Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 12:10 PM JST

PDB ID	:	5Z79
Title	:	Crystal Structure Analysis of the HPPK-DHPS in complex with substrates
Authors	:	Manickam, Y.; Karl, H.; Sharma, A.
Deposited on	:	2018-01-27
Resolution	:	2.90 Å(reported)

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

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

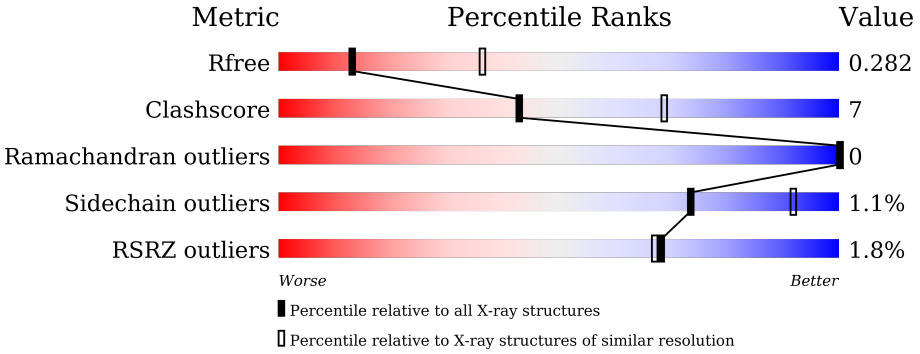
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	717	2% 68% 14% 18%
1	B	717	.% 65% 13% 22%
1	C	717	2% 70% 13% 16%
1	D	717	.% 66% 14% • 20%
1	E	717	.% 73% 8% 19%
1	F	717	.% 65% 14% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PE0	D	1105	-	X	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 28924 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.

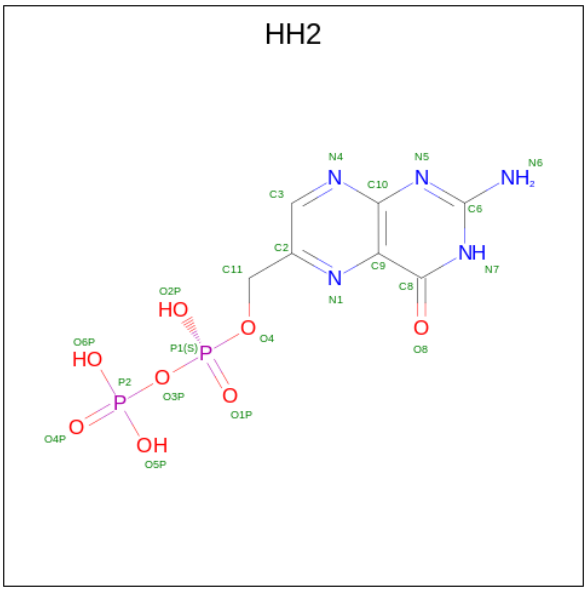
- Molecule 1 is a protein called Hydroxymethyldihydropterin pyrophosphokinase-dihydropter oate synthase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	588	4827	3106	807	893	21	0	0	0
1	B	562	4512	2909	746	838	19	0	0	0
1	C	599	4905	3154	822	908	21	0	0	0
1	D	577	4725	3047	789	870	19	0	0	0
1	E	584	4788	3082	800	885	21	0	0	0
1	F	566	4608	2973	770	846	19	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

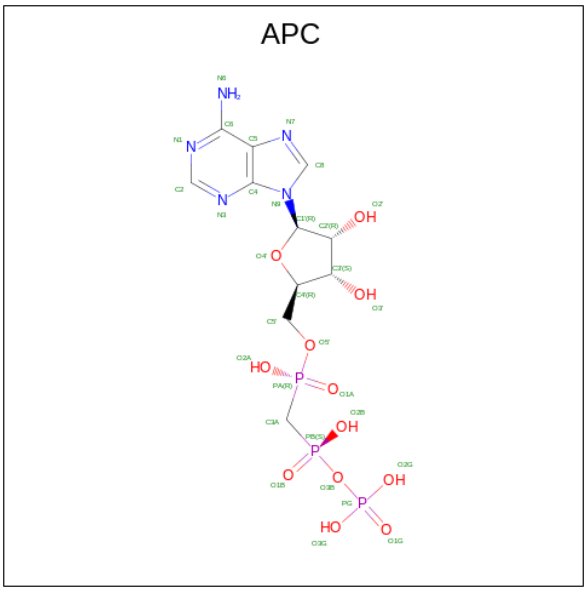
Chain	Residue	Modelled	Actual	Comment	Reference
A	383	ALA	GLY	see sequence details	UNP A0A1K9YMY7
B	383	ALA	GLY	see sequence details	UNP A0A1K9YMY7
C	383	ALA	GLY	see sequence details	UNP A0A1K9YMY7
D	383	ALA	GLY	see sequence details	UNP A0A1K9YMY7
E	383	ALA	GLY	see sequence details	UNP A0A1K9YMY7
F	383	ALA	GLY	see sequence details	UNP A0A1K9YMY7

- Molecule 2 is 6-HYDROXYMETHYLPTERIN-DIPHOSPHATE (three-letter code: HH2) (formula: $C_7H_9N_5O_8P_2$).



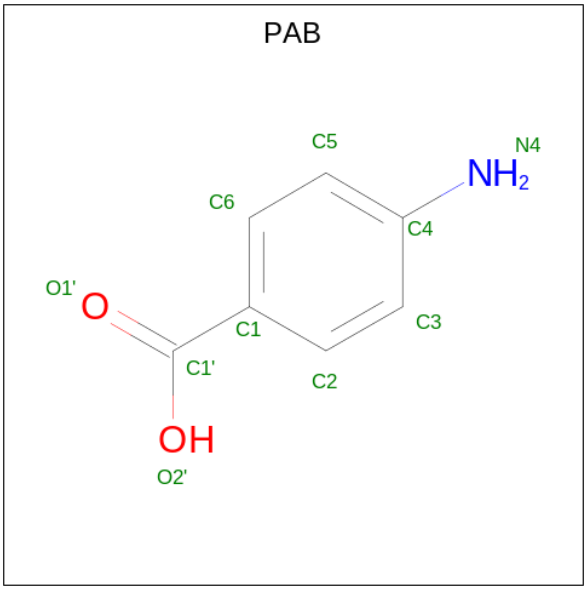
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	7	5	8	2		
2	B	1	Total	C	N	O	P	0	0
			22	7	5	8	2		
2	C	1	Total	C	N	O	P	0	0
			22	7	5	8	2		
2	D	1	Total	C	N	O	P	0	0
			22	7	5	8	2		
2	E	1	Total	C	N	O	P	0	0
			22	7	5	8	2		
2	F	1	Total	C	N	O	P	0	0
			22	7	5	8	2		

- Molecule 3 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	11	5	12	3	0	0
			Total	C	N	O	P		
3	C	1	31	11	5	12	3	0	0

- Molecule 4 is 4-AMINOBENZOIC ACID (three-letter code: PAB) (formula: $C_7H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	10	7	1	2	0	0
			Total	C	N	O		
4	B	1	10	7	1	2	0	0

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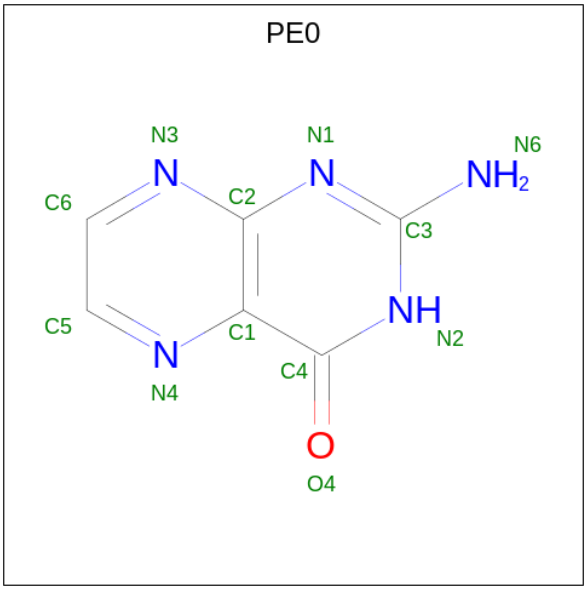
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	C	1	10	7	1	2	0	0
4	D	1	10	7	1	2	0	0
4	E	1	10	7	1	2	0	0
4	F	1	10	7	1	2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
5	C	1	1	1	0	0
5	D	1	1	1	0	0
5	E	1	1	1	0	0

- Molecule 6 is PTERINE (three-letter code: PE0) (formula: $C_6H_5N_5O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	12	6	5	1	0	0

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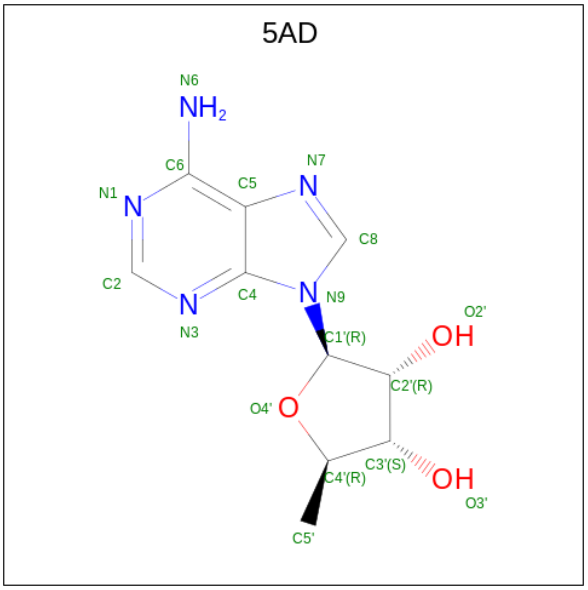
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	C	1	12	6	5	1	0	0
			Total	C	N	O		
6	D	1	12	6	5	1	0	0
			Total	C	N	O		
6	E	1	12	6	5	1	0	0

- Molecule 7 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	B	1	18	10	5	3	0	0
			Total	C	N	O		
7	D	1	18	10	5	3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	48	48	48	0	0
			Total	O		
8	B	16	16	16	0	0
			Total	O		
8	C	47	47	47	0	0
			Total	O		
8	D	50	50	50	0	0

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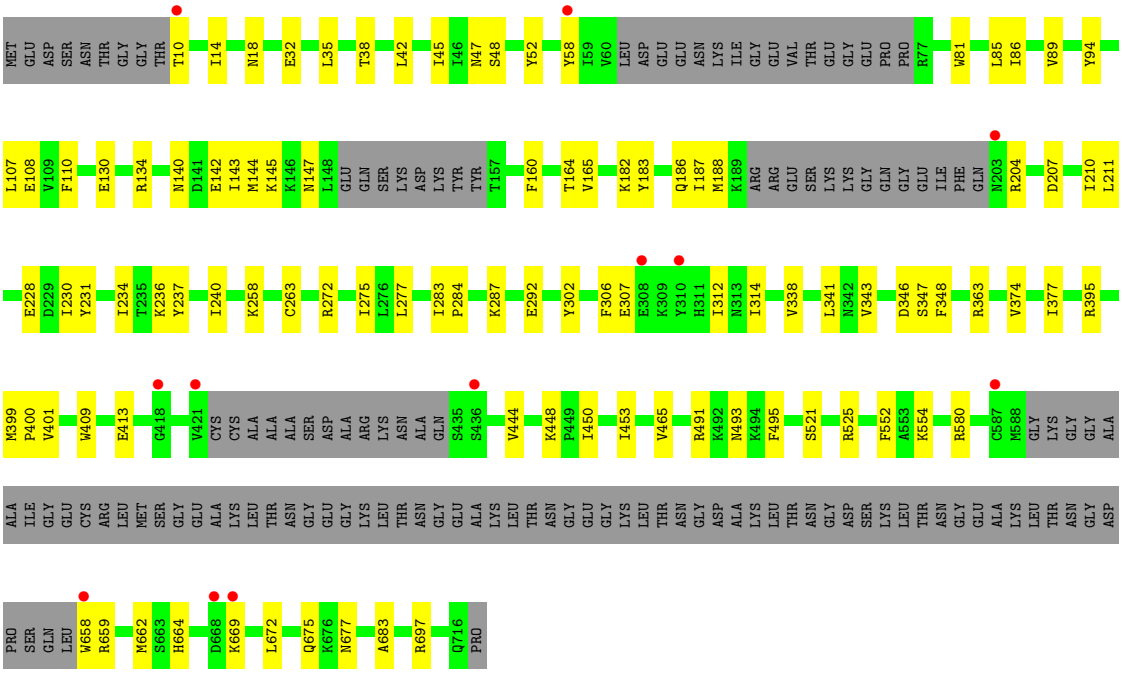
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	E	37	37	37	0	0
			Total	O		
8	F	19	19	19	0	0

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.

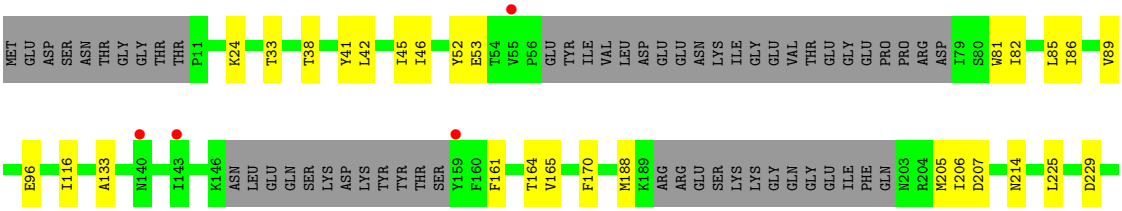
• Molecule 1: Hydroxymethyldihydropterin pyrophosphokinase-dihydropteroate synthase, putative

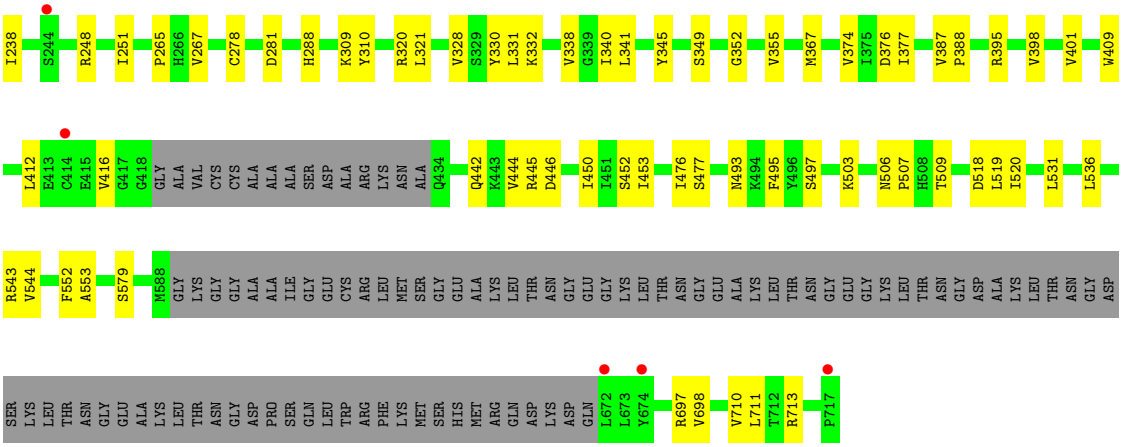
Chain A: 2% 68% 14% 18%



• Molecule 1: Hydroxymethyldihydropterin pyrophosphokinase-dihydropteroate synthase, putative

