Full wwPDB X-ray Structure Validation Report (i)

Jul 31, 2023 – 03:43 AM EDT

PDB ID	:	1ECB
Title	:	ESCHERICHIA COLI GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE (PRPP) AMIDOTRANSFERASE COMPLEXED WITH 2 GMP, 1 MG PER SUBUNIT
Authors	:	Krahn, J.M.; Smith, J.L.
Deposited on	:	1997-07-15
Resolution	:	2.70 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 (1)) were used in the production of this report:

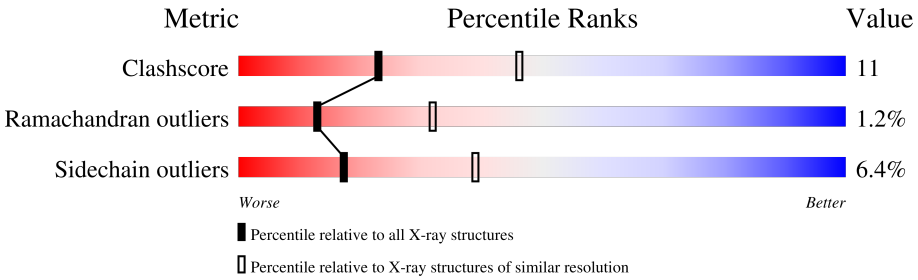
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	504	68% 25% • 6%
1	B	504	71% 21% • 7%
1	C	504	67% 24% • •
1	D	504	67% 24% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15139 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.

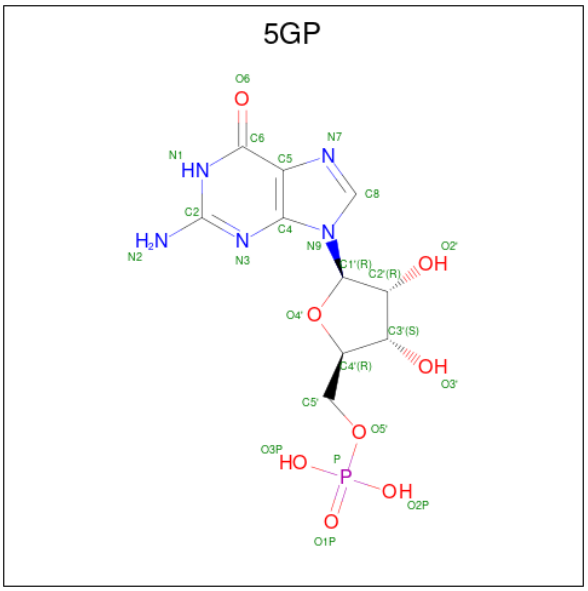
- Molecule 1 is a protein called GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3724	2345	657	705	17			
1	B	470	Total	C	N	O	S	0	0	0
			3685	2320	651	697	17			
1	C	482	Total	C	N	O	S	0	0	0
			3787	2381	675	714	17			
1	D	473	Total	C	N	O	S	0	0	0
			3708	2334	654	703	17			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	8	Total	O	0	0
			8	8		
4	C	13	Total	O	0	0
			13	13		
4	D	11	Total	O	0	0
			11	11		

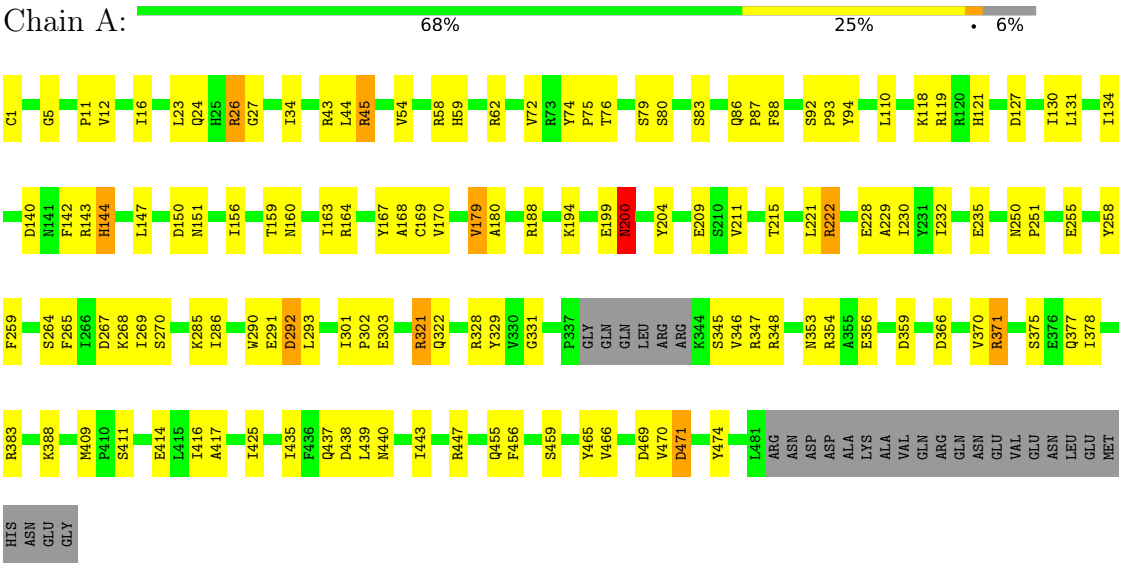
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

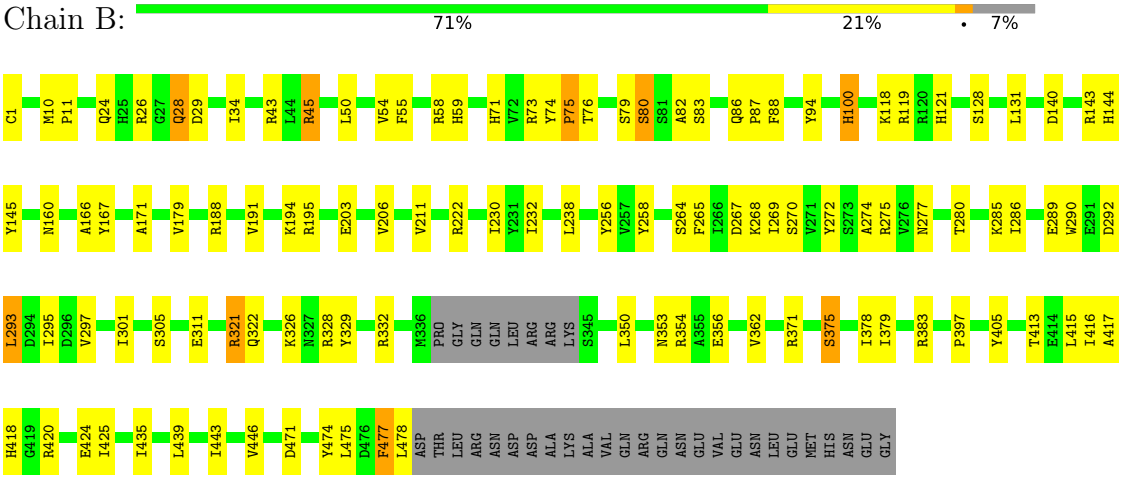
• Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE

Chain A:



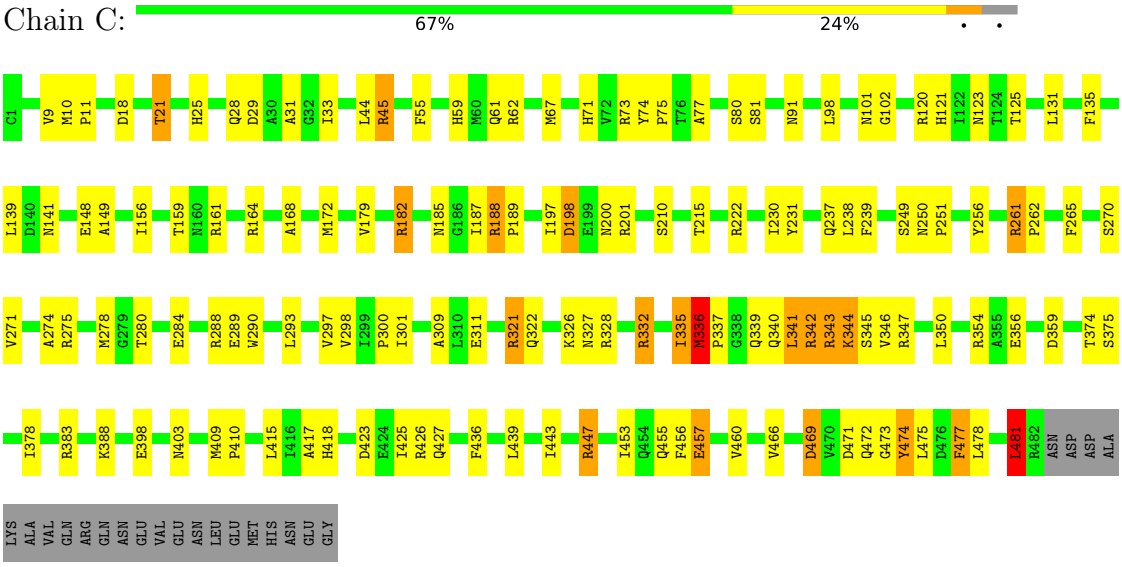
• Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE

Chain B:



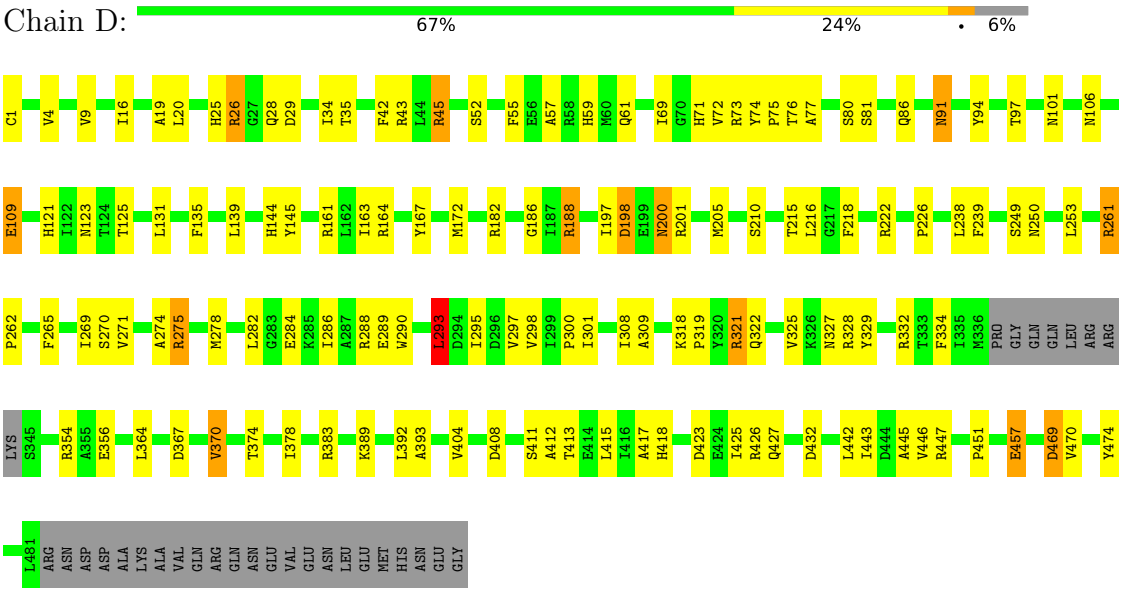
• Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE

Chain C:



• Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.80Å 113.20Å 199.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	97.7 (15.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.208 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15139	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5GP

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	0.62	0/3791	0.82	1/5133 (0.0%)
1	B	0.65	0/3751	0.82	0/5078
1	C	0.66	0/3855	0.85	2/5218 (0.0%)
1	D	0.65	1/3774 (0.0%)	0.84	3/5110 (0.1%)
All	All	0.65	1/15171 (0.0%)	0.83	6/20539 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	329	TYR	CE1-CZ	-5.12	1.31	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	293	LEU	CA-CB-CG	5.98	129.05	115.30
1	D	26	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	168	ALA	N-CA-C	-5.76	95.46	111.00
1	D	275	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	168	ALA	N-CA-C	-5.24	96.86	111.00
1	C	481	LEU	CA-CB-CG	5.22	127.32	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	145	TYR	Sidechain

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	3724	0	3687	89	0
1	B	3685	0	3645	82	0
1	C	3787	0	3757	96	0
1	D	3708	0	3667	85	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	48	0	22	6	0
3	B	48	0	22	2	0
3	C	48	0	21	2	0
3	D	48	0	22	3	0
4	A	7	0	0	0	0
4	B	8	0	0	0	0
4	C	13	0	0	1	0
4	D	11	0	0	0	0
All	All	15139	0	14843	342	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 11.

