



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:24 AM UTC

PDB ID : 5Z79 / pdb_00005z79
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

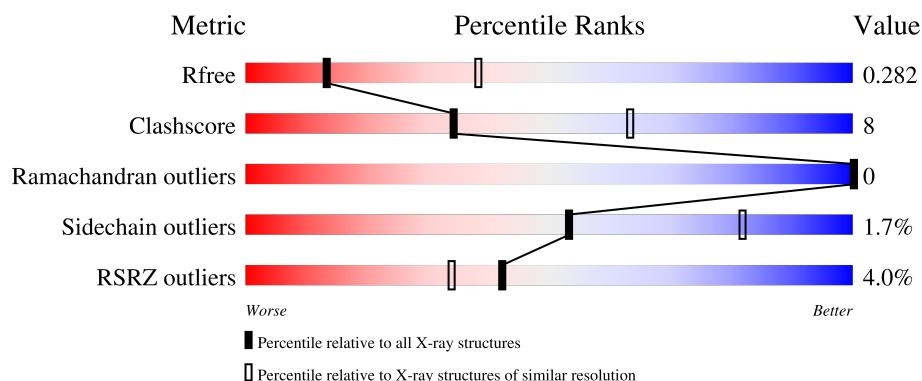
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	717	3% 65% 17% 18%
1	B	717	7% 63% 15% 22%
1	C	717	2% 67% 15% 16%
1	D	717	3% 63% 16% 20%
1	E	717	2% 72% 9% 19%

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Mol	Chain	Length	Quality of chain
1	F	717	3% 62% 16% • 21%

2 Entry composition

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.

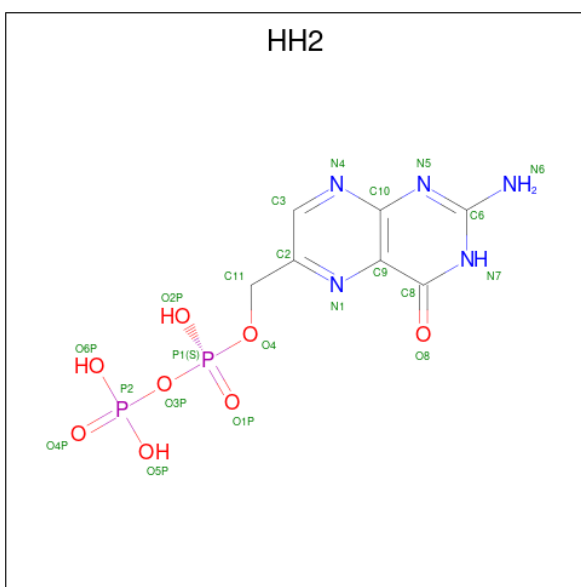
- Molecule 1 is a protein called Hydroxymethyldihydropterin pyrophosphokinase-dihydropter oate synthase, putative.

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

There are 6 discrepancies between the modelled and reference sequences:

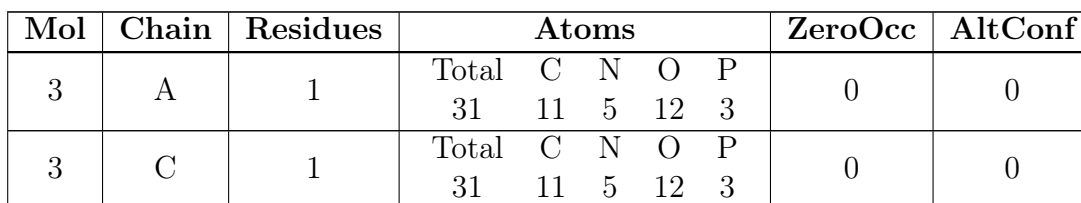
Chain	Residue	Modelled	Actual	Comment	Reference
A	383	ALA	GLY	see sequence details	UNP A0A1K9YMY7
B	383	ALA	GLY	see sequence details	UNP A0A1K9YMY7
C	383	ALA	GLY	see sequence details	UNP A0A1K9YMY7
D	383	ALA	GLY	see sequence details	UNP A0A1K9YMY7
E	383	ALA	GLY	see sequence details	UNP A0A1K9YMY7
F	383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

- Molecule 2 is 6-HYDROXYMETHYLPTERIN-DIPHOSPHATE (CCD ID: 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 (CCD ID: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



- PAB
-
- The chemical structure of PAB (4-aminobenzoic acid) is shown. It consists of a benzene ring with a carboxylic acid group (-COOH) at position 1 and an amino group (-NH₂) at position 4. The atoms are labeled as follows: C1, C2, C3, C4, C5, C6 for the benzene ring carbons; C1' for the carbonyl carbon; O1' for the carbonyl oxygen; O2' for the hydroxyl oxygen; and N4 for the amino group nitrogen. The labels are color-coded: C1-C6 are green, O1' and O2' are red, and N4 is blue.

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



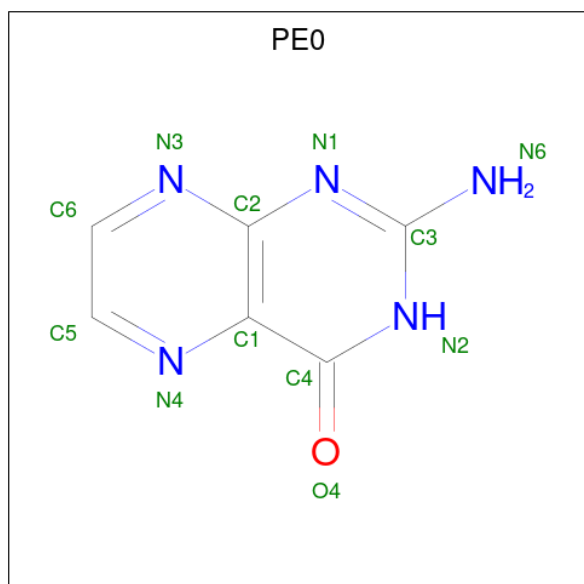
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			10	7	1	2		
4	D	1	Total	C	N	O	0	0
			10	7	1	2		
4	E	1	Total	C	N	O	0	0
			10	7	1	2		
4	F	1	Total	C	N	O	0	0
			10	7	1	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is PTERINE (CCD ID: PE0) (formula: C₆H₅N₅O).



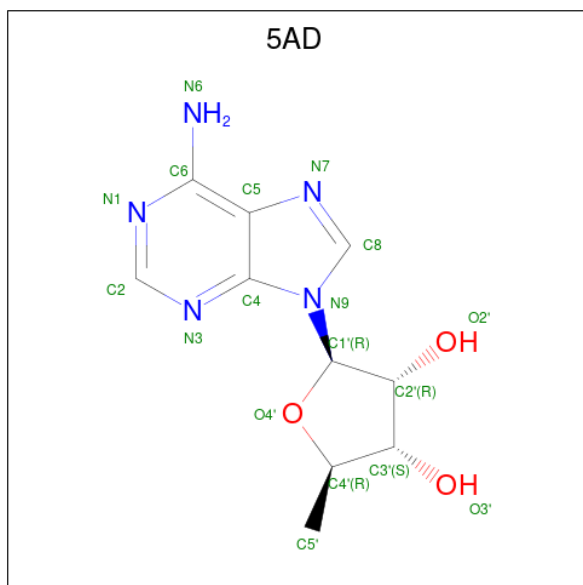
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	6	5	1		

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

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



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

- Molecule 8 is water.

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

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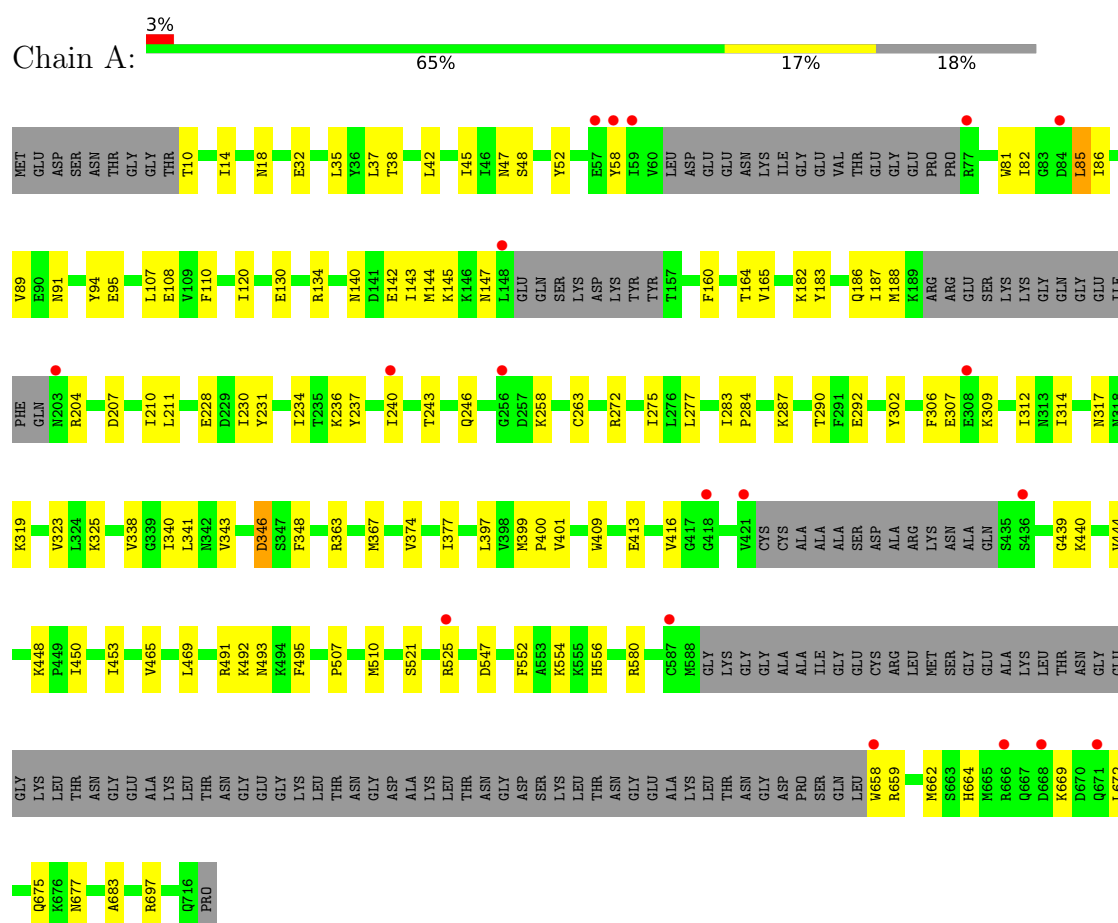
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	37	Total	O	0	0
			37	37		
8	F	19	Total	O	0	0
			19	19		

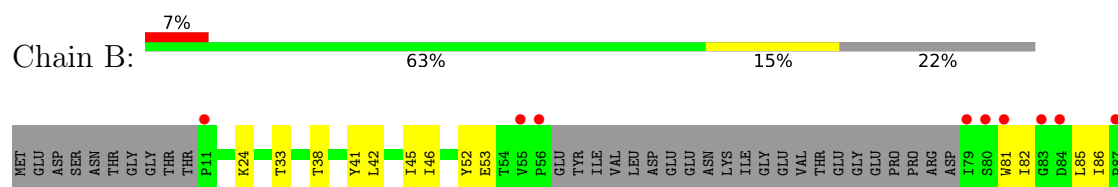
3 Residue-property plots

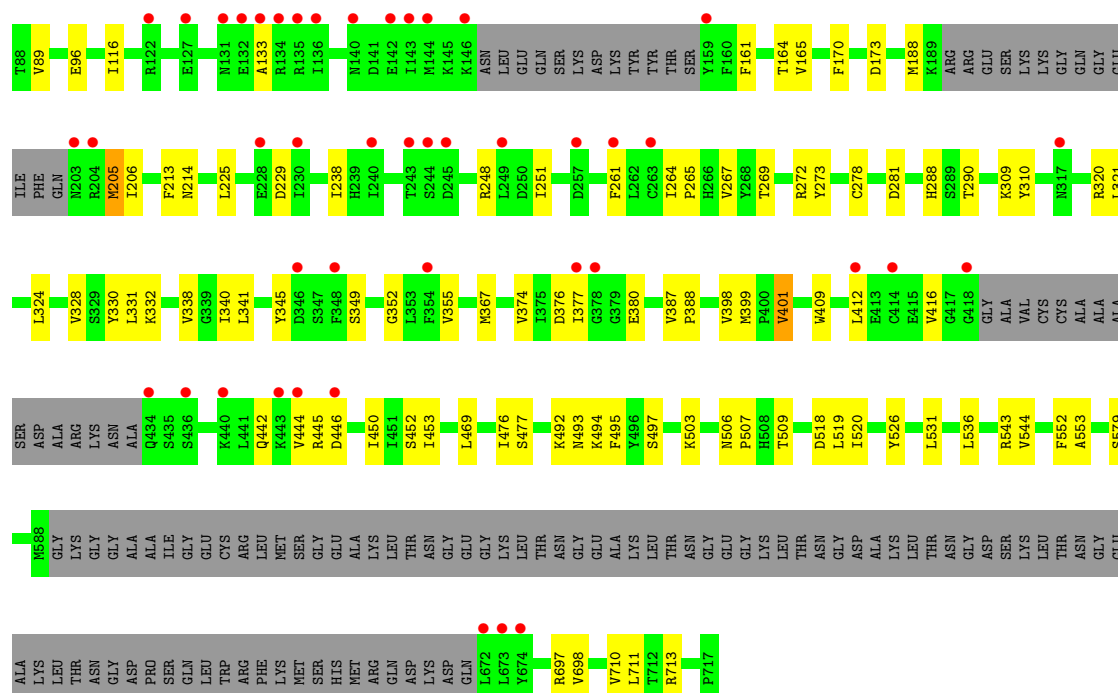
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

