:ASN:HA	1:E:276:PRO:HD2	1.85	0.43
1:B:33:GLN:HE22	1:B:72:ASN:ND2	2.05	0.43
3:B:1399:CX9:CAP	3:B:1399:CX9:C6	2.97	0.43
1:D:349:LEU:C	1:D:349:LEU:HD12	2.44	0.43
1:B:57:ALA:HA	1:B:58:PHE:HA	1.85	0.43
1:A:177:ARG:HG2	1:A:178:LEU:O	2.19	0.43
1:C:302:ALA:O	1:C:303:TYR:C	2.60	0.43
1:C:349:LEU:HD12	1:C:349:LEU:C	2.44	0.43
1:F:177:ARG:HG2	1:F:178:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASN:C	1:A:47:ASN:OD1	2.60	0.43
1:C:138:ASP:OD1	1:C:140:GLU:OE2	2.37	0.43
1:B:242:ASN:O	1:B:246:VAL:HG23	2.19	0.43
1:C:33:GLN:NE2	1:C:72:ASN:HD21	2.03	0.42
1:D:109:MET:HE1	1:D:158:LEU:CD2	2.49	0.42
3:D:1399:CX9:C6	3:D:1399:CX9:CAP	2.97	0.42
1:C:177:ARG:HG2	1:C:178:LEU:O	2.19	0.42
1:A:67:THR:HG23	1:A:68:THR:O	2.19	0.42
1:D:96:ILE:O	1:D:96:ILE:HG23	2.20	0.42
1:F:157:VAL:O	1:F:161:GLU:HG3	2.19	0.42
3:A:1399:CX9:HAL	3:A:1399:CX9:OAF	2.19	0.42
1:C:312:ASN:HD21	1:E:235:THR:CB	2.33	0.42
1:F:57:ALA:HA	1:F:58:PHE:HA	1.85	0.42
1:F:196:GLU:HB3	1:F:199:GLN:HE21	1.85	0.42
1:F:271:PHE:CD1	1:F:271:PHE:N	2.87	0.41
1:D:25:THR:O	1:D:358:MET:HA	2.20	0.41
1:B:99:TRP:HD1	1:B:100:ASN:HD22	1.68	0.41
1:C:84:LYS:NZ	1:C:131:GLU:O	2.53	0.41
1:A:95:ALA:HA	1:A:136:ASP:O	2.21	0.41
1:D:244:ASP:O	1:D:245:TYR:C	2.62	0.41
1:E:162:MET:HE3	1:E:162:MET:HB2	2.02	0.41
1:A:231:TYR:CD2	1:A:233:THR:HG22	2.36	0.41
1:C:344:ILE:CG1	1:F:38:LEU:HD21	2.49	0.41
1:E:172:GLN:O	1:E:173:ILE:CG2	2.68	0.41
1:C:116:ARG:O	1:C:120:ILE:HG13	2.20	0.41
1:B:290:PRO:HA	1:F:71:TRP:CD2	2.55	0.41
1:C:27:TYR:O	1:C:362:ILE:HG22	2.20	0.41
1:C:249:TYR:CD1	1:C:249:TYR:C	2.99	0.41
1:E:57:ALA:HA	1:E:58:PHE:HA	1.83	0.41
1:E:115:ASN:N	1:E:115:ASN:ND2	2.69	0.41
1:F:347:GLN:HE22	1:F:350:LYS:NZ	2.18	0.41
1:B:177:ARG:HG2	1:B:178:LEU:O	2.21	0.41
1:B:311:LYS:HE3	1:B:311:LYS:HB2	1.87	0.40
1:C:167:GLU:HG3	1:C:177:ARG:CD	2.51	0.40
1:D:247:MET:HE2	1:D:262:VAL:HG22	2.03	0.40
1:D:81:ASN:O	1:D:84:LYS:HB2	2.21	0.40
1:C:57:ALA:HA	1:C:58:PHE:HA	1.86	0.40
1:E:216:GLY:HA3	1:E:218:TRP:CH2	2.56	0.40
3:E:1398:CX9:HAA	3:E:1398:CX9:O6	2.21	0.40
1:F:211:THR:HB	1:F:243:VAL:HG22	2.04	0.40
1:A:227:PRO:HB2	1:A:322:GLN:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:390:GLN:HB2	4:E:2188:HOH:O	2.20	0.40
1:F:215:HIS:HB2	1:F:224:GLU:O	2.22	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	374/381 (98%)	363 (97%)	10 (3%)	1 (0%)	36	40
1	B	374/381 (98%)	365 (98%)	9 (2%)	0	100	100
1	C	374/381 (98%)	365 (98%)	9 (2%)	0	100	100
1	D	374/381 (98%)	366 (98%)	7 (2%)	1 (0%)	36	40
1	E	374/381 (98%)	362 (97%)	11 (3%)	1 (0%)	36	40
1	F	374/381 (98%)	362 (97%)	11 (3%)	1 (0%)	36	40
All	All	2244/2286 (98%)	2183 (97%)	57 (2%)	4 (0%)	43	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	173	ILE
1	A	173	ILE
1	F	131	GLU
1	D	265	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	311/314 (99%)	297 (96%)	14 (4%)	24	29
1	B	311/314 (99%)	301 (97%)	10 (3%)	34	43
1	C	311/314 (99%)	300 (96%)	11 (4%)	32	39
1	D	311/314 (99%)	299 (96%)	12 (4%)	28	35
1	E	311/314 (99%)	295 (95%)	16 (5%)	21	23
1	F	311/314 (99%)	293 (94%)	18 (6%)	18	19
All	All	1866/1884 (99%)	1785 (96%)	81 (4%)	26	31

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	62	GLN
1	A	78	GLN
1	A	90	LEU
1	A	96	ILE
1	A	162	MET
1	A	180	VAL
1	A	230	LYS
1	A	273	LEU
1	A	340	LYS
1	A	349	LEU
1	A	379	LEU
1	A	387	LEU
1	A	390	GLN
1	B	24	LEU
1	B	62	GLN
1	B	90	LEU
1	B	162	MET
1	B	172	GLN
1	B	230	LYS
1	B	273	LEU
1	B	349	LEU
1	B	379	LEU
1	B	387	LEU
1	C	24	LEU
1	C	62	GLN
1	C	78	GLN

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Mol	Chain	Res	Type
1	C	90	LEU
1	C	168	GLN
1	C	171	LYS
1	C	180	VAL
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	84	LYS
1	D	90	LEU
1	D	174	ASN
1	D	200	LEU
1	D	233	THR
1	D	273	LEU
1	D	337	ASP
1	D	349	LEU
1	D	379	LEU
1	D	387	LEU
1	E	24	LEU
1	E	90	LEU
1	E	114	GLU
1	E	167	GLU
1	E	172	GLN
1	E	174	ASN
1	E	180	VAL
1	E	200	LEU
1	E	230	LYS
1	E	233	THR
1	E	273	LEU
1	E	349	LEU
1	E	353	LYS
1	E	379	LEU
1	E	385	LYS
1	E	387	LEU
1	F	24	LEU
1	F	62	GLN
1	F	90	LEU
1	F	144	SER
1	F	147	SER
1	F	160	GLN

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Mol	Chain	Res	Type
1	F	172	GLN
1	F	180	VAL
1	F	200	LEU
1	F	201	SER
1	F	230	LYS
1	F	233	THR
1	F	271	PHE
1	F	273	LEU
1	F	337	ASP
1	F	349	LEU
1	F	379	LEU
1	F	387	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	78	GLN
1	A	85	ASN
1	A	100	ASN
1	A	160	GLN
1	A	174	ASN
1	A	192	GLN
1	A	199	GLN
1	A	278	ASN
1	A	312	ASN
1	A	347	GLN
1	A	374	GLN
1	B	33	GLN
1	B	78	GLN
1	B	85	ASN
1	B	100	ASN
1	B	115	ASN
1	B	129	GLN
1	B	192	GLN
1	B	238	ASN
1	B	248	ASN
1	B	312	ASN
1	C	33	GLN
1	C	85	ASN
1	C	100	ASN
1	C	115	ASN

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Mol	Chain	Res	Type
1	C	174	ASN
1	C	192	GLN
1	C	199	GLN
1	C	248	ASN
1	C	278	ASN
1	C	312	ASN
1	D	33	GLN
1	D	64	ASN
1	D	85	ASN
1	D	100	ASN
1	D	115	ASN
1	D	117	GLN
1	D	192	GLN
1	D	199	GLN
1	D	248	ASN
1	D	347	GLN
1	D	374	GLN
1	E	33	GLN
1	E	78	GLN
1	E	85	ASN
1	E	100	ASN
1	E	115	ASN
1	E	172	GLN
1	E	192	GLN
1	E	199	GLN
1	E	248	ASN
1	E	351	HIS
1	E	374	GLN
1	F	33	GLN
1	F	64	ASN
1	F	85	ASN
1	F	100	ASN
1	F	115	ASN
1	F	129	GLN
1	F	153	HIS
1	F	192	GLN
1	F	199	GLN
1	F	248	ASN
1	F	269	HIS
1	F	278	ASN
1	F	347	GLN
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 oligosaccharides 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	$\#\|Z\| > 2$
3	CX9	B	1399	-	31,31,31	1.51	6 (19%)	43,47,47	2.80	24 (55%)
3	CX9	E	1399	-	31,31,31	1.52	6 (19%)	43,47,47	2.52	22 (51%)
3	CX9	C	1398	-	31,31,31	1.61	7 (22%)	43,47,47	2.44	21 (48%)
2	GOL	F	1397	-	5,5,5	0.28	0	5,5,5	1.08	0
3	CX9	D	1398	-	31,31,31	1.69	8 (25%)	43,47,47	2.24	19 (44%)
2	GOL	C	1397	-	5,5,5	0.37	0	5,5,5	1.44	1 (20%)
2	GOL	A	1397	-	5,5,5	0.34	0	5,5,5	1.27	0
2	GOL	E	1397	-	5,5,5	0.50	0	5,5,5	1.24	1 (20%)
2	GOL	B	1397	-	5,5,5	0.39	0	5,5,5	1.13	0
3	CX9	A	1398	-	31,31,31	1.86	9 (29%)	43,47,47	2.33	18 (41%)
3	CX9	C	1399	-	31,31,31	1.72	7 (22%)	43,47,47	2.32	20 (46%)
3	CX9	D	1399	-	31,31,31	1.71	7 (22%)	43,47,47	2.35	21 (48%)
3	CX9	E	1398	-	31,31,31	1.82	8 (25%)	43,47,47	2.50	24 (55%)
3	CX9	B	1398	-	31,31,31	1.50	8 (25%)	43,47,47	2.24	20 (46%)
3	CX9	A	1399	-	31,31,31	1.66	10 (32%)	43,47,47	2.23	21 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	D	1397	-	5,5,5	0.49	0	5,5,5	1.03	0
3	CX9	F	1398	-	31,31,31	1.43	2 (6%)	43,47,47	2.32	19 (44%)
3	CX9	F	1399	-	31,31,31	1.73	10 (32%)	43,47,47	2.37	20 (46%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CX9	B	1399	-	-	3/6/6/6	0/4/4/4
3	CX9	E	1399	-	-	2/6/6/6	0/4/4/4
3	CX9	C	1398	-	-	0/6/6/6	0/4/4/4
2	GOL	F	1397	-	-	2/4/4/4	-
3	CX9	D	1398	-	-	0/6/6/6	0/4/4/4
2	GOL	C	1397	-	-	2/4/4/4	-
2	GOL	A	1397	-	-	2/4/4/4	-
2	GOL	E	1397	-	-	3/4/4/4	-
2	GOL	B	1397	-	-	2/4/4/4	-
3	CX9	A	1398	-	-	0/6/6/6	0/4/4/4
3	CX9	C	1399	-	-	2/6/6/6	0/4/4/4
3	CX9	D	1399	-	-	2/6/6/6	0/4/4/4
3	CX9	E	1398	-	-	0/6/6/6	0/4/4/4
3	CX9	B	1398	-	-	0/6/6/6	0/4/4/4
3	CX9	A	1399	-	-	4/6/6/6	0/4/4/4
2	GOL	D	1397	-	-	2/4/4/4	-
3	CX9	F	1398	-	-	0/6/6/6	0/4/4/4
3	CX9	F	1399	-	-	4/6/6/6	0/4/4/4