All (342) 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:C:336:MET:HB2	1:C:337:PRO:HD3	1.39	1.02
1:C:164:ARG:HD2	1:C:469:ASP:HB3	1.47	0.94
1:A:80:SER:HB2	1:A:83:SER:HB2	1.52	0.90
1:C:342:ARG:HA	1:C:342:ARG:NE	1.85	0.89
1:B:80:SER:HB2	1:B:83:SER:HB2	1.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ASP:HB2	1:D:75:PRO:HD3	1.58	0.83
1:C:341:LEU:HD13	1:C:342:ARG:N	1.98	0.78
1:C:29:ASP:HB2	1:C:75:PRO:HD3	1.64	0.77
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.49	0.77
1:C:383:ARG:HG3	1:C:383:ARG:HH11	1.50	0.76
1:B:301:ILE:HD13	1:B:378:ILE:HD13	1.68	0.76
1:A:76:THR:HG23	1:A:79:SER:HB2	1.67	0.75
1:B:383:ARG:HG3	1:B:383:ARG:HH11	1.50	0.75
1:D:383:ARG:HG3	1:D:383:ARG:HH11	1.50	0.74
1:D:182:ARG:HD2	1:D:188:ARG:O	1.88	0.74
1:C:410:PRO:HD2	1:C:415:LEU:HD21	1.72	0.72
1:C:332:ARG:HH12	1:C:343:ARG:NH2	1.86	0.71
1:A:383:ARG:HG3	1:A:383:ARG:HH11	1.54	0.71
1:B:45:ARG:HG3	1:B:59:HIS:HB3	1.71	0.71
1:A:265:PHE:CE2	1:A:270:SER:HB2	2.27	0.70
1:D:301:ILE:HD13	1:D:378:ILE:HD13	1.75	0.69
1:D:404:VAL:HG21	1:D:470:VAL:HG21	1.75	0.69
1:D:417:ALA:HA	1:D:425:ILE:HD11	1.75	0.69
1:C:182:ARG:HD2	1:C:188:ARG:O	1.92	0.69
1:B:417:ALA:HA	1:B:425:ILE:HD11	1.74	0.68
1:C:341:LEU:HD13	1:C:342:ARG:H	1.58	0.67
1:D:34:ILE:HD11	1:D:42:PHE:HB3	1.78	0.66
1:B:293:LEU:HD22	1:B:295:ILE:HG23	1.77	0.65
1:B:269:ILE:HD13	1:B:446:VAL:HG12	1.77	0.65
1:C:262:PRO:HA	1:C:271:VAL:HB	1.78	0.65
1:D:321:ARG:HG2	1:D:356:GLU:OE1	1.95	0.65
1:B:293:LEU:HD13	1:B:293:LEU:O	1.98	0.64
1:D:274:ALA:O	1:D:278:MET:HG3	1.97	0.63
1:B:76:THR:HG23	1:B:79:SER:HB2	1.79	0.63
1:B:119:ARG:HD2	1:D:94:TYR:CE1	2.34	0.63
1:B:321:ARG:HG2	1:B:321:ARG:HH11	1.63	0.62
1:A:58:ARG:HG2	1:A:58:ARG:NH1	2.13	0.62
1:A:321:ARG:HG2	1:A:356:GLU:OE1	1.99	0.62
1:C:301:ILE:HD13	1:C:378:ILE:HD13	1.79	0.62
1:C:321:ARG:HG2	1:C:356:GLU:OE1	2.00	0.62
1:A:86:GLN:HB3	1:A:87:PRO:HA	1.82	0.61
1:A:439:LEU:O	1:A:443:ILE:HG13	2.01	0.61
1:D:135:PHE:CZ	1:D:139:LEU:HD11	2.36	0.61
1:B:80:SER:CB	1:B:83:SER:HB2	2.27	0.61
1:B:58:ARG:HG2	1:B:58:ARG:HH11	1.66	0.60
1:C:336:MET:HB2	1:C:337:PRO:CD	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:TRP:O	1:A:292:ASP:N	2.34	0.60
1:C:188:ARG:HG3	1:C:188:ARG:HH11	1.67	0.60
1:D:370:VAL:HG13	3:D:505:5GP:O2P	2.02	0.59
1:B:321:ARG:HG2	1:B:356:GLU:OE1	2.02	0.59
1:A:371:ARG:HH11	1:A:371:ARG:HB3	1.66	0.59
1:C:417:ALA:HA	1:C:425:ILE:HD11	1.84	0.59
1:B:166:ALA:CB	1:B:405:TYR:HB3	2.32	0.59
1:D:121:HIS:HE1	1:D:123:ASN:OD1	1.86	0.59
1:B:256:TYR:O	1:B:275:ARG:HD2	2.02	0.58
1:C:45:ARG:HG2	1:C:55:PHE:CD1	2.39	0.58
1:D:94:TYR:HE1	1:D:145:TYR:HD2	1.52	0.58
1:B:474:TYR:O	1:B:478:LEU:HG	2.03	0.57
1:A:45:ARG:HG3	1:A:59:HIS:HB3	1.85	0.57
1:B:383:ARG:HG3	1:B:383:ARG:NH1	2.20	0.57
1:C:164:ARG:CD	1:C:469:ASP:HB3	2.28	0.57
1:B:100:HIS:HD1	1:B:128:SER:HG	1.51	0.56
1:D:238:LEU:HD12	1:D:239:PHE:N	2.19	0.56
1:B:45:ARG:HB3	1:B:55:PHE:HE1	1.70	0.56
1:D:94:TYR:CE1	1:D:145:TYR:HD2	2.23	0.56
1:C:453:ILE:HG21	1:C:456:PHE:CE1	2.41	0.56
1:D:25:HIS:CE1	1:D:261:ARG:HG3	2.41	0.56
1:C:321:ARG:HG2	1:C:321:ARG:HH11	1.71	0.56
1:B:328:ARG:HD2	1:B:329:TYR:CE1	2.41	0.56
1:A:44:LEU:HG	1:A:45:ARG:N	2.21	0.55
1:D:200:ASN:N	1:D:200:ASN:ND2	2.54	0.55
1:D:262:PRO:HA	1:D:271:VAL:HB	1.88	0.55
1:D:289:GLU:O	1:D:290:TRP:HD1	1.90	0.55
1:B:179:VAL:HA	1:B:230:ILE:O	2.06	0.55
1:A:164:ARG:NH1	1:A:469:ASP:HB3	2.21	0.55
1:C:284:GLU:O	1:C:288:ARG:HG3	2.06	0.55
1:A:471:ASP:O	1:A:474:TYR:HB3	2.06	0.55
1:C:250:ASN:OD1	1:C:466:VAL:HG21	2.07	0.55
1:C:261:ARG:NH2	1:D:327:ASN:OD1	2.40	0.55
1:D:442:LEU:O	1:D:445:ALA:HB3	2.07	0.54
1:A:371:ARG:HD3	3:A:505:5GP:O2P	2.06	0.54
1:B:371:ARG:O	1:B:416:ILE:HB	2.07	0.54
1:B:267:ASP:O	1:B:268:LYS:HB2	2.07	0.54
1:A:86:GLN:HG2	1:A:88:PHE:CE2	2.43	0.54
1:B:160:ASN:ND2	1:B:167:TYR:OH	2.41	0.54
1:B:321:ARG:HH11	1:B:321:ARG:CG	2.21	0.54
1:D:443:ILE:O	1:D:447:ARG:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLU:HG2	1:A:229:ALA:N	2.23	0.53
1:A:301:ILE:HD13	1:A:378:ILE:HD13	1.91	0.53
1:C:332:ARG:HH12	1:C:343:ARG:HH22	1.52	0.53
1:A:265:PHE:HA	1:A:269:ILE:O	2.08	0.53
1:B:80:SER:HB2	1:B:83:SER:CB	2.32	0.53
1:B:285:LYS:HG2	1:B:435:ILE:HD11	1.90	0.53
1:B:45:ARG:HB3	1:B:55:PHE:CE1	2.43	0.53
1:C:238:LEU:HD12	1:C:239:PHE:N	2.23	0.53
1:D:163:ILE:HD11	1:D:167:TYR:CZ	2.44	0.53
1:A:80:SER:CB	1:A:83:SER:HB2	2.34	0.53
1:C:383:ARG:HG3	1:C:383:ARG:NH1	2.21	0.53
1:D:45:ARG:HG2	1:D:55:PHE:CD1	2.43	0.53
1:D:238:LEU:HD12	1:D:239:PHE:H	1.73	0.53
1:C:443:ILE:O	1:C:447:ARG:HB2	2.08	0.53
1:A:443:ILE:O	1:A:447:ARG:HB2	2.09	0.53
1:B:477:PHE:HD1	1:B:477:PHE:O	1.91	0.53
1:D:164:ARG:HB3	1:D:469:ASP:OD2	2.08	0.53
1:B:86:GLN:HB3	1:B:87:PRO:HA	1.92	0.52
1:D:282:LEU:O	1:D:286:ILE:HG13	2.09	0.52
1:C:415:LEU:O	1:C:418:HIS:HB3	2.10	0.52
1:C:135:PHE:CZ	1:C:139:LEU:HD11	2.44	0.52
1:A:169:CYS:O	1:A:180:ALA:HA	2.10	0.52
1:C:33:ILE:HG13	1:C:55:PHE:CZ	2.44	0.52
1:A:346:VAL:HG23	1:A:377:GLN:OE1	2.10	0.52
1:C:73:ARG:NH1	1:C:81:SER:HA	2.25	0.52
1:B:297:VAL:CG1	1:B:362:VAL:HG12	2.40	0.51
1:C:475:LEU:HD23	1:C:478:LEU:HD12	1.91	0.51
1:B:290:TRP:O	1:B:293:LEU:HD12	2.10	0.51
1:A:285:LYS:HG2	1:A:435:ILE:HD11	1.93	0.51
1:B:439:LEU:O	1:B:443:ILE:HG13	2.11	0.51
1:C:328:ARG:HH22	3:D:506:5GP:H5'2	1.76	0.51
1:A:23:LEU:HD21	1:A:209:GLU:HB2	1.91	0.51
1:C:251:PRO:HG2	1:C:456:PHE:CD1	2.46	0.51
1:D:282:LEU:HD21	1:D:393:ALA:HB1	1.92	0.51
1:C:439:LEU:HG	1:C:443:ILE:HD11	1.93	0.51
1:B:471:ASP:O	1:B:475:LEU:HG	2.10	0.50
1:D:269:ILE:HD13	1:D:446:VAL:HG12	1.93	0.50
1:C:342:ARG:O	1:C:344:LYS:N	2.44	0.50
1:C:344:LYS:HD3	1:C:345:SER:H	1.77	0.50
1:B:80:SER:C	1:B:82:ALA:H	2.14	0.50
1:B:195:ARG:NH1	1:B:203:GLU:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:LEU:HA	1:C:481:LEU:HD21	1.93	0.50
1:B:397:PRO:HG2	1:B:439:LEU:HA	1.93	0.50
1:C:18:ASP:HA	1:C:21:THR:OG1	2.12	0.50
1:C:256:TYR:O	1:C:275:ARG:HD2	2.12	0.50
1:C:188:ARG:HG3	1:C:189:PRO:HD2	1.93	0.50
1:B:28:GLN:HB3	1:B:50:LEU:HD23	1.93	0.50
1:B:94:TYR:O	1:D:121:HIS:HB2	2.12	0.50
1:C:73:ARG:HG2	1:C:74:TYR:N	2.27	0.49
1:D:250:ASN:O	1:D:457:GLU:HB2	2.12	0.49
1:D:71:HIS:ND1	1:D:86:GLN:HB2	2.28	0.49
1:A:118:LYS:O	1:A:119:ARG:HB2	2.13	0.49
1:D:253:LEU:HD21	1:D:442:LEU:HD23	1.94	0.49
1:A:251:PRO:HG2	1:A:456:PHE:CD1	2.48	0.49
1:D:389:LYS:HA	1:D:432:ASP:OD2	2.13	0.49
1:C:280:THR:N	1:C:311:GLU:HG2	2.28	0.49
1:B:166:ALA:HB2	1:B:405:TYR:HB3	1.95	0.48
1:B:265:PHE:CE2	1:B:270:SER:HB2	2.48	0.48
1:C:237:GLN:NE2	1:C:239:PHE:CZ	2.81	0.48
1:B:74:TYR:O	1:B:76:THR:N	2.46	0.48
1:A:321:ARG:HG3	1:B:272:TYR:HE2	1.79	0.48
1:B:24:GLN:O	1:B:24:GLN:HG3	2.14	0.48
1:B:280:THR:N	1:B:311:GLU:HG2	2.29	0.48
1:C:45:ARG:HD2	1:C:59:HIS:CD2	2.48	0.48
1:C:73:ARG:HH12	1:C:81:SER:HA	1.78	0.48
1:C:289:GLU:O	1:C:290:TRP:HD1	1.97	0.48
1:D:426:ARG:HG2	1:D:426:ARG:HH11	1.77	0.48
1:C:403:ASN:HB2	1:C:460:VAL:CG1	2.43	0.48
1:D:321:ARG:HG2	1:D:321:ARG:HH11	1.79	0.48
1:A:160:ASN:ND2	1:A:167:TYR:OH	2.47	0.47
1:C:25:HIS:CE1	1:C:261:ARG:HG3	2.49	0.47
1:A:74:TYR:OH	3:A:505:5GP:O6	2.33	0.47
1:A:411:SER:OG	1:A:414:GLU:HG3	2.15	0.47
1:A:370:VAL:HB	3:A:505:5GP:O2P	2.15	0.47
1:B:118:LYS:O	1:B:119:ARG:HB2	2.14	0.47
1:B:293:LEU:CD2	1:B:295:ILE:HG23	2.44	0.47
1:D:197:ILE:HB	1:D:201:ARG:O	2.15	0.47
1:D:284:GLU:O	1:D:288:ARG:HG3	2.15	0.47
1:D:383:ARG:HG3	1:D:383:ARG:NH1	2.23	0.47
1:A:328:ARG:HH22	3:B:506:5GP:H5'2	1.79	0.47
1:D:297:VAL:HG21	1:D:321:ARG:HB2	1.97	0.47
1:B:1:CYS:O	1:B:26:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:HIS:HE1	1:B:73:ARG:HB2	1.79	0.47
1:C:336:MET:CB	1:C:337:PRO:HD3	2.28	0.47
1:B:34:ILE:HA	1:B:43:ARG:O	2.14	0.46
1:D:34:ILE:HG23	1:D:172:MET:CE	2.45	0.46