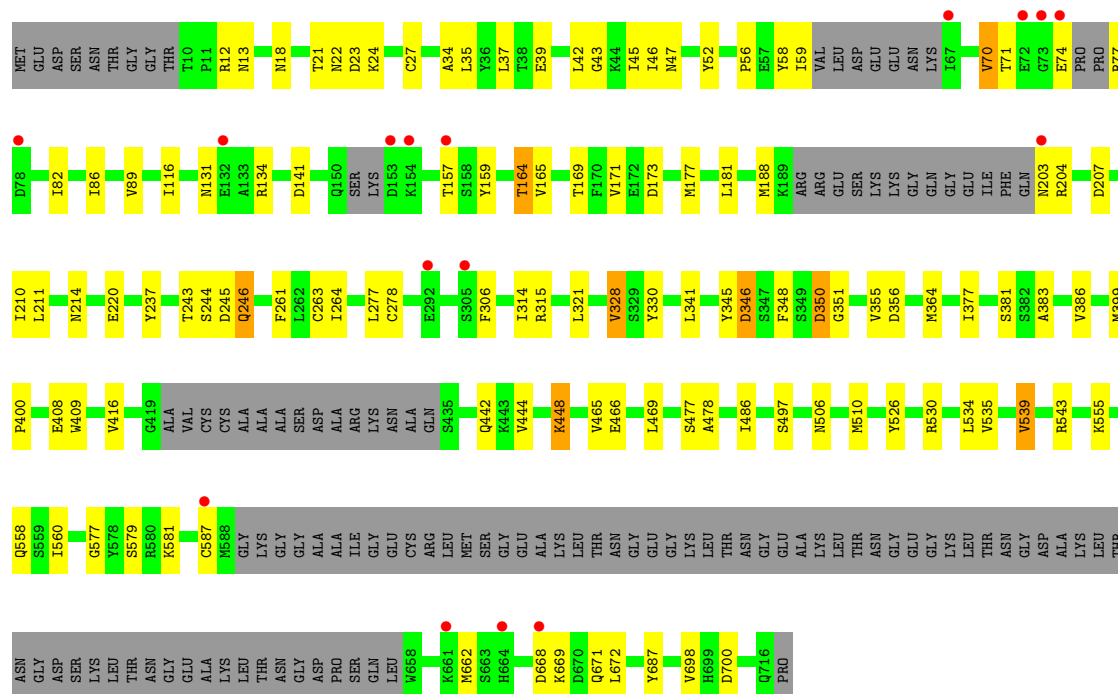


- Molecule 1: Hydroxymethyldihydropterin pyrophosphokinase-dihydropteroate synthase, putative

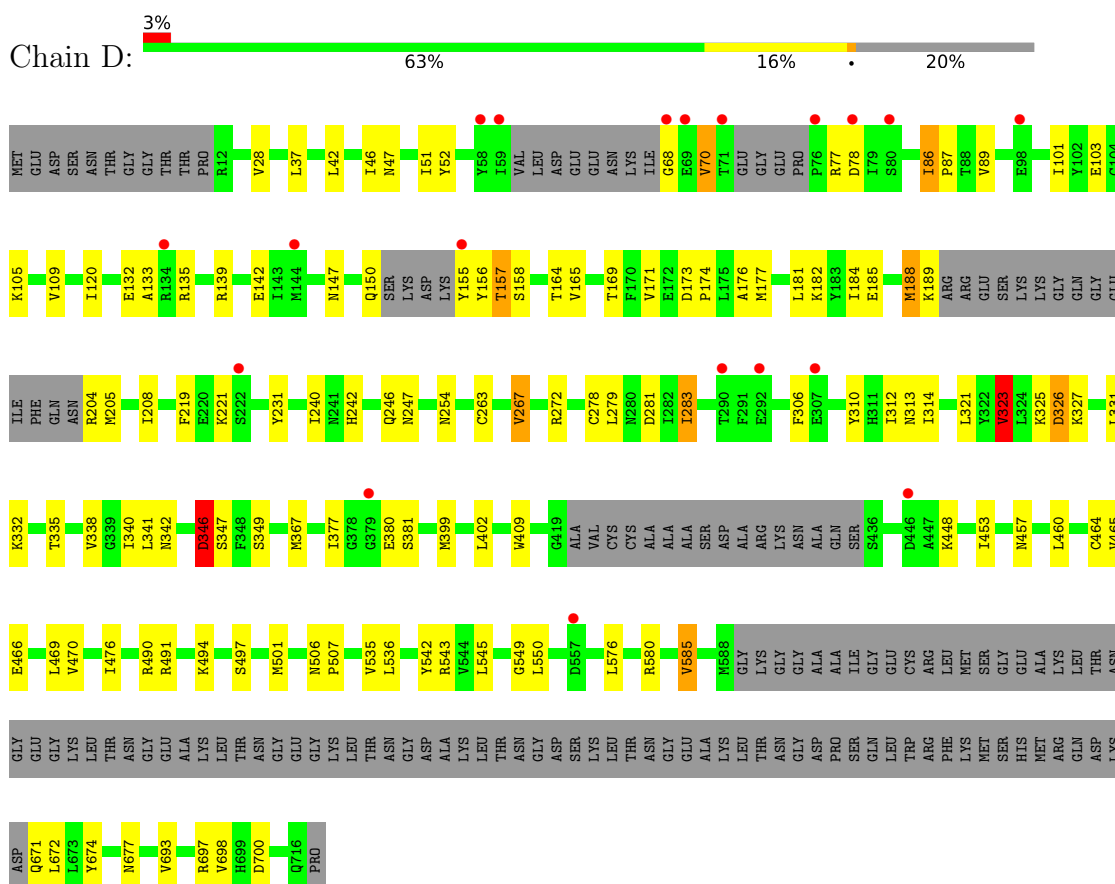




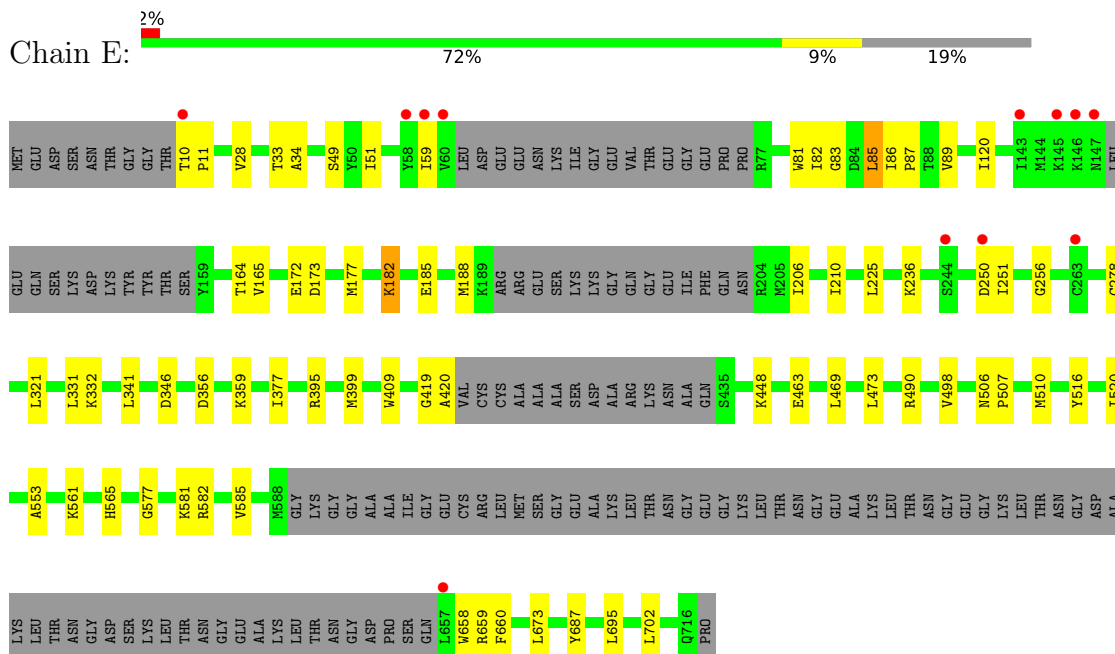
- Molecule 1: Hydroxymethyldihydropterin pyrophosphokinase-dihydropteroate synthase, putative



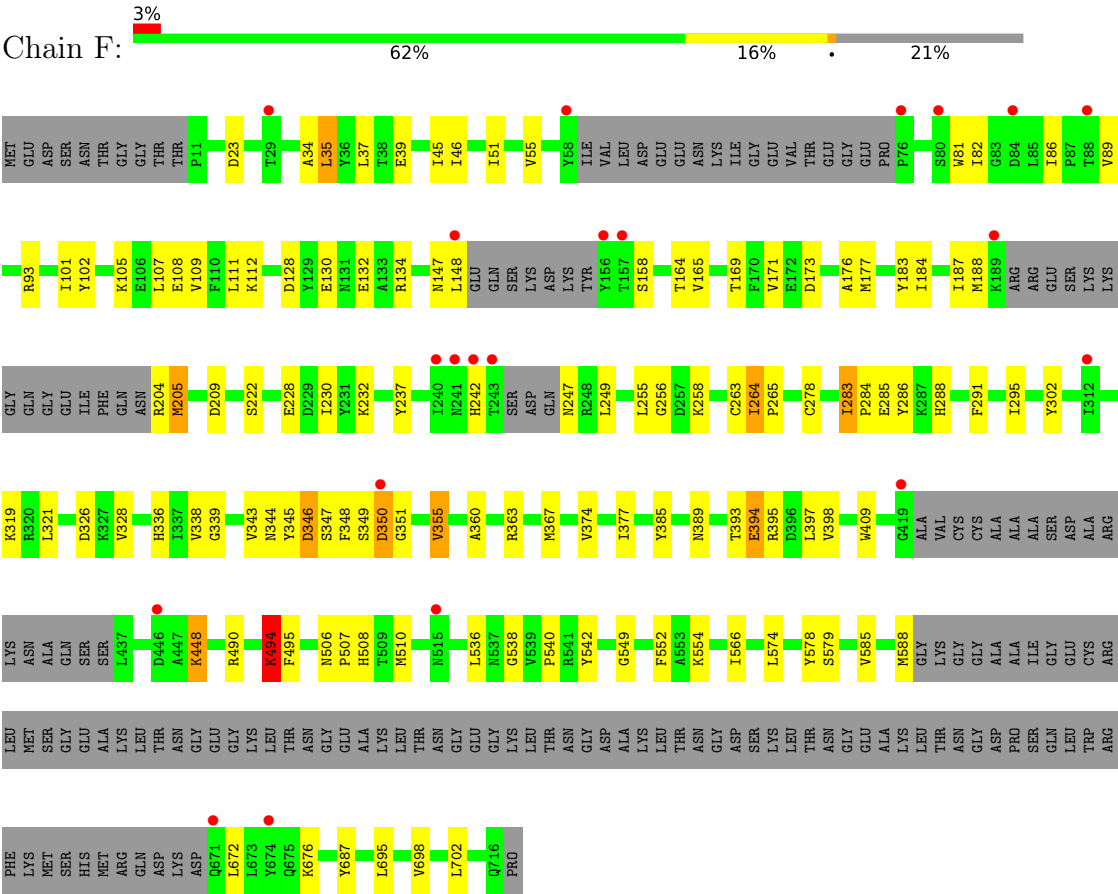
- Molecule 1: Hydroxymethyldihydropterin pyrophosphokinase-dihydropteroate synthase, putative



- Molecule 1: Hydroxymethyldihydropterin pyrophosphokinase-dihydropteroate synthase, putative



- Molecule 1: Hydroxymethyldihydropterin pyrophosphokinase-dihydropteroate synthase, putative



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 5AD, MG, PE0, PAB, HH2, APC

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	1.05	7/4920 (0.1%)	1.10	9/6638 (0.1%)
1	B	0.93	2/4601 (0.0%)	1.04	5/6230 (0.1%)
1	C	1.04	2/4999 (0.0%)	1.12	13/6746 (0.2%)
1	D	1.00	3/4815 (0.1%)	1.09	8/6498 (0.1%)
1	E	0.87	1/4881 (0.0%)	1.01	5/6591 (0.1%)
1	F	0.92	1/4697 (0.0%)	1.06	17/6342 (0.3%)
All	All	0.97	16/28913 (0.1%)	1.07	57/39045 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	324	LEU	CA-C	-8.13	1.42	1.52
1	A	547	ASP	C-O	-7.38	1.15	1.23
1	F	209	ASP	C-O	-5.73	1.16	1.23
1	A	85	LEU	C-O	-5.60	1.16	1.24
1	D	346	ASP	C-O	-5.46	1.17	1.24
1	A	246	GLN	C-O	-5.41	1.18	1.23
1	E	59	ILE	CA-CB	5.36	1.59	1.53
1	C	164	THR	C-O	-5.36	1.17	1.23
1	A	397	LEU	C-O	-5.26	1.18	1.24
1	A	323	VAL	C-O	-5.25	1.18	1.24
1	D	323	VAL	C-O	-5.24	1.18	1.24
1	A	325	LYS	C-O	-5.18	1.17	1.24
1	A	492	LYS	CA-C	5.18	1.58	1.53
1	C	442	GLN	C-O	-5.16	1.18	1.24
1	D	585	VAL	C-O	-5.14	1.17	1.24
1	B	213	PHE	C-O	-5.00	1.18	1.24