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1398	CX9	CAC-N3	5.77	1.57	1.47
3	C	1398	CX9	C5-N7	-4.50	1.30	1.38
3	E	1398	CX9	CAC-N3	4.48	1.54	1.47
3	E	1398	CX9	C5-N7	-3.98	1.31	1.38
3	F	1398	CX9	C5-N7	-3.90	1.31	1.38
3	E	1398	CX9	CAD-NAZ	3.78	1.53	1.47
3	C	1399	CX9	C2-N1	3.68	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1398	CX9	C5-N7	-3.66	1.31	1.38
3	D	1399	CX9	C2-N1	3.65	1.45	1.38
3	D	1398	CX9	CAC-N3	3.63	1.53	1.47
3	C	1398	CX9	CAC-N3	3.59	1.53	1.47
3	B	1399	CX9	C6-N1	3.44	1.46	1.40
3	D	1398	CX9	CAD-NAZ	3.38	1.53	1.47
3	F	1398	CX9	CAC-N3	3.37	1.52	1.47
3	D	1399	CX9	C5-N7	-3.27	1.32	1.38
3	A	1399	CX9	C6-N1	3.17	1.45	1.40
3	C	1399	CX9	CAV-CAP	-3.14	1.37	1.45
3	E	1399	CX9	CAR-N10	3.09	1.44	1.38
3	A	1399	CX9	CAC-N3	3.08	1.52	1.47
3	F	1399	CX9	CAT-NAZ	3.03	1.43	1.37
3	A	1399	CX9	CAV-CAP	-3.03	1.38	1.45
3	B	1398	CX9	CAC-N3	3.01	1.52	1.47
3	E	1399	CX9	CAV-CAP	-3.00	1.38	1.45
3	F	1399	CX9	CAR-N10	2.99	1.44	1.38
3	E	1398	CX9	C2-N3	2.99	1.44	1.39
3	F	1399	CX9	C2-N1	2.90	1.43	1.38
3	E	1399	CX9	C6-N1	2.89	1.45	1.40
3	B	1398	CX9	CAD-NAZ	2.85	1.52	1.47
3	A	1398	CX9	C4-N9	-2.83	1.30	1.36
3	A	1398	CX9	CAD-NAZ	2.82	1.52	1.47
3	D	1398	CX9	CAR-NAZ	-2.77	1.33	1.39
3	D	1399	CX9	CAT-NAZ	2.76	1.43	1.37
3	C	1399	CX9	CAV-NAX	-2.76	1.33	1.39
3	A	1399	CX9	C2-N1	2.75	1.43	1.38
3	E	1398	CX9	C4-N9	-2.74	1.30	1.36
3	C	1399	CX9	C6-N1	2.72	1.45	1.40
3	E	1399	CX9	CAD-NAZ	2.69	1.51	1.47
3	C	1398	CX9	CAV-NAX	-2.65	1.33	1.39
3	B	1399	CX9	C2-N1	2.64	1.43	1.38
3	C	1398	CX9	C2-N3	2.64	1.44	1.39
3	D	1398	CX9	C5-N7	-2.62	1.33	1.38
3	D	1398	CX9	CAV-NAX	-2.60	1.33	1.39
3	A	1398	CX9	CAV-CAP	-2.57	1.39	1.45
3	C	1398	CX9	CAV-CAP	-2.57	1.39	1.45
3	E	1398	CX9	CAR-N10	2.57	1.43	1.38
3	E	1398	CX9	CAV-CAP	-2.55	1.39	1.45
3	F	1399	CX9	CAV-NAX	-2.55	1.34	1.39
3	B	1399	CX9	CAT-NAZ	2.51	1.42	1.37
3	E	1399	CX9	CAC-N3	2.50	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1398	CX9	CAT-NAZ	2.47	1.42	1.37
3	C	1399	CX9	CAR-N10	2.47	1.43	1.38
3	F	1399	CX9	CAR-NAZ	2.46	1.43	1.39
3	B	1399	CX9	CAK-N1	2.40	1.52	1.47
3	B	1399	CX9	CAR-NAZ	2.40	1.43	1.39
3	C	1398	CX9	CAV-CAT	2.38	1.42	1.38
3	A	1398	CX9	OAF-CAP	2.35	1.27	1.23
3	D	1398	CX9	CAV-CAP	-2.34	1.39	1.45
3	B	1398	CX9	CAV-NAX	-2.33	1.34	1.39
3	B	1398	CX9	C5-N7	-2.31	1.34	1.38
3	A	1399	CX9	CAV-NAX	-2.30	1.34	1.39
3	B	1398	CX9	CAA-N7	2.29	1.51	1.46
3	A	1399	CX9	C5-N7	-2.29	1.34	1.38
3	E	1398	CX9	C5-C6	-2.28	1.37	1.43
3	F	1399	CX9	CAC-N3	2.26	1.51	1.47
3	A	1398	CX9	CAT-NAZ	2.25	1.42	1.37
3	F	1399	CX9	CAK-N1	2.23	1.52	1.47
3	A	1399	CX9	CAR-N10	2.22	1.42	1.38
3	B	1398	CX9	C4-N9	-2.22	1.31	1.36
3	E	1399	CX9	CAV-NAX	-2.20	1.34	1.39
3	F	1399	CX9	C4-N3	2.19	1.41	1.38
3	A	1399	CX9	CAT-NAZ	2.18	1.42	1.37
3	C	1399	CX9	CAA-N7	2.16	1.51	1.46
3	B	1398	CX9	C4-N3	-2.16	1.34	1.38
3	A	1398	CX9	CAV-NAX	-2.15	1.34	1.39
3	C	1398	CX9	CAT-NAN	-2.14	1.32	1.36
3	B	1399	CX9	CAA-N7	2.14	1.50	1.46
3	A	1399	CX9	C4-N3	2.14	1.41	1.38
3	D	1398	CX9	C8-N9	2.13	1.38	1.32
3	F	1399	CX9	CAV-CAP	-2.12	1.40	1.45
3	A	1398	CX9	C4-N3	-2.12	1.34	1.38
3	D	1399	CX9	CA0-N10	2.11	1.52	1.47
3	F	1399	CX9	C6-N1	2.11	1.44	1.40
3	A	1399	CX9	CAD-NAZ	2.06	1.50	1.47
3	B	1398	CX9	C8-N9	2.06	1.38	1.32
3	D	1399	CX9	C6-N1	2.02	1.43	1.40
3	D	1399	CX9	CAC-N3	2.02	1.50	1.47
3	D	1399	CX9	CAR-NAZ	2.01	1.43	1.39
3	C	1399	CX9	CAC-N3	2.00	1.50	1.47