1:A:204:TYR:HB2	1:A:232:ILE:HD13	1.96	0.46
1:A:345:SER:O	1:A:348:ARG:HB2	2.16	0.46
1:C:321:ARG:HH11	1:C:321:ARG:CG	2.28	0.46
1:C:481:LEU:H	1:C:481:LEU:HD23	1.80	0.46
1:D:19:ALA:HB2	1:D:216:LEU:HD11	1.97	0.46
1:A:321:ARG:HG2	1:A:321:ARG:HH11	1.79	0.46
1:A:200:ASN:OD1	1:A:200:ASN:N	2.48	0.46
1:A:417:ALA:HA	1:A:425:ILE:HD11	1.98	0.46
1:D:321:ARG:HH11	1:D:321:ARG:CG	2.29	0.46
1:C:426:ARG:HD3	4:C:515:HOH:O	2.16	0.46
3:C:506:5GP:N2	1:D:325:VAL:HG13	2.31	0.46
1:D:4:VAL:HG11	1:D:16:ILE:HG23	1.98	0.46
1:C:332:ARG:NH1	1:C:343:ARG:NH2	2.60	0.45
1:D:28:GLN:N	1:D:28:GLN:OE1	2.49	0.45
1:A:371:ARG:O	1:A:416:ILE:HB	2.16	0.45
1:D:45:ARG:HG2	1:D:55:PHE:CE1	2.50	0.45
1:A:12:VAL:O	1:A:16:ILE:HG13	2.17	0.45
1:A:86:GLN:HG2	1:A:88:PHE:CD2	2.51	0.45
1:A:140:ASP:O	1:A:143:ARG:NH2	2.49	0.45
1:B:326:LYS:HA	1:B:350:LEU:HD23	1.98	0.45
1:B:420:ARG:HG2	1:B:424:GLU:CD	2.37	0.45
1:A:110:LEU:HD22	1:A:134:ILE:HD11	1.99	0.45
1:B:86:GLN:HG2	1:B:88:PHE:CD2	2.52	0.45
1:C:200:ASN:O	1:C:201:ARG:HG3	2.17	0.45
1:C:423:ASP:O	1:C:427:GLN:HG3	2.16	0.45
1:C:471:ASP:C	1:C:473:GLY:H	2.20	0.45
1:C:265:PHE:CE1	1:C:270:SER:HB2	2.52	0.45
1:C:398:GLU:HG3	1:C:436:PHE:CE2	2.51	0.45
1:B:121:HIS:HB3	1:D:91:ASN:O	2.17	0.45
1:B:171:ALA:HB3	1:B:179:VAL:HG22	1.99	0.45
1:A:163:ILE:HD11	1:A:167:TYR:CZ	2.52	0.45
1:C:74:TYR:OH	3:C:505:5GP:O6	2.34	0.45
1:C:346:VAL:HG21	1:C:374:THR:HA	1.99	0.45
1:A:34:ILE:HG23	1:A:34:ILE:O	2.17	0.45
1:A:45:ARG:NH1	1:A:54:VAL:O	2.50	0.45
1:A:222:ARG:NH2	1:A:228:GLU:OE2	2.50	0.45
1:B:45:ARG:NH1	1:B:54:VAL:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ILE:O	1:B:290:TRP:HB2	2.17	0.45
1:C:121:HIS:HE1	1:C:123:ASN:OD1	1.99	0.45
1:C:197:ILE:O	1:C:198:ASP:HB3	2.17	0.45
1:D:74:TYR:HE2	1:D:408:ASP:HB3	1.82	0.45
1:B:274:ALA:O	1:B:277:ASN:HB2	2.18	0.44
1:B:301:ILE:HD13	1:B:378:ILE:CD1	2.44	0.44
1:C:327:ASN:OD1	1:D:261:ARG:NH2	2.49	0.44
1:C:332:ARG:HH21	1:D:57:ALA:HB2	1.82	0.44
1:D:1:CYS:O	1:D:26:ARG:HD3	2.17	0.44
1:D:293:LEU:HD13	1:D:295:ILE:HG23	1.98	0.44
1:D:374:THR:HG22	1:D:378:ILE:CD1	2.47	0.44
1:A:211:VAL:HG13	1:A:264:SER:OG	2.18	0.44
1:A:302:PRO:HA	1:A:303:GLU:HA	1.70	0.44
1:D:364:LEU:O	1:D:392:LEU:HD12	2.18	0.44
1:A:43:ARG:NH1	1:A:62:ARG:O	2.50	0.44
1:A:321:ARG:HH11	1:A:321:ARG:CG	2.31	0.44
1:B:232:ILE:HG12	1:B:238:LEU:HD13	1.98	0.44
1:A:110:LEU:HD22	1:A:134:ILE:CD1	2.47	0.44
1:A:121:HIS:HB3	1:C:91:ASN:O	2.16	0.44
1:C:250:ASN:HA	1:C:455:GLN:O	2.18	0.44
1:D:328:ARG:O	1:D:328:ARG:HG2	2.17	0.44
1:A:371:ARG:NH1	1:A:414:GLU:HB3	2.33	0.44
1:D:200:ASN:H	1:D:200:ASN:HD22	1.65	0.44
1:D:45:ARG:HD2	1:D:59:HIS:CG	2.52	0.44
1:D:265:PHE:CE1	1:D:270:SER:HB2	2.53	0.44
1:D:297:VAL:HG23	1:D:319:PRO:O	2.17	0.44
1:A:267:ASP:O	1:A:268:LYS:HB2	2.18	0.43
1:D:367:ASP:OD1	3:D:505:5GP:O3'	2.37	0.43
1:B:140:ASP:O	1:B:143:ARG:NH2	2.50	0.43
1:A:1:CYS:HA	1:A:72:VAL:O	2.18	0.43
1:B:80:SER:C	1:B:82:ALA:N	2.72	0.43
1:C:474:TYR:HA	1:C:477:PHE:HB3	1.99	0.43
1:D:69:ILE:HD11	1:D:97:THR:HG23	2.01	0.43
3:A:506:5GP:H5'2	1:B:328:ARG:HH22	1.83	0.43
1:B:10:MET:HB2	1:B:11:PRO:HD2	2.01	0.43
1:C:59:HIS:O	1:C:62:ARG:HG2	2.18	0.43
1:C:156:ILE:O	1:C:159:THR:HB	2.18	0.43
1:C:475:LEU:HD23	1:C:475:LEU:HA	1.87	0.43
1:C:28:GLN:N	1:C:28:GLN:OE1	2.52	0.43
1:C:342:ARG:HA	1:C:342:ARG:HE	1.79	0.43
1:D:73:ARG:NH1	1:D:81:SER:HA	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLN:O	1:A:24:GLN:HG3	2.19	0.43
1:A:250:ASN:HA	1:A:455:GLN:O	2.19	0.43
1:B:29:ASP:HB2	1:B:75:PRO:HD3	2.00	0.43
1:C:300:PRO:HB3	1:C:309:ALA:HB3	2.00	0.43
1:B:211:VAL:HG13	1:B:264:SER:OG	2.19	0.43
1:C:335:ILE:HG22	1:C:340:GLN:H	1.83	0.43
1:A:34:ILE:HA	1:A:43:ARG:O	2.19	0.43
1:C:403:ASN:HB2	1:C:460:VAL:HG13	2.00	0.43
1:D:20:LEU:HD22	1:D:72:VAL:HG13	2.00	0.43
1:B:285:LYS:HE3	1:B:289:GLU:OE1	2.18	0.43
1:A:383:ARG:HG3	1:A:383:ARG:NH1	2.29	0.42
1:A:459:SER:HB2	1:A:465:TYR:CE2	2.53	0.42
1:D:94:TYR:CE1	1:D:145:TYR:CD2	3.05	0.42
1:D:205:MET:HG2	1:D:218:PHE:CD2	2.55	0.42
1:D:447:ARG:NH1	1:D:451:PRO:O	2.52	0.42
1:B:265:PHE:HA	1:B:269:ILE:O	2.19	0.42
1:C:44:LEU:HG	1:C:45:ARG:N	2.34	0.42
1:C:179:VAL:HA	1:C:230:ILE:O	2.20	0.42
1:C:359:ASP:O	1:C:388:LYS:HE2	2.20	0.42
1:D:163:ILE:O	1:D:163:ILE:HG13	2.19	0.42
1:D:197:ILE:HG21	1:D:201:ARG:HE	1.85	0.42
1:A:24:GLN:HG2	1:B:329:TYR:CD2	2.54	0.42
1:A:286:ILE:O	1:A:290:TRP:HB2	2.20	0.42
1:B:415:LEU:O	1:B:418:HIS:HB3	2.20	0.42
1:A:301:ILE:HD12	1:A:366:ASP:HB2	2.01	0.42
1:B:34:ILE:HG23	1:B:34:ILE:O	2.18	0.42
1:B:166:ALA:HB3	1:B:405:TYR:HB3	2.01	0.42
1:C:439:LEU:HG	1:C:443:ILE:CD1	2.49	0.42
1:C:102:GLY:HA2	1:C:188:ARG:HD2	2.02	0.42
1:A:93:PRO:HB2	1:A:94:TYR:CD2	2.55	0.42
1:A:94:TYR:OH	1:A:147:LEU:HD21	2.20	0.42
1:A:127:ASP:HA	1:A:130:ILE:HG13	2.00	0.42
1:D:186:GLY:HA3	1:D:226:PRO:HG3	2.01	0.42
1:A:290:TRP:CG	1:A:293:LEU:HD12	2.55	0.42
1:A:359:ASP:O	1:A:388:LYS:HE2	2.20	0.42
1:C:297:VAL:HG22	1:C:298:VAL:N	2.34	0.42
1:C:326:LYS:HA	1:C:350:LEU:HD23	2.02	0.42
1:C:383:ARG:NH1	1:C:383:ARG:CG	2.82	0.42
1:A:465:TYR:CG	1:A:470:VAL:HG11	2.54	0.41
3:A:506:5GP:O4'	1:B:328:ARG:NH2	2.52	0.41
1:C:31:ALA:HA	1:C:71:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ASN:O	1:C:457:GLU:HB2	2.20	0.41
1:D:34:ILE:HG23	1:D:172:MET:HE1	2.01	0.41
1:B:230:ILE:HG23	1:B:238:LEU:HD11	2.02	0.41
1:A:331:GLY:H	1:A:348:ARG:HH12	1.67	0.41
1:A:359:ASP:C	1:A:388:LYS:HE2	2.41	0.41
1:B:375:SER:O	1:B:379:ILE:HD12	2.20	0.41
1:D:415:LEU:HB2	1:D:418:HIS:HB2	2.01	0.41
1:D:275:ARG:O	1:D:308:ILE:HG12	2.21	0.41
1:C:185:ASN:HB2	1:C:187:ILE:HG13	2.02	0.41
1:A:383:ARG:NH1	1:A:383:ARG:CG	2.83	0.41
1:B:258:TYR:CE1	3:B:505:5GP:H2'	2.55	0.41
1:C:29:ASP:OD2	1:C:81:SER:HB3	2.20	0.41
1:C:478:LEU:HA	1:C:481:LEU:CD2	2.50	0.41
1:D:383:ARG:NH1	1:D:383:ARG:CG	2.83	0.41
1:A:179:VAL:HA	1:A:230:ILE:O	2.21	0.41
1:A:221:LEU:O	1:A:222:ARG:HB3	2.20	0.41
1:D:198:ASP:OD1	1:D:200:ASN:ND2	2.53	0.41
1:D:297:VAL:HG22	1:D:298:VAL:N	2.35	0.41
1:D:300:PRO:HB3	1:D:309:ALA:CB	2.50	0.41
1:C:335:ILE:HD12	1:C:335:ILE:H	1.85	0.41
1:D:106:ASN:HB2	1:D:109:GLU:HG2	2.02	0.41
1:A:43:ARG:HH11	1:A:62:ARG:HG2	1.84	0.41
1:A:92:SER:HB3	1:C:120:ARG:HA	2.02	0.41
1:A:142:PHE:CD2	1:A:151:ASN:HB3	2.56	0.41
1:D:332:ARG:HG3	1:D:334:PHE:CZ	2.56	0.41
1:D:470:VAL:HG13	1:D:474:TYR:HD2	1.85	0.41
1:A:26:ARG:NH2	1:A:255:GLU:OE1	2.54	0.41
1:A:144:HIS:O	1:A:144:HIS:ND1	2.54	0.41
1:A:290:TRP:CD2	1:A:293:LEU:HD12	2.56	0.41
1:B:86:GLN:HG2	1:B:88:PHE:CE2	2.56	0.41
1:B:230:ILE:CG2	1:B:238:LEU:HD11	2.51	0.41
1:C:148:GLU:O	1:C:149:ALA:C	2.60	0.41
1:D:318:LYS:HD3	1:D:318:LYS:HA	1.92	0.41
1:A:74:TYR:O	1:A:76:THR:N	2.53	0.40
1:A:438:ASP:HB3	1:A:440:ASN:OD1	2.21	0.40
1:B:474:TYR:O	1:B:477:PHE:HB3	2.21	0.40
1:A:328:ARG:HD2	1:A:329:TYR:CE1	2.56	0.40
1:B:321:ARG:CG	1:B:321:ARG:NH1	2.80	0.40
1:C:10:MET:HB2	1:C:11:PRO:HD2	2.03	0.40
1:D:423:ASP:O	1:D:427:GLN:HG3	2.21	0.40
1:A:156:ILE:O	1:A:159:THR:HB	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:TYR:CE1	3:A:505:5GP:H2'	2.57	0.40
1:C:67:MET:HG2	1:C:172:MET:SD	2.62	0.40
1:C:274:ALA:O	1:C:278:MET:HG3	2.21	0.40
1:D:411:SER:O	1:D:412:ALA:C	2.59	0.40
1:A:5:GLY:HA3	1:A:170:VAL:HG21	2.04	0.40
1:D:35:THR:OG1	1:D:43:ARG:HB2	2.22	0.40
1:A:27:GLY:HA2	1:A:74:TYR:HA	2.03	0.40
1:B:191:VAL:O	1:B:206:VAL:HA	2.21	0.40
1:C:179:VAL:HG12	1:C:231:TYR:HD1	1.86	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	471/504 (94%)	427 (91%)	38 (8%)	6 (1%)	12	30
1	B	466/504 (92%)	427 (92%)	36 (8%)	3 (1%)	25	50
1	C	480/504 (95%)	431 (90%)	39 (8%)	10 (2%)	7	18
1	D	469/504 (93%)	431 (92%)	35 (8%)	3 (1%)	25	50
All	All	1886/2016 (94%)	1716 (91%)	148 (8%)	22 (1%)	13	32