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	205	MET	N-CA-C	10.92	123.19	111.28
1	C	70	VAL	N-CA-C	9.64	122.02	109.58
1	F	494	LYS	N-CA-C	9.02	123.63	110.28
1	F	222	SER	N-CA-C	7.76	120.72	111.02
1	F	264	ILE	CB-CA-C	-7.68	102.68	110.13
1	C	668	ASP	N-CA-C	7.58	119.62	111.36
1	B	173	ASP	CA-C-N	6.77	126.28	119.24
1	B	173	ASP	C-N-CA	6.77	126.28	119.24
1	F	158	SER	N-CA-C	6.48	123.56	113.72
1	B	205	MET	N-CA-C	6.39	118.12	111.03
1	F	448	LYS	CA-C-N	-6.39	113.09	119.99
1	F	448	LYS	C-N-CA	-6.39	113.09	119.99
1	A	243	THR	N-CA-C	6.32	120.58	109.96
1	A	246	GLN	N-CA-C	6.32	118.33	107.28
1	D	70	VAL	N-CA-C	6.23	116.89	108.17
1	C	539	VAL	CA-C-N	-6.12	113.64	119.76
1	C	539	VAL	C-N-CA	-6.12	113.64	119.76
1	A	323	VAL	N-CA-C	6.10	116.90	108.12
1	D	86	ILE	CA-C-N	-6.04	113.41	120.12
1	D	86	ILE	C-N-CA	-6.04	113.41	120.12
1	D	188	MET	N-CA-C	-5.94	101.67	110.46
1	B	492	LYS	CB-CA-C	-5.88	109.81	116.63
1	A	319	LYS	N-CA-C	5.87	118.96	109.40
1	E	346	ASP	N-CA-C	5.72	119.62	107.67
1	C	86	ILE	CB-CA-C	-5.69	106.55	114.00
1	C	346	ASP	N-CA-C	5.69	117.88	108.49
1	F	687	TYR	N-CA-C	-5.64	105.05	111.14
1	C	173	ASP	N-CA-C	5.62	113.19	108.13
1	A	346	ASP	N-CA-C	5.59	117.19	109.54
1	E	173	ASP	N-CA-C	5.58	114.72	108.25
1	F	204	ARG	CA-C-N	5.58	127.76	120.28
1	F	204	ARG	C-N-CA	5.58	127.76	120.28
1	F	355	VAL	N-CA-C	-5.56	105.69	111.58
1	A	416	VAL	CB-CA-C	-5.52	104.91	111.97
1	C	350	ASP	CB-CA-C	-5.49	100.57	109.13
1	F	173	ASP	CA-C-N	5.40	124.73	118.85
1	F	173	ASP	C-N-CA	5.40	124.73	118.85
1	E	28	VAL	N-CA-C	5.40	115.60	110.53
1	C	687	TYR	N-CA-C	-5.38	105.50	111.36
1	A	556	HIS	N-CA-C	5.37	116.81	111.07
1	E	185	GLU	N-CA-C	5.33	116.78	111.07
1	C	157	THR	N-CA-C	-5.33	101.96	109.96
1	D	254	ASN	N-CA-C	5.31	119.39	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	395	ARG	N-CA-C	5.21	116.64	111.07
1	B	269	THR	N-CA-C	5.20	116.95	111.28
1	D	283	ILE	CA-C-N	5.20	125.00	119.28
1	D	283	ILE	C-N-CA	5.20	125.00	119.28
1	D	677	ASN	N-CA-C	5.16	116.59	111.07
1	E	687	TYR	N-CA-C	-5.15	105.35	110.97
1	C	356	ASP	CA-C-N	-5.12	113.64	119.28
1	C	356	ASP	C-N-CA	-5.12	113.64	119.28
1	A	91	ASN	N-CA-C	5.11	117.28	110.53
1	C	246	GLN	N-CA-C	5.11	116.74	108.26
1	F	394	GLU	CA-C-N	5.10	127.07	120.44
1	F	394	GLU	C-N-CA	5.10	127.07	120.44
1	A	317	ASN	N-CA-C	5.04	119.38	112.88
1	F	350	ASP	N-CA-C	-5.00	108.92	114.62

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	78	0
1	B	4512	0	4436	72	0
1	C	4905	0	4895	84	0
1	D	4725	0	4740	75	0
1	E	4788	0	4785	47	0
1	F	4608	0	4606	84	0
2	A	22	0	6	1	0
2	B	22	0	6	0	0
2	C	22	0	6	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	435	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 8.

All (435) 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:B:340:ILE:O	1:B:367:MET:HE1	1.62	0.97
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
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:D:340:ILE:O	1:D:367:MET:HE1	1.84	0.76
1:C:204:ARG:CD	1:C:207:ASP:HB2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.73	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:F:37:LEU:HD12	1:F:188:MET:HE2	1.75	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:F:585:VAL:HA	1:F:588:MET:HE3	1.79	0.65
1:C:364:MET:HE3	1:C:377:ILE:HD11	1.77	0.65
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:B:320:ARG:C	1:B:321:LEU:HD12	2.22	0.64
1:B:399:MET:HE1	1:B:469:LEU:HD13	1.79	0.64
1:A:210:ILE:H	3:A:1102:APC:HN61	1.45	0.64
1:C:34:ALA:HA	1:C:188:MET:HE1	1.79	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:B:33:THR:HG22	1:B:188:MET:HE3	1.82	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:VAL:HG11	1:D:491:ARG:HD2	1.83	0.60
1:E:577:GLY:HA3	2:E:1101:HH2:O8	2.02	0.59
1:F:176:ALA:O	1:F:177:MET:C	2.44	0.59
1:B:53:GLU:HG3	1:B:161:PHE:CE2	2.36	0.59
1:A:37:LEU:HD12	1:A:188:MET:HE2	1.86	0.58
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:D:37:LEU:HD12	1:D:188:MET:HE2	1.85	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:A:340:ILE:O	1:A:367:MET:HE1	2.05	0.57
1:D:77:ARG:HG2	1:D:78:ASP:N	2.19	0.57
1:A:399:MET:HE1	1:A:469:LEU:CD1	2.34	0.56
1:C:12:ARG:HG3	1:C:12:ARG:HH11	1.70	0.56
1:C:34:ALA:CA	1:C:188:MET:HE1	2.34	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:B:387:VAL:O	1:B:388:PRO:C	2.48	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: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:399:MET:HE1	1:E:469:LEU:CD1	2.36	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:F:147:ASN:O	1:F:148:LEU:C	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:399:MET:HE1	1:D:469:LEU:CD1	2.38	0.53
1:C:116:ILE:HD12	1:C:214:ASN:CG	2.33	0.53
1:C:526:TYR:O	1:C:530:ARG:HG2	2.09	0.53
1:D:399:MET:HE1	1:D:469:LEU:HD13	1.90	0.53
1:F:702:LEU:C	1:F:702:LEU:HD23	2.33	0.53
1:A:491:ARG:NH1	1:A:491:ARG:CB	2.72	0.53
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:F:34:ALA:HA	1:F:188:MET:HE1	1.91	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:A:107:LEU:O	1:A:108:GLU:C	2.51	0.52
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: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:C:399:MET:HE1	1:C:469:LEU:HD13	1.91	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:A:363:ARG:HH21	1:A:367:MET:HE3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:476:ILE:HB	1:D:501:MET:HE2	1.93	0.51
1:B:476:ILE:O	1:B:477:SER:CB	2.58	0.51
1:C:399:MET:HE1	1:C:469:LEU:CD1	2.40	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
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: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:C:246:GLN:HG3	1:C:246:GLN:O	2.11	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: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:A:507:PRO:HA	1:A:510:MET:HE3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:516:TYR:OH	1:E:553:ALA:O	2.31	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:C:662:MET:HE3	1:C:671:GLN:OE1	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:B:518:ASP:O	1:B:519:LEU:C	2.55	0.48
1:C:530:ARG:O	1:C:534:LEU:HD23	2.13	0.48
1:B:506:ASN:OD1	1:B:509:THR:HG22	2.14	0.48
1:C:497:SER:HA	1:C:543:ARG:HB3	1.95	0.48
1:A:160:PHE:CD1	6:A:1105:PEO:O4	2.67	0.47
1:A:399:MET:HE1	1:A:469:LEU:HD11	1.94	0.47
1:D:176:ALA:O	1:D:177:MET:C	2.57	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:E:506:ASN:C	1:E:506:ASN:OD1	2.58	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:33:THR:HG22	1:B:188:MET:CE	2.44	0.47
1:B:338:VAL:HB	1:B:697:ARG:HA	1.95	0.47
1:E:82:ILE:O	1:E:83:GLY:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ARG:NH2	1:A:367:MET:HE3	2.30	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:34:ALA:CA	1:E:188:MET:HE1	2.44	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:132:GLU:O	1:D:133:ALA:C	2.58	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:F:264:ILE:HA	1:F:265:PRO:C	2.39	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:510:MET:HE1	1:F:552:PHE:CD2	2.50	0.46
1:C:171:VAL:CG2	1:C:177:MET:HE3	2.45	0.46
1:C:381:SER:OG	2:C:1101:HH2:O4P	2.30	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
1:D:342:ASN:ND2	2:D:1101:HH2:O1P	2.37	0.46
1:A:204:ARG:HH22	1:A:207:ASP:CG	2.24	0.45
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:A:164:THR:C	1:A:165:VAL:HG23	2.42	0.45
1:A:302:TYR:CD1	1:A:302:TYR:C	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:672:LEU:HD23	1:A:672:LEU:C	2.42	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:F:263:CYS:C	1:F:264:ILE:HD12	2.42	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:F:344:ASN:CG	1:F:347:SER:HG	2.25	0.45
1:A:399:MET:N	1:A:400:PRO:CD	2.80	0.45
1:D:313:ASN:O	1:D:314:ILE:C	2.60	0.45
1:F:350:ASP:O	1:F:351:GLY:C	2.60	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: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:D:184:ILE:HG22	1:D:188:MET:HE3	1.98	0.44
1:C:13:ASN:O	1:C:169:THR:HG22	2.18	0.44
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:93:ARG:HG3	1:F:237:TYR:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:272:ARG:O	1:B:273:TYR:C	2.61	0.43
1:F:23:ASP:C	1:F:23:ASP:OD1	2.61	0.43
1:D:549:GLY:O	1:D:550:LEU:C	2.61	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: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: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:E:33:THR:HG22	1:E:188:MET:HE2	1.99	0.43
1:A:263:CYS:HB3	3:A:1102:APC:H2	2.00	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:D:52:TYR:OH	1:D:281:ASP:OD2	2.35	0.43
1:E:507:PRO:HA	1:E:510:MET:HE3	2.00	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:B:261:PHE:CD1	1:B:261:PHE:C	2.96	0.42
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:B:321:LEU:HD23	1:B:328:VAL:CB	2.45	0.42
1:C:350:ASP:O	1:C:351:GLY:C	2.63	0.42
1:D:247:ASN:OD1	1:D:247:ASN:C	2.62	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:171:VAL:HG21	1:C:177:MET:HE3	2.01	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:F:348:PHE:O	1:F:348:PHE:CD1	2.72	0.42
1:F:578:TYR:O	1:F:579:SER:C	2.62	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:264:ILE:HA	1:B:265:PRO:C	2.45	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:A:439:GLY:O	1:A:440:LYS:C	2.63	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:34:ALA:HA	1:E:188:MET:HE1	2.01	0.41
1:F:255:LEU:O	1:F:258:LYS:HB2	2.21	0.41
1:F:264:ILE:HD12	1:F:264:ILE:N	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: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:81:TRP:CD1	1:B:81:TRP:H	2.38	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:81:TRP:CD1	1:E:81:TRP:H	2.39	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:465:VAL:CG1	1:A:491:ARG:HD3	2.49	0.41
1:B:399:MET:HE1	1:B:469:LEU:CD1	2.50	0.41
1:B:526:TYR:CD1	1:B:526:TYR:C	2.98	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: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:D:185:GLU:OE1	1:D:204:ARG:NH2	2.54	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:477:SER:O	1:C:478:ALA:C	2.64	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
1:F:302:TYR:CD1	1:F:302:TYR:C	2.99	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 ⓘ

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%)	534 (98%)	8 (2%)	57	84
1	B	494/647 (76%)	488 (99%)	6 (1%)	63	86
1	C	546/647 (84%)	538 (98%)	8 (2%)	57	84
1	D	526/647 (81%)	509 (97%)	17 (3%)	34	68
1	E	534/647 (82%)	528 (99%)	6 (1%)	65	88
1	F	510/647 (79%)	502 (98%)	8 (2%)	55	83
All	All	3152/3882 (81%)	3099 (98%)	53 (2%)	53	82

