Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 02:06 AM EDT

PDB ID	:	1CJB
Title	:	MALARIAL PURINE PHOSPHORIBOSYLTRANSFERASE
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Deposited on	:	1999-04-08
Resolution	:	2.00 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:

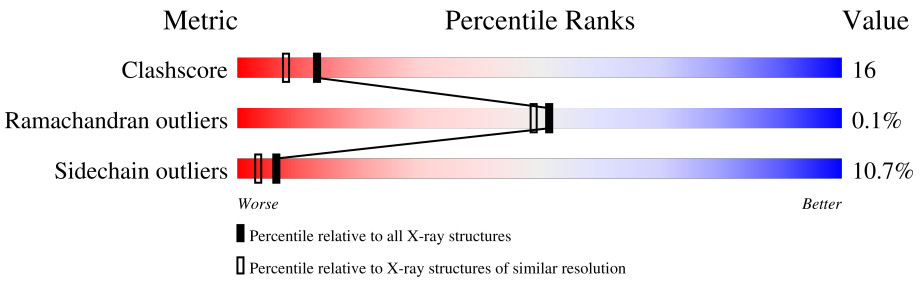
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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	231	70% 24% 5% •
1	B	231	68% 26% • •
1	C	231	67% 29% •
1	D	231	64% 30% 5% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7876 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.

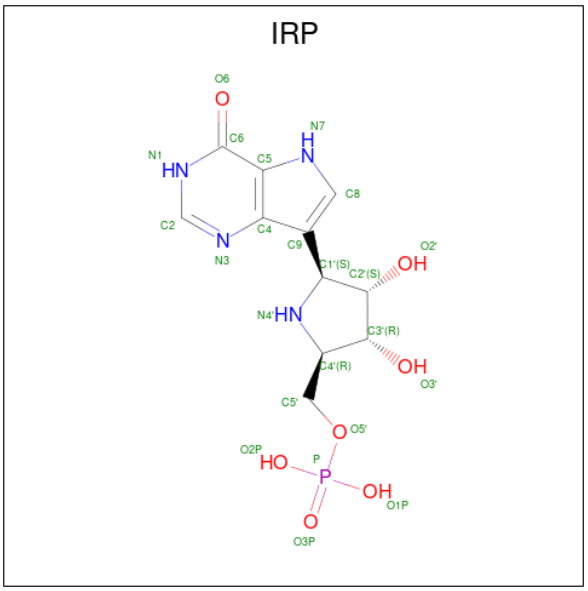
- Molecule 1 is a protein called PROTEIN (HYPOXANTHINE-GUANINE PHOSPHORIBO SYLTRANSFERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	228	1828	1186	301	333	8	0	0	1
1	B	228	1828	1186	301	333	8	0	0	1
1	C	230	1849	1199	303	339	8	0	0	0
1	D	228	1828	1186	301	333	8	0	0	1

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

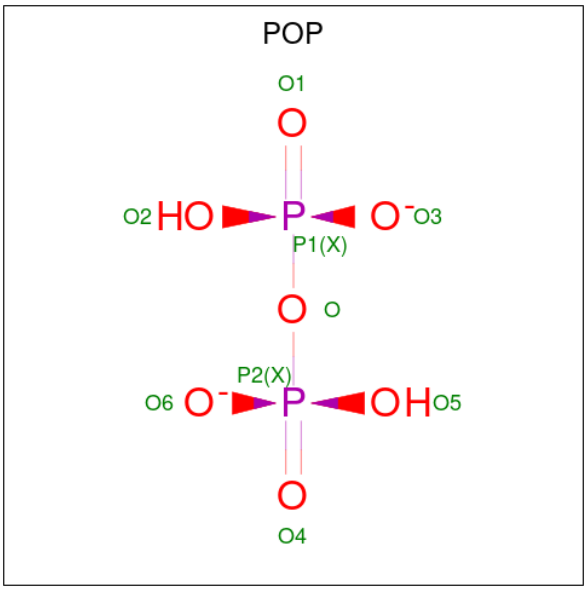
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0

- Molecule 3 is (1S)-1(9-DEAZAHYPOXANTHIN-9YL)1,4-DIDEOXY-1,4-IMINO-D-RIBIT OL-5-PHOSPHATE (three-letter code: IRP) (formula: $C_{11}H_{15}N_4O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	23	11	4	7	1	0	0
			Total	C	N	O	P		
3	B	1	23	11	4	7	1	0	0
			Total	C	N	O	P		
3	C	1	23	11	4	7	1	0	0
			Total	C	N	O	P		
3	D	1	23	11	4	7	1	0	0