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1398	CX9	CAP-N10-CAR	-6.64	117.45	125.62
3	B	1399	CX9	C6-N1-C2	-6.41	117.73	125.62
3	D	1399	CX9	CAP-N10-CAR	-6.10	118.11	125.62
3	A	1398	CX9	N1-C2-N3	5.83	123.91	116.72
3	F	1398	CX9	CAC-N3-C2	5.80	127.44	117.33
3	B	1399	CX9	CAP-N10-CAR	-5.68	118.63	125.62
3	C	1398	CX9	OAH-CAR-N10	-5.62	114.41	121.98
3	E	1399	CX9	C6-N1-C2	-5.60	118.73	125.62
3	F	1399	CX9	C6-N1-C2	-5.35	119.04	125.62
3	F	1399	CX9	CAP-N10-CAR	-5.35	119.04	125.62
3	A	1398	CX9	C6-N1-C2	-5.32	119.08	125.62
3	A	1399	CX9	C6-N1-C2	-5.25	119.16	125.62
3	B	1398	CX9	N1-C2-N3	5.23	123.17	116.72
3	E	1399	CX9	CAK-N1-C6	5.06	124.34	117.18
3	E	1398	CX9	NAN-CAJ-NAX	-4.95	107.23	112.98
3	D	1398	CX9	N10-CAR-NAZ	4.91	122.78	116.72
3	C	1399	CX9	C6-N1-C2	-4.86	119.64	125.62
3	B	1399	CX9	CAK-N1-C6	4.77	123.93	117.18
3	E	1399	CX9	CAP-N10-CAR	-4.74	119.79	125.62
3	B	1398	CX9	C6-N1-C2	-4.73	119.80	125.62
3	D	1399	CX9	C6-N1-C2	-4.69	119.84	125.62
3	C	1398	CX9	C6-N1-C2	-4.58	119.98	125.62
3	C	1399	CX9	CAA-N7-C8	-4.52	117.83	126.28
3	B	1399	CX9	C5-C6-N1	4.49	120.68	112.23
3	B	1399	CX9	NAN-CAJ-NAX	-4.47	107.80	112.98
3	E	1399	CX9	NAN-CAJ-NAX	-4.41	107.86	112.98
3	B	1398	CX9	CAP-N10-CAR	-4.38	120.23	125.62
3	A	1398	CX9	NAN-CAJ-NAX	-4.35	107.93	112.98
3	B	1399	CX9	OAH-CAR-N10	-4.35	116.13	121.98
3	A	1398	CX9	CAC-N3-C2	4.29	124.81	117.33
3	B	1399	CX9	O6-C6-C5	-4.29	117.59	126.38
3	D	1398	CX9	OAH-CAR-NAZ	-4.24	115.47	121.33
3	B	1398	CX9	CAC-N3-C2	4.22	124.69	117.33
3	F	1398	CX9	CAP-N10-CAR	-4.18	120.47	125.62
3	C	1399	CX9	CAP-N10-CAR	-4.18	120.48	125.62
3	C	1398	CX9	N10-CAR-NAZ	4.15	121.84	116.72
3	F	1398	CX9	NAN-CAJ-NAX	-4.13	108.19	112.98
3	A	1399	CX9	CAP-N10-CAR	-4.13	120.54	125.62
3	B	1399	CX9	CA0-N10-CAP	4.09	122.97	117.18
3	C	1398	CX9	N1-C2-N3	4.08	121.75	116.72
3	E	1398	CX9	N1-C2-N3	4.08	121.75	116.72
3	F	1399	CX9	C5-C6-N1	4.06	119.88	112.23
3	D	1399	CX9	CA0-N10-CAP	4.03	122.88	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1398	CX9	N1-C2-N3	4.00	121.65	116.72
3	D	1398	CX9	NAN-CAJ-NAX	-3.98	108.37	112.98
3	E	1398	CX9	CAC-N3-C2	3.96	124.23	117.33
3	C	1399	CX9	C5-C6-N1	3.95	119.66	112.23
3	B	1399	CX9	NAN-CAT-NAZ	3.95	133.54	127.81
3	A	1399	CX9	CAK-N1-C6	3.93	122.74	117.18
3	D	1398	CX9	CAJ-NAX-CAV	3.84	109.58	104.38
3	E	1399	CX9	C5-C6-N1	3.83	119.44	112.23
3	A	1398	CX9	CAJ-NAX-CAV	3.81	109.53	104.38
3	F	1398	CX9	CAC-N3-C4	-3.80	115.14	120.75
3	E	1398	CX9	C6-N1-C2	-3.80	120.94	125.62
3	F	1399	CX9	NAN-CAJ-NAX	-3.80	108.58	112.98
3	D	1399	CX9	NAN-CAT-NAZ	3.76	133.27	127.81
3	C	1398	CX9	NAN-CAJ-NAX	-3.72	108.67	112.98
3	C	1398	CX9	CAP-N10-CAR	-3.67	121.10	125.62
3	E	1398	CX9	O6-C6-C5	-3.67	118.86	126.38
3	E	1399	CX9	CAA-N7-C8	-3.66	119.43	126.28
3	B	1399	CX9	CAJ-NAX-CAV	3.66	109.33	104.38
3	D	1398	CX9	C6-N1-C2	-3.65	121.12	125.62
3	A	1399	CX9	N1-C2-N3	3.62	121.18	116.72
3	A	1399	CX9	C5-C6-N1	3.61	119.02	112.23
3	A	1398	CX9	NAN-CAT-NAZ	3.58	133.00	127.81
3	C	1399	CX9	CAK-N1-C6	3.56	122.22	117.18
3	F	1399	CX9	NAN-CAT-NAZ	3.53	132.94	127.81
3	E	1399	CX9	N1-C2-N3	3.53	121.07	116.72
3	C	1398	CX9	OAF-CAP-N10	-3.52	114.28	119.99
3	E	1399	CX9	OAH-CAR-NAZ	-3.51	116.48	121.33
3	F	1398	CX9	O2-C2-N1	-3.50	117.27	121.98
3	D	1399	CX9	N10-CAR-NAZ	3.49	121.03	116.72
3	D	1398	CX9	CAP-N10-CAR	-3.49	121.32	125.62
3	F	1399	CX9	CAJ-NAX-CAV	3.49	109.10	104.38
3	D	1399	CX9	C5-C6-N1	3.49	118.80	112.23
3	E	1398	CX9	N10-CAR-NAZ	3.48	121.01	116.72
3	C	1399	CX9	C6-C5-C4	-3.46	118.56	122.92
3	B	1398	CX9	CA0-CAL-CAK	-3.45	101.21	112.91
3	E	1398	CX9	CA0-N10-CAR	3.45	122.73	117.64
3	D	1398	CX9	N7-C8-N9	-3.40	107.32	113.48
3	E	1399	CX9	CAJ-NAX-CAV	3.39	108.97	104.38
3	A	1399	CX9	NAN-CAT-NAZ	3.38	132.72	127.81
3	F	1398	CX9	CAJ-NAX-CAV	3.36	108.92	104.38
3	D	1399	CX9	NAN-CAJ-NAX	-3.33	109.12	112.98
3	D	1398	CX9	N1-C2-N3	3.31	120.80	116.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1399	CX9	O2-C2-N3	-3.31	116.76	121.33
3	B	1398	CX9	O2-C2-N1	-3.30	117.53	121.98
3	E	1398	CX9	C2-N3-C4	-3.28	115.36	119.58
3	C	1398	CX9	CAC-N3-C2	3.28	123.04	117.33
3	F	1398	CX9	C8-N7-C5	3.25	111.69	105.59
3	F	1399	CX9	CAK-N1-C6	3.24	121.77	117.18
3	D	1398	CX9	CA0-CAL-CAK	-3.23	101.98	112.91
3	B	1398	CX9	NAN-CAJ-NAX	-3.20	109.27	112.98
3	A	1398	CX9	N10-CAR-NAZ	3.20	120.67	116.72
3	F	1399	CX9	N10-CAR-NAZ	3.19	120.66	116.72
3	B	1399	CX9	N7-C8-N9	-3.19	107.69	113.48
3	A	1398	CX9	CA0-CAL-CAK	-3.19	102.10	112.91
3	F	1398	CX9	OAH-CAR-NAZ	-3.17	116.94	121.33
3	B	1399	CX9	CAA-N7-C8	-3.15	120.39	126.28
3	E	1398	CX9	O2-C2-N1	-3.14	117.75	121.98
3	E	1399	CX9	N10-CAR-NAZ	3.14	120.59	116.72
3	F	1399	CX9	N1-C2-N3	3.13	120.58	116.72
3	D	1398	CX9	NAN-CAT-NAZ	3.12	132.34	127.81
3	C	1398	CX9	CAJ-NAX-CAV	3.09	108.56	104.38
3	C	1398	CX9	NAN-CAT-NAZ	3.08	132.28	127.81
3	B	1399	CX9	N10-CAR-NAZ	3.08	120.52	116.72
3	A	1398	CX9	CAK-N1-C2	3.06	122.16	117.64
3	C	1399	CX9	O6-C6-C5	-3.06	120.12	126.38
3	A	1398	CX9	O2-C2-N3	-3.05	117.12	121.33
3	A	1399	CX9	O6-C6-C5	-3.03	120.17	126.38
3	D	1398	CX9	CAA-N7-C5	-3.03	120.56	127.77
3	E	1399	CX9	C6-C5-C4	-3.02	119.11	122.92
3	C	1399	CX9	N7-C8-N9	-3.00	108.04	113.48
3	F	1399	CX9	O6-C6-C5	-2.99	120.26	126.38
3	F	1398	CX9	NAN-CAT-NAZ	2.98	132.14	127.81
3	A	1399	CX9	N7-C8-N9	-2.98	108.08	113.48
3	B	1399	CX9	N1-C2-N3	2.98	120.39	116.72
3	E	1399	CX9	C6-C5-N7	2.97	137.07	131.10
3	E	1398	CX9	NAN-CAT-NAZ	2.95	132.10	127.81
3	D	1399	CX9	O6-C6-C5	-2.94	120.35	126.38
3	F	1398	CX9	CAA-N7-C5	-2.94	120.77	127.77
3	A	1399	CX9	CAA-N7-C8	-2.88	120.89	126.28
3	C	1399	CX9	OAF-CAP-CAV	-2.88	117.17	124.59
3	C	1398	CX9	C5-C6-N1	2.86	117.61	112.23
3	C	1398	CX9	CAD-NAZ-CAR	2.86	122.31	117.33
3	C	1398	CX9	O2-C2-N1	-2.84	118.15	121.98
3	B	1399	CX9	C6-C5-C4	-2.83	119.35	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1399	CX9	C6-C5-N7	2.83	136.79	131.10
3	E	1399	CX9	CAL-CA0-N10	-2.83	105.66	112.36
3	D	1399	CX9	CAK-N1-C2	2.82	121.81	117.64
3	F	1398	CX9	N10-CAR-NAZ	2.81	120.19	116.72
3	F	1399	CX9	N7-C8-N9	-2.80	108.40	113.48
3	A	1398	CX9	CAP-N10-CAR	-2.79	122.18	125.62
3	F	1398	CX9	CA0-CAL-CAK	-2.79	103.46	112.91
3	D	1399	CX9	OAH-CAR-N10	-2.79	118.23	121.98
3	D	1399	CX9	N7-C8-N9	-2.78	108.44	113.48
3	E	1399	CX9	NAN-CAT-NAZ	2.78	131.85	127.81
3	E	1399	CX9	O2-C2-N3	-2.77	117.50	121.33
3	E	1398	CX9	C5-C6-N1	2.77	117.44	112.23
3	A	1398	CX9	CAD-NAZ-CAT	2.76	124.78	120.98
3	C	1398	CX9	N3-C4-N9	2.76	130.61	126.27
3	D	1399	CX9	CAJ-NAX-CAV	2.74	108.09	104.38
3	B	1398	CX9	CA0-N10-CAR	2.73	121.67	117.64
3	D	1398	CX9	C8-N7-C5	2.73	110.72	105.59
3	F	1398	CX9	N7-C8-N9	-2.73	108.54	113.48
3	A	1399	CX9	N10-CAR-NAZ	2.72	120.08	116.72
2	E	1397	GOL	C3-C2-C1	-2.70	101.89	111.80
3	F	1399	CX9	N3-C4-N9	2.69	130.50	126.27
3	B	1398	CX9	C5-C6-N1	2.69	117.29	112.23
3	F	1398	CX9	C6-N1-C2	-2.68	122.32	125.62
3	D	1399	CX9	OAF-CAP-CAV	-2.66	117.72	124.59
3	E	1398	CX9	N3-C4-N9	2.65	130.44	126.27
3	A	1399	CX9	NAN-CAJ-NAX	-2.64	109.91	112.98
3	E	1399	CX9	O6-C6-C5	-2.63	121.00	126.38
3	D	1399	CX9	N3-C4-N9	2.62	130.40	126.27
3	C	1399	CX9	CAD-NAZ-CAR	2.62	121.90	117.33
3	E	1399	CX9	OAF-CAP-CAV	-2.59	117.91	124.59
3	A	1399	CX9	C8-N7-C5	2.59	110.46	105.59
3	F	1399	CX9	CA0-N10-CAP	2.59	120.85	117.18
3	F	1399	CX9	C8-N7-C5	2.59	110.45	105.59
3	B	1398	CX9	CAJ-NAX-CAV	2.57	107.86	104.38
3	C	1398	CX9	N7-C8-N9	-2.57	108.81	113.48
3	B	1398	CX9	OAF-CAP-N10	-2.57	115.81	119.99
3	B	1398	CX9	CAD-NAZ-CAT	-2.57	117.45	120.98
3	A	1398	CX9	C2-N3-C4	-2.56	116.28	119.58
3	E	1398	CX9	N7-C8-N9	-2.56	108.84	113.48
3	E	1398	CX9	CA0-CAL-CAK	-2.56	104.25	112.91
3	B	1399	CX9	C8-N9-C4	2.55	109.09	102.98
3	C	1399	CX9	OAF-CAP-N10	2.53	124.10	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1399	CX9	CA0-CAL-CAK	2.51	121.40	112.91
3	B	1399	CX9	CAC-N3-C2	2.50	121.68	117.33
3	C	1399	CX9	NAN-CAT-NAZ	2.49	131.43	127.81
3	A	1398	CX9	C5-C6-N1	2.49	116.92	112.23
3	F	1398	CX9	CAL-CAK-N1	2.49	118.25	112.36
3	E	1399	CX9	C8-N7-C5	2.48	110.26	105.59
3	C	1398	CX9	CAL-CAK-N1	2.48	118.23	112.36
3	F	1399	CX9	CAC-N3-C2	2.48	121.65	117.33
3	D	1398	CX9	CA0-N10-CAP	2.47	120.68	117.18
3	C	1399	CX9	C8-N9-C4	2.47	108.91	102.98
3	C	1398	CX9	C8-N7-C5	2.46	110.21	105.59
3	D	1398	CX9	CAK-N1-C2	2.46	121.27	117.64
3	E	1398	CX9	CAJ-NAX-CAV	2.45	107.70	104.38
3	B	1399	CX9	CAV-CAP-N10	2.44	121.57	115.48
3	F	1399	CX9	CAA-N7-C8	-2.43	121.75	126.28
3	D	1398	CX9	N3-C4-N9	2.42	130.07	126.27
3	E	1398	CX9	OAF-CAP-CAV	-2.41	118.37	124.59
3	B	1399	CX9	C8-N7-C5	2.41	110.13	105.59
3	B	1398	CX9	C2-N3-C4	-2.41	116.47	119.58
3	D	1399	CX9	N1-C2-N3	2.39	119.66	116.72
3	E	1399	CX9	OAF-CAP-N10	2.39	123.87	119.99
3	D	1399	CX9	CAC-N3-C2	2.38	121.47	117.33
3	A	1399	CX9	C8-N9-C4	2.37	108.66	102.98
3	A	1399	CX9	OAF-CAP-CAV	-2.35	118.52	124.59
3	C	1399	CX9	C8-N7-C5	2.35	110.01	105.59
3	A	1399	CX9	C6-C5-C4	-2.35	119.96	122.92
3	D	1399	CX9	CAV-CAP-N10	2.34	121.32	115.48
3	B	1399	CX9	N3-C4-N9	2.34	129.94	126.27
3	E	1398	CX9	CAV-CAP-N10	2.33	121.28	115.48
3	A	1399	CX9	N3-C4-N9	2.32	129.91	126.27
3	E	1399	CX9	N7-C8-N9	-2.31	109.30	113.48
3	D	1398	CX9	CAC-N3-C2	2.31	121.36	117.33
2	C	1397	GOL	O2-C2-C1	2.30	118.72	109.18
3	A	1398	CX9	O2-C2-N1	-2.30	118.88	121.98
3	C	1399	CX9	CAL-CA0-N10	-2.29	106.95	112.36
3	C	1398	CX9	CA0-N10-CAR	2.28	121.01	117.64
3	E	1398	CX9	O6-C6-N1	2.27	123.68	119.99
3	A	1398	CX9	O6-C6-C5	-2.27	121.73	126.38
3	A	1399	CX9	CAD-NAZ-CAR	2.27	121.29	117.33
3	A	1398	CX9	CA0-N10-CAP	2.27	120.39	117.18
3	A	1399	CX9	O2-C2-N3	-2.26	118.22	121.33
3	C	1399	CX9	N10-CAR-NAZ	2.25	119.50	116.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1399	CX9	C6-C5-N7	2.25	135.62	131.10
3	D	1399	CX9	C8-N7-C5	2.25	109.82	105.59
3	F	1398	CX9	CA0-N10-CAR	2.25	120.95	117.64
3	D	1399	CX9	CAD-NAZ-CAR	2.24	121.24	117.33
3	E	1398	CX9	OAH-CAR-NAZ	-2.24	118.24	121.33
3	C	1398	CX9	CAK-N1-C2	2.23	120.94	117.64
3	C	1398	CX9	CAA-N7-C5	-2.23	122.46	127.77
3	B	1398	CX9	N10-CAR-NAZ	2.21	119.44	116.72
3	F	1399	CX9	OAF-CAP-CAV	-2.20	118.92	124.59
3	B	1398	CX9	CAK-N1-C2	2.20	120.89	117.64
3	B	1398	CX9	N7-C8-N9	-2.19	109.50	113.48
3	C	1399	CX9	CA0-N10-CAR	2.19	120.88	117.64
3	E	1398	CX9	CAK-N1-C6	2.19	120.28	117.18
3	A	1399	CX9	CAC-N3-C2	2.19	121.14	117.33
3	B	1399	CX9	CAD-NAZ-CAR	2.17	121.12	117.33
3	D	1398	CX9	C5-C6-N1	2.17	116.31	112.23
3	B	1398	CX9	NAN-CAT-NAZ	2.16	130.95	127.81
3	F	1399	CX9	C8-N9-C4	2.15	108.14	102.98
3	D	1399	CX9	O2-C2-N3	-2.15	118.37	121.33
3	B	1398	CX9	OAH-CAR-N10	-2.14	119.10	121.98
3	C	1398	CX9	CAT-CAV-NAX	-2.14	106.49	109.26
3	A	1398	CX9	N7-C8-N9	-2.13	109.62	113.48
3	B	1398	CX9	CAD-NAZ-CAR	2.13	121.04	117.33
3	E	1398	CX9	C5-C4-N9	-2.12	107.90	112.10
3	D	1398	CX9	CAT-CAV-NAX	-2.12	106.51	109.26
3	E	1399	CX9	CAD-NAZ-CAR	2.11	121.00	117.33
3	F	1399	CX9	C6-C5-C4	-2.10	120.27	122.92
3	A	1399	CX9	C5-C4-N9	-2.09	107.97	112.10
3	E	1399	CX9	CA0-N10-CAP	2.07	120.12	117.18
3	D	1398	CX9	O2-C2-N3	-2.07	118.47	121.33
3	E	1398	CX9	C8-N9-C4	2.05	107.89	102.98
3	A	1399	CX9	C6-C5-N7	2.05	135.21	131.10
3	F	1398	CX9	CAL-CA0-N10	-2.04	107.53	112.36
3	B	1399	CX9	C5-C4-N9	-2.04	108.07	112.10
3	B	1398	CX9	CAP-CAV-NAX	2.03	133.87	129.36
3	D	1399	CX9	C5-C4-N9	-2.02	108.09	112.10
3	F	1399	CX9	C6-C5-N7	2.02	135.15	131.10
3	E	1398	CX9	CAD-NAZ-CAR	2.01	120.84	117.33
3	B	1399	CX9	OAF-CAP-CAV	-2.01	119.40	124.59
3	F	1398	CX9	CAT-CAV-NAX	-2.01	106.66	109.26

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1397	GOL	C1-C2-C3-O3
2	A	1397	GOL	O2-C2-C3-O3
2	B	1397	GOL	C1-C2-C3-O3
2	C	1397	GOL	O1-C1-C2-C3
2	D	1397	GOL	C1-C2-C3-O3
2	D	1397	GOL	O2-C2-C3-O3
3	E	1399	CX9	CAL-CA0-N10-CAP
3	B	1399	CX9	CAL-CAK-N1-C6
3	E	1399	CX9	CAL-CA0-N10-CAR
3	B	1399	CX9	CAL-CAK-N1-C2
3	D	1399	CX9	CAL-CAK-N1-C6
3	F	1399	CX9	CAL-CA0-N10-CAP
3	C	1399	CX9	CAL-CA0-N10-CAP
2	C	1397	GOL	O1-C1-C2-O2
3	A	1399	CX9	CAL-CA0-N10-CAP
2	B	1397	GOL	O2-C2-C3-O3
3	A	1399	CX9	CAL-CAK-N1-C6
2	E	1397	GOL	O1-C1-C2-O2
3	D	1399	CX9	CAL-CAK-N1-C2
3	F	1399	CX9	CAL-CA0-N10-CAR
3	F	1399	CX9	CAL-CAK-N1-C6
2	E	1397	GOL	O1-C1-C2-C3
2	F	1397	GOL	C1-C2-C3-O3
3	A	1399	CX9	CAL-CAK-N1-C2
3	A	1399	CX9	CAL-CA0-N10-CAR
2	E	1397	GOL	O2-C2-C3-O3
2	F	1397	GOL	O2-C2-C3-O3
3	C	1399	CX9	CAL-CA0-N10-CAR
3	B	1399	CX9	N10-CA0-CAL-CAK
3	F	1399	CX9	CAL-CAK-N1-C2

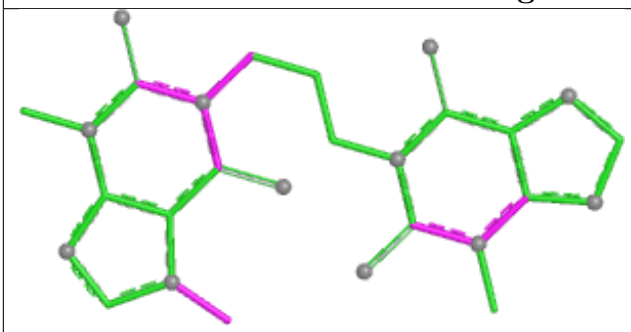
There are no ring outliers.