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ILE
1	A	85	LEU
1	A	95	GLU
1	A	120	ILE
1	A	290	THR
1	A	309	LYS
1	A	346	ASP
1	A	453	ILE
1	B	85	LEU
1	B	290	THR
1	B	380	GLU
1	B	401	VAL
1	B	453	ILE
1	B	494	LYS
1	C	82	ILE
1	C	203	ASN
1	C	328	VAL
1	C	346	ASP
1	C	448	LYS
1	C	535	VAL
1	C	672	LEU
1	C	700	ASP

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Mol	Chain	Res	Type
1	D	28	VAL
1	D	157	THR
1	D	165	VAL
1	D	267	VAL
1	D	272	ARG
1	D	323	VAL
1	D	326	ASP
1	D	346	ASP
1	D	347	SER
1	D	380	GLU
1	D	453	ILE
1	D	490	ARG
1	D	494	LYS
1	D	576	LEU
1	D	672	LEU
1	D	698	VAL
1	D	700	ASP
1	E	85	LEU
1	E	165	VAL
1	E	182	LYS
1	E	206	ILE
1	E	490	ARG
1	E	695	LEU
1	F	35	LEU
1	F	55	VAL
1	F	205	MET
1	F	242	HIS
1	F	283	ILE
1	F	346	ASP
1	F	494	LYS
1	F	672	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	317	ASN
1	A	336	HIS
1	A	586	HIS
1	A	664	HIS
1	B	113	ASN
1	B	515	ASN

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Mol	Chain	Res	Type
1	B	556	HIS
1	B	565	HIS
1	B	567	HIS
1	C	117	ASN
1	C	482	ASN
1	C	556	HIS
1	D	254	ASN
1	D	288	HIS
1	D	336	HIS
1	D	442	GLN
1	D	482	ASN
1	D	493	ASN
1	D	556	HIS
1	D	675	GLN
1	E	246	GLN
1	E	254	ASN
1	E	481	HIS
1	E	556	HIS
1	F	186	GLN
1	F	247	ASN
1	F	266	HIS
1	F	313	ASN
1	F	481	HIS

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](#)

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
2	HH2	D	1101	5	22,23,23	1.33	3 (13%)	26,35,35	1.40	5 (19%)
3	APC	A	1102	-	29,33,33	0.74	2 (6%)	44,52,52	0.60	0
6	PE0	E	1104	-	13,13,13	1.49	2 (15%)	15,18,18	1.86	5 (33%)
2	HH2	E	1101	5	22,23,23	1.41	3 (13%)	26,35,35	1.85	8 (30%)
2	HH2	B	1101	-	22,23,23	1.33	3 (13%)	26,35,35	1.39	6 (23%)
4	PAB	D	1103	-	10,10,10	0.66	0	13,13,13	1.14	0
4	PAB	B	1103	-	10,10,10	0.67	0	13,13,13	1.21	0
4	PAB	A	1103	-	10,10,10	0.69	0	13,13,13	1.07	0
6	PE0	C	1105	-	13,13,13	1.62	3 (23%)	15,18,18	2.06	6 (40%)
2	HH2	A	1101	5	22,23,23	1.24	3 (13%)	26,35,35	1.43	4 (15%)
4	PAB	C	1103	-	10,10,10	0.65	0	13,13,13	1.27	1 (7%)
2	HH2	F	1101	-	22,23,23	1.41	3 (13%)	26,35,35	1.60	5 (19%)
6	PE0	A	1105	-	13,13,13	1.39	1 (7%)	15,18,18	1.71	5 (33%)
3	APC	C	1102	-	29,33,33	0.72	2 (6%)	44,52,52	0.63	1 (2%)
6	PE0	D	1105	-	13,13,13	1.45	3 (23%)	15,18,18	1.89	4 (26%)
2	HH2	C	1101	5	22,23,23	1.41	4 (18%)	26,35,35	1.82	6 (23%)
4	PAB	F	1102	-	10,10,10	0.75	0	13,13,13	0.84	0
7	5AD	D	1102	-	20,20,20	1.47	2 (10%)	28,30,30	2.28	7 (25%)
7	5AD	B	1102	-	20,20,20	1.65	4 (20%)	28,30,30	2.31	13 (46%)
4	PAB	E	1102	-	10,10,10	0.67	0	13,13,13	1.11	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
2	HH2	D	1101	5	-	6/12/12/12	0/2/2/2
3	APC	A	1102	-	-	5/19/38/38	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	B	1101	-	-	4/12/12/12	0/2/2/2
4	PAB	D	1103	-	-	0/4/4/4	0/1/1/1
4	PAB	B	1103	-	-	0/4/4/4	0/1/1/1
4	PAB	A	1103	-	-	0/4/4/4	0/1/1/1
6	PE0	C	1105	-	-	-	0/2/2/2
2	HH2	A	1101	5	-	4/12/12/12	0/2/2/2
4	PAB	C	1103	-	-	0/4/4/4	0/1/1/1
2	HH2	F	1101	-	-	6/12/12/12	0/2/2/2
6	PE0	A	1105	-	-	-	0/2/2/2
3	APC	C	1102	-	-	8/19/38/38	0/3/3/3
6	PE0	D	1105	-	-	-	0/2/2/2
2	HH2	C	1101	5	-	6/12/12/12	0/2/2/2
4	PAB	F	1102	-	-	0/4/4/4	0/1/1/1
7	5AD	D	1102	-	-	0/4/20/20	0/3/3/3
7	5AD	B	1102	-	-	0/4/20/20	0/3/3/3
4	PAB	E	1102	-	-	0/4/4/4	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1102	5AD	C5-C4	4.70	1.47	1.39
2	B	1101	HH2	C9-C10	4.04	1.48	1.40
6	C	1105	PE0	C4-N2	-4.02	1.31	1.37
2	E	1101	HH2	P1-O3P	3.94	1.63	1.59
2	F	1101	HH2	C9-C10	3.81	1.48	1.40
6	E	1104	PE0	C4-N2	-3.79	1.32	1.37
2	A	1101	HH2	C9-C10	3.74	1.48	1.40
7	D	1102	5AD	C5-C4	3.69	1.45	1.39
2	D	1101	HH2	C9-C10	3.64	1.48	1.40
6	D	1105	PE0	C4-N2	-3.55	1.32	1.37
2	D	1101	HH2	P1-O3P	3.48	1.63	1.59
2	C	1101	HH2	C8-N7	-3.36	1.32	1.37
7	D	1102	5AD	C5-N7	-3.32	1.33	1.39
6	A	1105	PE0	C4-N2	-3.28	1.32	1.37
7	B	1102	5AD	C5-C6	3.16	1.49	1.41
2	C	1101	HH2	P1-O3P	2.97	1.62	1.59
7	B	1102	5AD	C8-N7	2.87	1.37	1.31
2	F	1101	HH2	P1-O3P	2.84	1.62	1.59
2	B	1101	HH2	P1-O3P	2.79	1.62	1.59
6	E	1104	PE0	C1-C2	2.62	1.45	1.40
2	F	1101	HH2	C8-N7	-2.58	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1101	HH2	C8-N7	-2.55	1.33	1.37
6	D	1105	PE0	C1-C2	2.49	1.45	1.40
2	C	1101	HH2	C6-N7	-2.42	1.31	1.37
3	A	1102	APC	PB-O2B	-2.42	1.50	1.56
6	C	1105	PE0	C3-N2	-2.36	1.31	1.37
3	C	1102	APC	PB-O2B	-2.33	1.50	1.56
2	D	1101	HH2	C8-N7	-2.26	1.34	1.37
2	B	1101	HH2	C8-N7	-2.22	1.34	1.37
3	C	1102	APC	PA-O2A	-2.20	1.51	1.56
2	A	1101	HH2	P1-O3P	2.18	1.61	1.59
3	A	1102	APC	PA-O2A	-2.17	1.51	1.56
7	B	1102	5AD	C4-N9	-2.15	1.33	1.37
6	D	1105	PE0	C3-N2	-2.12	1.32	1.37
2	C	1101	HH2	C9-C10	2.09	1.44	1.40
2	A	1101	HH2	C8-N7	-2.09	1.34	1.37
6	C	1105	PE0	C1-C2	2.07	1.44	1.40
2	E	1101	HH2	C6-N7	-2.03	1.32	1.37

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1102	5AD	C5-C4-N3	-7.04	117.03	126.72
2	C	1101	HH2	C3-C2-N1	-5.42	117.35	120.87
7	D	1102	5AD	N3-C4-N9	5.18	135.98	127.17
7	B	1102	5AD	C5-C4-N3	-5.11	119.69	126.72
2	E	1101	HH2	C3-C2-N1	-4.88	117.70	120.87
7	B	1102	5AD	C4-C5-N7	-4.33	105.63	110.58
7	D	1102	5AD	C2-N3-C4	4.22	122.15	111.83
6	C	1105	PE0	C1-C2-N1	-4.00	117.58	123.19
2	C	1101	HH2	C8-C9-N1	3.97	126.04	118.17
7	B	1102	5AD	C2-N3-C4	3.85	121.25	111.83
6	E	1104	PE0	C4-C1-N4	3.74	124.94	118.38
7	B	1102	5AD	N3-C2-N1	-3.68	123.00	128.58
2	E	1101	HH2	C8-C9-N1	3.62	125.34	118.17
2	F	1101	HH2	C8-C9-N1	3.51	125.12	118.17
6	D	1105	PE0	C1-C2-N1	-3.47	118.33	123.19
7	B	1102	5AD	N3-C4-N9	3.44	133.01	127.17
6	D	1105	PE0	C4-C1-N4	3.41	124.37	118.38
7	D	1102	5AD	N3-C2-N1	-3.40	123.44	128.58
2	D	1101	HH2	C9-C10-N5	-3.31	118.54	123.19
7	B	1102	5AD	C6-C5-N7	3.31	138.48	132.09
6	E	1104	PE0	C1-C2-N1	-3.28	118.58	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1105	PE0	C4-C1-N4	3.22	124.03	118.38
2	C	1101	HH2	C9-C10-N5	-3.10	118.84	123.19
2	F	1101	HH2	C11-C2-N1	3.08	121.91	115.69
6	C	1105	PE0	C4-C1-N4	3.02	123.69	118.38
7	B	1102	5AD	C5-N7-C8	2.94	108.06	103.45
4	C	1103	PAB	O2'-C1'-C1	2.93	122.36	114.84
7	B	1102	5AD	C4-N9-C8	2.83	108.71	105.74
2	F	1101	HH2	C9-C10-N5	-2.81	119.24	123.19
2	A	1101	HH2	C8-C9-N1	2.79	123.70	118.17
7	B	1102	5AD	C2'-C3'-C4'	2.75	106.42	102.36
7	D	1102	5AD	C5'-C4'-C3'	-2.71	112.85	115.70
2	C	1101	HH2	C11-C2-N1	2.70	121.13	115.69
2	F	1101	HH2	C9-C8-N7	2.58	118.99	114.07
7	B	1102	5AD	N9-C8-N7	-2.57	110.29	113.94
2	B	1101	HH2	C9-C10-N5	-2.54	119.62	123.19
2	E	1101	HH2	C9-C10-N5	-2.53	119.64	123.19
2	D	1101	HH2	C8-C9-N1	2.49	123.11	118.17
2	B	1101	HH2	C11-C2-N1	2.49	120.71	115.69
2	A	1101	HH2	C11-C2-N1	2.45	120.63	115.69
2	E	1101	HH2	N6-C6-N7	2.45	121.92	116.76
6	C	1105	PE0	N3-C2-N1	2.45	123.52	116.41
6	C	1105	PE0	C1-C4-N2	2.43	118.70	114.07
2	E	1101	HH2	O8-C8-C9	-2.43	119.51	124.32
2	A	1101	HH2	C9-C10-N5	-2.40	119.82	123.19
6	A	1105	PE0	C6-N3-C2	2.38	121.29	115.14
6	C	1105	PE0	O4-C4-C1	-2.38	119.60	124.32
2	B	1101	HH2	O6P-P2-O5P	2.37	116.70	107.80
2	B	1101	HH2	C9-C8-N7	2.35	118.56	114.07
2	B	1101	HH2	C8-C9-N1	2.34	122.81	118.17
6	D	1105	PE0	C1-C4-N2	2.34	118.54	114.07
6	A	1105	PE0	C5-N4-C1	2.33	121.33	116.80
7	D	1102	5AD	C4-C5-N7	-2.28	107.97	110.58
6	A	1105	PE0	C2-C1-N4	-2.27	118.65	122.95
2	E	1101	HH2	C11-C2-N1	2.27	120.26	115.69
7	B	1102	5AD	C5'-C4'-C3'	-2.26	113.32	115.70
6	A	1105	PE0	C1-C2-N1	-2.19	120.11	123.19
7	D	1102	5AD	C2'-C3'-C4'	2.19	105.60	102.36
2	D	1101	HH2	C9-C8-N7	2.19	118.24	114.07
2	F	1101	HH2	O6P-P2-O5P	2.17	115.92	107.80
2	E	1101	HH2	N4-C10-N5	2.15	122.65	116.41
6	E	1104	PE0	N3-C2-N1	2.11	122.55	116.41
6	E	1104	PE0	C2-C1-N4	-2.10	118.97	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1102	5AD	C2-N1-C6	2.10	122.18	118.73
7	B	1102	5AD	C4-N9-C1'	-2.08	121.76	126.63
6	E	1104	PE0	C1-C4-N2	2.08	118.04	114.07
2	D	1101	HH2	C11-C2-N1	2.06	119.84	115.69
2	D	1101	HH2	N4-C10-N5	2.06	122.39	116.41
6	C	1105	PE0	C2-C1-N4	-2.06	119.06	122.95
6	D	1105	PE0	N3-C2-N1	2.05	122.38	116.41
3	C	1102	APC	O2B-PB-O1B	2.05	116.63	109.95
2	C	1101	HH2	N6-C6-N7	2.04	121.06	116.76
2	E	1101	HH2	C9-C8-N7	2.02	117.92	114.07
2	B	1101	HH2	N4-C10-N5	2.02	122.27	116.41
2	C	1101	HH2	N4-C10-N5	2.01	122.25	116.41
2	A	1101	HH2	O3P-P1-O1P	-2.01	104.66	110.70

There are no chirality outliers.