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
4	A	1	9	7	2	0	0
4	B	1	9	7	2	0	0
4	C	1	9	7	2	0	0
4	D	1	9	7	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	118	118	118	0	0
5	B	128	128	128	0	0
5	C	92	92	92	0	0
5	D	69	69	69	0	0

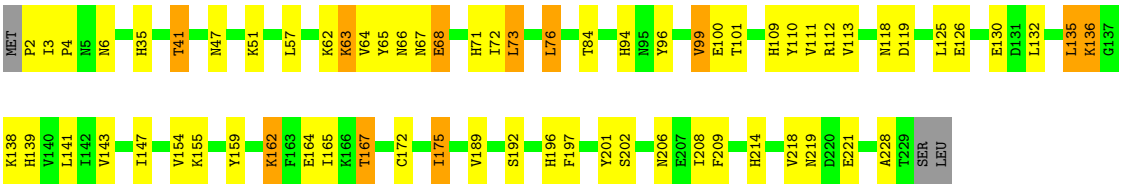
3 Residue-property plots (i)

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

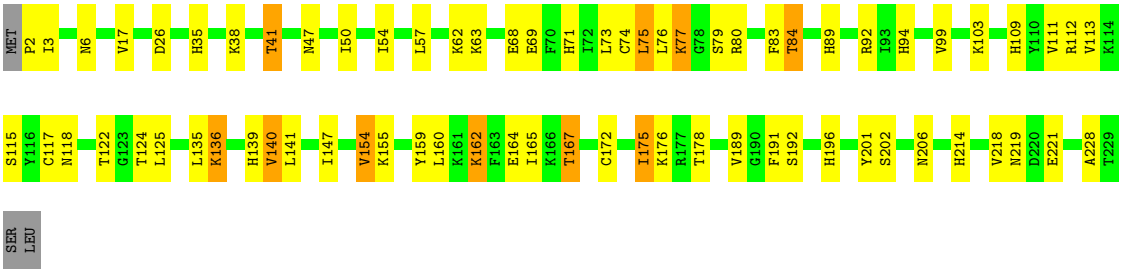
• Molecule 1: PROTEIN (HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE)

Chain A:



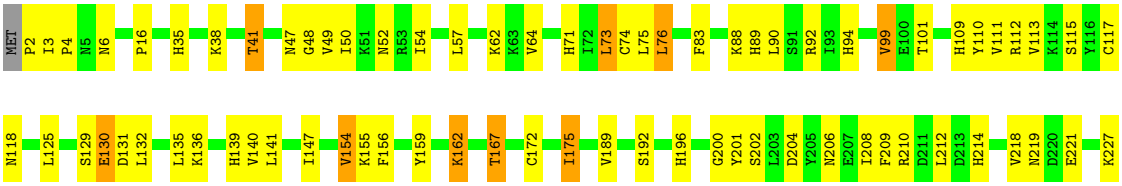
• Molecule 1: PROTEIN (HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE)

Chain B:



• Molecule 1: PROTEIN (HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE)

Chain C:



A228 T229 S230 L231

• Molecule 1: PROTEIN (HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE)

Chain D: 64% 30% 5% •

MET P2 I3 N6 H35 T41 N47 G48 V49 I50 K51 N52 L57 K62 K63 E69 F70 H71 I72 L73 C74 L75 L76 K77 F83 H94 N95 Y96 V99 E100 T101 H109 Y110 V111 R112 V113 K114 S115 Y116 C117 N118 D119 Q120 S121 T122 G123 T124 L125 E126

I127 V128 S129 E130 D131 L132 S133 C134 L135 K136 G137 K138 H139 V140 L141 I142 I147 L153 V154 K162 I165 K166 T167 I170 A171 C172 I175 T178 W181 K185 V189 S192 H196 F197 Y201 S202 Y205 N206 E207 I208 H214 V218 N219 D220

E221 G222 K223 Y226 K227 A228 T229 SER LEU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	105.49Å 110.39Å 173.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	98.0 (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.196 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7876	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