6 monomers are involved in 8 short contacts:

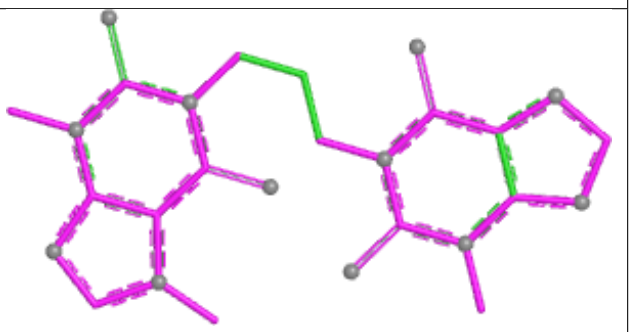
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1399	CX9	1	0
3	E	1399	CX9	1	0
3	D	1399	CX9	2	0
3	E	1398	CX9	1	0
3	A	1399	CX9	2	0
3	F	1399	CX9	1	0

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.

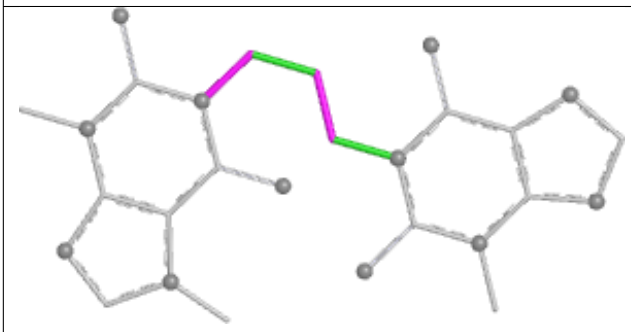
Ligand CX9 B 1399



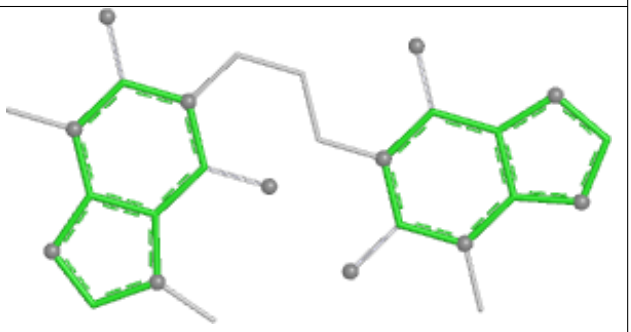
Bond lengths



Bond angles

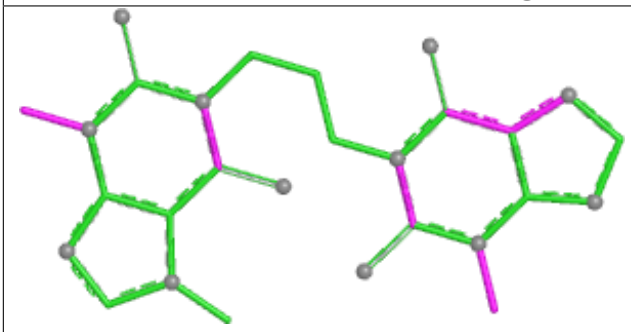


Torsions

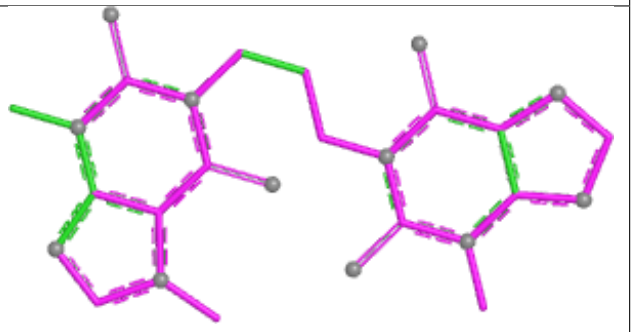


Rings

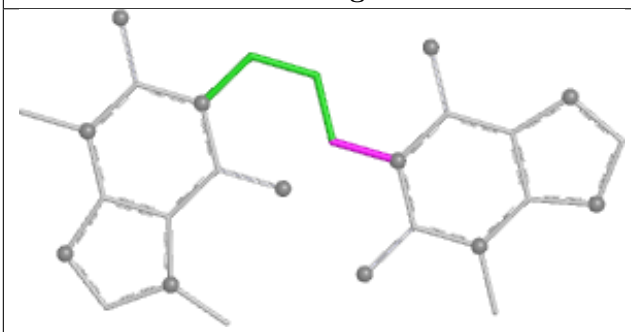
Ligand CX9 E 1399



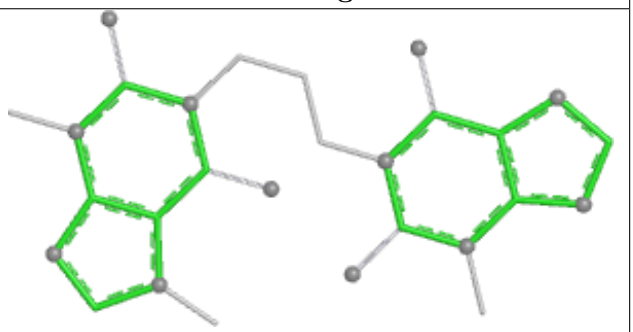
Bond lengths



Bond angles

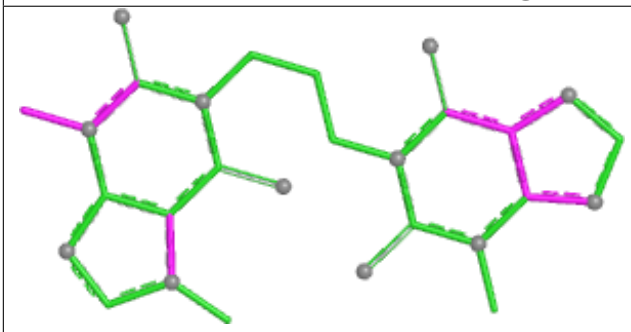


Torsions

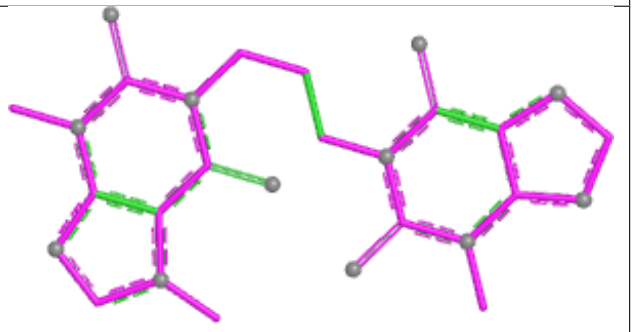


Rings

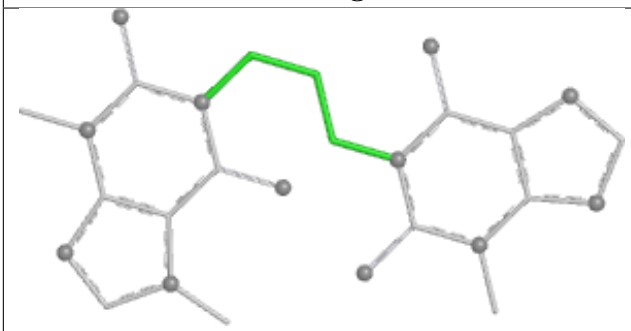
Ligand CX9 C 1398



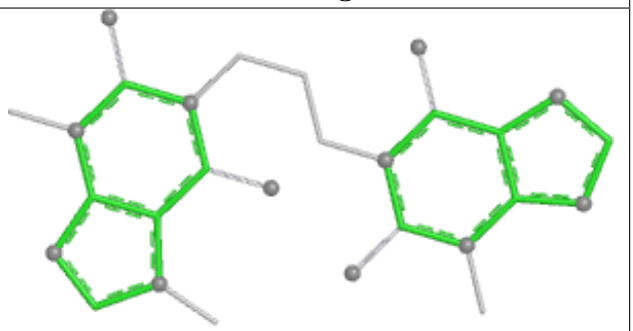
Bond lengths



Bond angles

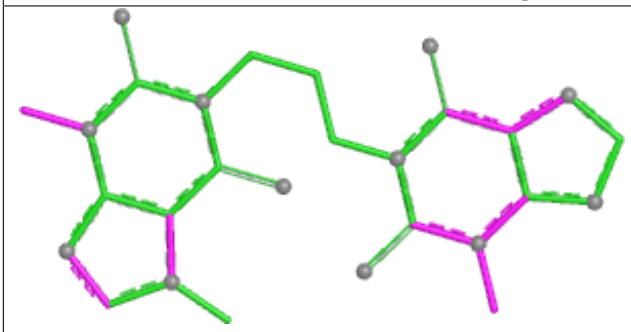


Torsions

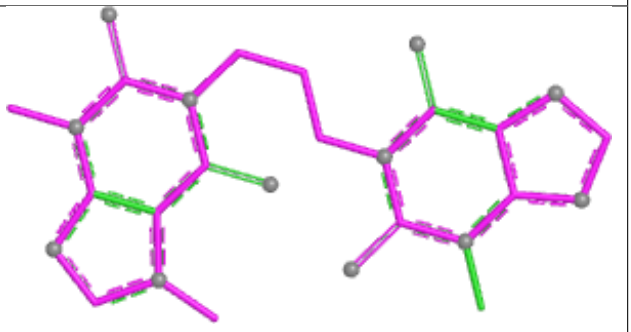


Rings

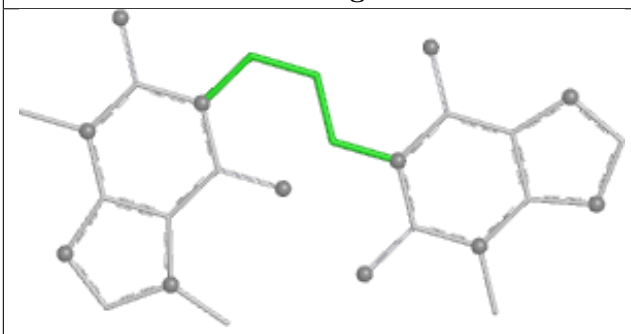
Ligand CX9 D 1398



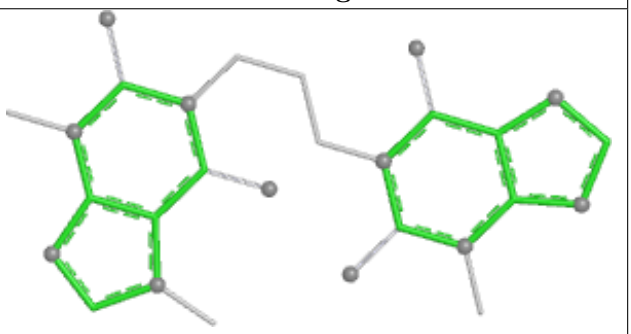
Bond lengths



Bond angles

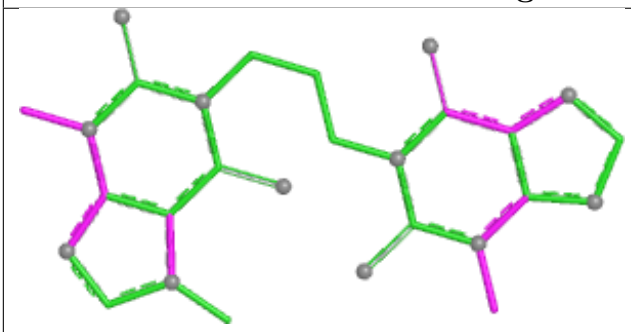


Torsions

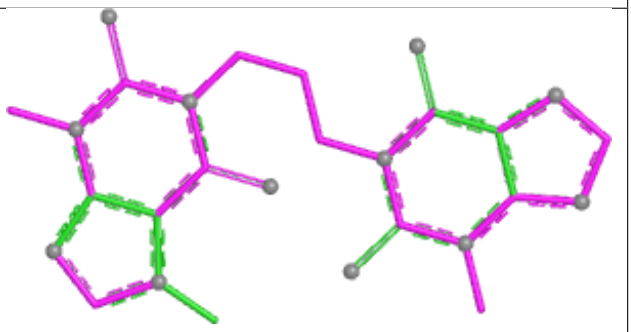


Rings

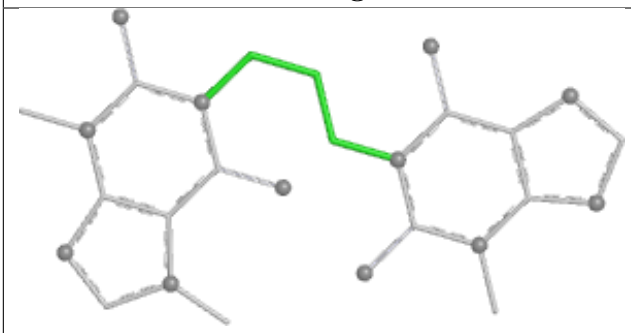