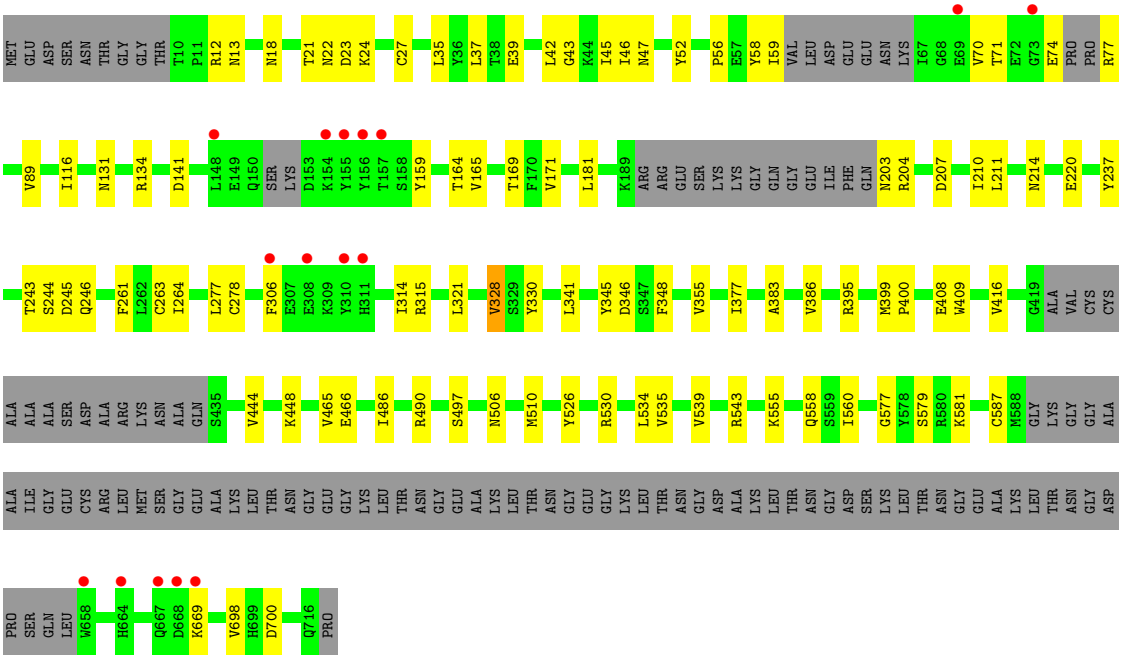
Chain B: % 65% 13% 22%





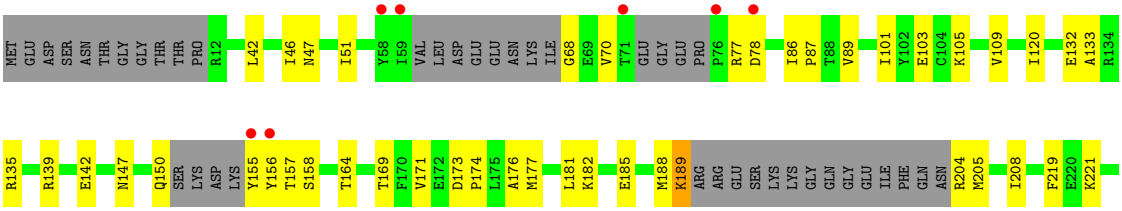
• Molecule 1: Hydroxymethyldihydropterin pyrophosphokinase-dihydropteroate synthase, putative

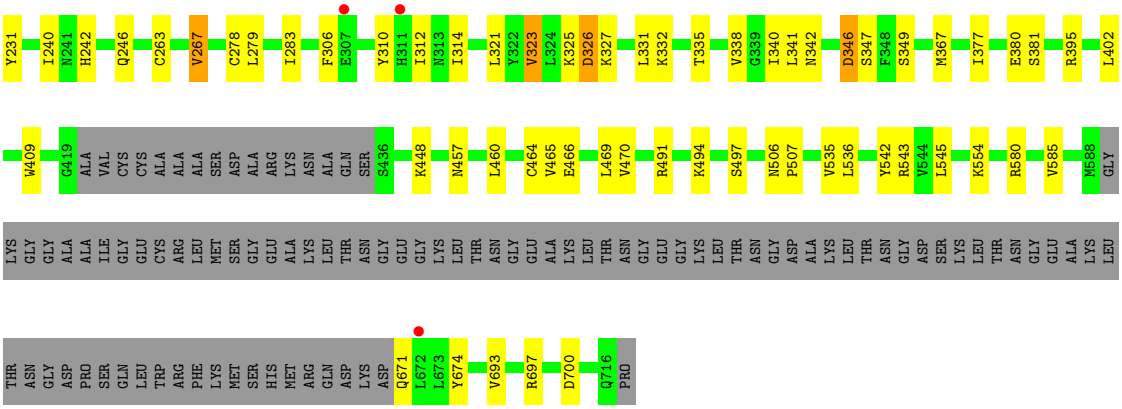
Chain C:



• Molecule 1: Hydroxymethyldihydropterin pyrophosphokinase-dihydropteroate synthase, putative

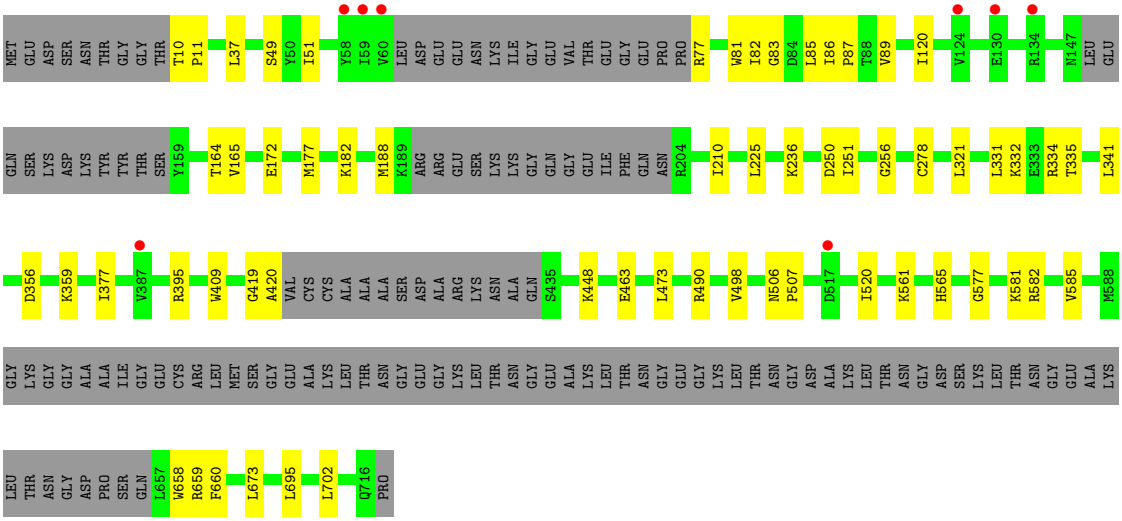
Chain D:





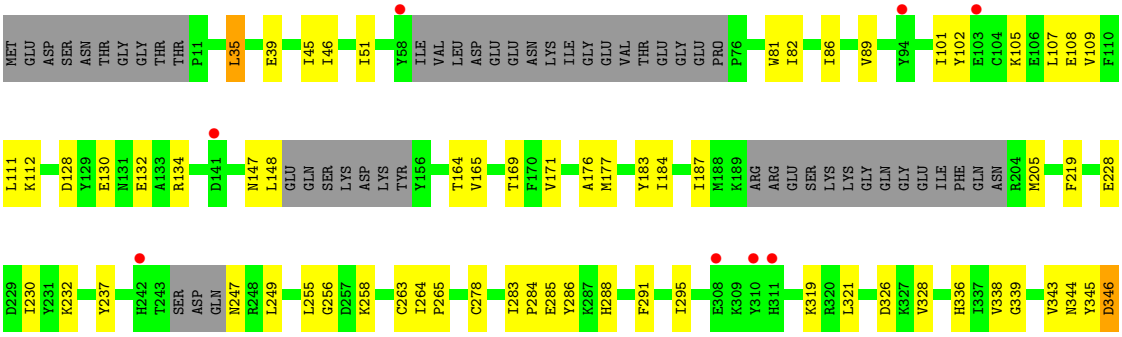
• Molecule 1: Hydroxymethyldihydropterin pyrophosphokinase-dihydropteroate synthase, putative

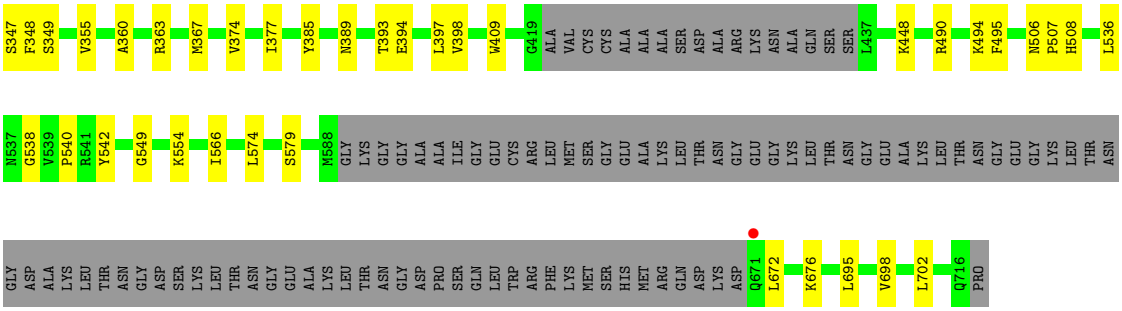
Chain E:



• Molecule 1: Hydroxymethyldihydropterin pyrophosphokinase-dihydropteroate synthase, putative

Chain F:




S347
F348
S349
V355
A360
R363
M367
V374
I377
Y385
N389
T393
E394
L397
V398
W409
G419
ALA
VAL
CYS
CYS
ALA
ALA
ALA
SER
ASP
ALA
ARG
LYS
ASN
ALA
GLN
SER
SER
L437
K448
R490
K494
F495
N506
P507
H508
L536
N537
G538
V539
P540
R541
Y542
G549
K554
I566
L574
S579
M588
GLY
LYS
GLY
GLY
ALA
ALA
ILE
GLY
GLU
CYS
ARG
LEU
MET
SER
GLY
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LEU
TRP
ARG
PHE
LYS
MET
SER
HIS
MET
ARG
GLN
ASP
LYS
ASP
Q671
L672
K676
L695
V698
L702
Q716
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.05Å 113.89Å 172.39Å 90.00° 94.24° 90.00°	Depositor
Resolution (Å)	49.82 – 2.90 49.82 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.82-2.90) 99.7 (49.82-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.242 , 0.285 0.248 , 0.282	Depositor DCC
R_{free} test set	2006 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	28924	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.36% 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: 5AD, APC, HH2, PE0, PAB, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.78	0/4920	0.85	0/6638
1	B	0.67	0/4601	0.78	0/6230
1	C	0.79	0/4999	0.86	0/6746
1	D	0.75	0/4815	0.83	0/6498
1	E	0.64	0/4881	0.77	0/6591
1	F	0.69	0/4697	0.79	0/6342
All	All	0.72	0/28913	0.81	0/39045

There are no bond length outliers.

There are no bond angle outliers.

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	4827	0	4848	70	0
1	B	4512	0	4436	66	0
1	C	4905	0	4895	73	0
1	D	4725	0	4740	67	0
1	E	4788	0	4785	42	0
1	F	4608	0	4606	76	0
2	A	22	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	22	0	6	0	0
2	C	22	0	6	0	0
2	D	22	0	6	1	0
2	E	22	0	6	2	0
2	F	22	0	6	2	0
3	A	31	0	14	4	0
3	C	31	0	14	3	0
4	A	10	0	6	0	0
4	B	10	0	6	0	0
4	C	10	0	6	0	0
4	D	10	0	6	0	0
4	E	10	0	6	1	0
4	F	10	0	6	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	12	0	5	1	0
6	C	12	0	5	0	0
6	D	12	0	5	0	0
6	E	12	0	5	0	0
7	B	18	0	13	0	0
7	D	18	0	13	2	0
8	A	48	0	0	1	0
8	B	16	0	0	0	0
8	C	47	0	0	1	0
8	D	50	0	0	3	0
8	E	37	0	0	0	0
8	F	19	0	0	0	0
All	All	28924	0	28456	389	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 7.