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: POP, IRP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.37	0/1872	0.63	1/2529 (0.0%)
1	B	0.39	0/1872	0.64	1/2529 (0.0%)
1	C	0.35	0/1893	0.61	1/2556 (0.0%)
1	D	0.38	0/1872	0.61	1/2529 (0.0%)
All	All	0.37	0/7509	0.62	4/10143 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	2	PRO	N-CA-CB	5.30	109.66	103.30
1	A	2	PRO	N-CA-CB	5.18	109.51	103.30
1	C	2	PRO	N-CA-CB	5.06	109.37	103.30
1	B	2	PRO	N-CA-CB	5.05	109.36	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1828	0	1822	61	0
1	B	1828	0	1822	57	0
1	C	1849	0	1845	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1828	0	1822	73	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	23	0	12	0	0
3	B	23	0	11	0	0
3	C	23	0	12	0	0
3	D	23	0	12	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
4	C	9	0	0	0	0
4	D	9	0	0	0	0
5	A	118	0	0	6	0
5	B	128	0	0	7	0
5	C	92	0	0	4	0
5	D	69	0	0	5	0
All	All	7876	0	7358	241	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 16.

All (241) 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:118:ASN:HD21	1:C:228:ALA:H	1.10	0.99
1:C:47:ASN:H	1:C:214:HIS:HD2	1.07	0.96
1:D:47:ASN:H	1:D:214:HIS:HD2	1.10	0.94
1:C:48:GLY:H	1:D:52:ASN:HD21	1.13	0.94
1:B:118:ASN:HD21	1:B:228:ALA:H	1.09	0.94
1:C:52:ASN:HD21	1:D:48:GLY:H	1.15	0.92
1:A:47:ASN:H	1:A:214:HIS:HD2	1.06	0.92
1:C:139:HIS:HD2	1:C:167:THR:HB	1.33	0.90
1:D:118:ASN:HD21	1:D:228:ALA:H	1.15	0.90
1:B:113:VAL:HG13	1:B:125:LEU:HD11	1.51	0.89
1:D:118:ASN:HD22	1:D:206:ASN:HD21	1.20	0.88
1:A:41:THR:HG22	1:A:219:ASN:HB3	1.56	0.88
1:B:47:ASN:H	1:B:214:HIS:HD2	1.23	0.87
1:D:111:VAL:HG13	1:D:129:SER:HB3	1.56	0.87
1:C:41:THR:HG22	1:C:219:ASN:HB3	1.59	0.84
1:D:47:ASN:H	1:D:214:HIS:CD2	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:THR:HG22	1:B:219:ASN:HB3	1.60	0.83
1:A:118:ASN:HD22	1:A:206:ASN:HD21	1.26	0.82
1:B:113:VAL:CG1	1:B:125:LEU:HD11	2.10	0.82
1:B:139:HIS:HD2	1:B:167:THR:HB	1.44	0.81
1:C:118:ASN:HD22	1:C:206:ASN:HD21	1.27	0.81
1:A:118:ASN:HD21	1:A:228:ALA:H	1.24	0.81
1:C:47:ASN:H	1:C:214:HIS:CD2	1.98	0.79
1:A:139:HIS:HD2	1:A:167:THR:HB	1.48	0.78
1:C:113:VAL:CG1	1:C:125:LEU:HD11	2.15	0.77
1:C:52:ASN:ND2	1:D:48:GLY:H	1.81	0.76
1:C:48:GLY:H	1:D:52:ASN:ND2	1.84	0.76
1:A:118:ASN:ND2	1:A:206:ASN:HD21	1.83	0.76
1:B:38:LYS:HE3	5:B:804:HOH:O	1.87	0.74
1:D:118:ASN:ND2	1:D:206:ASN:HD21	1.85	0.74
1:A:47:ASN:H	1:A:214:HIS:CD2	1.99	0.73
1:C:62:LYS:NZ	1:C:94:HIS:HD2	1.86	0.72
1:C:49:VAL:HG22	1:D:49:VAL:HG23	1.70	0.72
1:A:71:HIS:HD2	1:A:109:HIS:HE1	1.38	0.71