Ligand CX9 A 1398



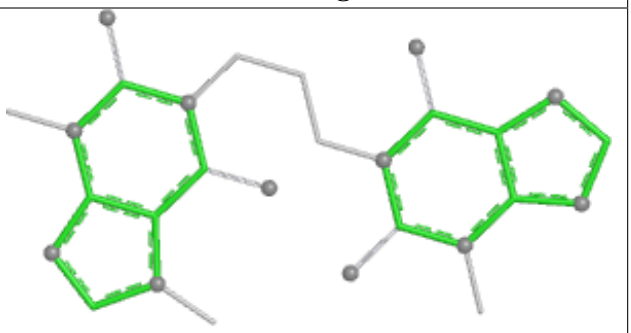
Bond lengths



Bond angles

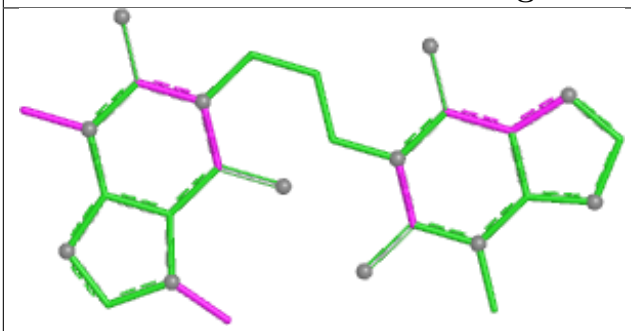


Torsions

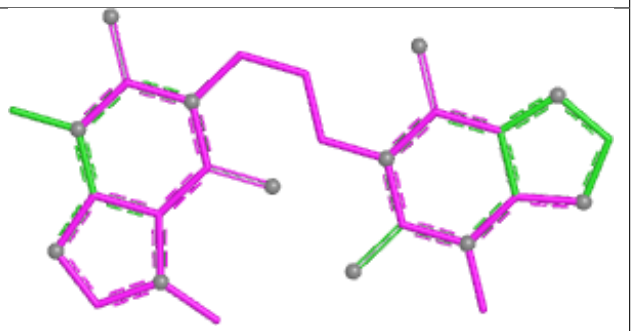


Rings

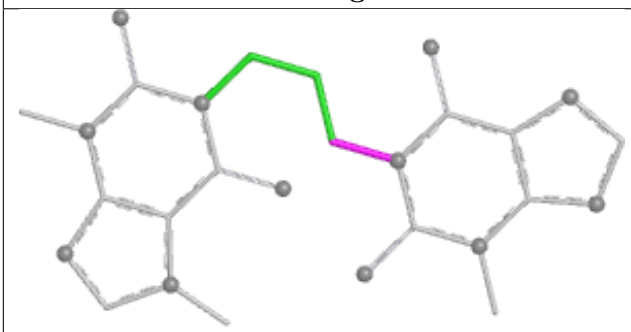
Ligand CX9 C 1399



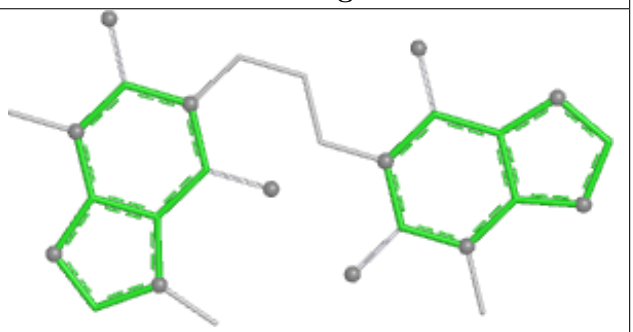
Bond lengths



Bond angles

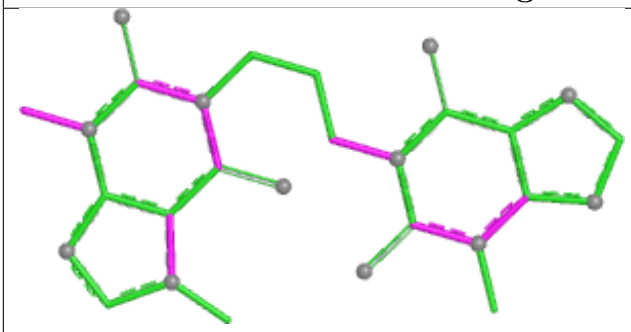


Torsions

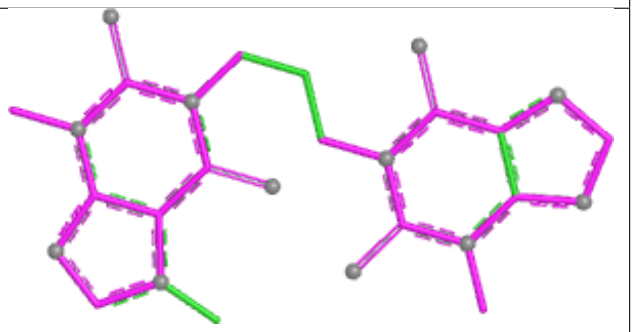


Rings

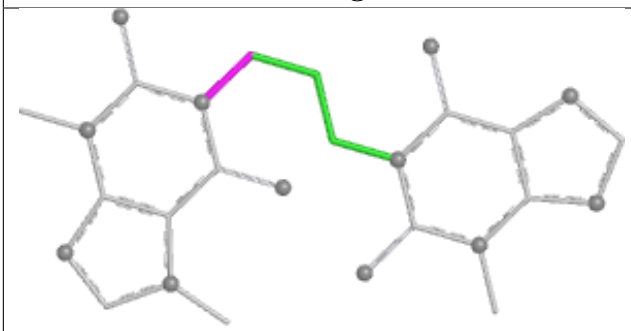
Ligand CX9 D 1399



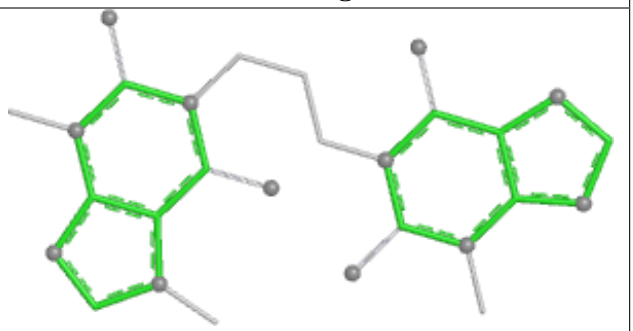
Bond lengths



Bond angles

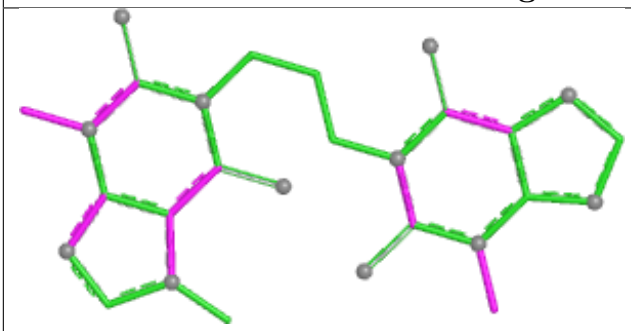


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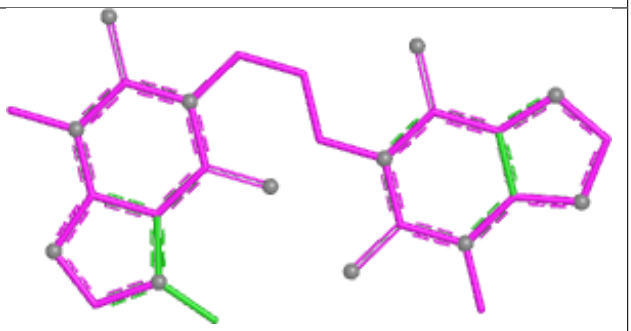


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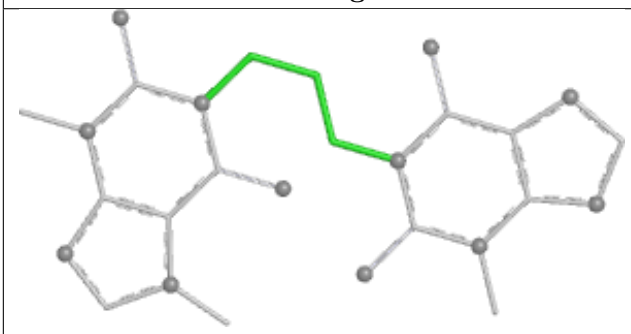
Ligand CX9 E 1398



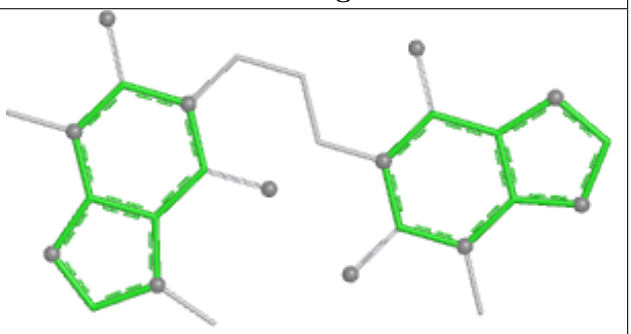
Bond lengths



Bond angles

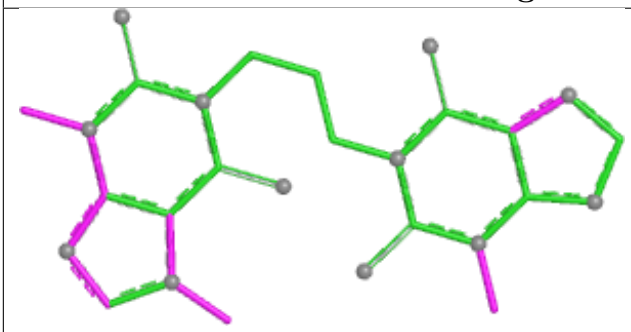


Torsions

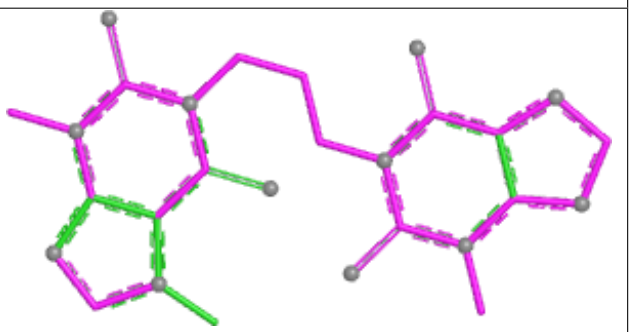


Rings

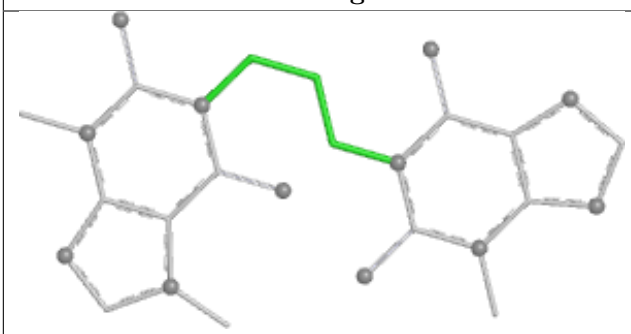
Ligand CX9 B 1398



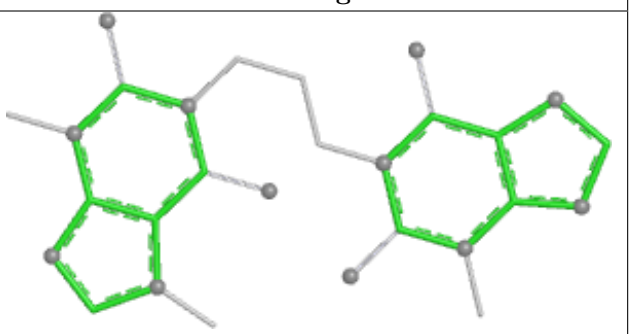
Bond lengths



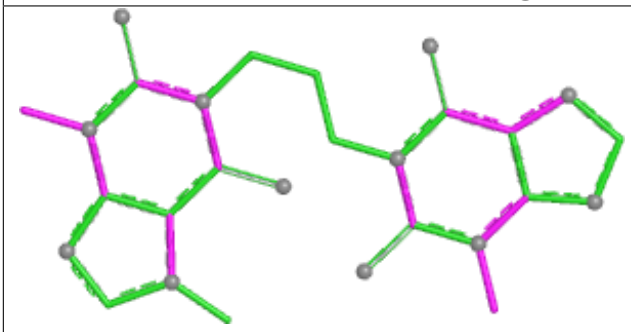
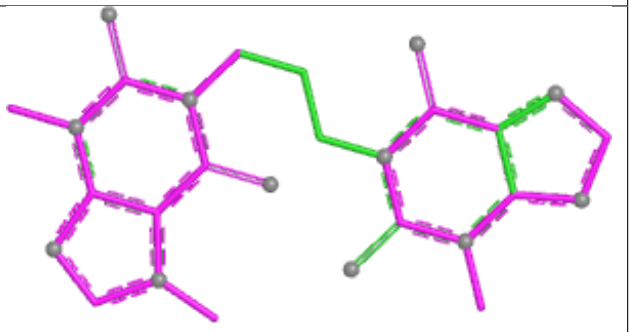
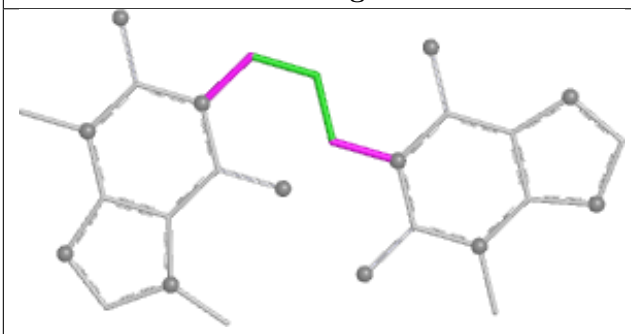
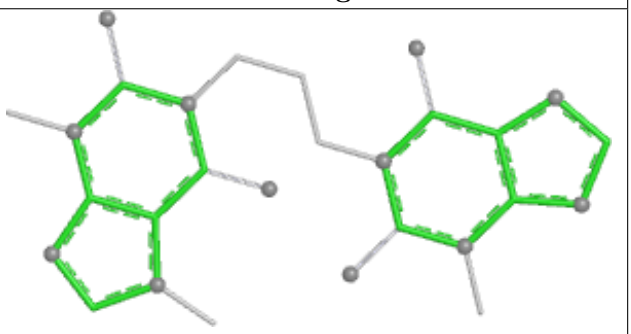
Bond angles