All (389) 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:133:ALA:HB1	1:B:267:VAL:HG21	1.32	1.12
1:C:164:THR:HG23	1:C:278:CYS:HB3	1.46	0.98
1:F:336:HIS:HB2	1:F:695:LEU:HD23	1.50	0.93
1:C:164:THR:HG23	1:C:278:CYS:CB	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:PHE:O	1:C:669:LYS:HE3	1.72	0.87
1:B:133:ALA:CB	1:B:267:VAL:HG21	2.07	0.85
1:F:35:LEU:HD23	1:F:45:ILE:CD1	2.10	0.82
1:F:35:LEU:HD23	1:F:45:ILE:HD13	1.62	0.81
1:D:77:ARG:NH1	1:D:205:MET:HG3	2.00	0.77
1:C:204:ARG:CD	1:C:207:ASP:HB2	2.15	0.76
1:C:164:THR:CG2	1:C:278:CYS:HB3	2.17	0.75
1:F:490:ARG:HD2	1:F:538:GLY:O	1.85	0.75
1:D:341:LEU:HD23	1:D:377:ILE:HD12	1.70	0.73
1:A:186:GLN:NE2	1:A:258:LYS:HE2	2.04	0.73
1:C:164:THR:CG2	1:C:278:CYS:CB	2.67	0.72
1:C:204:ARG:HD2	1:C:207:ASP:HB2	1.68	0.72
1:D:77:ARG:HH12	1:D:205:MET:HG3	1.55	0.72
1:C:243:THR:HG21	1:C:245:ASP:OD1	1.91	0.71
1:A:58:TYR:HB3	1:A:144:MET:HG2	1.72	0.71
1:D:164:THR:OG1	1:D:278:CYS:HB3	1.90	0.71
1:F:339:GLY:HA3	1:F:367:MET:HE3	1.72	0.70
1:D:51:ILE:HG22	1:D:321:LEU:HD12	1.74	0.70
1:A:465:VAL:HG11	1:A:491:ARG:HD3	1.74	0.68
1:C:169:THR:OG1	1:C:171:VAL:HG22	1.94	0.66
1:D:263:CYS:SG	1:D:267:VAL:HG23	2.36	0.66
1:C:210:ILE:H	3:C:1102:APC:HN61	1.42	0.66
1:A:341:LEU:HD23	1:A:377:ILE:HG13	1.78	0.66
1:A:86:ILE:O	1:A:89:VAL:HG22	1.96	0.65
1:F:35:LEU:HD21	1:F:165:VAL:HG21	1.79	0.65
1:D:188:MET:O	1:D:189:LYS:HG2	1.97	0.65
1:A:210:ILE:H	3:A:1102:APC:HN61	1.45	0.64
1:C:39:GLU:HG3	1:C:43:GLY:O	1.98	0.63
1:B:38:THR:HG23	1:B:42:LEU:HD12	1.81	0.63
1:B:321:LEU:HD23	1:B:328:VAL:HB	1.81	0.62
1:F:385:TYR:HA	1:F:508:HIS:CD2	2.35	0.62
1:E:331:LEU:HG	1:E:332:LYS:HG2	1.80	0.62
1:C:579:SER:HB2	1:C:698:VAL:HA	1.82	0.61
1:B:331:LEU:HG	1:B:332:LYS:HG2	1.81	0.61
1:D:323:VAL:HG13	1:D:327:LYS:O	1.99	0.61
1:E:419:GLY:O	1:E:420:ALA:HB2	2.01	0.61
1:B:24:LYS:HE3	1:B:330:TYR:OH	2.02	0.60
1:B:476:ILE:O	1:B:477:SER:HB3	2.01	0.60
1:C:263:CYS:HB3	3:C:1102:APC:H2	1.82	0.60
1:D:402:LEU:HB3	1:D:469:LEU:HD22	1.84	0.60
1:D:465:VAL:HG11	1:D:491:ARG:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:577:GLY:HA3	2:E:1101:HH2:O8	2.02	0.59
1:B:320:ARG:C	1:B:321:LEU:HD12	2.22	0.59
1:B:53:GLU:HG3	1:B:161:PHE:CE2	2.36	0.59
1:F:348:PHE:CE1	2:F:1101:HH2:O2P	2.56	0.57
1:F:86:ILE:O	1:F:89:VAL:HG22	2.03	0.57
1:E:395:ARG:NH1	1:E:463:GLU:OE2	2.36	0.57
1:F:81:TRP:CZ3	1:F:82:ILE:HD13	2.40	0.57
1:C:506:ASN:O	1:C:510:MET:HG2	2.05	0.57
1:D:77:ARG:HG2	1:D:78:ASP:N	2.19	0.57
1:C:12:ARG:HG3	1:C:12:ARG:HH11	1.70	0.56
1:D:279:LEU:HD22	1:D:283:ILE:HD11	1.88	0.56
1:C:243:THR:CG2	1:C:245:ASP:OD1	2.54	0.56
1:D:585:VAL:HG12	1:D:585:VAL:O	2.05	0.56
1:D:323:VAL:HG23	1:D:542:TYR:CD1	2.41	0.55
1:B:45:ILE:HG23	1:B:165:VAL:CG2	2.36	0.55
1:A:662:MET:HG3	1:A:675:GLN:OE1	2.07	0.55
1:F:506:ASN:HB2	1:F:507:PRO:CD	2.36	0.55
1:D:323:VAL:HG23	1:D:542:TYR:HD1	1.72	0.55
1:F:183:TYR:O	1:F:187:ILE:HD13	2.07	0.55
1:E:473:LEU:O	1:E:498:VAL:HA	2.06	0.55
1:F:176:ALA:O	1:F:177:MET:C	2.44	0.55
1:B:205:MET:HG3	1:B:206:ILE:HG22	1.89	0.55
1:B:320:ARG:HD2	1:B:331:LEU:HD22	1.89	0.55
1:E:585:VAL:HG21	1:E:673:LEU:HD11	1.89	0.54
1:E:81:TRP:HZ3	1:E:85:LEU:HD12	1.72	0.54
1:A:236:LYS:HD3	1:A:237:TYR:CE2	2.43	0.54
1:B:321:LEU:HD12	1:B:321:LEU:N	2.23	0.54
1:B:497:SER:OG	1:B:543:ARG:NH1	2.40	0.54
1:C:131:ASN:HA	1:C:134:ARG:NH1	2.23	0.54
1:D:346:ASP:O	1:D:381:SER:HB2	2.07	0.54
1:B:86:ILE:O	1:B:89:VAL:HG22	2.06	0.54
1:C:37:LEU:HD21	1:C:89:VAL:HG11	1.89	0.54
1:C:465:VAL:HG23	1:C:466:GLU:N	2.22	0.54
1:E:658:TRP:CG	1:F:349:SER:HB2	2.42	0.54
1:F:490:ARG:HE	1:F:495:PHE:HE2	1.54	0.54
1:D:466:GLU:HG2	1:D:491:ARG:HH12	1.73	0.54
1:A:231:TYR:CE2	1:A:240:ILE:HD11	2.43	0.53
1:C:383:ALA:HB3	1:C:386:VAL:HG21	1.90	0.53
1:B:340:ILE:O	1:B:367:MET:CE	2.56	0.53
1:C:526:TYR:O	1:C:530:ARG:HG2	2.09	0.53
1:A:491:ARG:NH1	1:A:491:ARG:CB	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:SER:O	1:A:525:ARG:HG3	2.09	0.53
1:C:52:TYR:CD2	1:C:277:LEU:HD21	2.44	0.53
1:A:658:TRP:CD1	1:B:349:SER:HA	2.44	0.53
1:D:173:ASP:HB2	1:D:174:PRO:HD2	1.90	0.53
1:C:345:TYR:CZ	1:C:355:VAL:HG11	2.44	0.52
1:A:491:ARG:HB3	1:A:491:ARG:CZ	2.38	0.52
1:C:18:ASN:HB2	1:C:211:LEU:HD11	1.90	0.52
1:B:96:GLU:OE2	1:B:170:PHE:HD2	1.93	0.52
1:A:272:ARG:HB2	1:A:275:ILE:HD12	1.92	0.52
1:B:86:ILE:HG12	1:B:493:ASN:HB2	1.92	0.52
1:C:534:LEU:HD12	1:C:539:VAL:HG21	1.91	0.52
1:F:409:TRP:CE2	1:F:448:LYS:HG3	2.45	0.52
1:C:243:THR:HG22	1:C:245:ASP:H	1.75	0.52
1:F:230:ILE:HD11	1:F:256:GLY:N	2.24	0.52
1:C:341:LEU:HD23	1:C:377:ILE:HG13	1.92	0.52
1:B:579:SER:HB2	1:B:698:VAL:HA	1.91	0.52
1:D:42:LEU:CD2	1:D:171:VAL:HG21	2.40	0.52
1:D:331:LEU:HG	1:D:332:LYS:HG2	1.92	0.52
1:D:263:CYS:N	7:D:1102:5AD:H2	2.25	0.51
1:B:387:VAL:O	1:B:388:PRO:C	2.48	0.51
1:A:409:TRP:CZ2	1:A:448:LYS:HB2	2.46	0.51
1:A:38:THR:HG23	1:A:42:LEU:HD12	1.93	0.51
1:B:442:GLN:O	1:B:446:ASP:CB	2.58	0.51
1:C:74:GLU:O	1:C:74:GLU:HG2	2.10	0.51
1:C:243:THR:HG22	1:C:244:SER:N	2.26	0.51
1:F:393:THR:HG22	1:F:394:GLU:N	2.25	0.51
1:E:377:ILE:HD12	1:E:377:ILE:N	2.25	0.51
1:C:204:ARG:HD3	1:C:207:ASP:HB2	1.93	0.51
1:B:267:VAL:HG22	1:B:267:VAL:O	2.10	0.51
1:D:242:HIS:HB2	8:D:1203:HOH:O	2.11	0.51
1:D:464:CYS:HB3	1:D:470:VAL:HG22	1.92	0.51
1:B:476:ILE:O	1:B:477:SER:CB	2.58	0.51
1:D:155:TYR:N	1:D:157:THR:HG23	2.26	0.51
1:E:172:GLU:OE2	1:E:236:LYS:NZ	2.41	0.51
1:E:182:LYS:HE2	1:E:182:LYS:HA	1.94	0.50
1:A:580:ARG:HA	1:A:677:ASN:OD1	2.11	0.50
1:A:81:TRP:CH2	1:A:188:MET:O	2.64	0.50
1:F:348:PHE:HE1	2:F:1101:HH2:O2P	1.93	0.50
1:A:52:TYR:CD2	1:A:277:LEU:HD21	2.46	0.50
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.76	0.50
1:F:108:GLU:O	1:F:112:LYS:HE3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:ASN:CG	1:F:347:SER:HG	2.14	0.50
1:F:346:ASP:OD2	1:F:389:ASN:N	2.44	0.50
1:C:35:LEU:HD21	1:C:165:VAL:HG21	1.94	0.50
1:F:35:LEU:CD2	1:F:45:ILE:HD13	2.38	0.50
1:F:232:LYS:HE2	1:F:232:LYS:HA	1.94	0.50
1:C:486:ILE:HG12	1:C:534:LEU:HD11	1.92	0.50
1:C:246:GLN:HG3	1:C:246:GLN:O	2.11	0.50
1:D:409:TRP:CD1	1:D:448:LYS:HE2	2.47	0.50
1:B:86:ILE:N	1:B:86:ILE:HD12	2.27	0.49
1:D:306:PHE:CG	1:D:314:ILE:HD12	2.47	0.49
1:A:186:GLN:OE1	1:A:186:GLN:HA	2.11	0.49
1:A:348:PHE:O	1:A:669:LYS:HE3	2.12	0.49
1:F:147:ASN:O	1:F:148:LEU:C	2.50	0.49
1:E:520:ILE:HD11	1:E:561:LYS:HG2	1.94	0.49
1:A:144:MET:O	1:A:147:ASN:O	2.29	0.49
1:C:164:THR:CG2	1:C:278:CYS:HB2	2.41	0.49
1:A:86:ILE:HG13	1:A:493:ASN:HB2	1.95	0.49
1:C:42:LEU:HD11	1:C:181:LEU:HD21	1.95	0.49
1:D:47:ASN:OD1	1:D:535:VAL:HG11	2.13	0.49
1:D:147:ASN:O	1:D:150:GLN:O	2.31	0.49
1:A:45:ILE:HD13	1:A:165:VAL:HG11	1.94	0.49
1:F:360:ALA:O	1:F:363:ARG:HB3	2.13	0.49
1:A:228:GLU:OE1	1:A:228:GLU:N	2.45	0.48
1:C:321:LEU:HD13	1:C:328:VAL:HG21	1.95	0.48
1:B:52:TYR:OH	1:B:281:ASP:OD2	2.27	0.48
1:B:519:LEU:HD23	1:B:520:ILE:CD1	2.43	0.48
1:E:419:GLY:O	1:E:420:ALA:CB	2.61	0.48
1:B:164:THR:HG23	1:B:278:CYS:CB	2.43	0.48
1:D:42:LEU:O	1:D:169:THR:HA	2.14	0.48
1:D:219:PHE:HE1	1:D:221:LYS:HG2	1.76	0.48
1:E:164:THR:OG1	1:E:278:CYS:HB3	2.14	0.48
1:C:116:ILE:HD12	1:C:214:ASN:CG	2.33	0.48
1:F:702:LEU:C	1:F:702:LEU:HD23	2.33	0.48
1:D:68:GLY:HA3	1:D:156:TYR:OH	2.14	0.48
1:B:248:ARG:HB3	1:B:251:ILE:HD12	1.95	0.48
1:C:59:ILE:HA	1:C:141:ASP:OD1	2.14	0.48
1:A:18:ASN:HB2	1:A:211:LEU:HD11	1.96	0.48
1:A:552:PHE:O	1:A:554:LYS:HD2	2.13	0.48
1:C:530:ARG:O	1:C:534:LEU:HD23	2.13	0.48
1:A:107:LEU:O	1:A:108:GLU:C	2.51	0.48
1:B:506:ASN:OD1	1:B:509:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:SER:HA	1:C:543:ARG:HB3	1.95	0.48
1:A:160:PHE:CD1	6:A:1105:PE0:O4	2.67	0.47
1:B:33:THR:HG22	1:B:188:MET:CE	2.44	0.47
1:C:12:ARG:NH1	8:C:1202:HOH:O	2.48	0.47
1:D:338:VAL:HB	1:D:697:ARG:HA	1.96	0.47
1:F:107:LEU:O	1:F:111:LEU:HD23	2.14	0.47
1:C:220:GLU:O	1:C:261:PHE:HB2	2.14	0.47
1:C:131:ASN:HA	1:C:134:ARG:HH12	1.79	0.47
1:D:86:ILE:HB	1:D:87:PRO:HD3	1.95	0.47
1:E:356:ASP:HB3	1:E:359:LYS:HE3	1.97	0.47
1:B:506:ASN:HB2	1:B:507:PRO:CD	2.44	0.47
1:F:566:ILE:HD11	1:F:574:LEU:HD21	1.96	0.47
1:C:314:ILE:CG2	1:C:315:ARG:N	2.78	0.47
1:A:140:ASN:HA	1:A:143:ILE:HD12	1.95	0.47
1:A:374:VAL:HG13	1:A:450:ILE:HG22	1.97	0.47
1:B:338:VAL:HB	1:B:697:ARG:HA	1.95	0.47
1:F:343:VAL:HG12	1:F:343:VAL:O	2.15	0.47
1:F:344:ASN:ND2	1:F:347:SER:OG	2.48	0.47
1:F:348:PHE:O	1:F:348:PHE:CG	2.67	0.47
1:C:71:THR:HG23	1:C:71:THR:O	2.14	0.47
1:C:560:ILE:HD11	1:C:587:CYS:SG	2.55	0.47
1:F:494:LYS:HE2	1:F:494:LYS:HA	1.97	0.47
1:B:398:VAL:O	1:B:401:VAL:HG22	2.15	0.47
1:D:335:THR:OG1	1:D:693:VAL:O	2.20	0.47
1:E:659:ARG:CG	1:E:660:PHE:N	2.78	0.47
1:C:35:LEU:HD22	1:C:45:ILE:CD1	2.45	0.47
1:D:219:PHE:CE1	1:D:221:LYS:HG2	2.50	0.46
1:A:409:TRP:CH2	1:A:448:LYS:HA	2.50	0.46
1:D:101:ILE:HD12	1:D:103:GLU:O	2.15	0.46
1:D:70:VAL:HG13	1:D:158:SER:HA	1.98	0.46
1:D:135:ARG:O	1:D:139:ARG:HG2	2.15	0.46
1:E:177:MET:HG2	1:E:210:ILE:HD11	1.98	0.46
1:F:579:SER:HB2	1:F:698:VAL:HA	1.96	0.46
1:B:477:SER:HB2	1:B:503:LYS:HE2	1.97	0.46
1:C:116:ILE:HD12	1:C:214:ASN:OD1	2.15	0.46
1:A:47:ASN:OD1	1:A:48:SER:N	2.49	0.46
1:A:130:GLU:O	1:A:134:ARG:HG2	2.16	0.46
1:B:46:ILE:O	1:B:536:LEU:HA	2.16	0.46
1:F:130:GLU:O	1:F:134:ARG:HG2	2.15	0.46
1:A:142:GLU:HA	1:A:145:LYS:HE3	1.97	0.46
1:C:12:ARG:HG3	1:C:12:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ASN:ND2	2:D:1101:HH2:O1P	2.37	0.46
1:B:377:ILE:HG21	1:B:398:VAL:HG13	1.97	0.45
1:B:412:LEU:O	1:B:416:VAL:HG23	2.15	0.45
1:C:377:ILE:HD12	1:C:377:ILE:N	2.29	0.45
1:F:169:THR:OG1	1:F:171:VAL:HG22	2.15	0.45
1:C:21:THR:OG1	1:C:22:ASN:N	2.49	0.45
1:C:45:ILE:HG23	1:C:165:VAL:HG13	1.98	0.45
1:E:702:LEU:HD11	1:F:676:LYS:HE2	1.98	0.45
1:A:491:ARG:NH1	1:A:491:ARG:HB3	2.31	0.45
1:C:204:ARG:NH2	3:C:1102:APC:O2B	2.50	0.45
1:E:582:ARG:O	1:E:585:VAL:HG12	2.16	0.45
1:F:286:TYR:O	1:F:295:ILE:HG12	2.16	0.45
1:D:310:TYR:HB3	1:D:312:ILE:HD12	1.97	0.45
1:F:345:TYR:CZ	1:F:355:VAL:HG11	2.52	0.45
1:D:671:GLN:HA	1:D:674:TYR:CD2	2.51	0.45
1:E:250:ASP:OD1	1:E:251:ILE:HG13	2.17	0.45
1:F:39:GLU:OE1	1:F:490:ARG:NH2	2.50	0.45
1:C:306:PHE:CE2	1:C:314:ILE:HD12	2.51	0.45
1:C:171:VAL:HA	1:C:237:TYR:CE1	2.52	0.45
1:D:181:LEU:HD22	1:D:208:ILE:HG21	1.99	0.45
1:A:338:VAL:HB	1:A:697:ARG:HA	1.98	0.45
1:D:182:LYS:HA	1:D:182:LYS:HE2	1.99	0.45
1:E:409:TRP:NE1	1:E:448:LYS:HD3	2.32	0.45
1:A:399:MET:N	1:A:400:PRO:CD	2.80	0.45
1:B:81:TRP:CZ3	1:B:82:ILE:HD13	2.50	0.45
1:B:376:ASP:HA	1:B:452:SER:O	2.17	0.45
1:F:169:THR:HG21	1:F:177:MET:HE3	1.99	0.45
1:C:70:VAL:HG11	1:C:159:TYR:CD2	2.52	0.44
1:F:328:VAL:HG23	1:F:328:VAL:O	2.16	0.44
1:F:377:ILE:HG21	1:F:398:VAL:HG13	1.99	0.44
1:F:536:LEU:HD23	1:F:536:LEU:O	2.17	0.44
1:B:81:TRP:CH2	1:B:82:ILE:HD11	2.52	0.44
1:C:555:LYS:O	1:C:558:GLN:HB2	2.17	0.44
1:D:105:LYS:O	1:D:109:VAL:HG23	2.17	0.44
1:A:10:THR:N	8:A:1209:HOH:O	2.50	0.44
1:A:35:LEU:HD21	1:A:165:VAL:HG21	1.98	0.44
1:A:186:GLN:HE22	1:A:258:LYS:HE2	1.76	0.44
1:D:506:ASN:HB2	1:D:507:PRO:CD	2.47	0.44
1:F:247:ASN:HD22	1:F:249:LEU:HG	1.83	0.44
1:C:35:LEU:HD22	1:C:45:ILE:HD13	1.98	0.44
1:C:13:ASN:O	1:C:169:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:ILE:N	1:E:120:ILE:HD12	2.33	0.44
1:E:225:LEU:O	1:E:256:GLY:HA3	2.18	0.44
1:F:128:ASP:O	1:F:132:GLU:HG2	2.18	0.44
1:A:230:ILE:HG22	1:A:234:ILE:HD12	2.00	0.44
1:D:46:ILE:O	1:D:536:LEU:HA	2.18	0.44
1:A:182:LYS:O	1:A:186:GLN:HG2	2.17	0.44
1:B:506:ASN:H	1:B:509:THR:HG22	1.82	0.44
1:F:265:PRO:HD3	1:F:288:HIS:CE1	2.53	0.44
1:D:340:ILE:O	1:D:367:MET:HE1	2.17	0.43
1:E:82:ILE:O	1:E:83:GLY:C	2.55	0.43
1:E:581:LYS:NZ	2:E:1101:HH2:O8	2.47	0.43
1:A:14:ILE:HG21	1:A:110:PHE:CG	2.53	0.43
1:B:116:ILE:HD12	1:B:214:ASN:OD1	2.18	0.43
1:B:225:LEU:HD22	1:B:229:ASP:HB3	2.01	0.43
1:B:518:ASP:O	1:B:519:LEU:C	2.55	0.43
1:F:45:ILE:HG23	1:F:165:VAL:HG13	2.00	0.43
1:D:465:VAL:CG1	1:D:491:ARG:HD2	2.47	0.43
1:E:37:LEU:HD12	1:E:188:MET:HE2	2.01	0.43
1:F:264:ILE:HA	1:F:265:PRO:C	2.39	0.43
1:F:285:GLU:OE1	1:F:285:GLU:N	2.37	0.43
1:B:309:LYS:HE3	1:B:310:TYR:CZ	2.54	0.43
1:C:314:ILE:HG23	1:C:315:ARG:N	2.34	0.43
1:D:139:ARG:O	1:D:142:GLU:HG2	2.19	0.43
1:D:263:CYS:H	7:D:1102:5AD:H2	1.83	0.43
1:D:349:SER:HB2	1:D:580:ARG:HH11	1.84	0.43
1:A:263:CYS:HB3	3:A:1102:APC:H2	2.00	0.43
1:D:176:ALA:O	1:D:177:MET:C	2.57	0.43
1:F:105:LYS:O	1:F:109:VAL:HG23	2.19	0.43
1:F:283:ILE:N	1:F:284:PRO:CD	2.82	0.43
2:A:1101:HH2:O6P	2:A:1101:HH2:H112	2.19	0.43
1:F:540:PRO:HB3	1:F:542:TYR:CE2	2.54	0.43
1:A:186:GLN:HE21	1:A:258:LYS:HG3	1.84	0.43
1:F:326:ASP:N	1:F:326:ASP:OD1	2.52	0.43
1:F:393:THR:O	1:F:397:LEU:HD12	2.19	0.43
1:A:45:ILE:HG23	1:A:165:VAL:HG13	2.01	0.42
1:A:413:GLU:HG2	1:A:444:VAL:HG11	2.01	0.42
1:A:683:ALA:HB3	1:B:710:VAL:HG11	2.00	0.42
1:B:374:VAL:HG13	1:B:450:ILE:HG22	2.01	0.42
1:D:246:GLN:O	1:D:246:GLN:HG3	2.19	0.42
1:E:506:ASN:C	1:E:506:ASN:OD1	2.58	0.42
1:B:321:LEU:HD23	1:B:328:VAL:CB	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:PHE:CG	1:A:314:ILE:HD13	2.54	0.42
1:C:56:PRO:HB3	1:C:58:TYR:CZ	2.54	0.42
1:E:582:ARG:HE	4:E:1102:PAB:C1'	2.31	0.42
1:A:204:ARG:NH2	3:A:1102:APC:O2B	2.52	0.42
1:A:263:CYS:N	3:A:1102:APC:H2	2.34	0.42
1:A:307:GLU:HG2	1:A:312:ILE:O	2.19	0.42
1:C:46:ILE:O	1:C:47:ASN:HB2	2.20	0.42
1:D:86:ILE:O	1:D:89:VAL:HG22	2.20	0.42
1:E:658:TRP:CD1	1:F:349:SER:HA	2.54	0.42
1:B:265:PRO:HD3	1:B:288:HIS:CE1	2.54	0.42
1:B:340:ILE:N	1:B:367:MET:HE1	2.34	0.42
1:C:577:GLY:O	1:C:581:LYS:HE3	2.18	0.42
1:F:164:THR:OG1	1:F:278:CYS:HB3	2.19	0.42
1:F:494:LYS:CE	1:F:494:LYS:CA	2.98	0.42
1:A:659:ARG:HA	1:A:659:ARG:NE	2.35	0.42
1:B:164:THR:HG23	1:B:278:CYS:HB2	2.00	0.42
1:F:338:VAL:HG22	1:F:374:VAL:HB	2.02	0.42
1:B:345:TYR:CD1	1:B:355:VAL:HG11	2.55	0.42
1:B:531:LEU:HD13	1:B:544:VAL:HG11	2.02	0.42
1:D:132:GLU:O	1:D:133:ALA:C	2.58	0.42
1:F:348:PHE:O	1:F:348:PHE:CD1	2.72	0.42
1:B:352:GLY:HA2	1:B:355:VAL:HG13	2.01	0.42
1:B:41:TYR:CD1	1:B:238:ILE:HD12	2.55	0.42
1:B:495:PHE:CD1	1:B:495:PHE:N	2.88	0.42
1:C:416:VAL:HG21	1:C:444:VAL:HG21	2.02	0.42
1:D:70:VAL:CG1	1:D:158:SER:HA	2.50	0.42
1:E:506:ASN:HB2	1:E:507:PRO:CD	2.50	0.42
1:F:494:LYS:HA	1:F:494:LYS:CE	2.50	0.42
1:B:340:ILE:O	1:B:367:MET:HE3	2.19	0.41
1:C:23:ASP:HB2	1:C:77:ARG:HE	1.85	0.41
1:D:323:VAL:CG2	1:D:542:TYR:CD1	3.02	0.41
1:D:457:ASN:HB3	1:D:460:LEU:HB3	2.02	0.41
1:F:51:ILE:HG13	1:F:542:TYR:CD2	2.55	0.41
1:F:101:ILE:HG13	1:F:536:LEU:CD2	2.50	0.41
1:A:32:GLU:HB3	1:A:495:PHE:CE1	2.55	0.41
1:B:713:ARG:O	1:B:713:ARG:NH1	2.48	0.41
1:E:334:ARG:HG3	1:E:335:THR:N	2.35	0.41
1:E:520:ILE:HG12	1:E:565:HIS:HB2	2.01	0.41
1:F:46:ILE:O	1:F:536:LEU:HA	2.20	0.41
1:F:184:ILE:O	1:F:187:ILE:HB	2.20	0.41
1:A:186:GLN:HE22	1:A:258:LYS:CE	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:TYR:CE1	1:D:240:ILE:HD11	2.55	0.41
1:D:335:THR:HB	8:D:1236:HOH:O	2.19	0.41
1:F:102:TYR:CD1	1:F:102:TYR:N	2.87	0.41
1:A:287:LYS:NZ	1:A:292:GLU:O	2.54	0.41
1:A:363:ARG:NH1	1:A:664:HIS:CD2	2.87	0.41
1:B:340:ILE:HG22	1:B:341:LEU:N	2.36	0.41
1:B:409:TRP:HZ2	1:B:444:VAL:O	2.04	0.41
1:C:24:LYS:HE3	1:C:330:TYR:OH	2.19	0.41
1:C:399:MET:HB2	1:C:400:PRO:HD3	2.03	0.41
1:F:255:LEU:O	1:F:258:LYS:HB2	2.21	0.41
1:F:264:ILE:N	1:F:264:ILE:HD12	2.35	0.41
1:F:319:LYS:O	1:F:321:LEU:HD13	2.21	0.41
1:A:283:ILE:N	1:A:284:PRO:CD	2.83	0.41
1:C:321:LEU:HD13	1:C:328:VAL:CG2	2.51	0.41
1:D:340:ILE:N	1:D:367:MET:HE1	2.34	0.41
1:E:120:ILE:HD12	1:E:120:ILE:H	1.85	0.41
1:F:549:GLY:O	1:F:554:LYS:CE	2.69	0.41
1:A:183:TYR:CE2	1:A:187:ILE:HD11	2.56	0.41
1:B:552:PHE:O	1:B:553:ALA:HB3	2.21	0.41
1:E:51:ILE:HG22	1:E:321:LEU:HD12	2.03	0.41
1:E:86:ILE:HB	1:E:87:PRO:HD3	2.02	0.41
1:F:336:HIS:CB	1:F:695:LEU:HD23	2.36	0.41
1:C:164:THR:HG21	1:C:278:CYS:HB2	2.03	0.41
1:E:341:LEU:HD23	1:E:377:ILE:HG13	2.02	0.41
1:E:658:TRP:CD1	1:F:349:SER:CB	3.04	0.41
1:F:228:GLU:O	1:F:232:LYS:HG2	2.21	0.41
1:A:164:THR:C	1:A:165:VAL:HG23	2.42	0.41
1:A:204:ARG:HH22	1:A:207:ASP:CG	2.24	0.41
1:A:465:VAL:CG1	1:A:491:ARG:HD3	2.49	0.41
1:C:23:ASP:O	1:C:27:CYS:HB2	2.21	0.41
1:D:325:LYS:HE2	1:D:326:ASP:OD2	2.21	0.41
1:A:187:ILE:O	1:A:187:ILE:CG2	2.69	0.41
1:D:120:ILE:N	8:D:1207:HOH:O	2.54	0.41
1:D:497:SER:HA	1:D:543:ARG:HB3	2.02	0.41
1:E:81:TRP:CZ3	1:E:85:LEU:HD12	2.54	0.41
1:A:302:TYR:CD1	1:A:302:TYR:C	2.95	0.40
1:B:133:ALA:HB1	1:B:267:VAL:CG2	2.25	0.40
1:F:171:VAL:HG12	1:F:237:TYR:CZ	2.56	0.40
1:A:343:VAL:HG11	1:A:401:VAL:HG21	2.02	0.40
1:A:672:LEU:HD23	1:A:672:LEU:C	2.42	0.40
1:D:185:GLU:OE1	1:D:204:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:THR:N	1:E:11:PRO:HD2	2.35	0.40
1:E:49:SER:HB3	1:E:164:THR:OG1	2.22	0.40
1:C:408:GLU:HA	1:C:408:GLU:OE1	2.21	0.40
1:E:82:ILE:O	1:E:85:LEU:HB2	2.21	0.40
1:F:263:CYS:C	1:F:264:ILE:HD12	2.42	0.40
1:F:288:HIS:HB3	1:F:291:PHE:HD1	1.87	0.40
1:B:82:ILE:O	1:B:82:ILE:CG2	2.70	0.40
1:B:445:ARG:HH11	1:B:445:ARG:HD3	1.69	0.40
1:B:711:LEU:HD23	1:B:711:LEU:HA	1.87	0.40
1:C:409:TRP:CE2	1:C:448:LYS:HG3	2.56	0.40
1:E:86:ILE:O	1:E:89:VAL:HG22	2.22	0.40
1:A:94:TYR:N	1:A:94:TYR:CD1	2.90	0.40
1:A:491:ARG:CB	1:A:491:ARG:HH11	2.35	0.40
1:C:264:ILE:N	1:C:264:ILE:HD12	2.37	0.40
1:D:135:ARG:HD3	1:D:139:ARG:HH21	1.87	0.40
1:D:545:LEU:HD12	1:D:545:LEU:N	2.37	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	576/717 (80%)	544 (94%)	32 (6%)	0	100	100
1	B	550/717 (77%)	513 (93%)	37 (7%)	0	100	100
1	C	585/717 (82%)	548 (94%)	37 (6%)	0	100	100
1	D	563/717 (78%)	536 (95%)	27 (5%)	0	100	100
1	E	572/717 (80%)	530 (93%)	42 (7%)	0	100	100
1	F	552/717 (77%)	509 (92%)	43 (8%)	0	100	100
All	All	3398/4302 (79%)	3180 (94%)	218 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	542/647 (84%)	537 (99%)	5 (1%)	78	93
1	B	494/647 (76%)	490 (99%)	4 (1%)	81	94
1	C	546/647 (84%)	539 (99%)	7 (1%)	69	90
1	D	526/647 (81%)	515 (98%)	11 (2%)	53	81
1	E	534/647 (82%)	530 (99%)	4 (1%)	84	95
1	F	510/647 (79%)	505 (99%)	5 (1%)	76	92
All	All	3152/3882 (81%)	3116 (99%)	36 (1%)	73	92