All (44) 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	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'
3	C	1102	APC	C3'-C4'-C5'-O5'
2	A	1101	HH2	O4-C11-C2-N1
2	B	1101	HH2	O4-C11-C2-N1

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Mol	Chain	Res	Type	Atoms
2	C	1101	HH2	O4-C11-C2-N1
2	C	1101	HH2	P2-O3P-P1-O2P
2	A	1101	HH2	O4-C11-C2-C3
2	B	1101	HH2	O4-C11-C2-C3
2	C	1101	HH2	O4-C11-C2-C3
2	D	1101	HH2	C11-O4-P1-O3P
3	C	1102	APC	PA-C3A-PB-O2B
3	C	1102	APC	PB-C3A-PA-O2A
2	C	1101	HH2	P1-O3P-P2-O4P
2	A	1101	HH2	P2-O3P-P1-O2P
2	A	1101	HH2	P2-O3P-P1-O1P
3	C	1102	APC	PA-C3A-PB-O1B
3	C	1102	APC	C4'-C5'-O5'-PA
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
3	C	1102	APC	C2'-C1'-N9-C8
2	C	1101	HH2	P2-O3P-P1-O1P

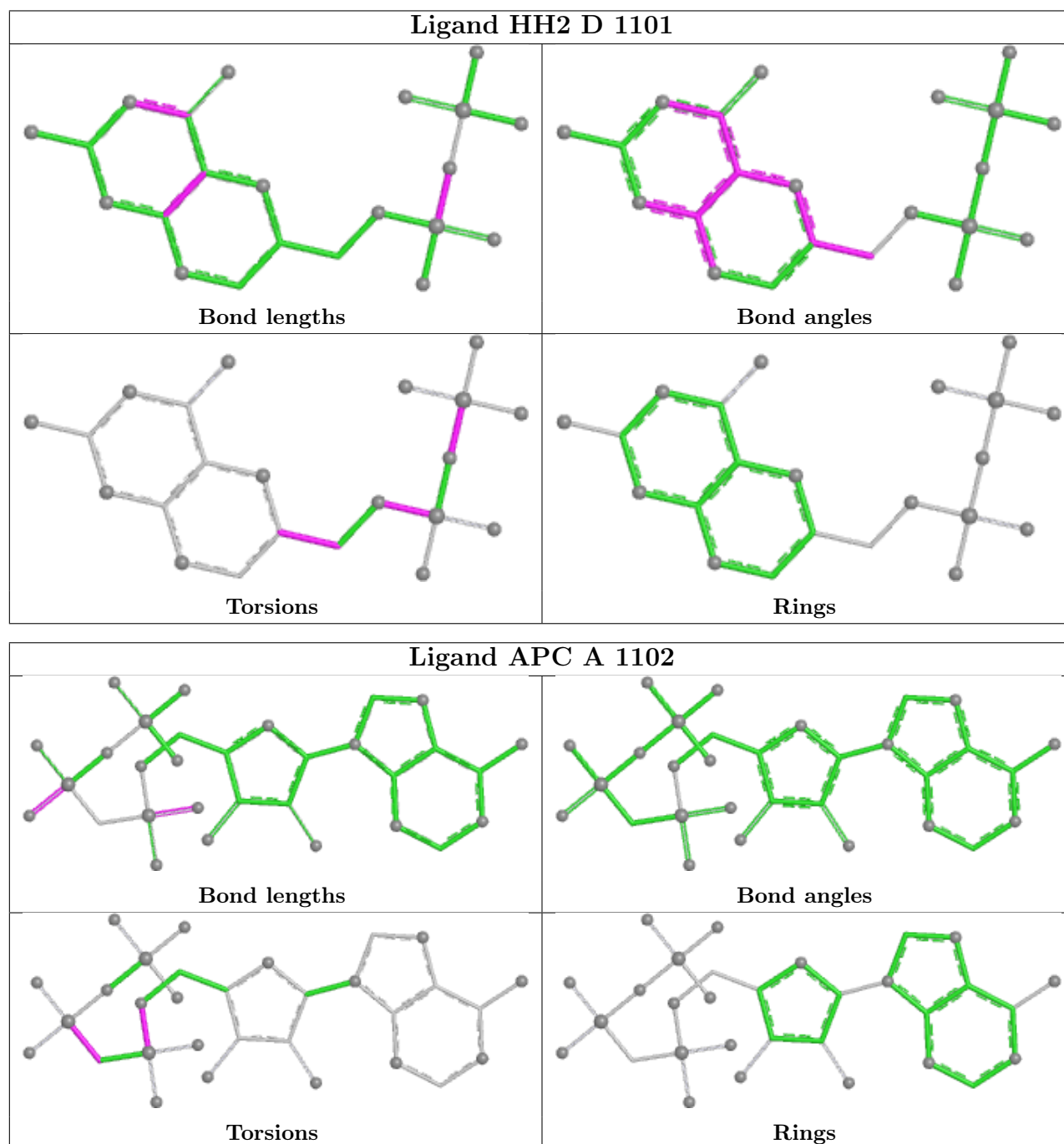
There are no ring outliers.

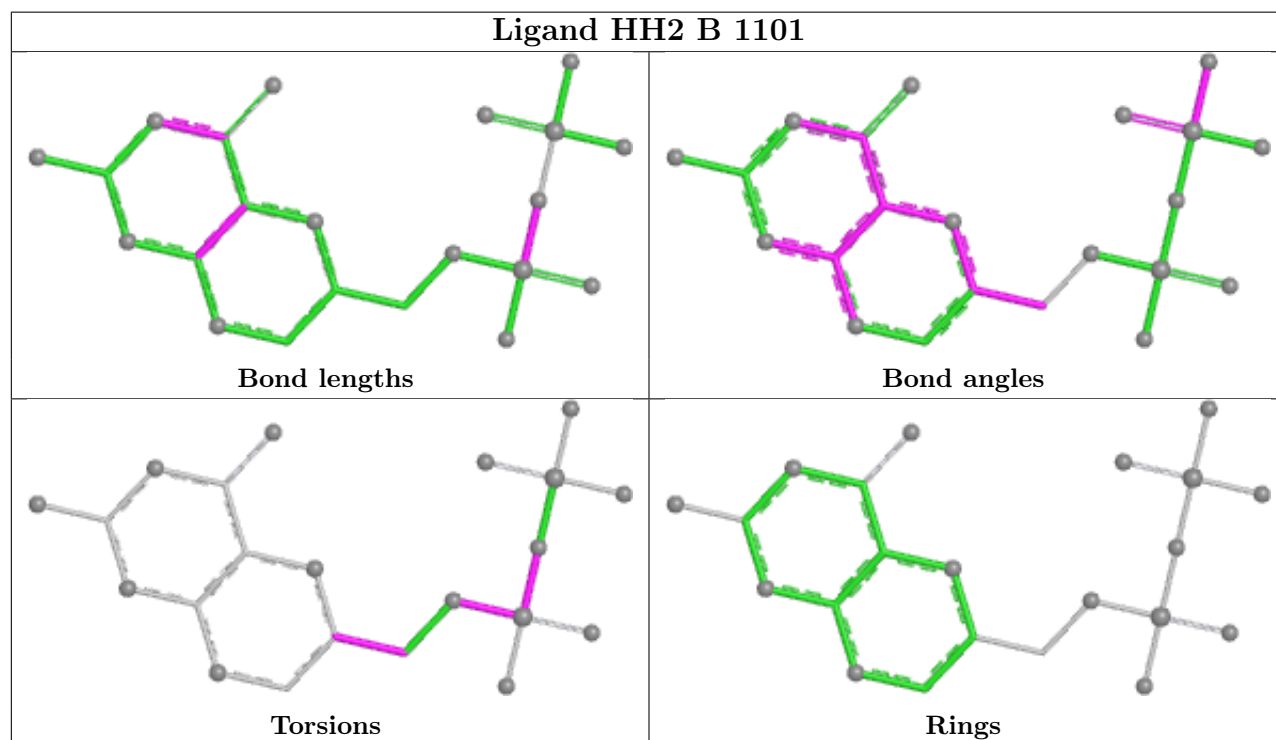
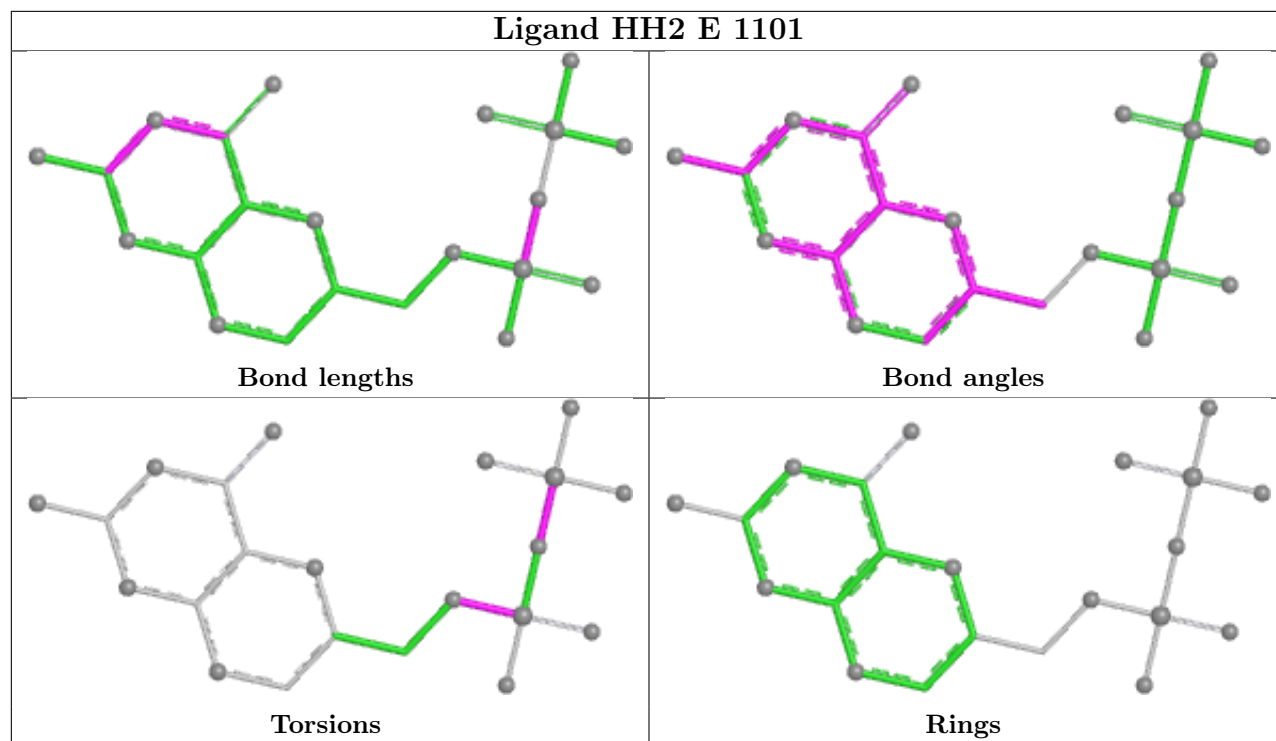
10 monomers are involved in 18 short contacts:

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

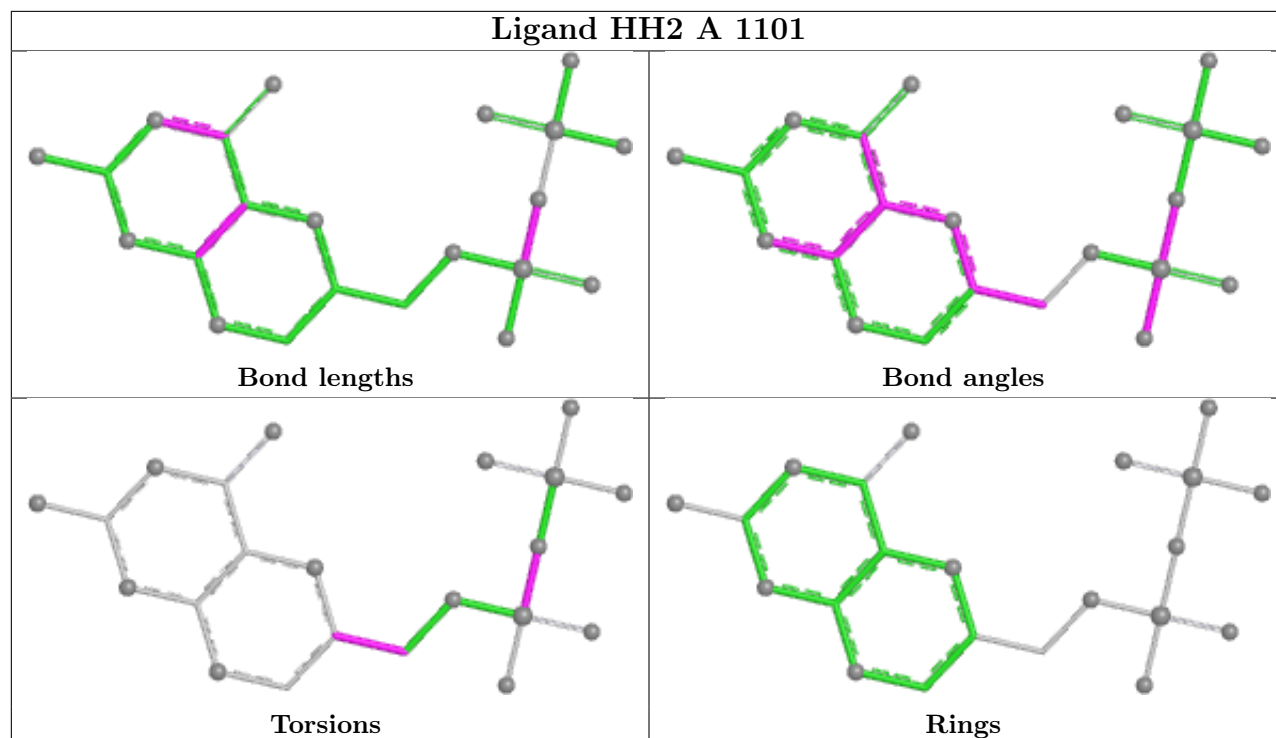
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