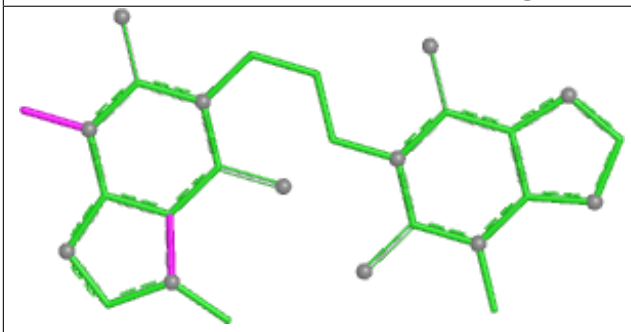
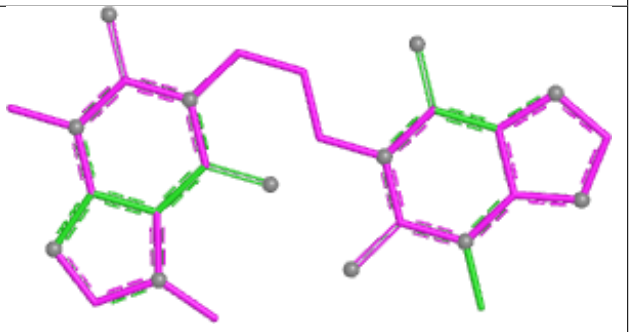
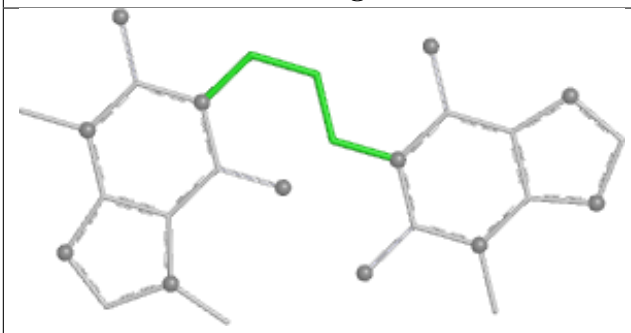
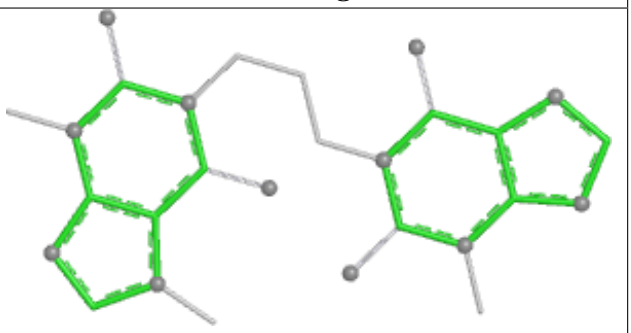


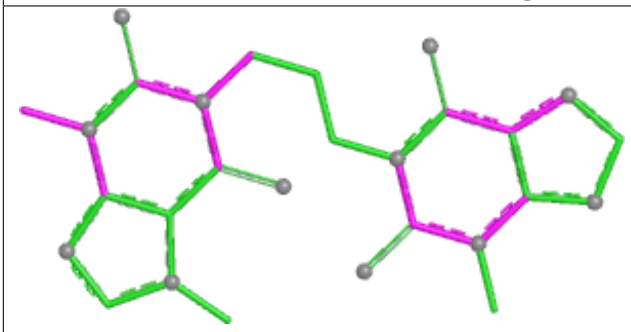
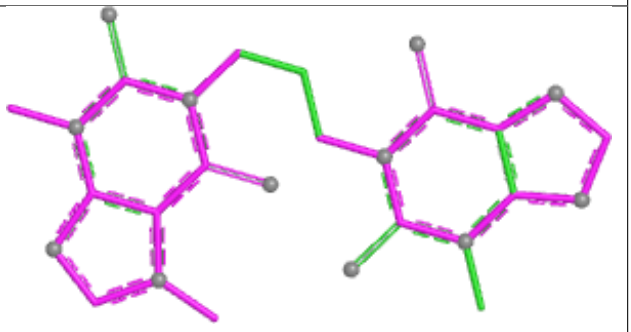
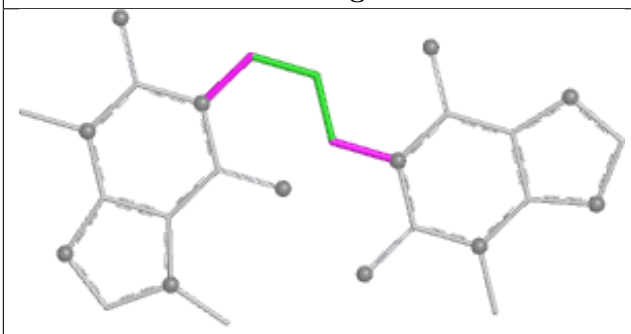
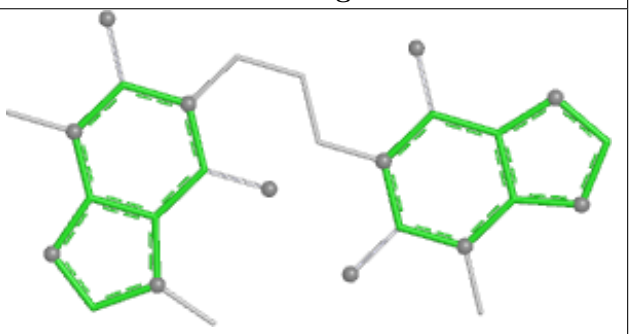
Torsions



Rings

Ligand CX9 A 1399	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CX9 F 1398	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CX9 F 1399	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	376/381 (98%)	-0.70	2 (0%)	87	88	13, 22, 42, 65	0
1	B	376/381 (98%)	-0.79	2 (0%)	87	88	12, 22, 37, 53	0
1	C	376/381 (98%)	-0.64	1 (0%)	90	90	12, 24, 44, 70	0
1	D	376/381 (98%)	-0.57	4 (1%)	78	79	13, 27, 50, 73	0
1	E	376/381 (98%)	-0.53	1 (0%)	90	90	11, 26, 48, 74	0
1	F	376/381 (98%)	-0.22	6 (1%)	70	71	16, 37, 62, 80	0
All	All	2256/2286 (98%)	-0.57	16 (0%)	84	85	11, 26, 51, 80	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	396	ALA	4.1
1	B	396	ALA	3.8
1	C	396	ALA	3.7
1	F	21	ALA	3.2
1	D	396	ALA	2.9
1	A	396	ALA	2.9
1	A	21	ALA	2.6
1	F	173	ILE	2.4
1	F	221	TYR	2.3
1	F	233	THR	2.3
1	E	396	ALA	2.3
1	D	21	ALA	2.2
1	D	392	ALA	2.2
1	D	221	TYR	2.1
1	F	168	GLN	2.0
1	B	21	ALA	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)

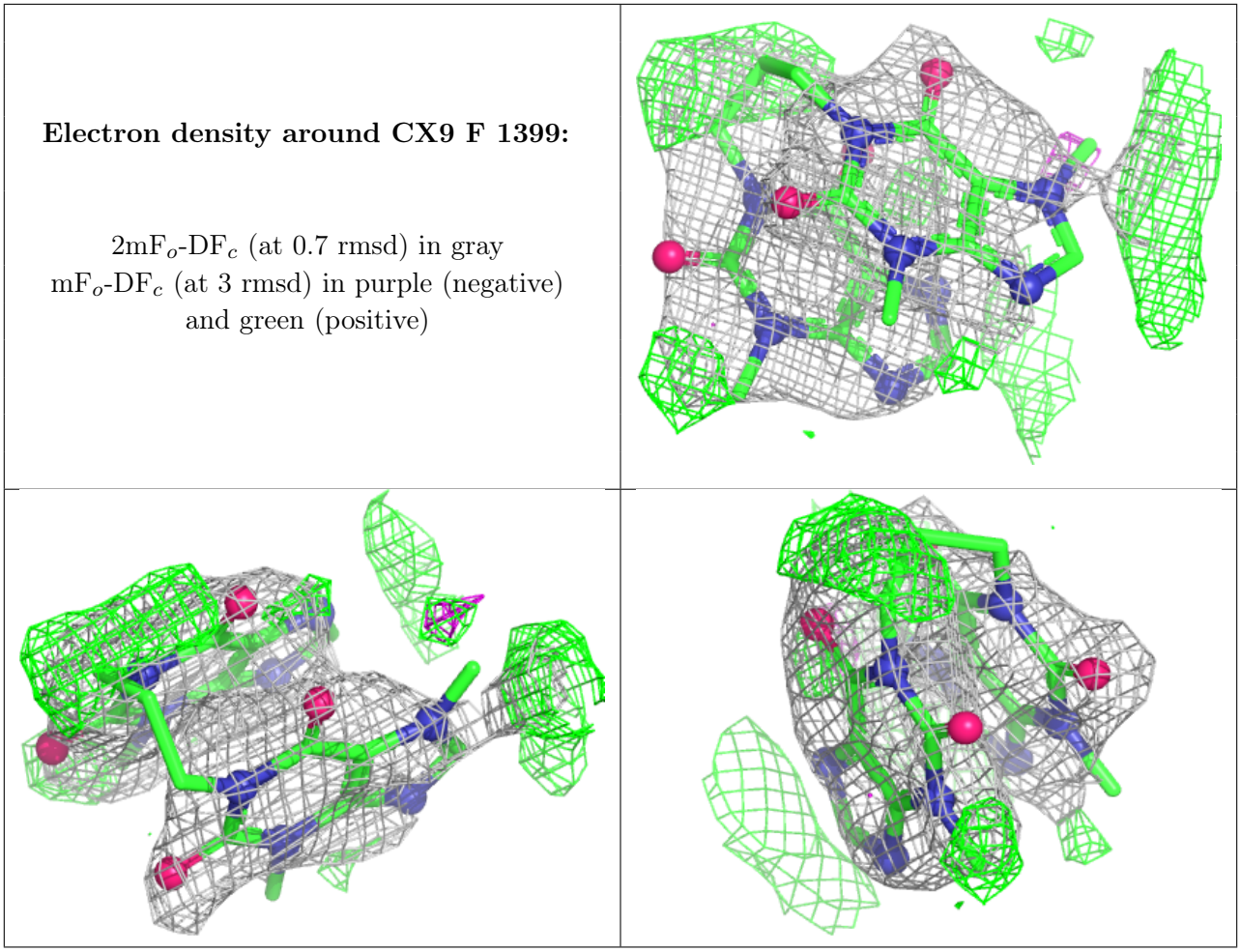
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CX9	F	1399	28/28	0.65	0.25	65,69,74,75	28
3	CX9	A	1399	28/28	0.75	0.19	50,53,57,58	28
3	CX9	B	1399	28/28	0.76	0.19	48,54,59,60	28
3	CX9	D	1399	28/28	0.77	0.19	48,50,54,56	28
3	CX9	C	1399	28/28	0.77	0.20	40,46,50,51	28
3	CX9	E	1399	28/28	0.80	0.18	40,46,50,51	28
2	GOL	E	1397	6/6	0.93	0.08	25,35,39,42	0
2	GOL	C	1397	6/6	0.94	0.09	28,38,43,52	0
2	GOL	A	1397	6/6	0.95	0.07	22,31,33,38	0
2	GOL	B	1397	6/6	0.95	0.08	28,34,38,41	0
2	GOL	F	1397	6/6	0.95	0.07	32,38,40,47	0
3	CX9	F	1398	28/28	0.96	0.05	21,28,31,32	0
3	CX9	B	1398	28/28	0.97	0.05	9,18,29,32	0
3	CX9	E	1398	28/28	0.97	0.05	14,24,35,37	0
3	CX9	A	1398	28/28	0.97	0.05	11,16,27,28	0
2	GOL	D	1397	6/6	0.97	0.06	22,31,35,41	0
3	CX9	D	1398	28/28	0.97	0.05	14,18,22,23	0
3	CX9	C	1398	28/28	0.98	0.04	13,21,33,34	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.