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	346	ASP
1	A	347	SER
1	A	395	ARG
1	A	453	ILE
1	B	85	LEU
1	B	207	ASP
1	B	395	ARG
1	B	453	ILE
1	C	203	ASN
1	C	328	VAL
1	C	346	ASP
1	C	395	ARG
1	C	490	ARG
1	C	535	VAL
1	C	700	ASP
1	D	189	LYS
1	D	267	VAL
1	D	323	VAL

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Mol	Chain	Res	Type
1	D	326	ASP
1	D	346	ASP
1	D	347	SER
1	D	380	GLU
1	D	395	ARG
1	D	494	LYS
1	D	554	LYS
1	D	700	ASP
1	E	77	ARG
1	E	165	VAL
1	E	490	ARG
1	E	695	LEU
1	F	35	LEU
1	F	205	MET
1	F	219	PHE
1	F	346	ASP
1	F	672	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	247	ASN

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)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 for Mogul analysis.

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	$\#\|Z\| > 2$
7	5AD	D	1102	-	17,20,20	1.00	0	15,30,30	1.49	3 (20%)
3	APC	C	1102	-	27,33,33	0.94	2 (7%)	31,52,52	0.91	1 (3%)
6	PE0	E	1104	-	13,13,13	1.70	3 (23%)	15,18,18	3.72	9 (60%)
2	HH2	E	1101	5	21,23,23	1.52	2 (9%)	27,35,35	3.43	13 (48%)
2	HH2	F	1101	-	21,23,23	1.73	5 (23%)	27,35,35	2.83	11 (40%)
2	HH2	B	1101	-	21,23,23	1.58	3 (14%)	27,35,35	2.46	9 (33%)
6	PE0	C	1105	-	13,13,13	1.23	2 (15%)	15,18,18	3.49	10 (66%)
4	PAB	D	1103	-	10,10,10	0.65	0	13,13,13	1.08	0
7	5AD	B	1102	-	17,20,20	1.11	1 (5%)	15,30,30	1.79	5 (33%)
4	PAB	E	1102	-	10,10,10	0.67	0	13,13,13	1.05	0
4	PAB	C	1103	-	10,10,10	0.64	0	13,13,13	1.24	1 (7%)
4	PAB	B	1103	-	10,10,10	0.66	0	13,13,13	1.15	0
2	HH2	D	1101	5	21,23,23	1.50	2 (9%)	27,35,35	2.49	9 (33%)
2	HH2	C	1101	5	21,23,23	1.55	5 (23%)	27,35,35	3.54	13 (48%)
3	APC	A	1102	-	27,33,33	0.97	2 (7%)	31,52,52	0.88	1 (3%)
2	HH2	A	1101	5	21,23,23	1.59	2 (9%)	27,35,35	2.61	10 (37%)
6	PE0	D	1105	-	13,13,13	1.67	4 (30%)	15,18,18	3.51	10 (66%)
6	PE0	A	1105	-	13,13,13	1.58	3 (23%)	15,18,18	3.39	10 (66%)
4	PAB	F	1102	-	10,10,10	0.74	0	13,13,13	0.80	0
4	PAB	A	1103	-	10,10,10	0.68	0	13,13,13	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	5AD	D	1102	-	-	0/0/20/20	0/3/3/3
3	APC	C	1102	-	-	5/15/38/38	0/3/3/3
6	PE0	E	1104	-	-	-	0/2/2/2
2	HH2	E	1101	5	-	5/12/12/12	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HH2	F	1101	-	-	6/12/12/12	0/2/2/2
2	HH2	B	1101	-	-	5/12/12/12	0/2/2/2
6	PE0	C	1105	-	-	-	0/2/2/2
4	PAB	D	1103	-	-	0/4/4/4	0/1/1/1
7	5AD	B	1102	-	-	0/0/20/20	0/3/3/3
4	PAB	E	1102	-	-	0/4/4/4	0/1/1/1
4	PAB	C	1103	-	-	0/4/4/4	0/1/1/1
4	PAB	B	1103	-	-	0/4/4/4	0/1/1/1
2	HH2	D	1101	5	-	6/12/12/12	0/2/2/2
2	HH2	C	1101	5	-	6/12/12/12	0/2/2/2
3	APC	A	1102	-	-	5/15/38/38	0/3/3/3
2	HH2	A	1101	5	-	4/12/12/12	0/2/2/2
6	PE0	D	1105	-	-	-	0/2/2/2
6	PE0	A	1105	-	-	-	0/2/2/2
4	PAB	F	1102	-	-	0/4/4/4	0/1/1/1
4	PAB	A	1103	-	-	0/4/4/4	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1101	HH2	C9-C8	4.61	1.49	1.41
2	E	1101	HH2	C10-N4	-4.53	1.30	1.37
2	B	1101	HH2	C9-C10	4.33	1.48	1.40
2	A	1101	HH2	C9-C8	4.28	1.48	1.41
6	E	1104	PE0	C1-C4	4.16	1.48	1.41
2	D	1101	HH2	C9-C8	4.15	1.48	1.41
2	F	1101	HH2	C9-C10	4.05	1.48	1.40
6	A	1105	PE0	C2-N3	-3.98	1.31	1.37
2	A	1101	HH2	C9-C10	3.97	1.48	1.40
2	C	1101	HH2	C9-C8	3.93	1.48	1.41
2	D	1101	HH2	C9-C10	3.85	1.48	1.40
2	B	1101	HH2	C9-C8	3.81	1.47	1.41
6	D	1105	PE0	C2-N3	-3.30	1.32	1.37
6	D	1105	PE0	C1-C4	3.12	1.46	1.41
2	E	1101	HH2	C9-C8	3.05	1.46	1.41
2	C	1101	HH2	C10-N4	-2.97	1.33	1.37
2	F	1101	HH2	C2-N1	2.67	1.37	1.32
6	E	1104	PE0	C1-C2	2.65	1.45	1.40
6	A	1105	PE0	C1-C4	2.60	1.45	1.41
6	E	1104	PE0	C2-N3	-2.52	1.33	1.37
3	A	1102	APC	PB-O2B	-2.51	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1105	PE0	C1-C2	2.50	1.45	1.40
7	B	1102	5AD	C5-C4	2.48	1.47	1.40
3	C	1102	APC	PB-O2B	-2.42	1.50	1.56
2	C	1101	HH2	C10-N5	-2.35	1.32	1.36
3	C	1102	APC	PA-O2A	-2.29	1.51	1.56
6	A	1105	PE0	C2-N1	-2.28	1.32	1.36
3	A	1102	APC	PA-O2A	-2.25	1.51	1.56
6	D	1105	PE0	C2-N1	-2.20	1.32	1.36
6	C	1105	PE0	C2-N3	-2.18	1.34	1.37
2	F	1101	HH2	C9-N1	2.15	1.36	1.33
2	B	1101	HH2	C3-N4	2.14	1.35	1.31
2	C	1101	HH2	C6-N7	-2.06	1.31	1.35
2	C	1101	HH2	C9-C10	2.03	1.44	1.40
2	F	1101	HH2	C3-N4	2.03	1.35	1.31
6	C	1105	PE0	C1-C2	2.00	1.44	1.40