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	GLU
1	C	80	SER
1	C	339	GLN
1	C	343	ARG
1	D	80	SER
1	A	199	GLU

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Mol	Chain	Res	Type
1	C	336	MET
1	D	77	ALA
1	D	354	ARG
1	B	80	SER
1	C	198	ASP
1	C	354	ARG
1	A	200	ASN
1	A	354	ARG
1	C	341	LEU
1	B	75	PRO
1	B	354	ARG
1	C	141	ASN
1	C	472	GLN
1	C	77	ALA
1	A	75	PRO
1	A	11	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	397/422 (94%)	373 (94%)	24 (6%)	19 42
1	B	392/422 (93%)	374 (95%)	18 (5%)	27 54
1	C	403/422 (96%)	370 (92%)	33 (8%)	11 26
1	D	395/422 (94%)	368 (93%)	27 (7%)	16 36
All	All	1587/1688 (94%)	1485 (94%)	102 (6%)	17 39

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	45	ARG
1	A	131	LEU
1	A	144	HIS
1	A	150	ASP

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Mol	Chain	Res	Type
1	A	179	VAL
1	A	188	ARG
1	A	194	LYS
1	A	200	ASN
1	A	215	THR
1	A	222	ARG
1	A	235	GLU
1	A	259	PHE
1	A	292	ASP
1	A	321	ARG
1	A	322	GLN
1	A	347	ARG
1	A	353	ASN
1	A	371	ARG
1	A	375	SER
1	A	409	MET
1	A	437	GLN
1	A	466	VAL
1	A	471	ASP
1	B	28	GLN
1	B	45	ARG
1	B	100	HIS
1	B	131	LEU
1	B	144	HIS
1	B	188	ARG
1	B	194	LYS
1	B	222	ARG
1	B	292	ASP
1	B	293	LEU
1	B	305	SER
1	B	321	ARG
1	B	322	GLN
1	B	332	ARG
1	B	353	ASN
1	B	375	SER
1	B	413	THR
1	B	477	PHE
1	C	9	VAL
1	C	21	THR
1	C	45	ARG
1	C	61	GLN
1	C	98	LEU

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Mol	Chain	Res	Type
1	C	101	ASN
1	C	125	THR
1	C	131	LEU
1	C	161	ARG
1	C	182	ARG
1	C	188	ARG
1	C	210	SER
1	C	215	THR
1	C	222	ARG
1	C	249	SER
1	C	261	ARG
1	C	293	LEU
1	C	321	ARG
1	C	322	GLN
1	C	332	ARG
1	C	335	ILE
1	C	336	MET
1	C	342	ARG
1	C	344	LYS
1	C	347	ARG
1	C	375	SER
1	C	409	MET
1	C	447	ARG
1	C	457	GLU
1	C	469	ASP
1	C	474	TYR
1	C	477	PHE
1	C	481	LEU
1	D	9	VAL
1	D	45	ARG
1	D	52	SER
1	D	61	GLN
1	D	76	THR
1	D	91	ASN
1	D	101	ASN
1	D	109	GLU
1	D	125	THR
1	D	131	LEU
1	D	144	HIS
1	D	161	ARG
1	D	188	ARG
1	D	198	ASP