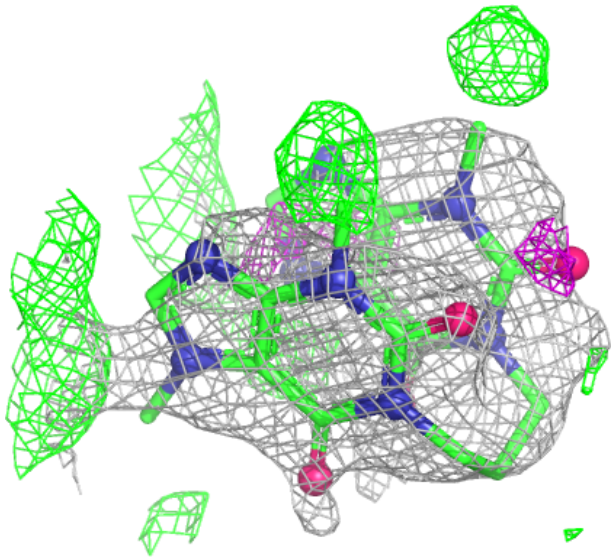
Electron density around CX9 F 1399:

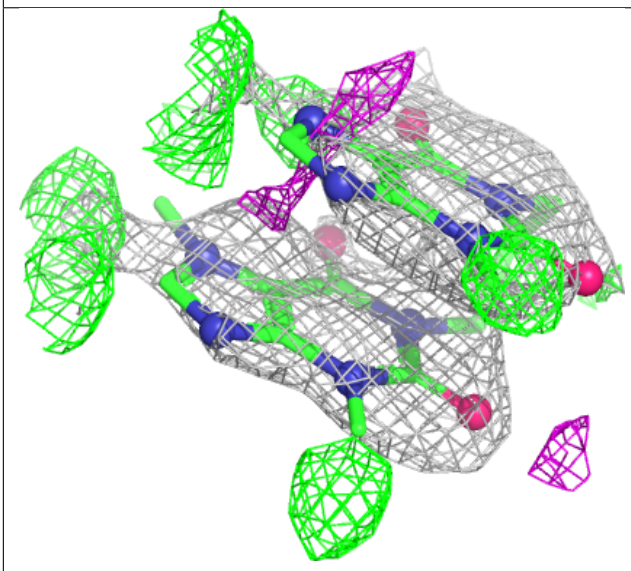
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

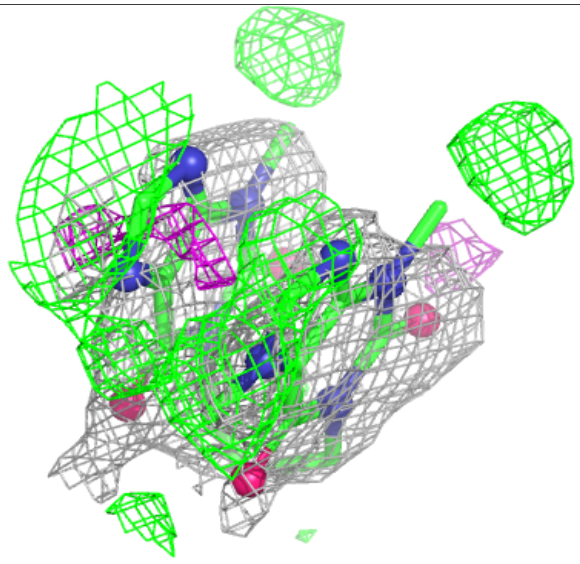


Electron density around CX9 A 1399:

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

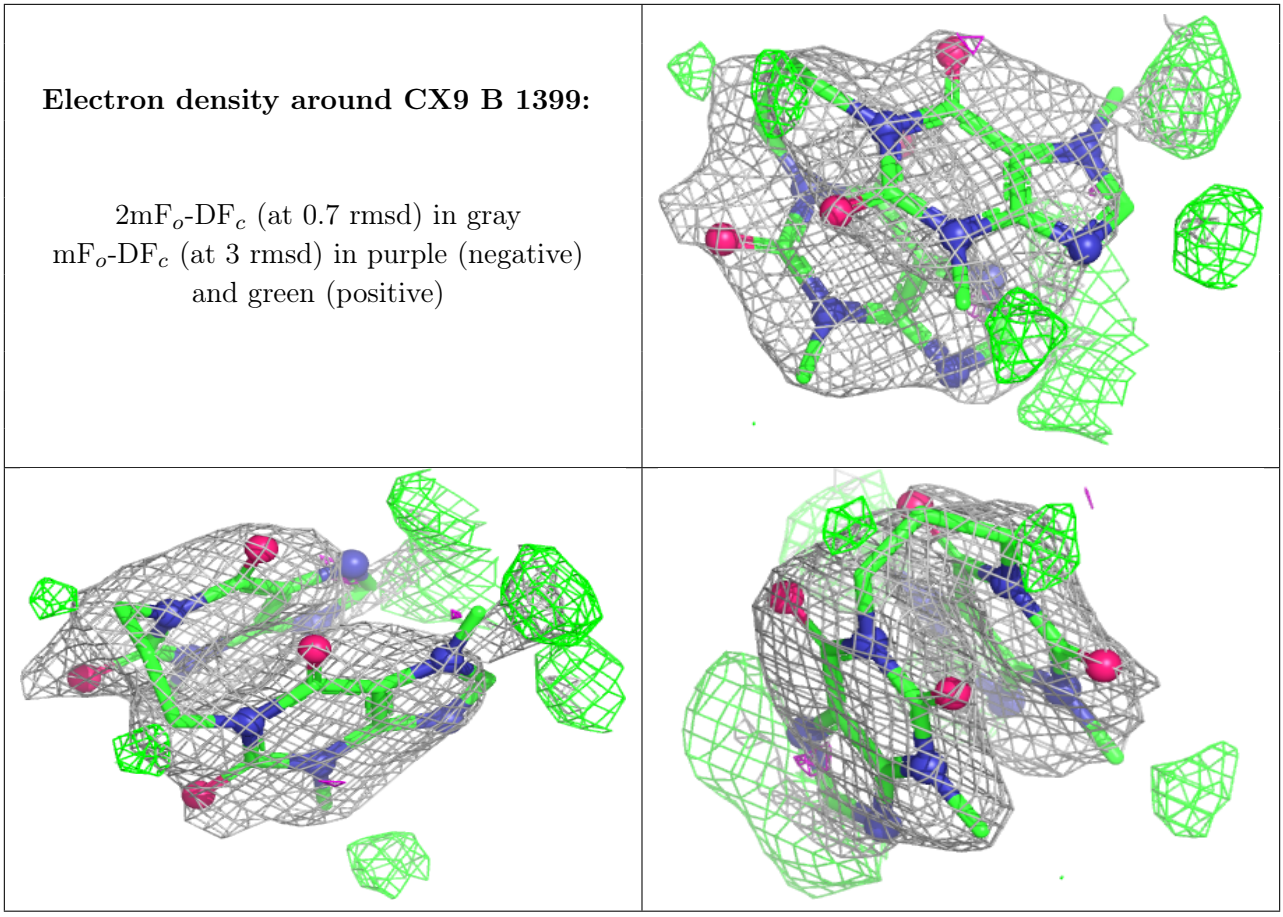






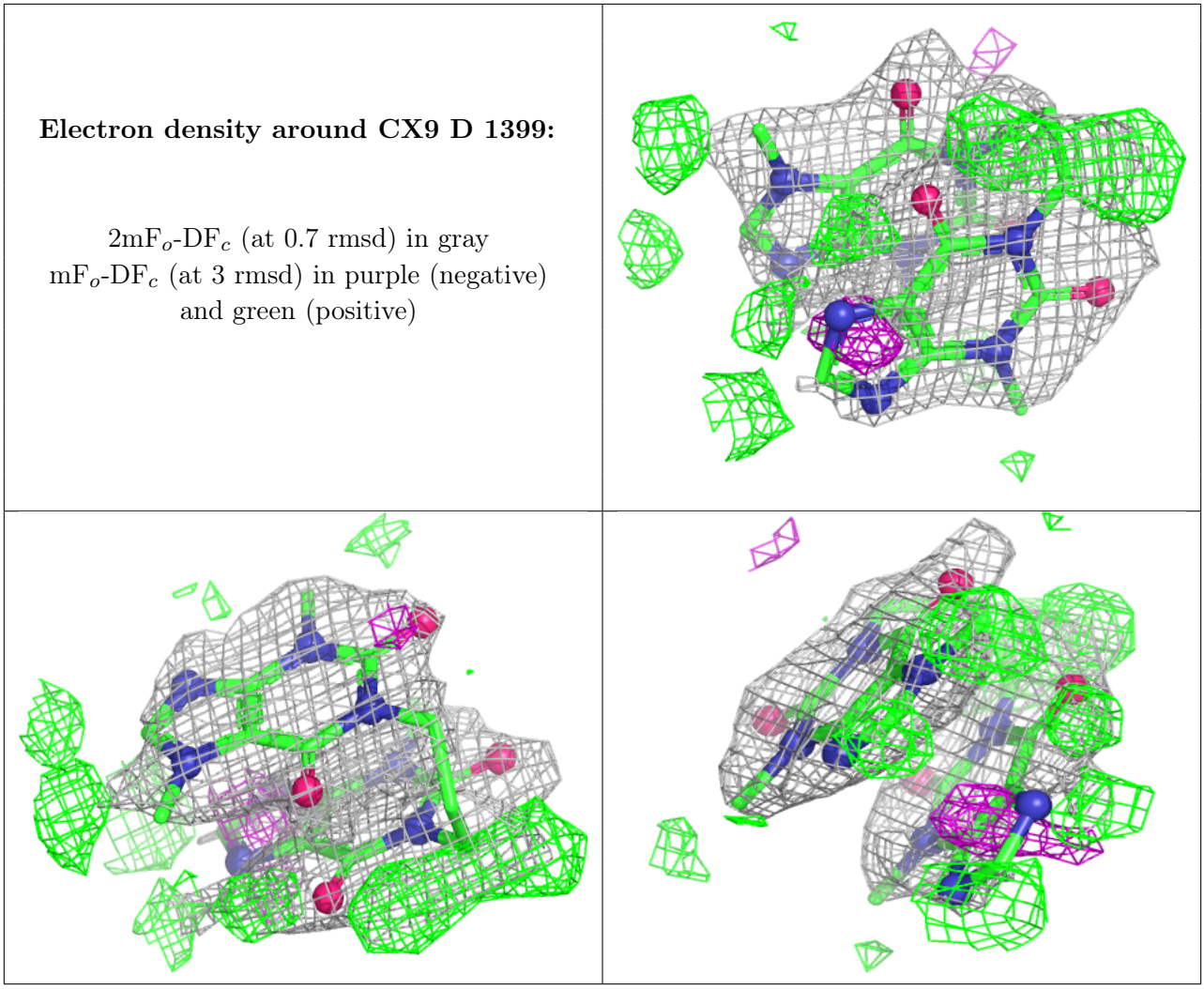
Electron density around CX9 B 1399:

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



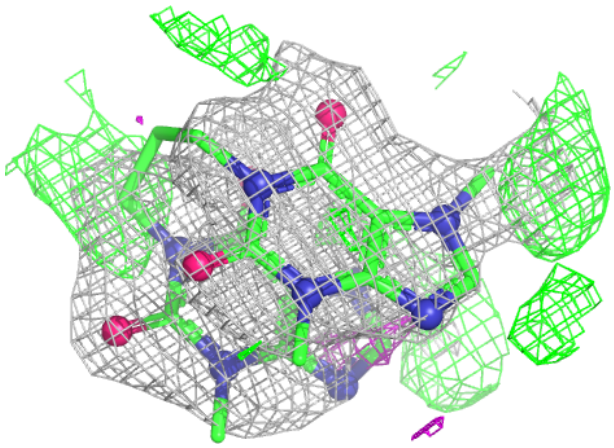
Electron density around CX9 D 1399:

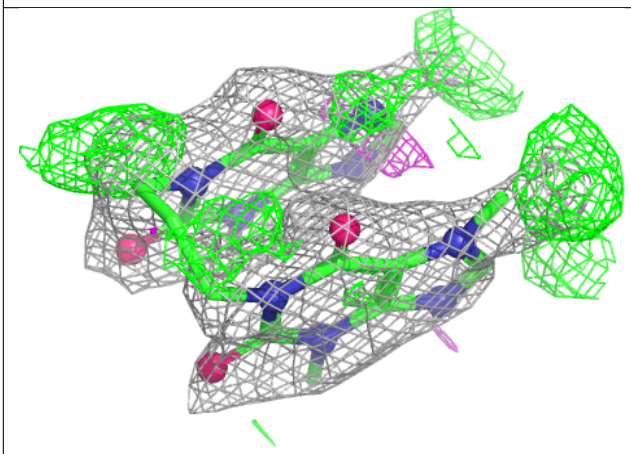
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

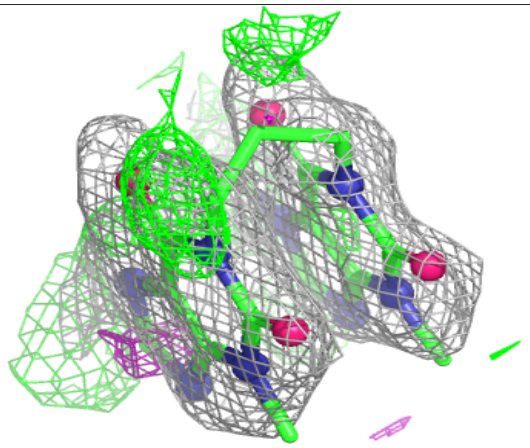


Electron density around CX9 C 1399:

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

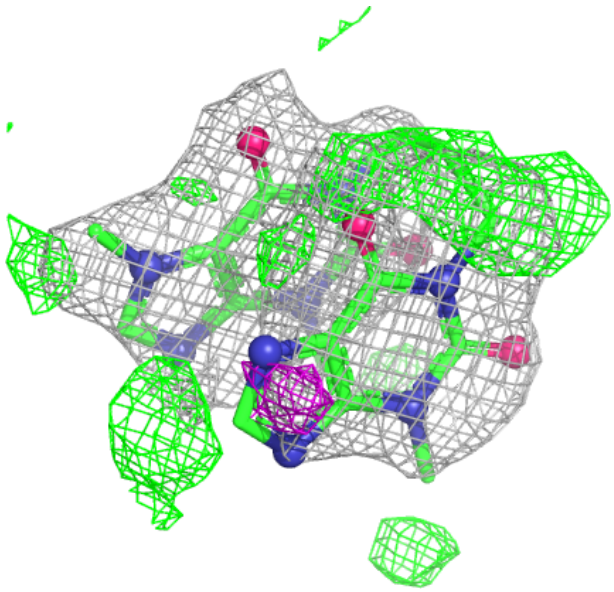


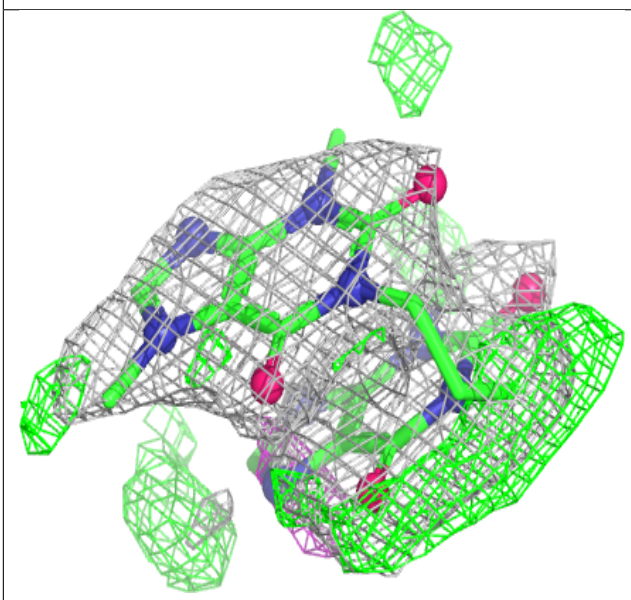


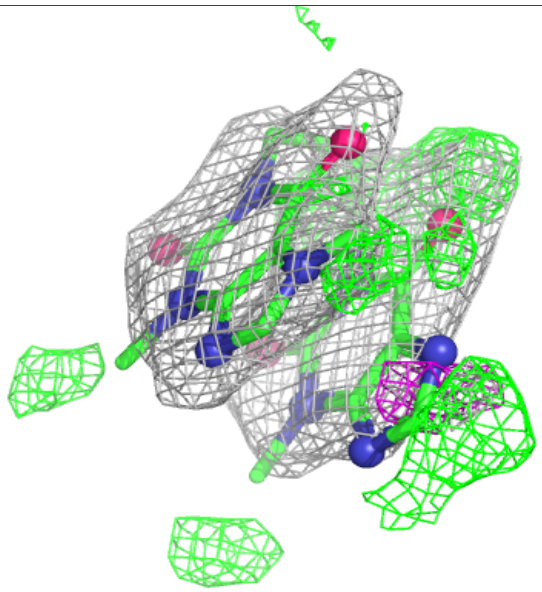


Electron density around CX9 E 1399:

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

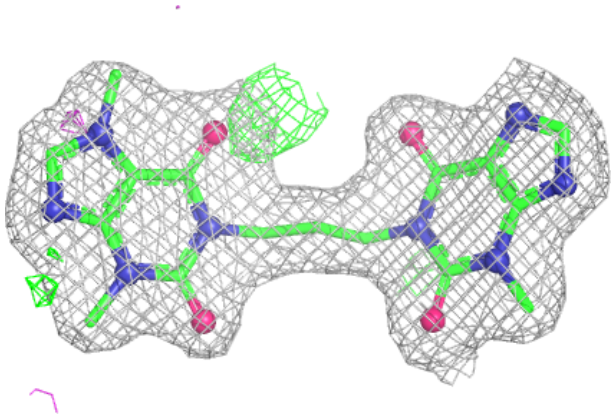


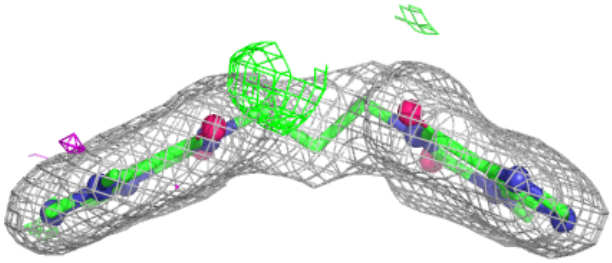


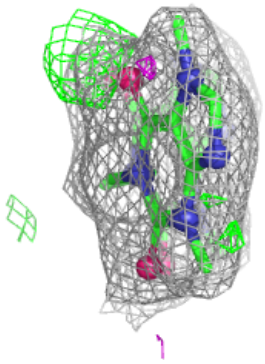


Electron density around CX9 F 1398:

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

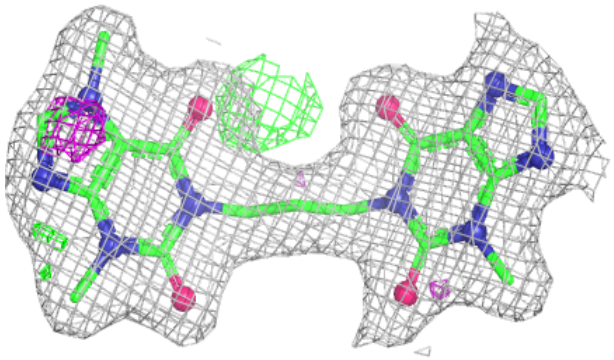


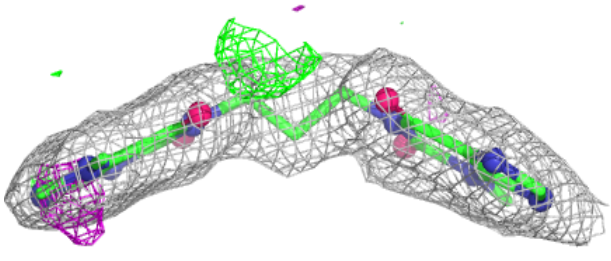


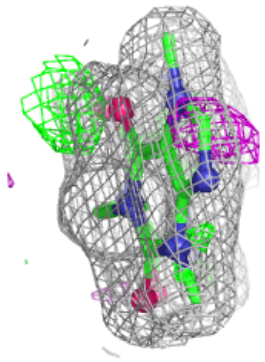


Electron density around CX9 B 1398:

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

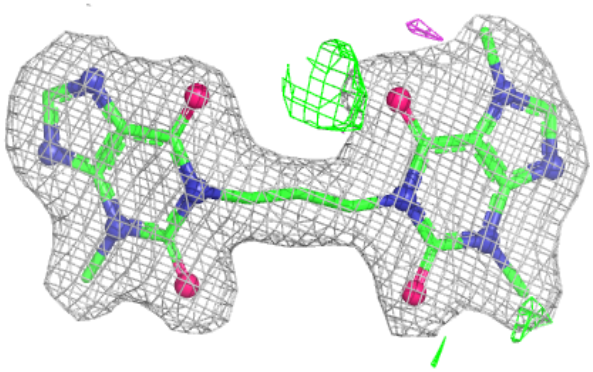


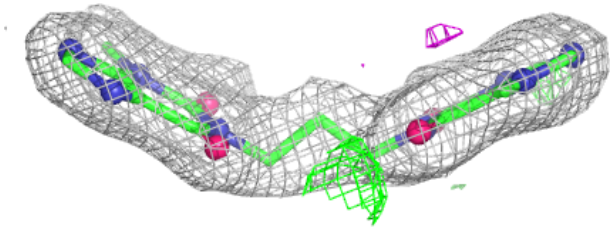


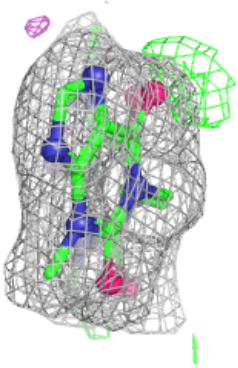


Electron density around CX9 E 1398:

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

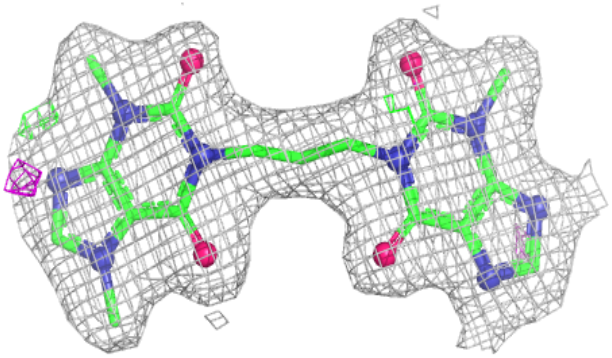


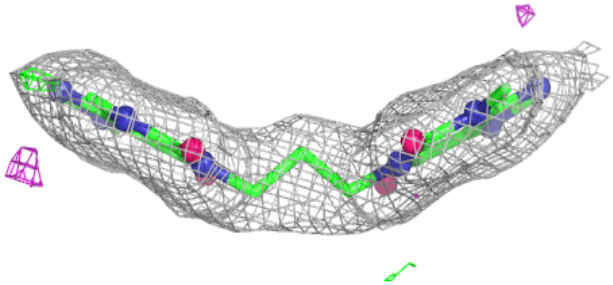


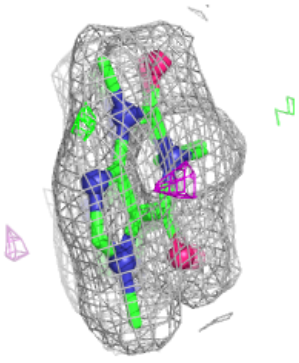


Electron density around CX9 A 1398:

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

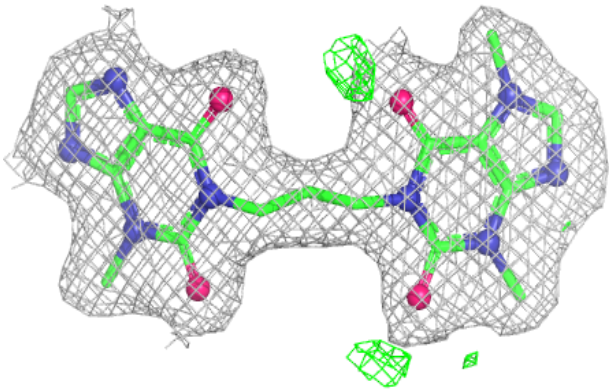


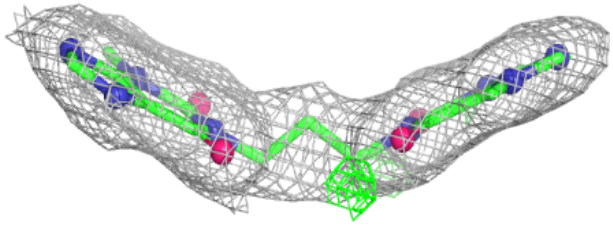


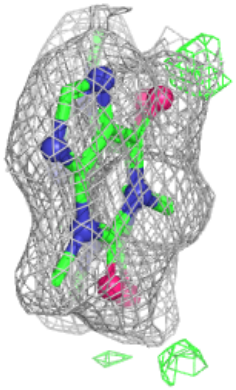


Electron density around CX9 D 1398:

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

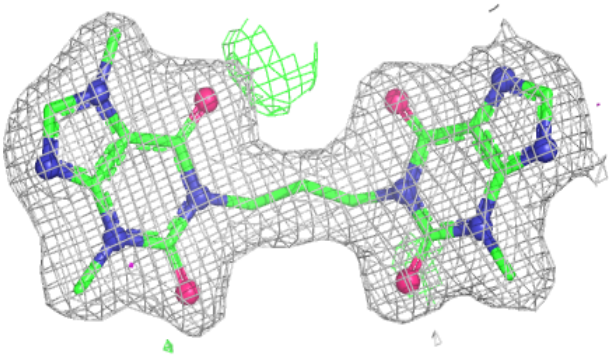


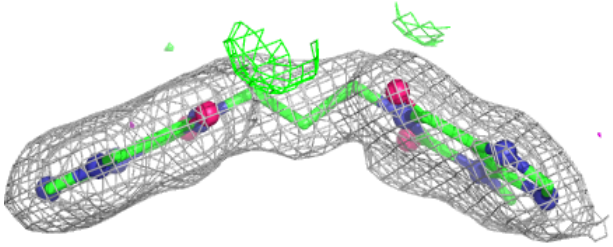


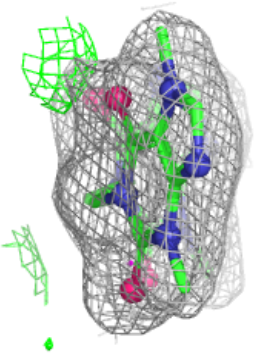


Electron density around CX9 C 1398:

$2mF_o$-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.