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1101	HH2	C6-N5-C10	6.91	123.25	115.36
6	C	1105	PE0	N3-C2-N1	6.74	123.52	115.82
2	E	1101	HH2	C6-N5-C10	6.59	122.88	115.36
2	F	1101	HH2	C10-C9-C8	-6.55	115.61	119.95
2	C	1101	HH2	C8-C9-N1	6.51	126.04	118.60
2	E	1101	HH2	C10-C9-C8	-6.36	115.74	119.95
6	D	1105	PE0	C3-N1-C2	6.00	122.21	115.36
2	E	1101	HH2	N4-C10-N5	5.98	122.65	115.82
2	E	1101	HH2	C8-C9-N1	5.90	125.34	118.60
6	E	1104	PE0	N3-C2-N1	5.90	122.55	115.82
6	E	1104	PE0	C3-N1-C2	5.89	122.08	115.36
2	B	1101	HH2	C10-C9-C8	-5.88	116.06	119.95
6	E	1104	PE0	C2-C1-C4	-5.86	116.07	119.95
2	D	1101	HH2	N4-C10-N5	5.76	122.39	115.82
6	D	1105	PE0	N3-C2-N1	5.75	122.38	115.82
2	C	1101	HH2	C6-N7-C8	5.71	125.00	115.93
2	F	1101	HH2	C8-C9-N1	5.71	125.12	118.60
2	E	1101	HH2	N5-C6-N7	-5.67	119.67	127.22
2	B	1101	HH2	N4-C10-N5	5.65	122.27	115.82
2	C	1101	HH2	N4-C10-N5	5.64	122.25	115.82
6	C	1105	PE0	C3-N1-C2	5.58	121.73	115.36
2	C	1101	HH2	C10-C9-C8	-5.48	116.33	119.95
2	F	1101	HH2	N4-C10-N5	5.39	121.98	115.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	1104	PE0	C4-C1-N4	5.38	124.94	118.24
2	C	1101	HH2	C3-C2-N1	-5.36	117.35	120.85
6	D	1105	PE0	C2-C1-C4	-5.29	116.45	119.95
2	C	1101	HH2	N5-C6-N7	-5.25	120.22	127.22
2	C	1101	HH2	C9-C8-N7	-5.18	116.34	123.43
2	D	1101	HH2	C6-N5-C10	5.14	121.23	115.36
2	E	1101	HH2	C6-N7-C8	5.14	124.09	115.93
2	F	1101	HH2	C6-N5-C10	5.10	121.19	115.36
2	E	1101	HH2	C3-N4-C10	5.06	121.78	116.69
2	A	1101	HH2	C10-C9-C8	-5.05	116.61	119.95
2	A	1101	HH2	N4-C10-N5	5.04	121.58	115.82
6	D	1105	PE0	C4-C1-N4	4.92	124.37	118.24
6	A	1105	PE0	N3-C2-N1	4.82	121.33	115.82
2	E	1101	HH2	C3-C2-N1	-4.82	117.70	120.85
6	A	1105	PE0	C1-C4-N2	-4.74	116.95	123.43
6	A	1105	PE0	C4-C1-N4	4.65	124.03	118.24
2	D	1101	HH2	C10-C9-C8	-4.52	116.96	119.95
2	A	1101	HH2	C6-N7-C8	4.50	123.07	115.93
2	A	1101	HH2	C8-C9-N1	4.46	123.70	118.60
2	A	1101	HH2	C9-C8-N7	-4.42	117.39	123.43
6	E	1104	PE0	C3-N2-C4	4.42	122.95	115.93
6	A	1105	PE0	C3-N2-C4	4.41	122.93	115.93
6	C	1105	PE0	C4-C1-N4	4.38	123.69	118.24
2	A	1101	HH2	C6-N5-C10	4.32	120.29	115.36
6	A	1105	PE0	C3-N1-C2	4.27	120.23	115.36
2	B	1101	HH2	C6-N5-C10	4.15	120.10	115.36
2	B	1101	HH2	C6-N7-C8	4.15	122.52	115.93
2	C	1101	HH2	C10-C9-N1	-4.14	117.64	122.33
6	C	1105	PE0	C2-C1-C4	-4.08	117.25	119.95
2	F	1101	HH2	C6-N7-C8	4.03	122.34	115.93
2	E	1101	HH2	C9-C8-N7	-4.03	117.92	123.43
6	A	1105	PE0	C2-C1-C4	-4.00	117.30	119.95
2	D	1101	HH2	C6-N7-C8	3.98	122.25	115.93
2	D	1101	HH2	C8-C9-N1	3.95	123.11	118.60
6	E	1104	PE0	C1-C4-N2	-3.94	118.04	123.43
6	C	1105	PE0	C3-N2-C4	3.90	122.13	115.93
6	A	1105	PE0	C6-N3-C2	3.80	121.29	116.60
2	C	1101	HH2	C3-N4-C10	3.80	120.51	116.69
2	D	1101	HH2	C9-C8-N7	-3.80	118.24	123.43
6	D	1105	PE0	C3-N2-C4	3.76	121.90	115.93
6	E	1104	PE0	N1-C3-N2	-3.72	122.27	127.22
2	C	1101	HH2	C2-N1-C9	3.72	122.83	118.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1101	HH2	C8-C9-N1	3.69	122.81	118.60
2	F	1101	HH2	C3-N4-C10	3.67	120.38	116.69
7	B	1102	5AD	N3-C2-N1	-3.63	123.00	128.68
7	B	1102	5AD	C4-C5-N7	-3.61	105.63	109.40
6	D	1105	PE0	C1-C4-N2	-3.58	118.54	123.43
6	A	1105	PE0	N1-C3-N2	-3.58	122.45	127.22
2	B	1101	HH2	C9-C8-N7	-3.56	118.56	123.43
6	D	1105	PE0	N1-C3-N2	-3.49	122.57	127.22
6	C	1105	PE0	N1-C3-N2	-3.48	122.58	127.22
6	C	1105	PE0	C1-C4-N2	-3.46	118.70	123.43
2	F	1101	HH2	N5-C6-N7	-3.44	122.63	127.22
2	A	1101	HH2	C3-N4-C10	3.40	120.11	116.69
7	D	1102	5AD	N3-C2-N1	-3.35	123.44	128.68
2	D	1101	HH2	N5-C6-N7	-3.32	122.79	127.22
2	A	1101	HH2	N5-C6-N7	-3.30	122.82	127.22
2	F	1101	HH2	C9-C8-N7	-3.25	118.99	123.43
6	A	1105	PE0	C2-C1-N4	-3.17	118.65	122.32
2	B	1101	HH2	N5-C6-N7	-3.06	123.14	127.22
2	E	1101	HH2	C10-C9-N1	-3.02	118.91	122.33
2	E	1101	HH2	N6-C6-N7	3.00	121.92	117.25
4	C	1103	PAB	O2'-C1'-C1	2.90	122.36	114.85
6	E	1104	PE0	C2-C1-N4	-2.89	118.97	122.32
2	E	1101	HH2	C2-N1-C9	2.83	121.79	118.45
6	C	1105	PE0	C2-C1-N4	-2.81	119.06	122.32
7	B	1102	5AD	C1'-N9-C4	-2.78	121.76	126.64
6	D	1105	PE0	C2-C1-N4	-2.71	119.18	122.32
7	D	1102	5AD	C5'-C4'-C3'	-2.71	112.85	115.70
2	F	1101	HH2	C10-C9-N1	-2.71	119.26	122.33
6	E	1104	PE0	C6-N3-C2	2.70	119.94	116.60
6	D	1105	PE0	C6-N3-C2	2.62	119.83	116.60
2	B	1101	HH2	C3-N4-C10	2.60	119.31	116.69
2	C	1101	HH2	P1-O3P-P2	-2.57	124.00	132.83
2	D	1101	HH2	C3-N4-C10	2.54	119.24	116.69
3	A	1102	APC	C5-C6-N6	2.52	124.18	120.35
6	C	1105	PE0	C1-C2-N1	-2.51	117.58	121.80
6	C	1105	PE0	C6-N3-C2	2.45	119.63	116.60
2	C	1101	HH2	N6-C6-N7	2.45	121.06	117.25
7	D	1102	5AD	C3'-C2'-C1'	2.38	104.57	100.98
2	B	1101	HH2	O6P-P2-O5P	2.37	116.70	107.64
6	A	1105	PE0	C5-N4-C1	2.36	121.33	117.12
2	A	1101	HH2	P1-O3P-P2	-2.34	124.80	132.83
2	A	1101	HH2	C10-C9-N1	-2.33	119.69	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1102	APC	C5-C6-N6	2.33	123.89	120.35
7	B	1102	5AD	C5'-C4'-C3'	-2.26	113.32	115.70
2	F	1101	HH2	P1-O3P-P2	-2.17	125.36	132.83
2	F	1101	HH2	O6P-P2-O5P	2.17	115.92	107.64
2	D	1101	HH2	C10-C9-N1	-2.12	119.93	122.33
6	D	1105	PE0	C1-C2-N1	-2.07	118.33	121.80
2	E	1101	HH2	P1-O3P-P2	-2.03	125.86	132.83
7	B	1102	5AD	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	HH2	C11-O4-P1-O1P
2	C	1101	HH2	C11-O4-P1-O3P
2	D	1101	HH2	O4-C11-C2-N1
2	D	1101	HH2	O4-C11-C2-C3
2	D	1101	HH2	C11-O4-P1-O1P
2	D	1101	HH2	C11-O4-P1-O2P
2	D	1101	HH2	C11-O4-P1-O3P
2	E	1101	HH2	C11-O4-P1-O1P
2	E	1101	HH2	C11-O4-P1-O2P
2	E	1101	HH2	C11-O4-P1-O3P
2	E	1101	HH2	P1-O3P-P2-O6P
2	F	1101	HH2	C11-O4-P1-O1P
2	F	1101	HH2	C11-O4-P1-O2P
2	F	1101	HH2	C11-O4-P1-O3P
2	F	1101	HH2	P1-O3P-P2-O6P
3	A	1102	APC	PA-C3A-PB-O1B
3	A	1102	APC	PA-C3A-PB-O2B
3	A	1102	APC	PA-C3A-PB-O3B
3	A	1102	APC	C5'-O5'-PA-O1A
3	A	1102	APC	C5'-O5'-PA-C3A
3	C	1102	APC	PB-C3A-PA-O5'
3	C	1102	APC	O4'-C4'-C5'-O5'
2	A	1101	HH2	O4-C11-C2-N1
2	B	1101	HH2	O4-C11-C2-N1
2	C	1101	HH2	O4-C11-C2-N1
2	B	1101	HH2	C11-O4-P1-O3P
3	C	1102	APC	C3'-C4'-C5'-O5'
2	A	1101	HH2	O4-C11-C2-C3
2	B	1101	HH2	O4-C11-C2-C3

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Mol	Chain	Res	Type	Atoms
2	C	1101	HH2	O4-C11-C2-C3
2	C	1101	HH2	P2-O3P-P1-O2P
2	C	1101	HH2	P1-O3P-P2-O4P
3	C	1102	APC	C4'-C5'-O5'-PA
2	A	1101	HH2	P2-O3P-P1-O2P
2	A	1101	HH2	P2-O3P-P1-O1P
3	C	1102	APC	PA-C3A-PB-O1B
2	F	1101	HH2	P1-O3P-P2-O4P
2	D	1101	HH2	P1-O3P-P2-O5P
2	E	1101	HH2	P1-O3P-P2-O5P
2	B	1101	HH2	P2-O3P-P1-O2P
2	F	1101	HH2	O4-C11-C2-C3
2	C	1101	HH2	C11-O4-P1-O1P

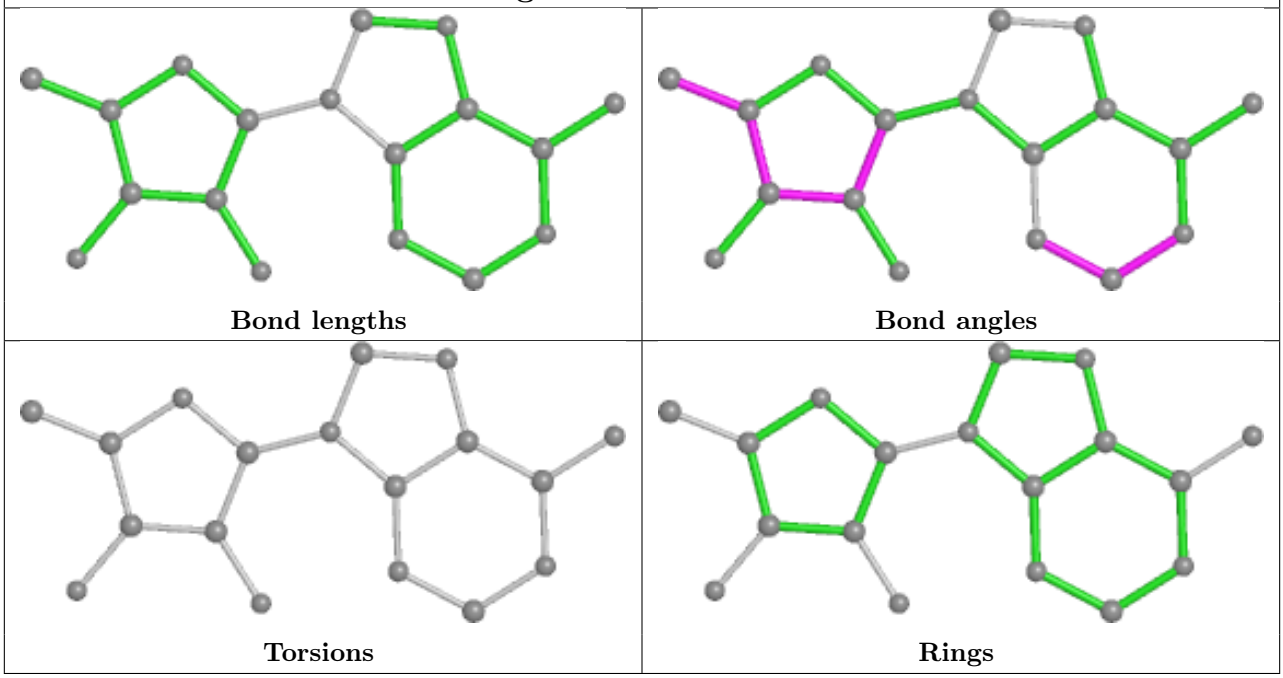
There are no ring outliers.