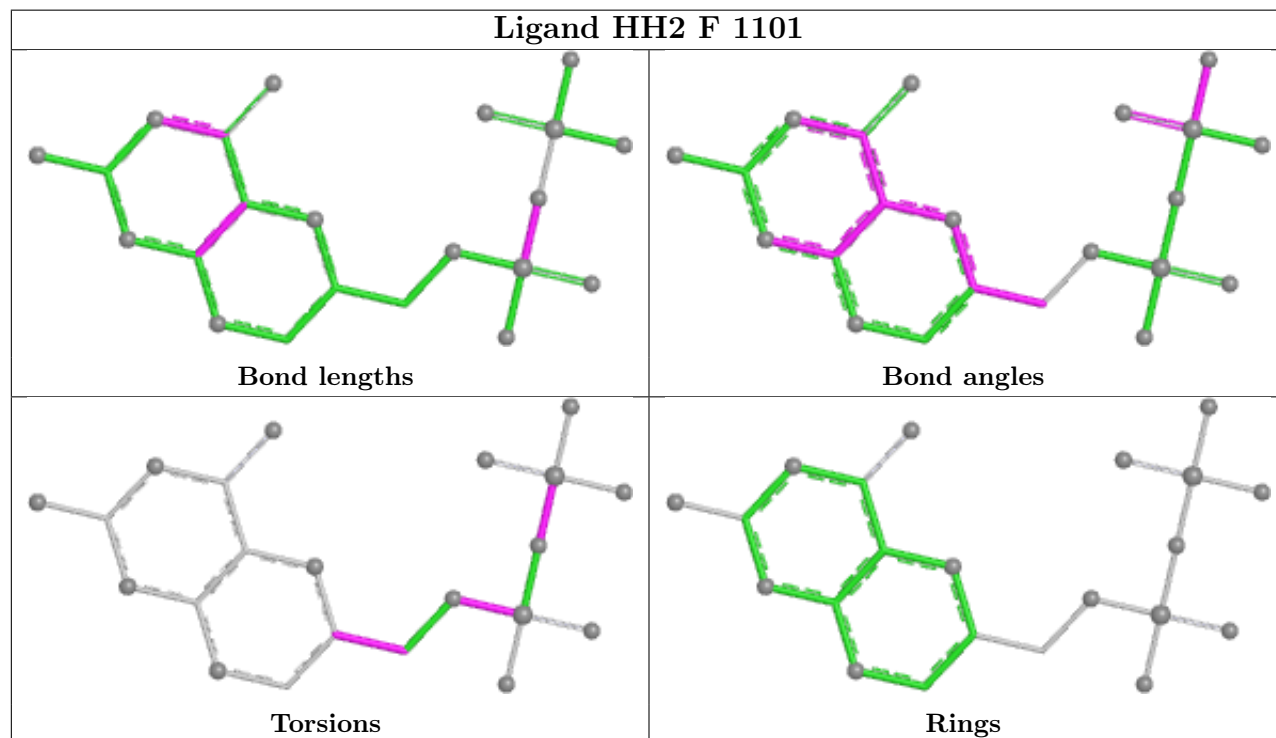




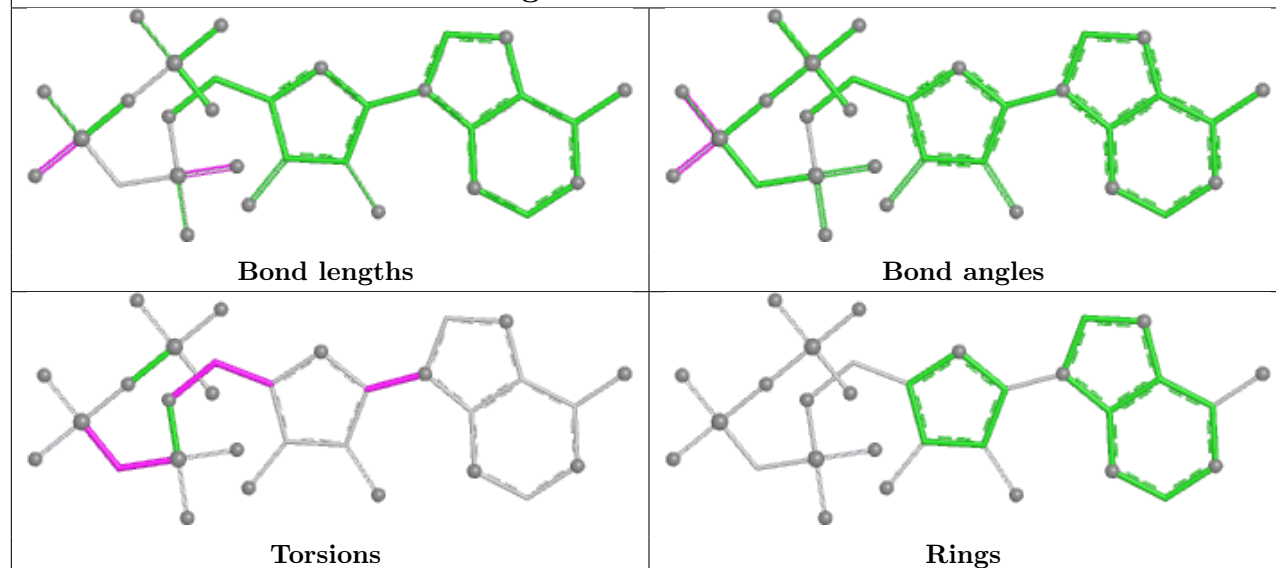
Ligand HH2 A 1101



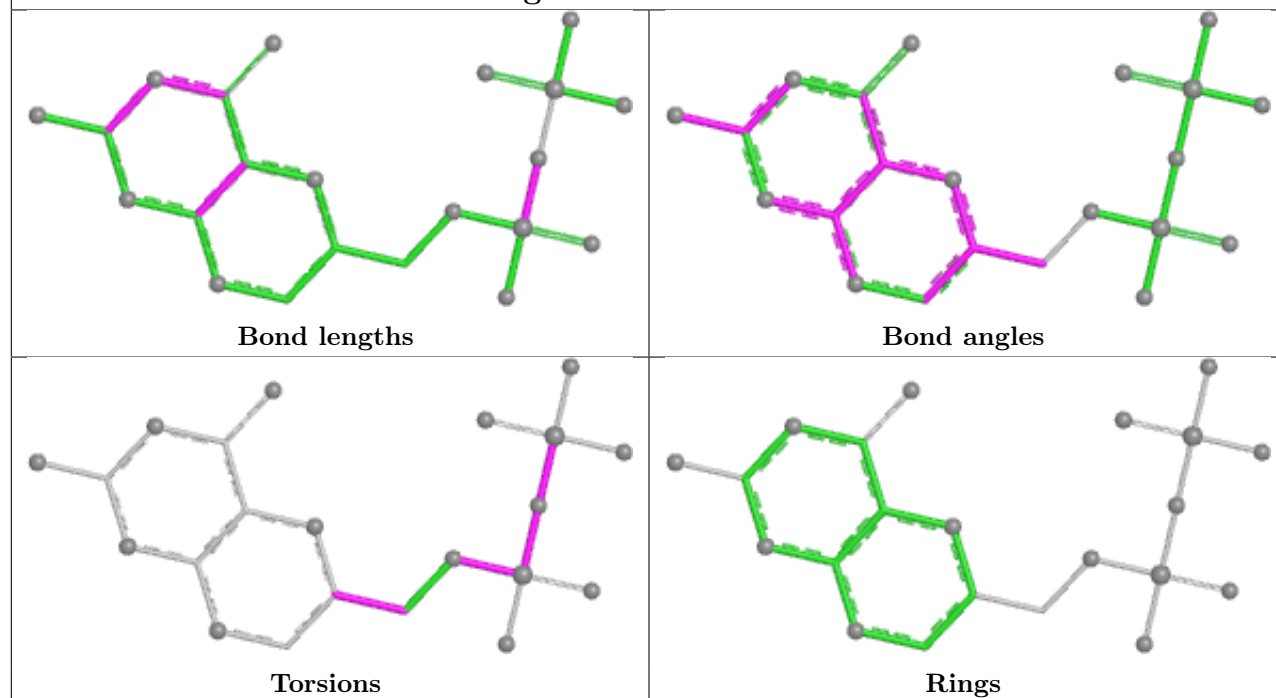
Ligand HH2 F 1101

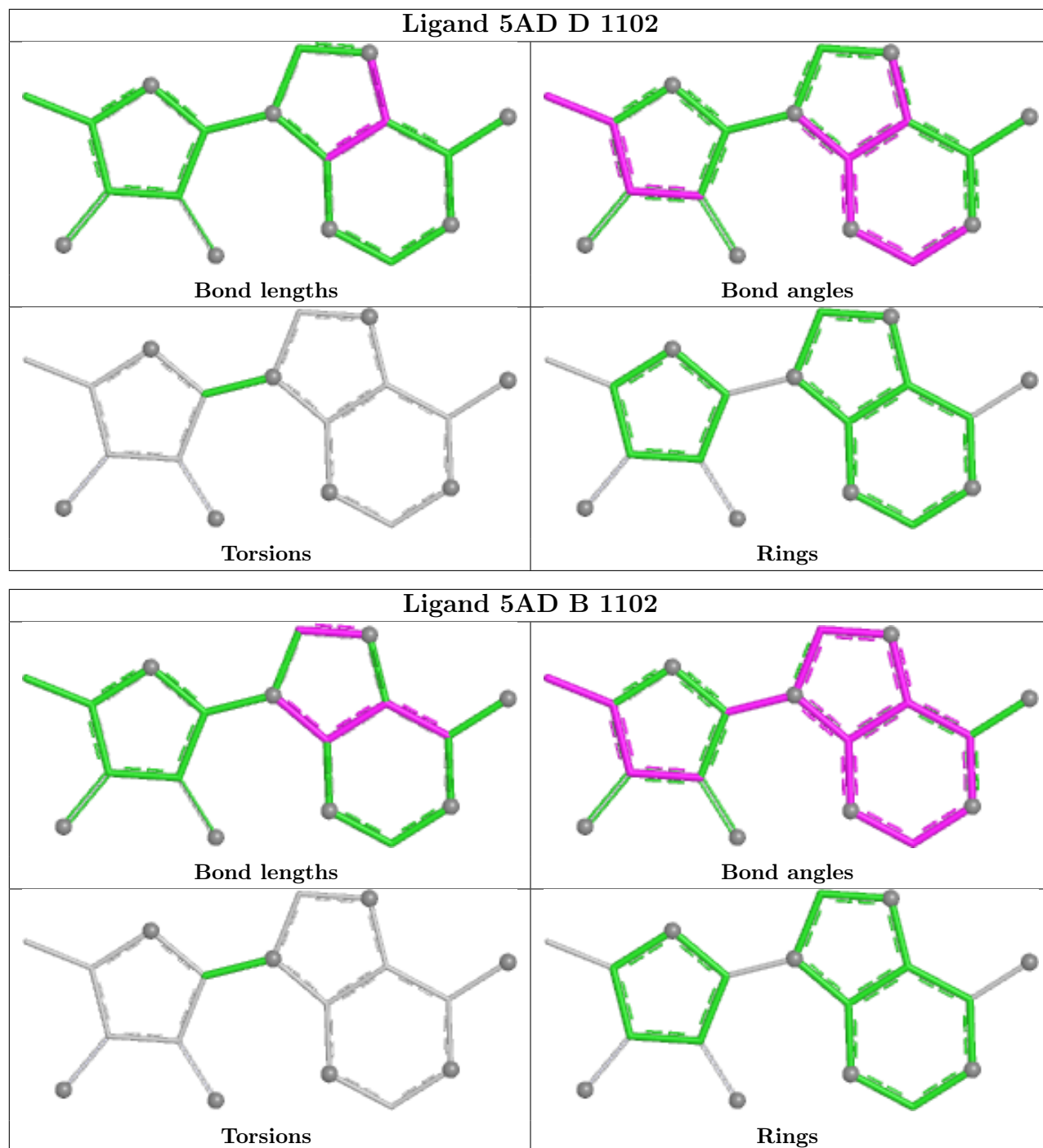


Ligand APC C 1102



Ligand HH2 C 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	588/717 (82%)	0.30	19 (3%)	50	41	26, 37, 51, 62	0
1	B	562/717 (78%)	0.70	53 (9%)	14	12	36, 53, 78, 93	0
1	C	599/717 (83%)	0.18	16 (2%)	56	47	23, 35, 52, 72	0
1	D	577/717 (80%)	0.33	19 (3%)	49	40	27, 36, 54, 68	0
1	E	584/717 (81%)	0.40	12 (2%)	63	54	35, 48, 65, 76	0
1	F	566/717 (78%)	0.39	21 (3%)	45	37	35, 47, 63, 72	0
All	All	3476/4302 (80%)	0.38	140 (4%)	42	34	23, 42, 65, 93	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	SER	6.2
1	F	243	THR	5.6
1	D	71	THR	5.5
1	B	672	LEU	5.2
1	E	147	ASN	5.1
1	A	203	ASN	4.9
1	C	153	ASP	4.8
1	E	657	LEU	4.5
1	C	668	ASP	4.1
1	B	418	GLY	4.1
1	F	148	LEU	4.1
1	A	58	TYR	3.9
1	C	154	LYS	3.8
1	F	241	ASN	3.8
1	B	228	GLU	3.8
1	E	146	LYS	3.8
1	A	436	SER	3.7
1	F	157	THR	3.7
1	A	148	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	414	CYS	3.6
1	D	69	GLU	3.6
1	A	59	ILE	3.6
1	B	240	ILE	3.6
1	F	240	ILE	3.6
1	A	658	TRP	3.6
1	B	434	GLN	3.5
1	B	143	ILE	3.4
1	B	674	TYR	3.4
1	F	58	TYR	3.4
1	B	133	ALA	3.4
1	B	134	ARG	3.3
1	C	73	GLY	3.3
1	D	76	PRO	3.3
1	B	81	TRP	3.3
1	B	146	LYS	3.2
1	F	76	PRO	3.2
1	B	131	ASN	3.2
1	E	10	THR	3.2
1	B	55	VAL	3.1
1	F	242	HIS	3.1
1	B	243	THR	3.1
1	C	72	GLU	3.0
1	D	144	MET	3.0
1	C	587	CYS	3.0
1	B	245	ASP	3.0
1	B	132	GLU	3.0
1	D	290	THR	3.0
1	D	59	ILE	2.9
1	B	249	LEU	2.9
1	B	84	ASP	2.9
1	C	67	ILE	2.9
1	A	587	CYS	2.9
1	B	136	ILE	2.9
1	A	418	GLY	2.9
1	F	189	LYS	2.9
1	D	446	ASP	2.9
1	B	122	ARG	2.8
1	E	59	ILE	2.8
1	A	525	ARG	2.8
1	E	244	SER	2.8
1	A	421	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	317	ASN	2.8
1	D	155	TYR	2.8
1	F	29	THR	2.8
1	D	68	GLY	2.7
1	A	77	ARG	2.7
1	D	307	GLU	2.7
1	D	58	TYR	2.7
1	E	58	TYR	2.7
1	F	419	GLY	2.7
1	B	203	ASN	2.6
1	F	515	ASN	2.6
1	F	312	ILE	2.6
1	B	346	ASP	2.6
1	D	292	GLU	2.6
1	B	673	LEU	2.6
1	D	78	ASP	2.6
1	F	446	ASP	2.5
1	C	157	THR	2.5
1	F	80	SER	2.5
1	B	127	GLU	2.5
1	B	142	GLU	2.5
1	B	440	LYS	2.4
1	F	156	TYR	2.4
1	B	446	ASP	2.4
1	E	143	ILE	2.4
1	C	74	GLU	2.4
1	B	444	VAL	2.4
1	E	263	CYS	2.4
1	B	56	PRO	2.4
1	B	443	LYS	2.3
1	B	354	PHE	2.3
1	D	222	SER	2.3
1	E	250	ASP	2.3
1	F	350	ASP	2.3
1	C	305	SER	2.3
1	B	230	ILE	2.3
1	F	674	TYR	2.3
1	D	134	ARG	2.3
1	B	80	SER	2.3
1	D	80	SER	2.3
1	F	88	THR	2.3
1	B	159	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	668	ASP	2.3
1	B	83	GLY	2.3
1	E	145	LYS	2.2
1	B	11	PRO	2.2
1	A	256	GLY	2.2
1	B	135	ARG	2.2
1	B	144	MET	2.2
1	B	261	PHE	2.2
1	B	140	ASN	2.2
1	A	240	ILE	2.2
1	C	78	ASP	2.2
1	D	557	ASP	2.2
1	F	84	ASP	2.2
1	B	87	PRO	2.2
1	D	379	GLY	2.2
1	A	57	GLU	2.2
1	B	436	SER	2.2
1	D	98	GLU	2.2
1	F	671	GLN	2.1
1	C	203	ASN	2.1
1	A	84	ASP	2.1
1	E	60	VAL	2.1
1	B	412	LEU	2.1
1	B	263	CYS	2.1
1	B	348	PHE	2.1
1	B	378	GLY	2.1
1	A	671	GLN	2.0
1	C	664	HIS	2.0
1	A	666	ARG	2.0
1	B	257	ASP	2.0
1	A	308	GLU	2.0
1	C	292	GLU	2.0
1	C	661	LYS	2.0
1	B	204	ARG	2.0
1	B	79	ILE	2.0
1	B	377	ILE	2.0
1	C	132	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

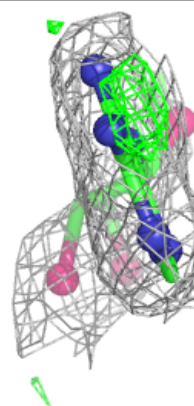
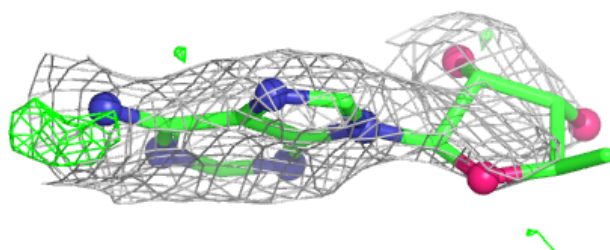
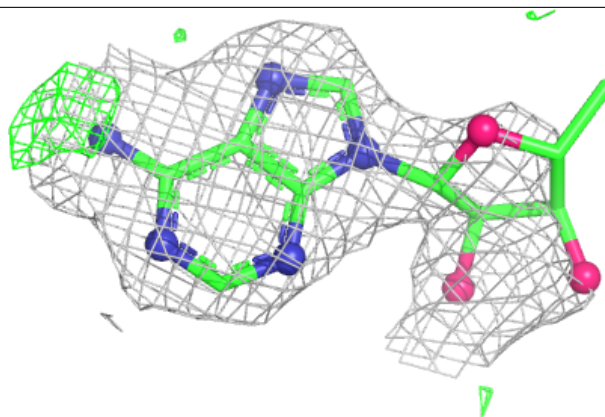
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PE0	D	1105	12/12	0.71	0.19	55,68,73,75	0
5	MG	A	1104	1/1	0.75	0.14	31,31,31,31	0
7	5AD	B	1102	18/18	0.75	0.27	29,41,55,57	18
3	APC	C	1102	31/31	0.76	0.21	39,77,109,115	31
7	5AD	D	1102	18/18	0.77	0.27	18,31,40,41	18
6	PE0	C	1105	12/12	0.80	0.18	44,51,59,63	12
3	APC	A	1102	31/31	0.81	0.17	17,49,94,109	31
5	MG	E	1103	1/1	0.82	0.10	28,28,28,28	0
6	PE0	A	1105	12/12	0.83	0.20	36,44,50,51	12
6	PE0	E	1104	12/12	0.84	0.16	28,32,34,35	12
2	HH2	B	1101	22/22	0.87	0.13	23,41,52,56	0
4	PAB	B	1103	10/10	0.87	0.17	39,48,55,84	0
4	PAB	E	1102	10/10	0.89	0.19	32,40,54,65	0
5	MG	D	1104	1/1	0.90	0.09	27,27,27,27	0
2	HH2	A	1101	22/22	0.90	0.12	22,28,51,56	0
4	PAB	F	1102	10/10	0.91	0.14	19,24,26,29	10
2	HH2	E	1101	22/22	0.92	0.11	27,43,56,60	0
2	HH2	F	1101	22/22	0.92	0.14	42,50,72,76	0
5	MG	C	1104	1/1	0.93	0.08	32,32,32,32	0
4	PAB	D	1103	10/10	0.93	0.16	23,38,59,88	0
4	PAB	A	1103	10/10	0.93	0.15	35,45,53,66	0
2	HH2	D	1101	22/22	0.94	0.10	23,31,38,44	0
2	HH2	C	1101	22/22	0.94	0.10	28,37,43,52	0
4	PAB	C	1103	10/10	0.95	0.12	14,22,28,41	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.

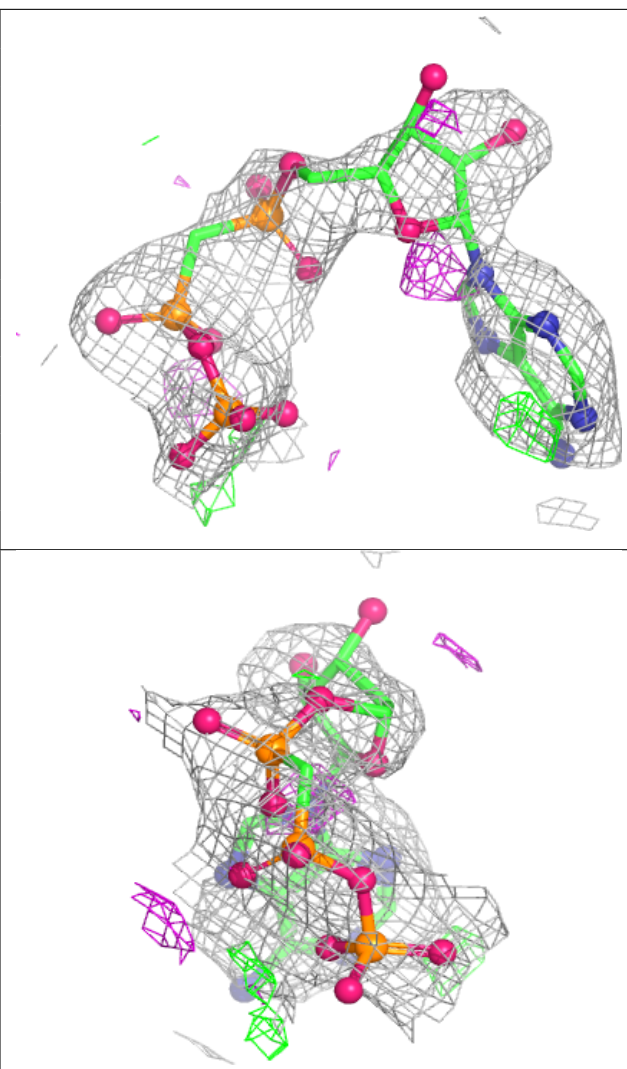
Electron density around 5AD B 1102:

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



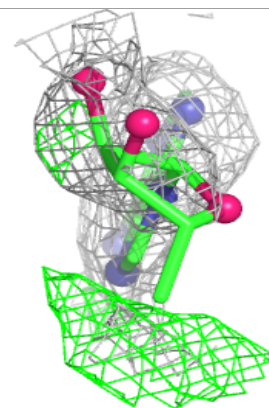
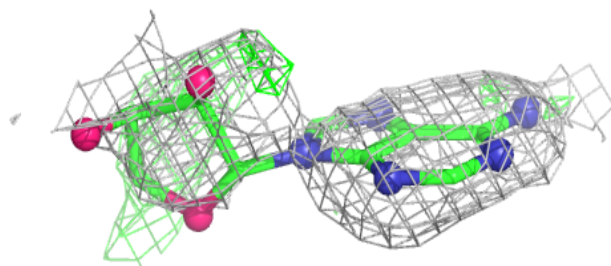
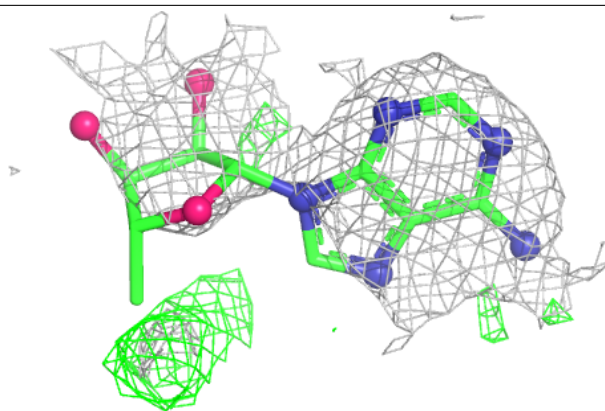
Electron density around APC C 1102:

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



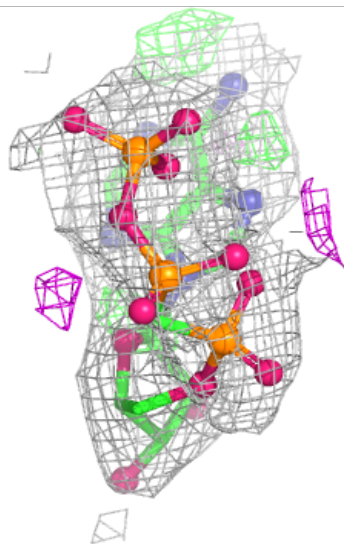
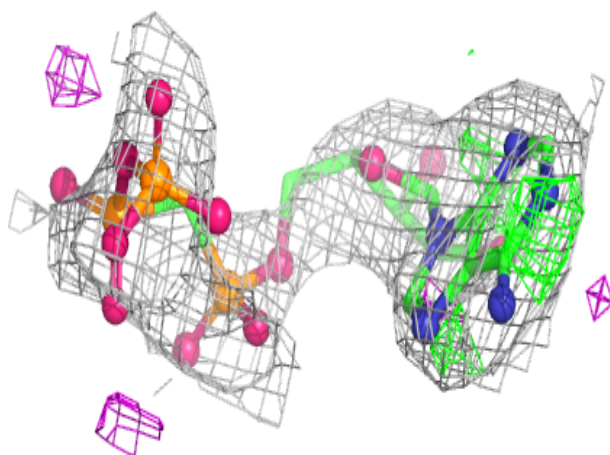
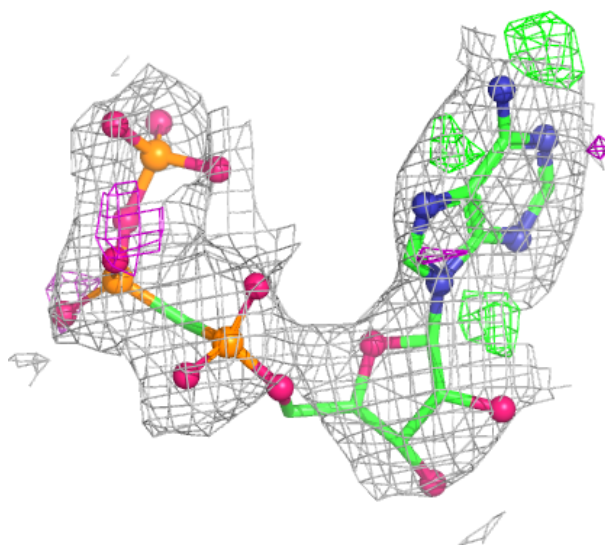
Electron density around 5AD D 1102:

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



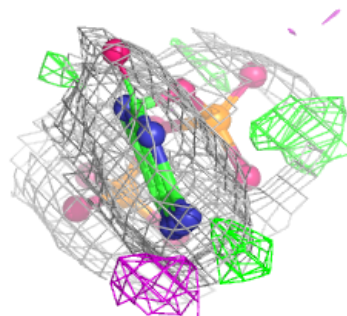
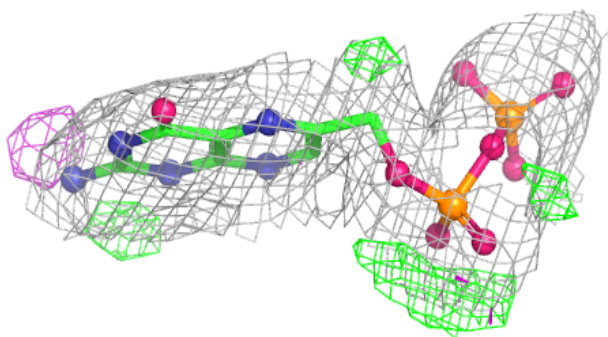
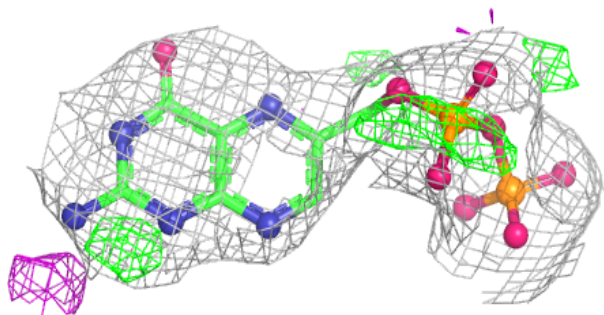
Electron density around APC A 1102:

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

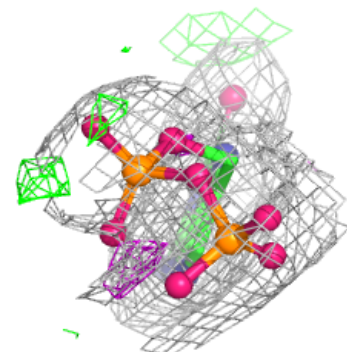
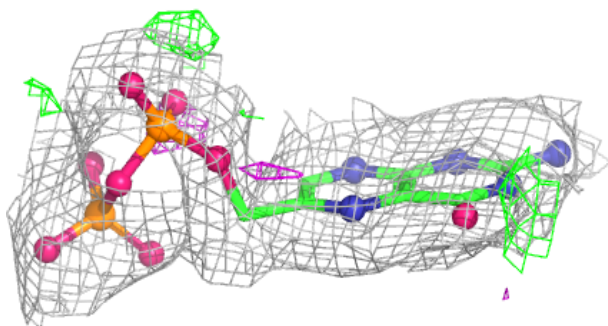
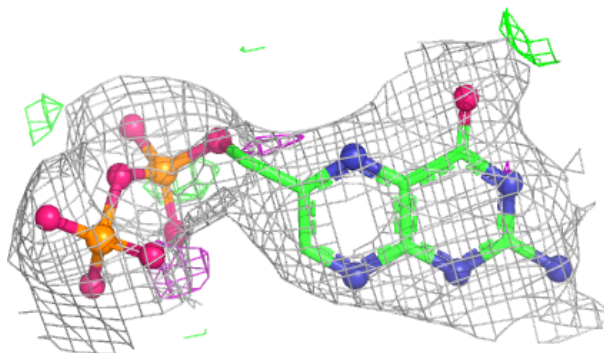


Electron density around HH2 B 1101:

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

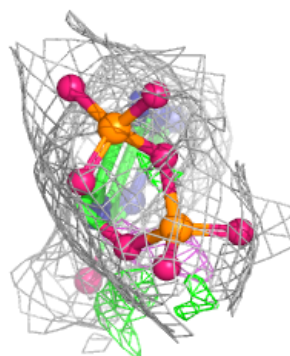
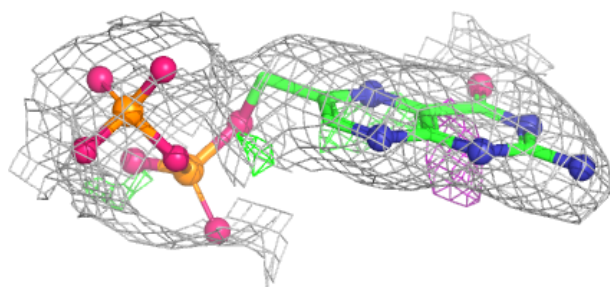
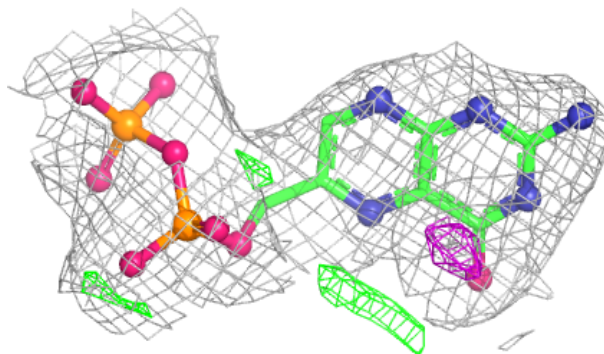
**Electron density around HH2 A 1101:**

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

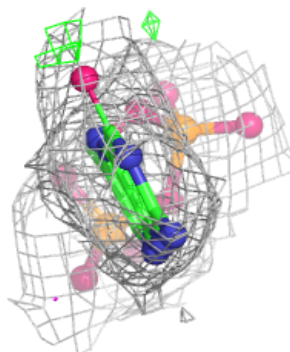
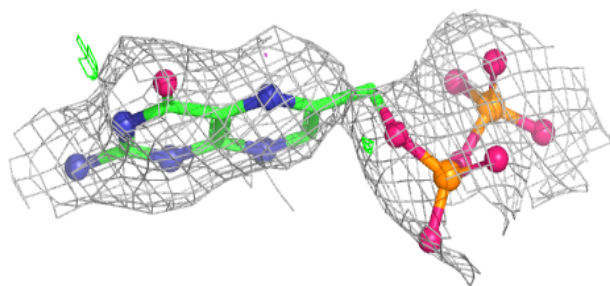
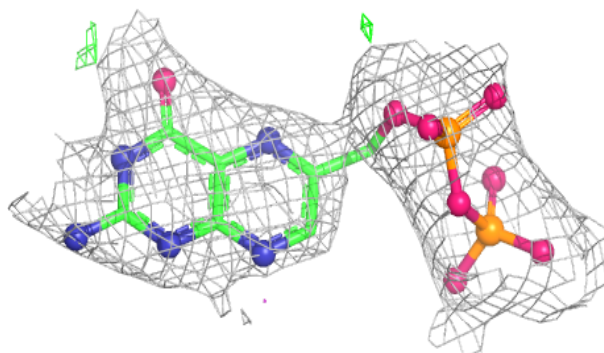


Electron density around HH2 E 1101:

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

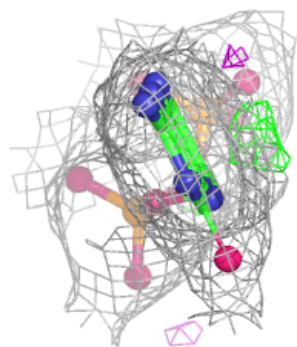
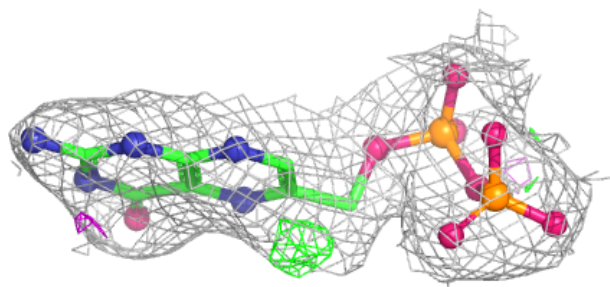
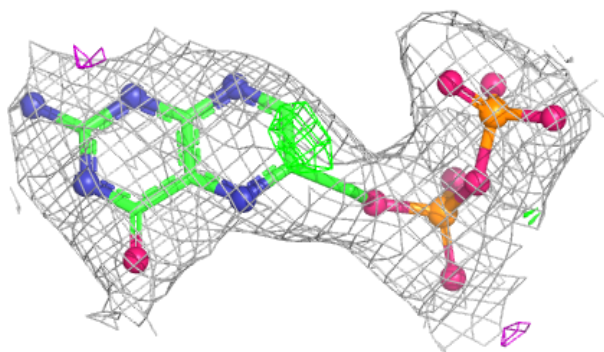
**Electron density around HH2 F 1101:**

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

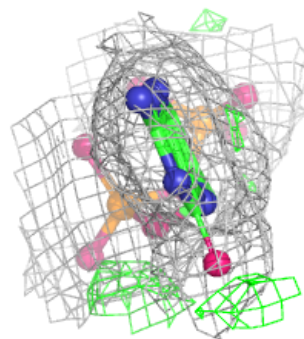
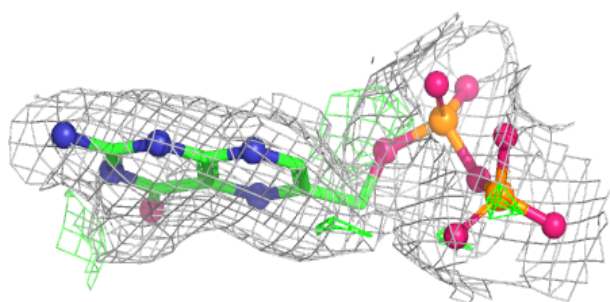
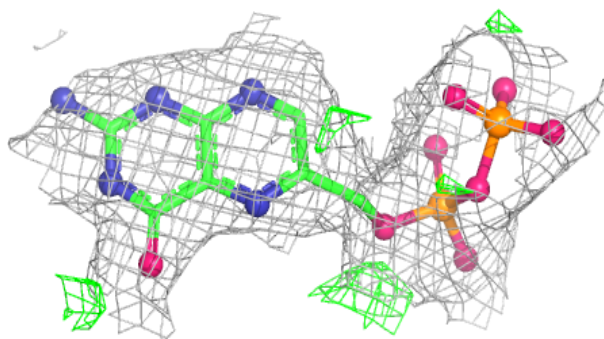


Electron density around HH2 D 1101:

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

**Electron density around HH2 C 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.