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Mol	Chain	Res	Type
1	D	200	ASN
1	D	210	SER
1	D	215	THR
1	D	222	ARG
1	D	249	SER
1	D	261	ARG
1	D	293	LEU
1	D	321	ARG
1	D	322	GLN
1	D	370	VAL
1	D	413	THR
1	D	457	GLU
1	D	469	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	160	ASN
1	A	185	ASN
1	A	250	ASN
1	A	322	GLN
1	A	353	ASN
1	A	454	GLN
1	B	101	ASN
1	B	160	ASN
1	B	185	ASN
1	B	250	ASN
1	B	322	GLN
1	B	353	ASN
1	C	101	ASN
1	C	121	HIS
1	C	237	GLN
1	C	322	GLN
1	D	101	ASN
1	D	121	HIS
1	D	200	ASN
1	D	322	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
3	5GP	C	506	-	22,26,26	1.73	4 (18%)	26,40,40	2.23	9 (34%)
3	5GP	C	505	2	22,26,26	1.74	5 (22%)	26,40,40	1.53	4 (15%)
3	5GP	A	505	2	22,26,26	1.76	5 (22%)	26,40,40	1.70	4 (15%)
3	5GP	B	506	-	22,26,26	1.97	8 (36%)	26,40,40	2.12	9 (34%)
3	5GP	D	506	-	22,26,26	1.58	3 (13%)	26,40,40	1.71	6 (23%)
3	5GP	D	505	2	22,26,26	1.72	5 (22%)	26,40,40	1.64	6 (23%)
3	5GP	B	505	2	22,26,26	1.71	6 (27%)	26,40,40	1.66	6 (23%)
3	5GP	A	506	-	22,26,26	1.80	5 (22%)	26,40,40	1.74	10 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5GP	C	506	-	-	6/6/26/26	0/3/3/3
3	5GP	C	505	2	-	0/6/26/26	0/3/3/3
3	5GP	A	505	2	-	0/6/26/26	0/3/3/3
3	5GP	B	506	-	-	6/6/26/26	0/3/3/3
3	5GP	D	506	-	-	6/6/26/26	0/3/3/3
3	5GP	D	505	2	-	0/6/26/26	0/3/3/3
3	5GP	B	505	2	-	0/6/26/26	0/3/3/3
3	5GP	A	506	-	-	5/6/26/26	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	505	5GP	O4'-C1'	4.51	1.47	1.41
3	A	505	5GP	C6-N1	4.50	1.44	1.37
3	D	505	5GP	C6-N1	4.22	1.44	1.37
3	C	505	5GP	C6-N1	4.12	1.44	1.37
3	A	506	5GP	C8-N7	-4.10	1.28	1.35
3	B	506	5GP	O4'-C1'	3.99	1.46	1.41
3	B	505	5GP	C6-N1	3.79	1.43	1.37
3	C	506	5GP	C8-N7	-3.68	1.28	1.35
3	A	506	5GP	O4'-C1'	3.55	1.46	1.41
3	D	505	5GP	O4'-C1'	3.47	1.45	1.41
3	D	505	5GP	C5-C6	-3.31	1.40	1.47
3	B	506	5GP	O4'-C4'	-3.31	1.37	1.45
3	B	506	5GP	C8-N7	-3.27	1.29	1.35
3	D	506	5GP	C8-N7	-3.22	1.29	1.35
3	C	506	5GP	C6-N1	3.17	1.42	1.37
3	D	506	5GP	O4'-C4'	-3.16	1.37	1.45
3	B	505	5GP	C5-C6	-3.11	1.41	1.47
3	C	506	5GP	C2'-C1'	-3.07	1.49	1.53
3	B	506	5GP	C5-C6	-2.93	1.41	1.47
3	B	505	5GP	O4'-C1'	2.81	1.45	1.41
3	B	505	5GP	C2'-C1'	2.79	1.58	1.53
3	A	505	5GP	O4'-C1'	2.79	1.45	1.41
3	C	505	5GP	C5-C6	-2.71	1.41	1.47
3	C	506	5GP	O2'-C2'	-2.68	1.36	1.43
3	D	505	5GP	C5-C4	-2.63	1.36	1.43
3	B	506	5GP	C5'-C4'	-2.61	1.43	1.51
3	C	505	5GP	C5-C4	-2.59	1.36	1.43
3	D	505	5GP	C8-N7	-2.53	1.30	1.35
3	A	506	5GP	O4'-C4'	-2.45	1.39	1.45
3	A	505	5GP	C2'-C1'	2.40	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	506	5GP	C5-C6	-2.33	1.42	1.47
3	B	506	5GP	O2'-C2'	-2.33	1.37	1.43
3	C	505	5GP	C8-N7	-2.32	1.31	1.35
3	A	505	5GP	C4-N3	2.29	1.42	1.37
3	B	505	5GP	C5-C4	-2.22	1.37	1.43
3	A	505	5GP	P-O5'	2.20	1.67	1.60
3	B	506	5GP	C2'-C1'	-2.18	1.50	1.53
3	A	506	5GP	C5-C4	-2.15	1.37	1.43
3	B	505	5GP	O2'-C2'	2.06	1.47	1.43
3	B	506	5GP	C5-C4	-2.04	1.37	1.43
3	D	506	5GP	C5'-C4'	-2.02	1.45	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	506	5GP	O4'-C1'-C2'	-5.60	98.74	106.93
3	C	506	5GP	O6-C6-N1	5.22	126.81	120.65
3	A	505	5GP	P-O5'-C5'	4.84	131.64	118.30
3	B	506	5GP	N2-C2-N3	-4.78	110.43	119.74
3	B	505	5GP	P-O5'-C5'	4.72	131.31	118.30
3	D	505	5GP	P-O5'-C5'	4.30	130.15	118.30
3	D	506	5GP	O6-C6-N1	4.15	125.55	120.65
3	B	506	5GP	O4'-C1'-C2'	-4.11	100.92	106.93
3	C	505	5GP	P-O5'-C5'	3.66	128.39	118.30
3	C	506	5GP	C3'-C2'-C1'	3.57	106.35	100.98
3	A	506	5GP	O4'-C4'-C5'	-3.52	97.80	109.37
3	D	505	5GP	C2'-C3'-C4'	3.47	109.39	102.64
3	C	506	5GP	C5-C6-N1	-3.40	107.95	113.95
3	A	505	5GP	C3'-C2'-C1'	3.33	106.00	100.98
3	C	505	5GP	C2'-C3'-C4'	3.14	108.74	102.64
3	B	506	5GP	O6-C6-N1	3.12	124.33	120.65
3	B	506	5GP	P-O5'-C5'	2.99	126.53	118.30
3	C	506	5GP	O2'-C2'-C1'	-2.93	100.03	110.85
3	A	505	5GP	O3P-P-O2P	2.92	118.80	107.64
3	D	506	5GP	O2'-C2'-C1'	-2.91	100.12	110.85
3	C	506	5GP	P-O5'-C5'	2.85	126.14	118.30
3	B	506	5GP	O2'-C2'-C1'	-2.82	100.45	110.85
3	B	506	5GP	C5-C6-N1	-2.80	109.00	113.95
3	D	506	5GP	O4'-C1'-C2'	-2.79	102.84	106.93
3	D	506	5GP	O4'-C4'-C5'	-2.77	100.27	109.37
3	B	505	5GP	O3P-P-O2P	2.77	118.21	107.64
3	D	505	5GP	O3'-C3'-C4'	-2.74	103.13	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	506	5GP	O4'-C4'-C5'	-2.74	100.37	109.37
3	A	506	5GP	N1-C2-N3	2.72	128.41	123.32
3	D	506	5GP	C5-C6-N1	-2.71	109.17	113.95
3	C	505	5GP	O3P-P-O2P	2.69	117.92	107.64
3	A	506	5GP	O2'-C2'-C1'	-2.67	100.99	110.85
3	B	506	5GP	N2-C2-N1	2.51	122.06	116.71
3	C	506	5GP	O4'-C4'-C5'	-2.43	101.38	109.37
3	D	505	5GP	O3P-P-O2P	2.42	116.88	107.64
3	A	506	5GP	O5'-P-O1P	-2.37	99.84	106.47
3	C	506	5GP	O3P-P-O5'	-2.36	100.45	106.73
3	D	505	5GP	O3P-P-O5'	-2.33	100.52	106.73
3	D	505	5GP	O6-C6-N1	2.32	123.39	120.65
3	B	505	5GP	O6-C6-N1	2.28	123.34	120.65
3	B	505	5GP	N2-C2-N1	2.27	121.54	116.71
3	A	506	5GP	O5'-C5'-C4'	-2.24	101.27	108.99
3	B	506	5GP	N1-C2-N3	2.24	127.51	123.32
3	B	505	5GP	C2'-C3'-C4'	2.23	106.97	102.64
3	A	506	5GP	O6-C6-N1	2.20	123.25	120.65
3	A	505	5GP	N2-C2-N1	2.19	121.38	116.71
3	C	505	5GP	N2-C2-N1	2.18	121.36	116.71
3	A	506	5GP	O4'-C1'-C2'	-2.16	103.78	106.93
3	A	506	5GP	O3P-P-O1P	2.15	119.10	110.68
3	D	506	5GP	P-O5'-C5'	2.12	124.12	118.30
3	B	505	5GP	O3P-P-O5'	-2.11	101.12	106.73
3	A	506	5GP	C5'-C4'-C3'	2.10	123.04	115.18
3	A	506	5GP	C5-C6-N1	-2.01	110.40	113.95
3	C	506	5GP	O5'-P-O1P	-2.01	100.84	106.47

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	506	5GP	C5'-O5'-P-O1P
3	A	506	5GP	C5'-O5'-P-O2P
3	A	506	5GP	C5'-O5'-P-O3P
3	B	506	5GP	C5'-O5'-P-O1P
3	B	506	5GP	C5'-O5'-P-O2P
3	B	506	5GP	C5'-O5'-P-O3P
3	C	506	5GP	C5'-O5'-P-O1P
3	C	506	5GP	C5'-O5'-P-O2P
3	C	506	5GP	C5'-O5'-P-O3P
3	D	506	5GP	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
3	D	506	5GP	C5'-O5'-P-O2P
3	D	506	5GP	C5'-O5'-P-O3P
3	D	506	5GP	O4'-C4'-C5'-O5'
3	B	506	5GP	C3'-C4'-C5'-O5'
3	D	506	5GP	C3'-C4'-C5'-O5'
3	B	506	5GP	O4'-C4'-C5'-O5'
3	A	506	5GP	O4'-C4'-C5'-O5'
3	C	506	5GP	C4'-C5'-O5'-P
3	C	506	5GP	O4'-C4'-C5'-O5'
3	D	506	5GP	C4'-C5'-O5'-P
3	C	506	5GP	C3'-C4'-C5'-O5'
3	A	506	5GP	C3'-C4'-C5'-O5'
3	B	506	5GP	C4'-C5'-O5'-P

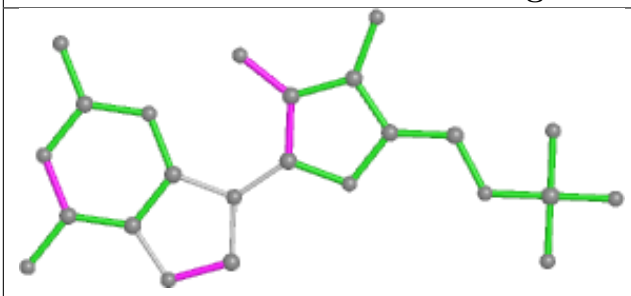
There are no ring outliers.

8 monomers are involved in 13 short contacts:

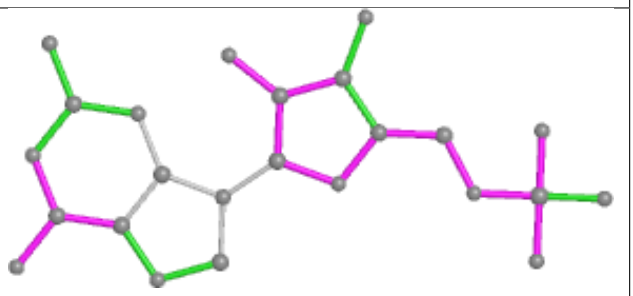
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	506	5GP	1	0
3	C	505	5GP	1	0
3	A	505	5GP	4	0
3	B	506	5GP	1	0
3	D	506	5GP	1	0
3	D	505	5GP	2	0
3	B	505	5GP	1	0
3	A	506	5GP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