9 monomers are involved in 17 short contacts:

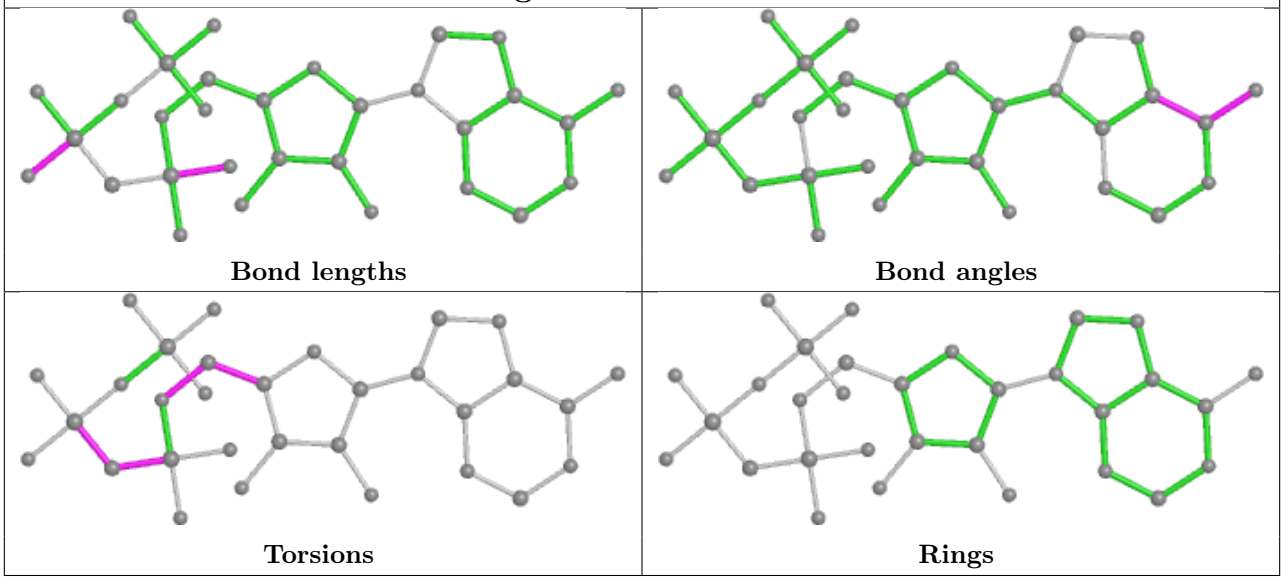
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1102	5AD	2	0
3	C	1102	APC	3	0
2	E	1101	HH2	2	0
2	F	1101	HH2	2	0
4	E	1102	PAB	1	0
2	D	1101	HH2	1	0
3	A	1102	APC	4	0
2	A	1101	HH2	1	0
6	A	1105	PE0	1	0

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.

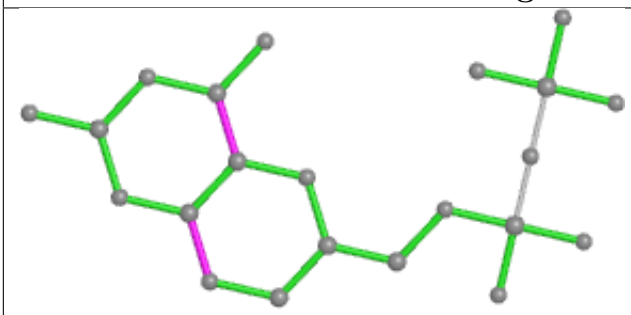
Ligand 5AD D 1102



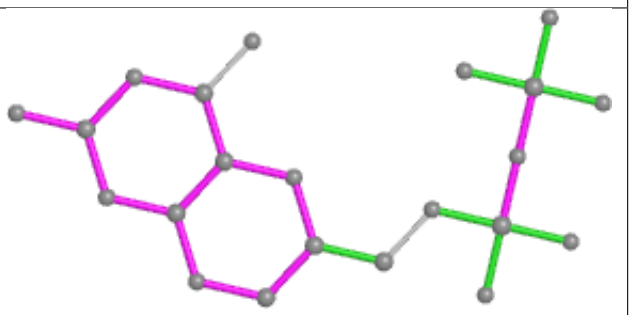
Ligand APC C 1102



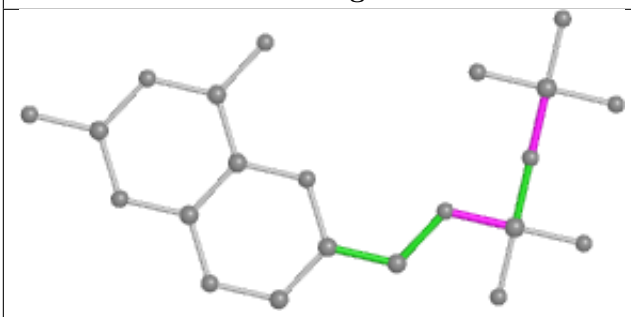
Ligand HH2 E 1101



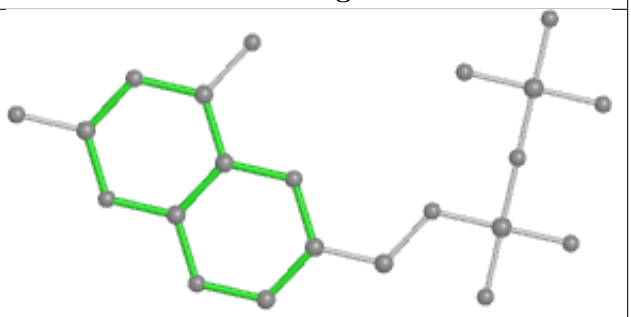
Bond lengths



Bond angles

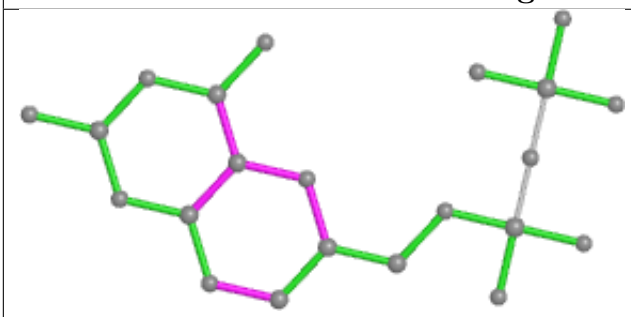


Torsions



Rings

Ligand HH2 F 1101



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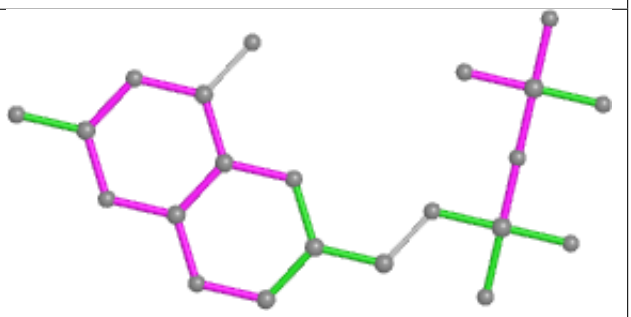
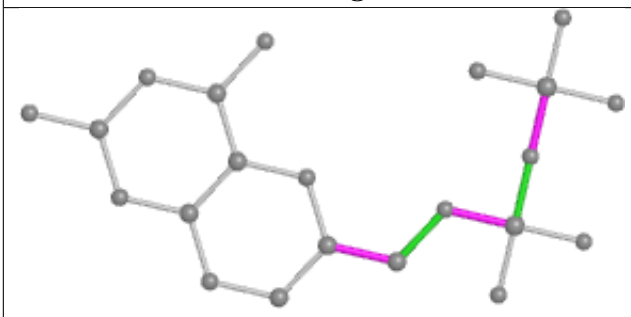


Bond angles



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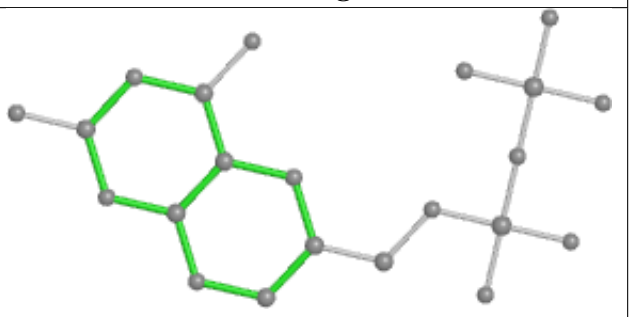
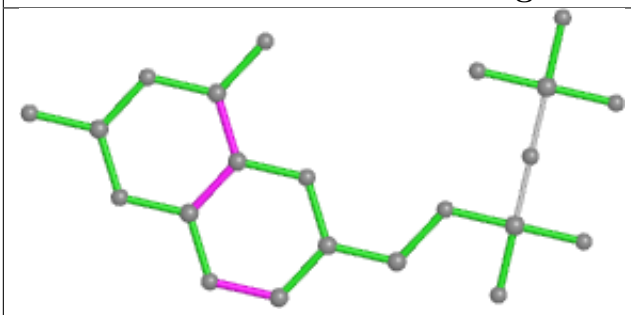
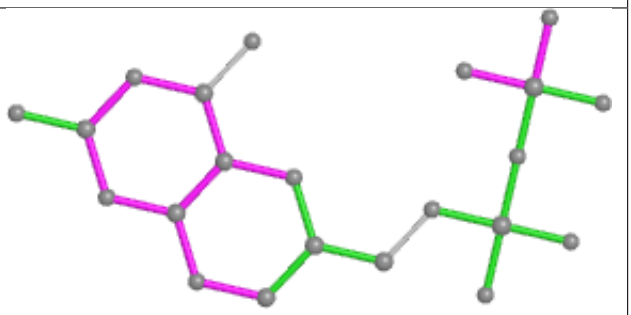


Rings

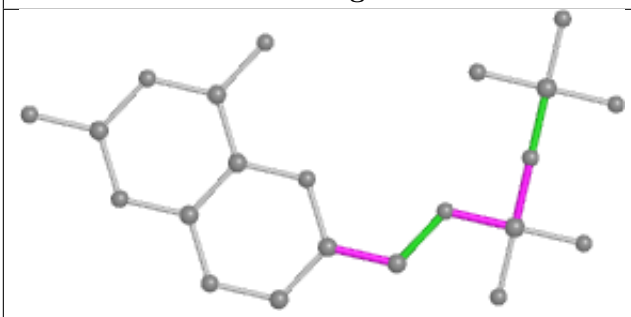
Ligand HH2 B 1101



Bond lengths



Bond angles



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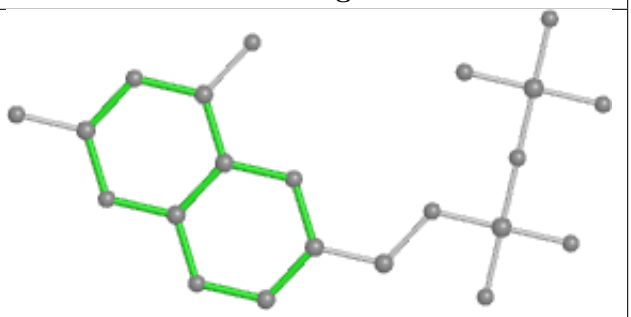
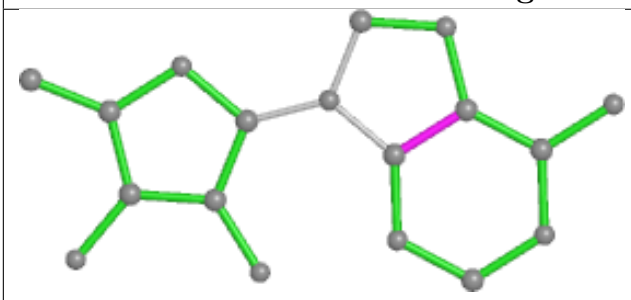
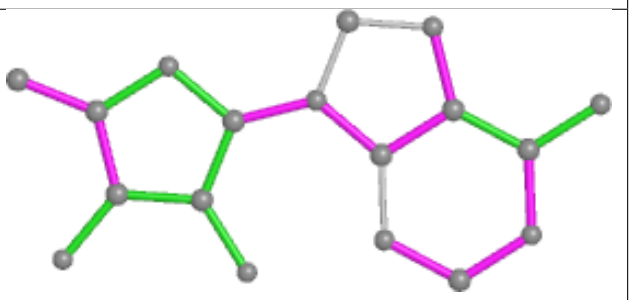


Rings

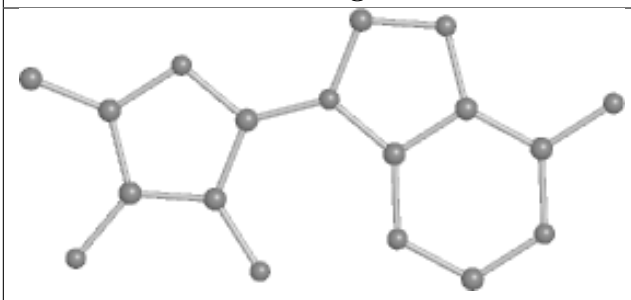
Ligand 5AD B 1102



Bond lengths



Bond angles



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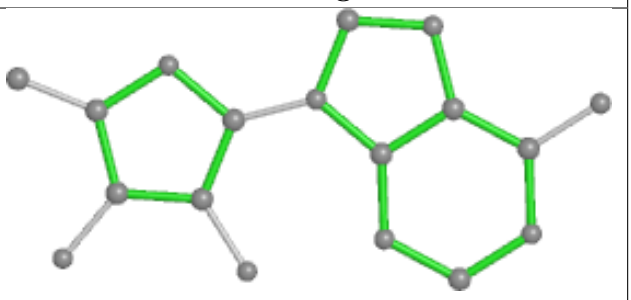
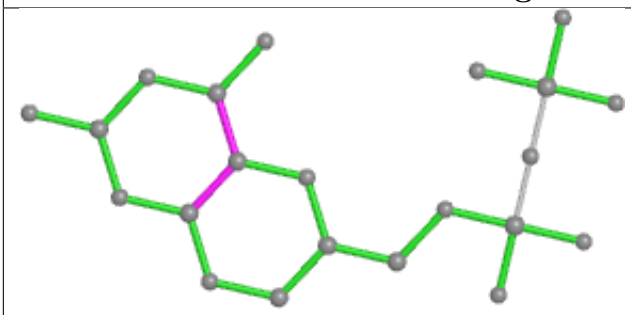
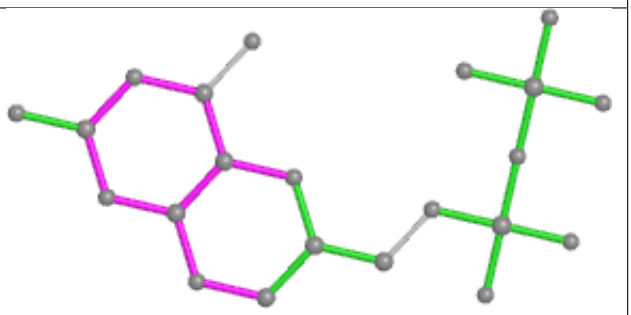


Rings

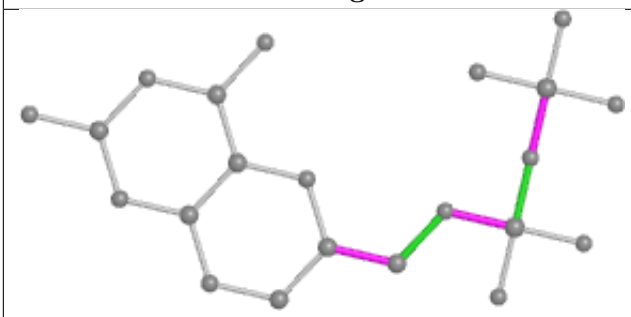
Ligand HH2 D 1101



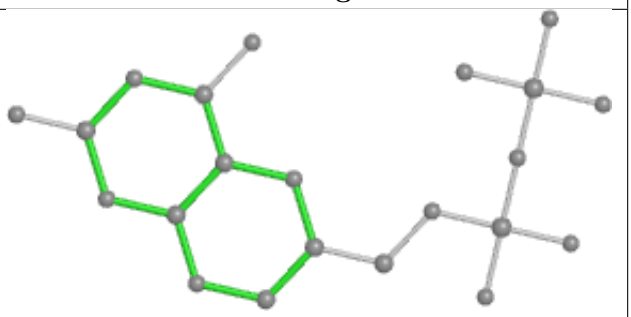
Bond lengths



Bond angles

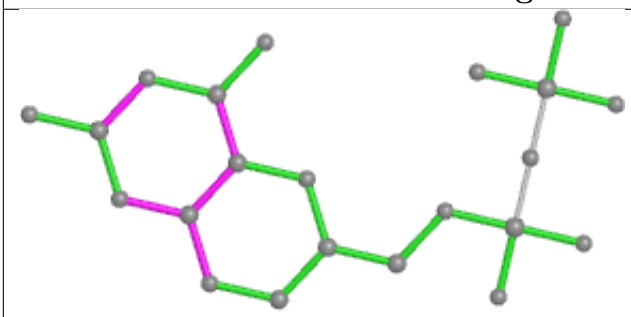


Torsions

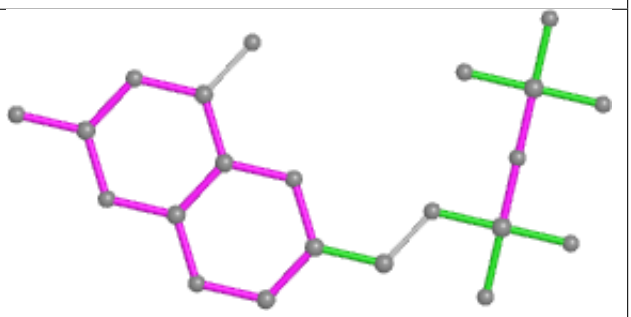


Rings

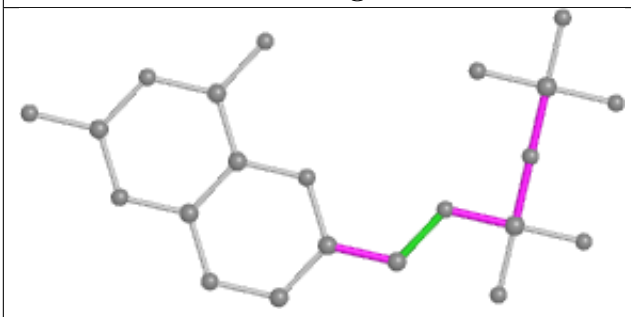
Ligand HH2 C 1101



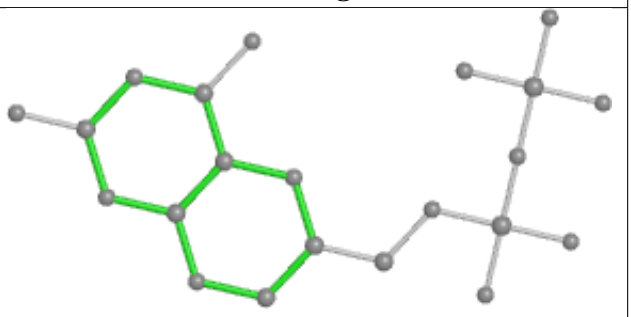
Bond lengths



Bond angles

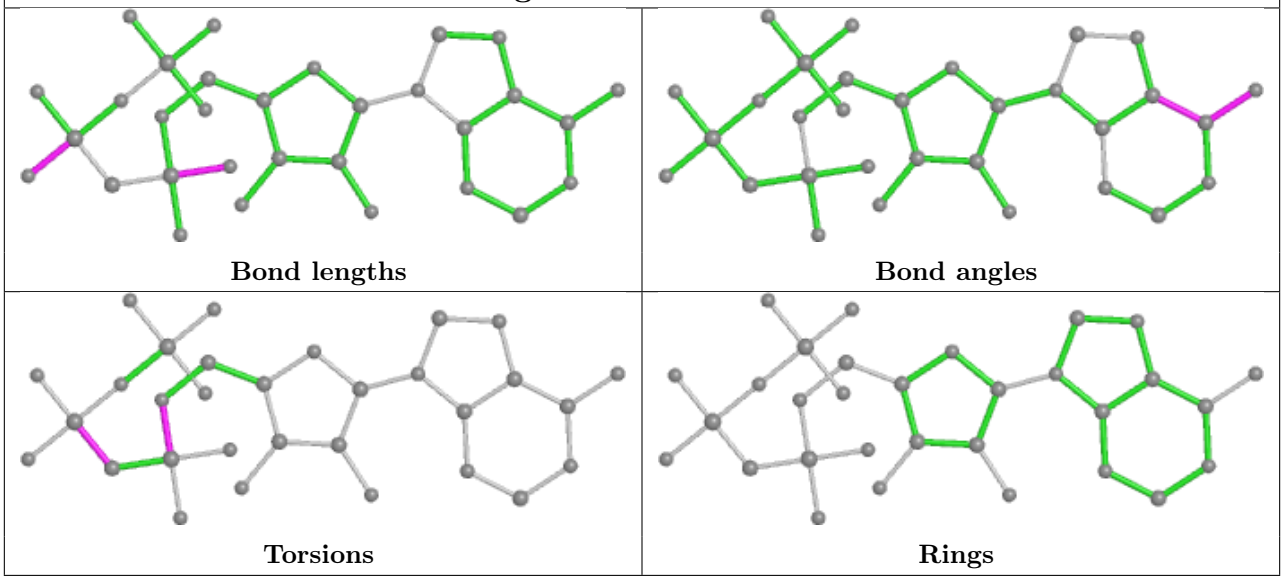


Torsions

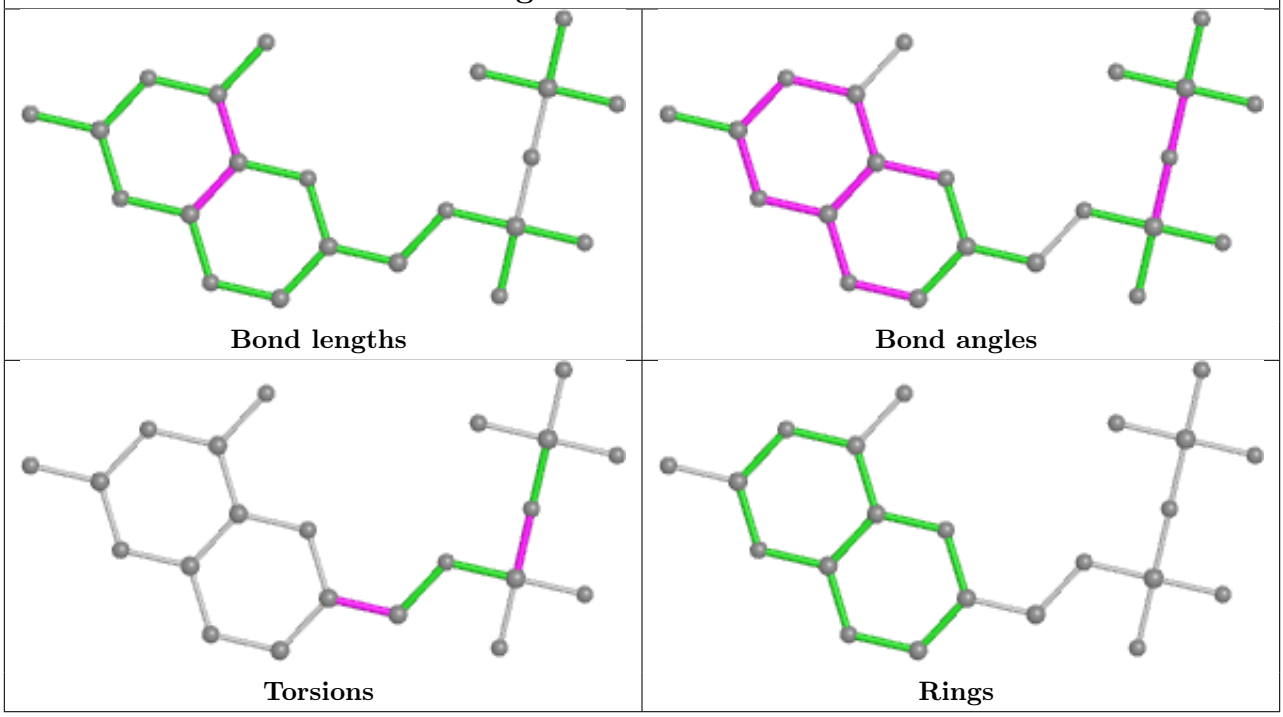


Rings

Ligand APC A 1102



Ligand HH2 A 1101



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	588/717 (82%)	-0.09	12 (2%)	65	63	26, 37, 51, 62	0
1	B	562/717 (78%)	0.10	9 (1%)	72	71	36, 53, 78, 93	0
1	C	599/717 (83%)	-0.13	16 (2%)	54	50	23, 35, 52, 72	0
1	D	577/717 (80%)	-0.12	10 (1%)	70	69	27, 36, 54, 68	0
1	E	584/717 (81%)	0.00	8 (1%)	75	75	35, 48, 65, 76	0
1	F	566/717 (78%)	0.00	9 (1%)	72	71	35, 47, 63, 72	0
All	All	3476/4302 (80%)	-0.04	64 (1%)	68	67	23, 42, 65, 93	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	414	CYS	4.3
1	A	58	TYR	4.0
1	D	76	PRO	3.9
1	F	58	TYR	3.8
1	D	155	TYR	3.7
1	A	418	GLY	3.6
1	C	73	GLY	3.6
1	C	667	GLN	3.6
1	F	311	HIS	3.3
1	D	71	THR	3.3
1	C	148	LEU	3.3
1	C	155	TYR	3.2
1	C	311	HIS	3.2
1	B	140	ASN	3.2
1	A	203	ASN	3.0
1	A	658	TRP	3.0
1	B	717	PRO	2.9
1	D	58	TYR	2.9
1	C	157	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	94	TYR	2.8
1	E	58	TYR	2.8
1	F	242	HIS	2.8
1	C	668	ASP	2.7
1	A	10	THR	2.7
1	E	59	ILE	2.7
1	D	307	GLU	2.6
1	C	306	PHE	2.6
1	A	668	ASP	2.5
1	D	311	HIS	2.5
1	C	154	LYS	2.5
1	F	671	GLN	2.4
1	D	59	ILE	2.4
1	A	308	GLU	2.4
1	A	421	VAL	2.4
1	C	69	GLU	2.4
1	C	310	TYR	2.4
1	E	387	VAL	2.3
1	F	310	TYR	2.3
1	E	134	ARG	2.3
1	B	674	TYR	2.3
1	F	141	ASP	2.3
1	E	130	GLU	2.3
1	A	436	SER	2.3
1	A	310	TYR	2.3
1	C	156	TYR	2.3
1	B	244	SER	2.2
1	A	669	LYS	2.2
1	B	672	LEU	2.2
1	F	308	GLU	2.2
1	D	78	ASP	2.1
1	C	658	TRP	2.1
1	B	143	ILE	2.1
1	C	308	GLU	2.1
1	B	159	TYR	2.1
1	D	156	TYR	2.1
1	B	55	VAL	2.0
1	F	103	GLU	2.0
1	D	672	LEU	2.0
1	C	664	HIS	2.0
1	E	517	ASP	2.0
1	A	587	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	60	VAL	2.0
1	E	124	VAL	2.0
1	C	669	LYS	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
7	5AD	B	1102	18/18	0.74	0.34	29,41,55,57	18
3	APC	C	1102	31/31	0.79	0.34	39,77,109,115	31
7	5AD	D	1102	18/18	0.81	0.36	18,31,40,41	18
5	MG	E	1103	1/1	0.83	0.11	28,28,28,28	0
6	PE0	D	1105	12/12	0.83	0.34	55,68,73,75	0
5	MG	A	1104	1/1	0.84	0.21	31,31,31,31	0
3	APC	A	1102	31/31	0.85	0.23	17,49,94,109	31
4	PAB	B	1103	10/10	0.89	0.26	39,48,55,84	0
6	PE0	E	1104	12/12	0.89	0.23	28,32,34,35	12
4	PAB	F	1102	10/10	0.89	0.30	19,24,26,29	10
6	PE0	A	1105	12/12	0.89	0.39	36,44,50,51	12
6	PE0	C	1105	12/12	0.90	0.18	44,51,59,63	12
4	PAB	E	1102	10/10	0.91	0.36	32,40,54,65	0
2	HH2	B	1101	22/22	0.92	0.19	23,41,52,56	0
4	PAB	D	1103	10/10	0.92	0.29	23,38,59,88	0
2	HH2	A	1101	22/22	0.94	0.16	22,28,51,56	0
2	HH2	F	1101	22/22	0.94	0.18	42,50,72,76	0
2	HH2	E	1101	22/22	0.95	0.16	27,43,56,60	0
5	MG	C	1104	1/1	0.95	0.09	32,32,32,32	0
4	PAB	A	1103	10/10	0.95	0.27	35,45,53,66	0

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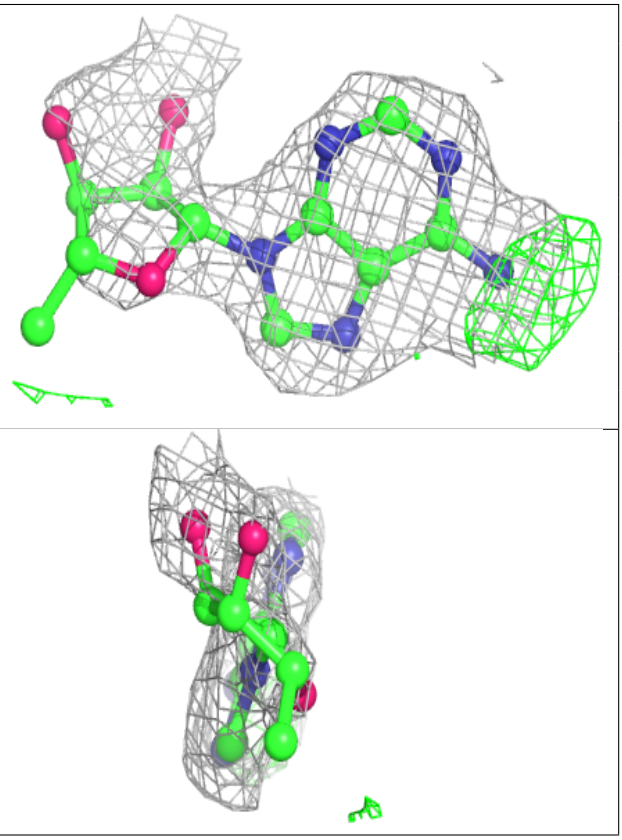
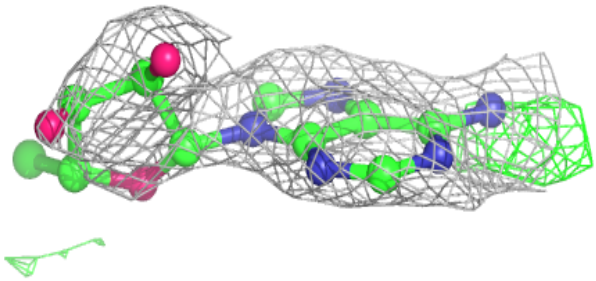
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	D	1104	1/1	0.96	0.10	27,27,27,27	0
4	PAB	C	1103	10/10	0.96	0.22	14,22,28,41	0
2	HH2	C	1101	22/22	0.96	0.14	28,37,43,52	0
2	HH2	D	1101	22/22	0.96	0.15	23,31,38,44	0

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 5AD B 1102:

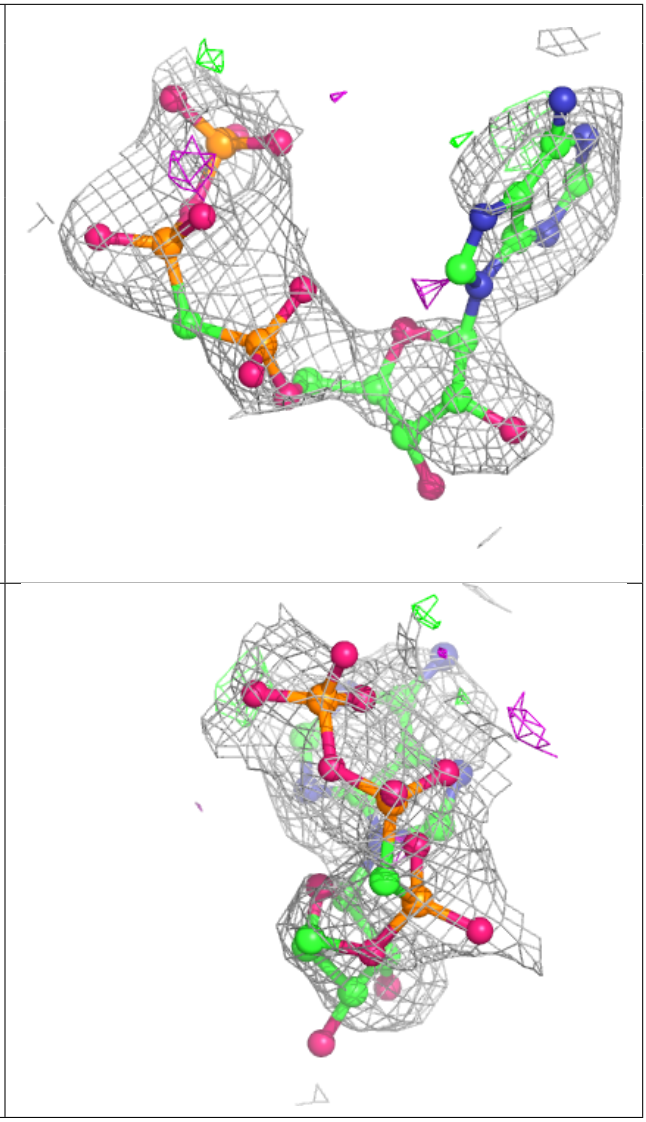
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)