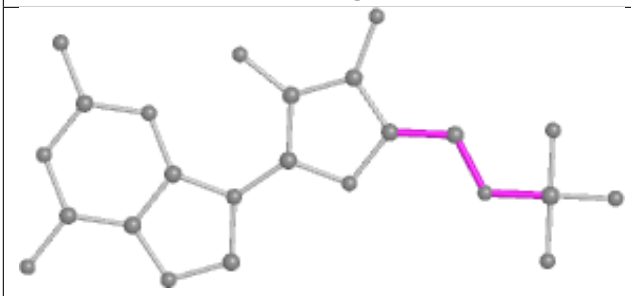
Ligand 5GP C 506



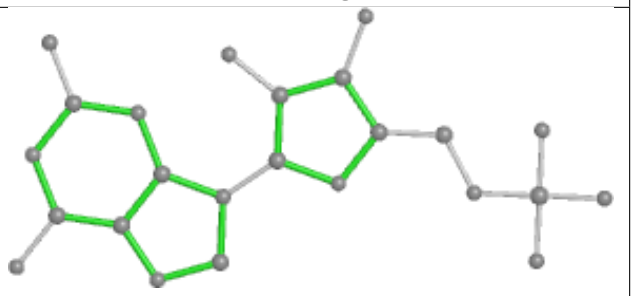
Bond lengths



Bond angles

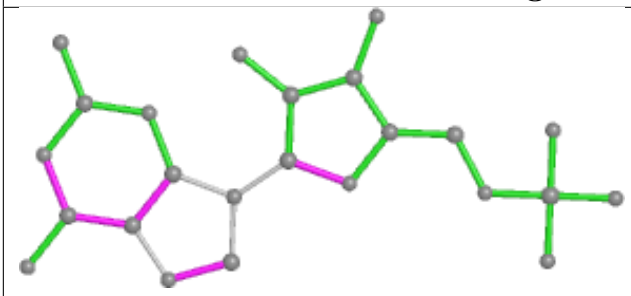


Torsions

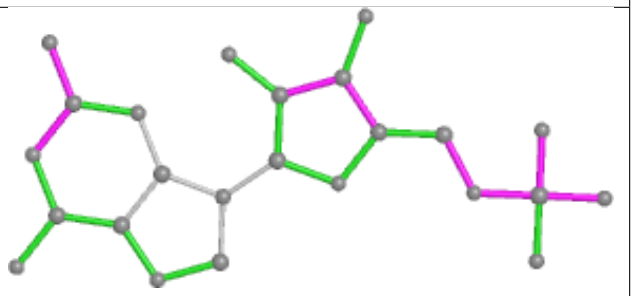


Rings

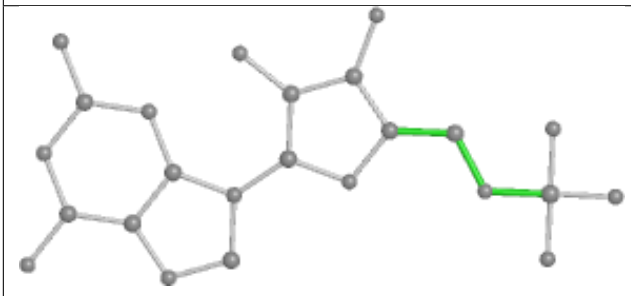
Ligand 5GP C 505



Bond lengths



Bond angles



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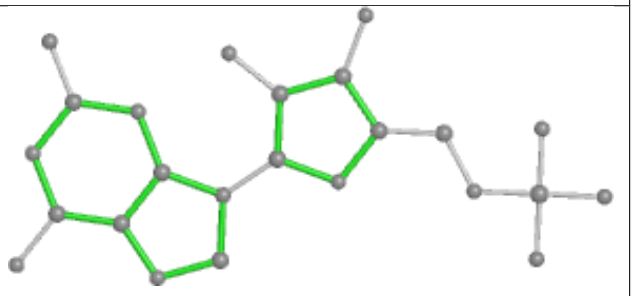
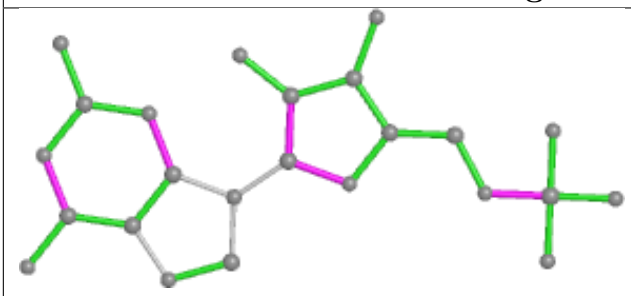
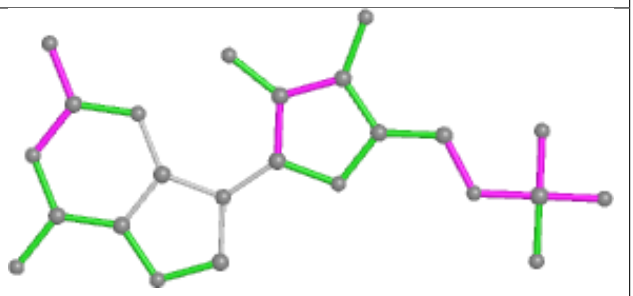