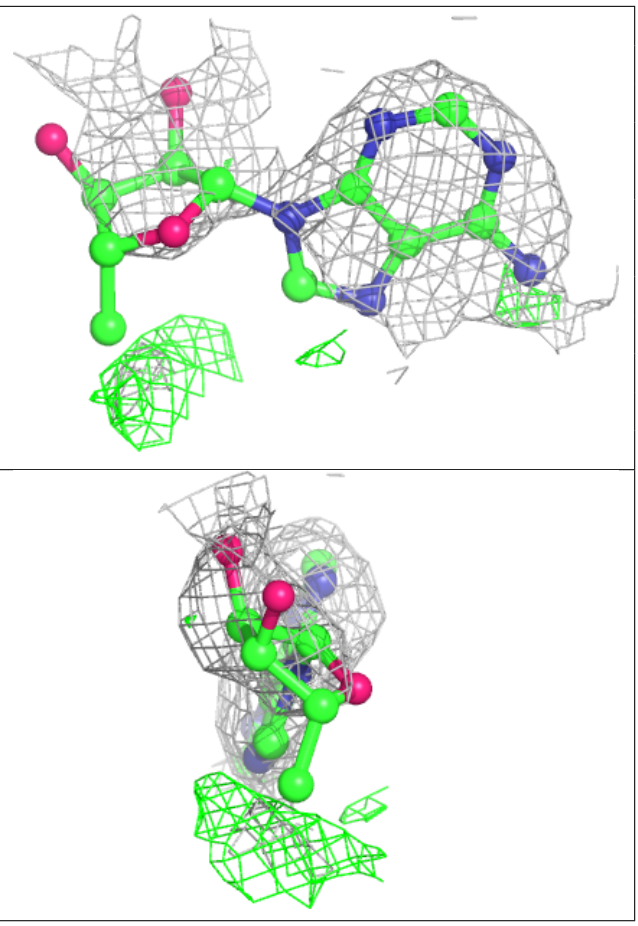
Electron density around APC C 1102:

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



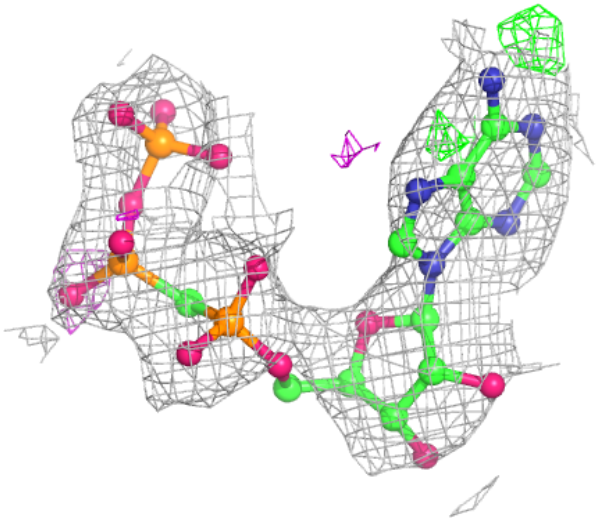
Electron density around 5AD D 1102:

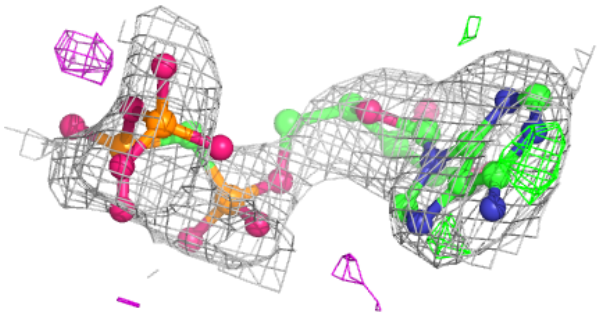
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

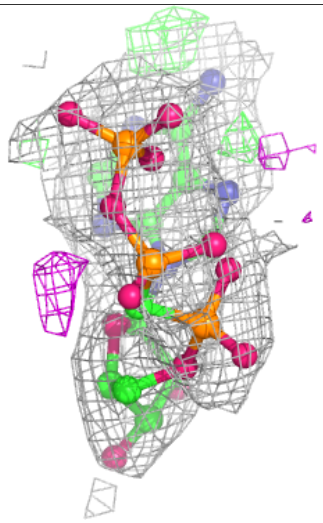


Electron density around APC A 1102:

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







Electron density around HH2 B 1101:

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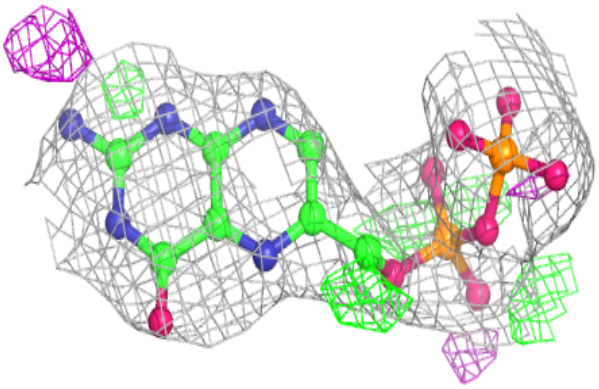
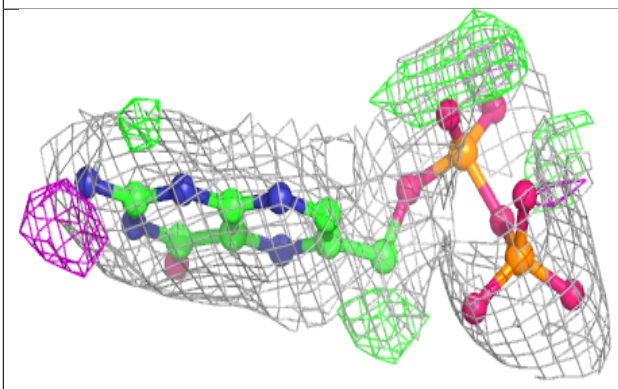
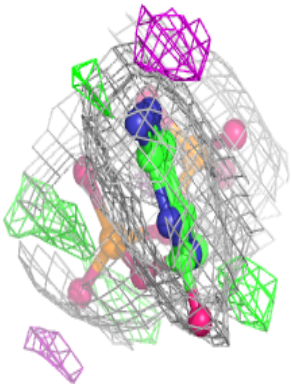
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

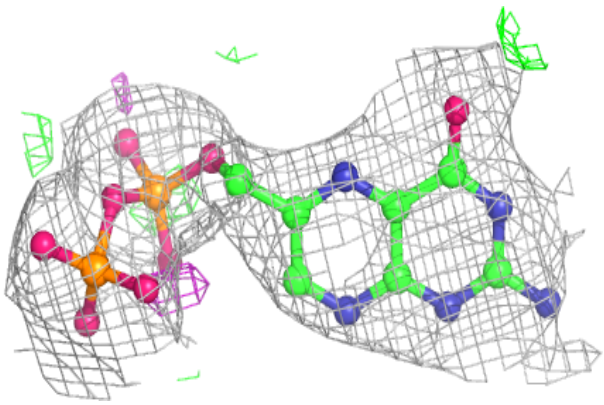


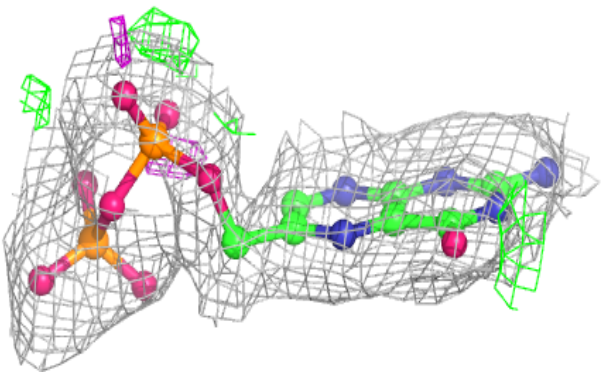


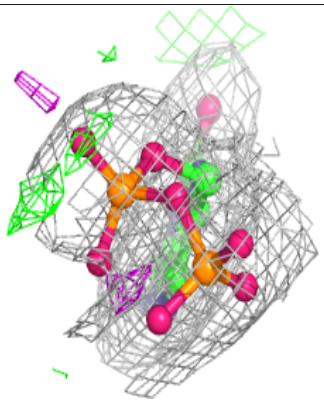


Electron density around HH2 A 1101:

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

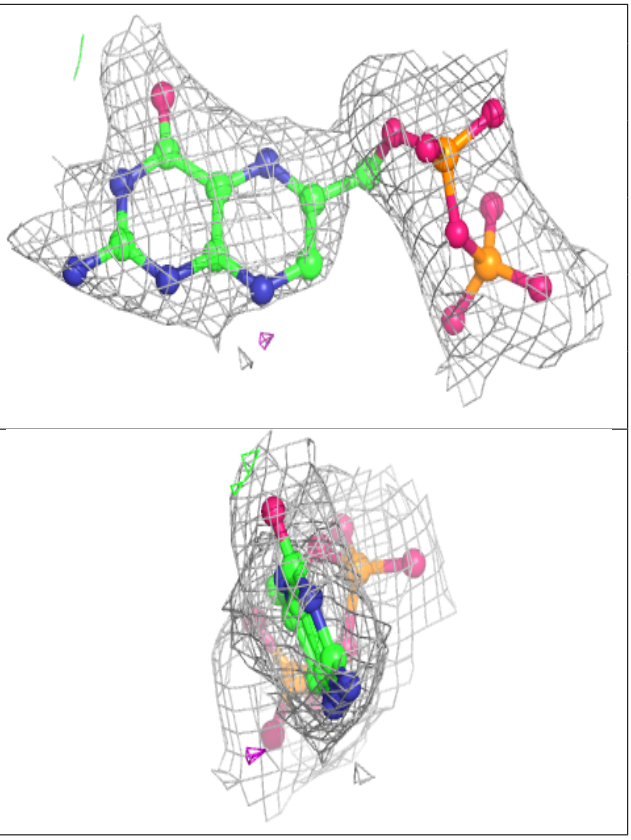


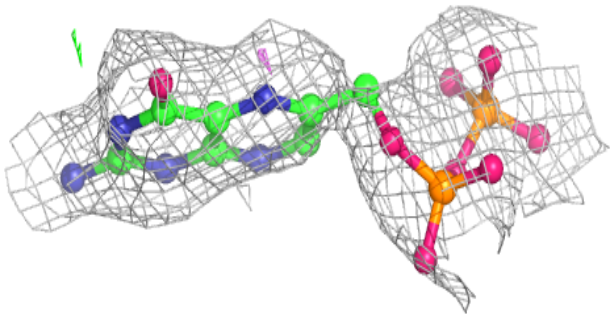




Electron density around HH2 F 1101:

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





Electron density around HH2 E 1101:

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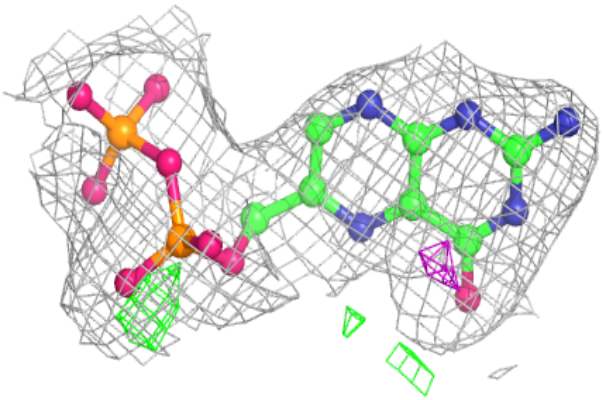
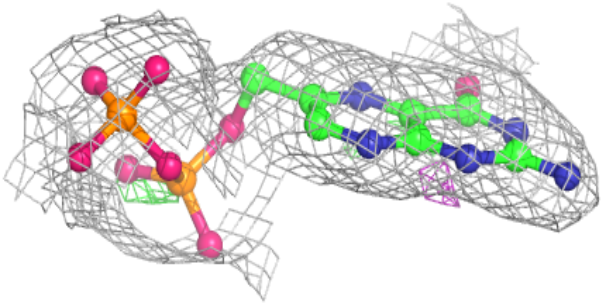
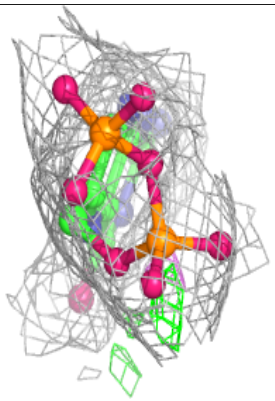
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HH2 C 1101:

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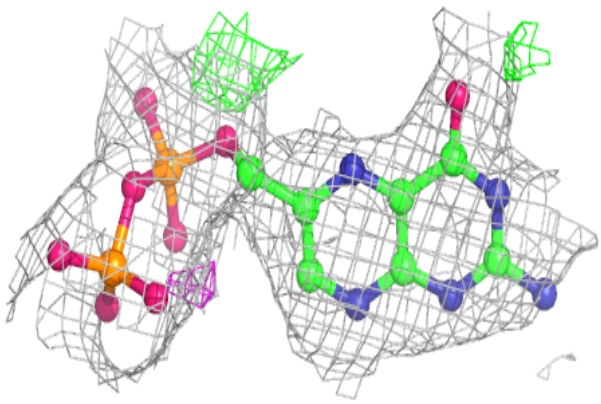
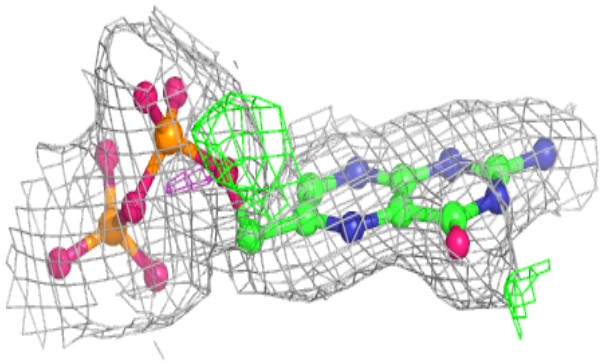
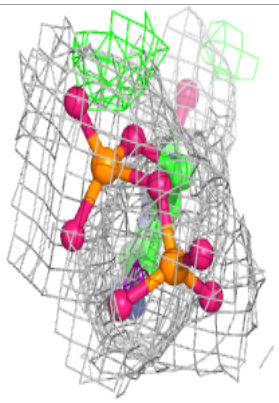
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

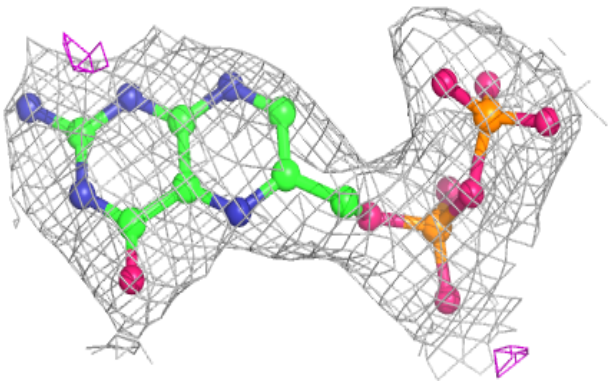


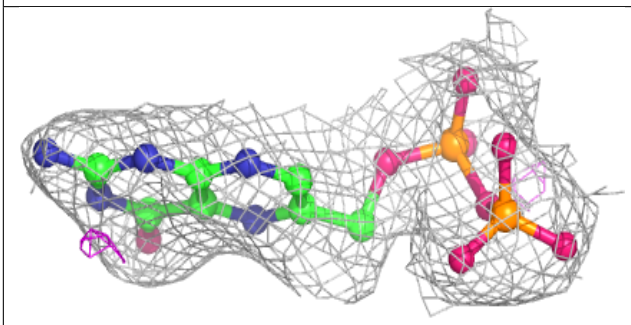


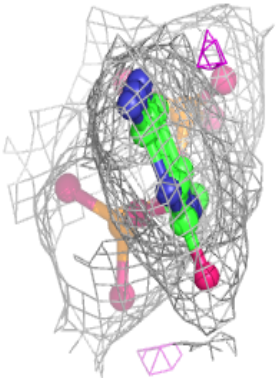


Electron density around HH2 D 1101:

$2mF_o$-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.