Rings

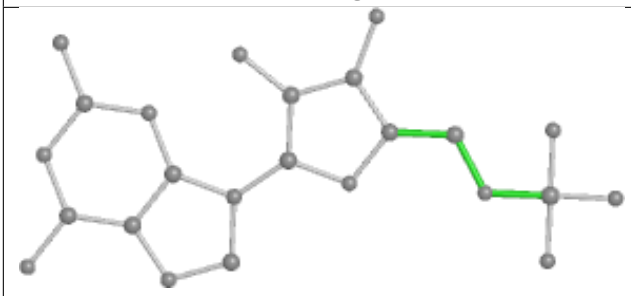
Ligand 5GP A 505



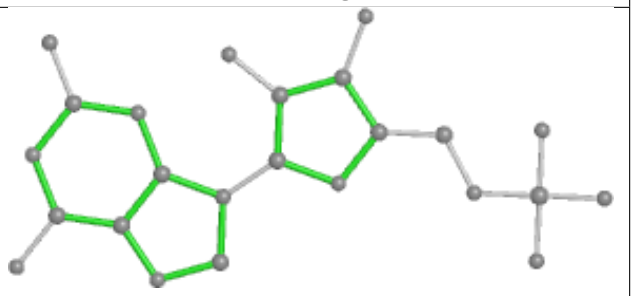
Bond lengths



Bond angles

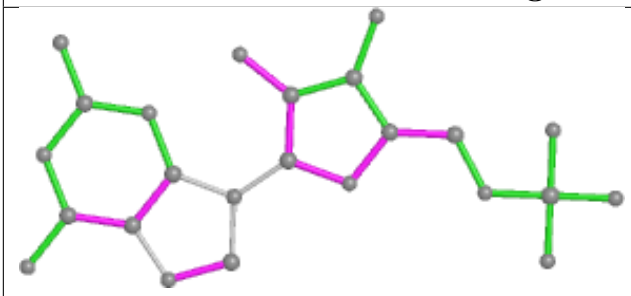


Torsions

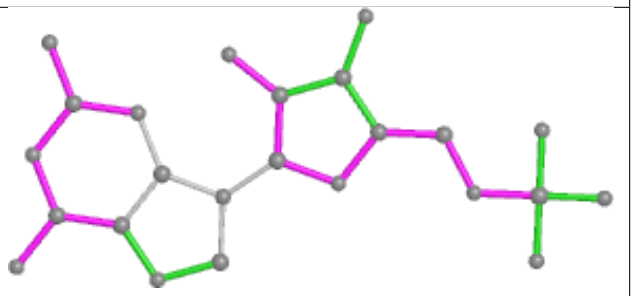


Rings

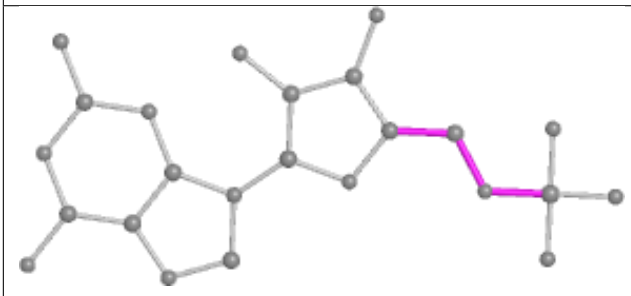
Ligand 5GP B 506



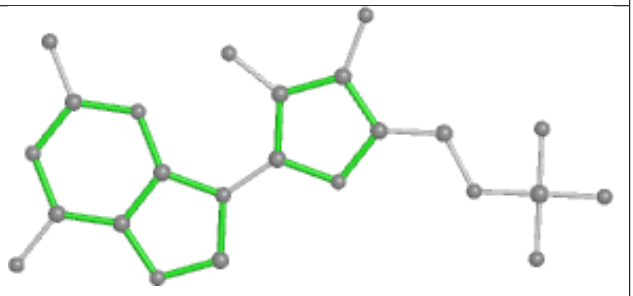
Bond lengths



Bond angles

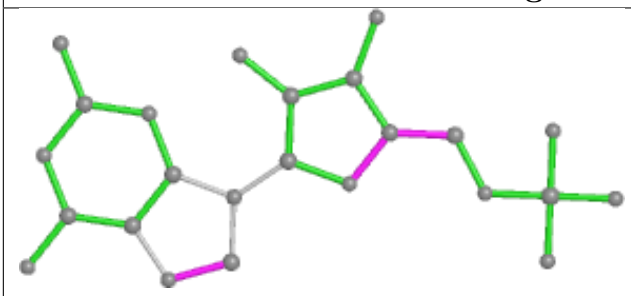


Torsions

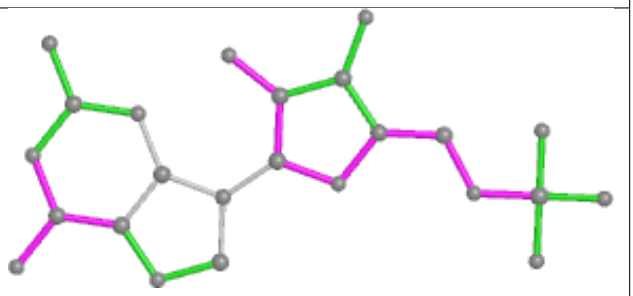


Rings

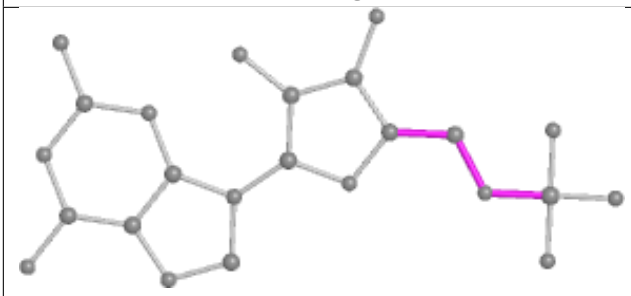
Ligand 5GP D 506



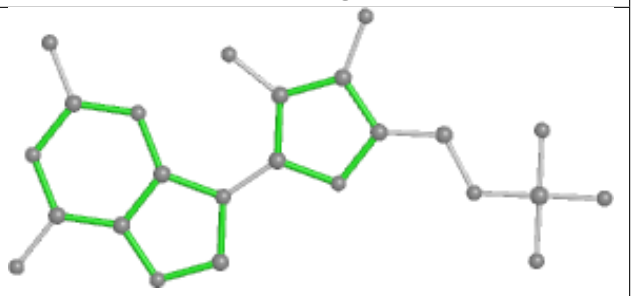
Bond lengths



Bond angles

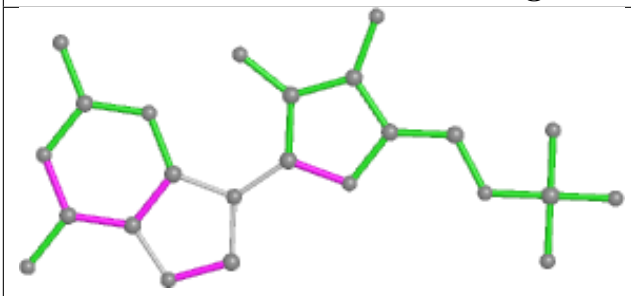


Torsions

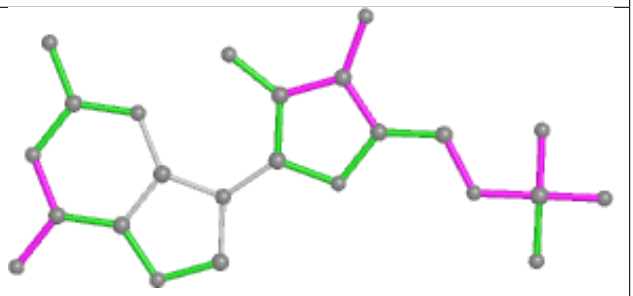


Rings

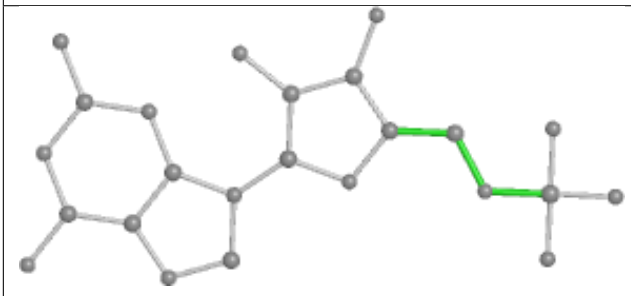
Ligand 5GP D 505



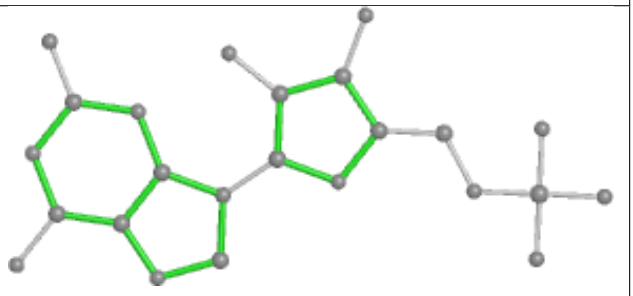
Bond lengths



Bond angles

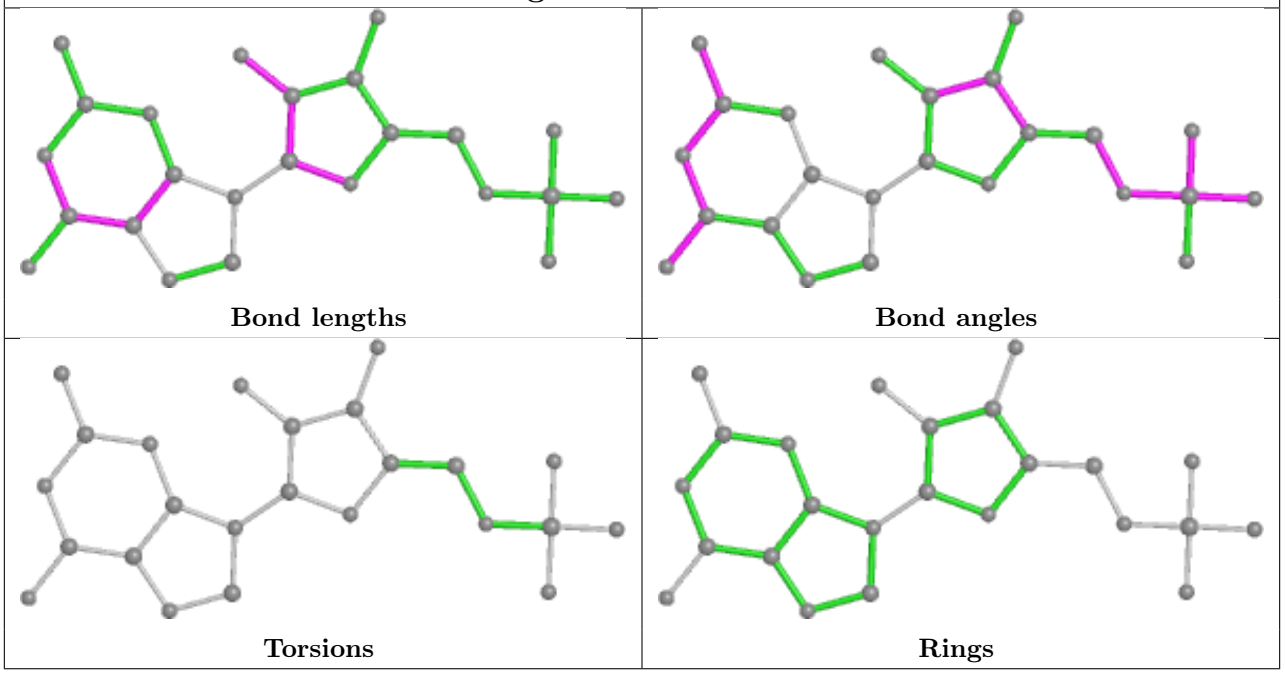


Torsions

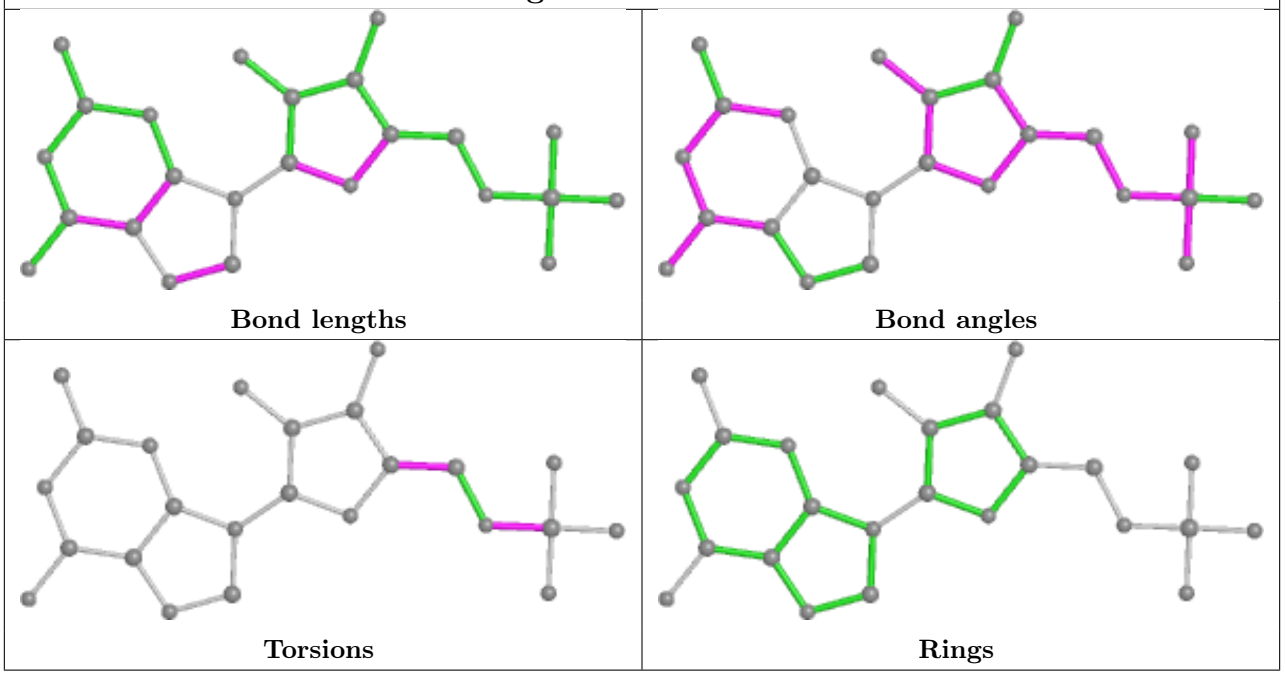


Rings

Ligand 5GP B 505



Ligand 5GP A 506



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.