1:C:167:THR:HG22	5:C:519:HOH:O	1.91	0.70
1:A:196:HIS:HE1	5:A:775:HOH:O	1.73	0.70
1:D:139:HIS:HA	1:D:167:THR:HG22	1.74	0.70
1:D:111:VAL:HG22	1:D:129:SER:HB2	1.74	0.69
1:C:71:HIS:CD2	1:C:109:HIS:HE1	2.09	0.69
1:D:71:HIS:HD2	1:D:109:HIS:HE1	1.41	0.69
1:B:118:ASN:ND2	1:B:206:ASN:HD21	1.91	0.68
1:C:118:ASN:ND2	1:C:228:ALA:H	1.88	0.68
1:B:118:ASN:HD22	1:B:206:ASN:HD21	1.42	0.67
1:D:41:THR:HG22	1:D:219:ASN:HB3	1.77	0.67
1:B:71:HIS:HD2	1:B:109:HIS:HE1	1.41	0.66
1:D:71:HIS:CD2	1:D:109:HIS:HE1	2.12	0.66
1:C:201:TYR:O	1:C:202:SER:HB2	1.95	0.66
1:C:71:HIS:HD2	1:C:109:HIS:HE1	1.41	0.66
1:A:71:HIS:CD2	1:A:109:HIS:HE1	2.14	0.66
1:C:113:VAL:HG13	1:C:125:LEU:HD11	1.78	0.66
1:C:52:ASN:HD21	1:D:48:GLY:N	1.92	0.65
1:C:38:LYS:HE3	5:C:587:HOH:O	1.96	0.65
1:C:49:VAL:HG22	1:D:49:VAL:CG2	2.27	0.65
1:C:147:ILE:HB	1:C:175:ILE:HG12	1.78	0.65
1:C:118:ASN:ND2	1:C:206:ASN:HD21	1.94	0.65
1:A:41:THR:HG21	5:A:901:HOH:O	1.97	0.64
1:A:3:ILE:HG21	1:A:167:THR:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:HIS:CD2	1:B:167:THR:HB	2.30	0.63
1:B:201:TYR:O	1:B:202:SER:HB2	1.98	0.62
1:B:62:LYS:NZ	1:B:94:HIS:HD2	1.97	0.62
1:A:62:LYS:NZ	1:A:94:HIS:HD2	1.96	0.62
1:D:175:ILE:HG22	1:D:192:SER:HA	1.82	0.61
1:A:136:LYS:HG3	1:A:164:GLU:HB2	1.81	0.61
1:B:47:ASN:H	1:B:214:HIS:CD2	2.11	0.61
1:C:62:LYS:HZ3	1:C:94:HIS:HD2	1.46	0.61
1:B:71:HIS:CD2	1:B:109:HIS:HE1	2.18	0.60
1:D:62:LYS:NZ	1:D:94:HIS:HD2	1.99	0.60
1:D:201:TYR:O	1:D:202:SER:HB2	2.01	0.60
1:A:147:ILE:HG13	1:A:172:CYS:SG	2.42	0.60
1:B:75:LEU:O	1:B:79:SER:HB2	2.01	0.59
1:A:41:THR:HG22	1:A:219:ASN:CB	2.32	0.59
1:C:73:LEU:HD21	1:C:111:VAL:HG23	1.85	0.59
1:B:160:LEU:HD22	1:B:165:ILE:CD1	2.33	0.58
1:B:139:HIS:HD2	1:B:167:THR:CB	2.15	0.58
1:C:48:GLY:N	1:D:52:ASN:HD21	1.94	0.58
1:C:74:CYS:HB2	1:C:83:PHE:CD1	2.38	0.58
1:D:181:TRP:HH2	1:D:185:LYS:HE3	1.68	0.58
1:B:118:ASN:HD21	1:B:228:ALA:N	1.92	0.58
1:B:167:THR:CG2	5:B:506:HOH:O	2.52	0.57
1:A:167:THR:CG2	5:A:525:HOH:O	2.51	0.57
1:A:35:HIS:H	1:A:35:HIS:CD2	2.22	0.57
1:D:47:ASN:N	1:D:214:HIS:HD2	1.91	0.57
1:B:35:HIS:CD2	1:B:35:HIS:H	2.23	0.56
1:B:175:ILE:HG22	1:B:192:SER:HA	1.87	0.56
1:C:16:PRO:HB3	1:C:189:VAL:HG13	1.87	0.56
1:B:69:GLU:OE2	1:B:71:HIS:HE1	1.87	0.56
1:A:147:ILE:HB	1:A:175:ILE:HG12	1.87	0.56
1:D:118:ASN:HD21	1:D:228:ALA:N	1.96	0.55
1:A:113:VAL:CG1	1:A:125:LEU:HD11	2.37	0.55
1:A:73:LEU:HD21	1:A:111:VAL:HG23	1.89	0.55
1:B:136:LYS:HE3	1:B:164:GLU:HB2	1.89	0.55
1:C:147:ILE:HG13	1:C:172:CYS:SG	2.47	0.55
1:D:116:TYR:CE1	1:D:121:SER:HB2	2.41	0.55
1:A:100:GLU:OE2	1:B:38:LYS:HE2	2.07	0.54
1:B:122:THR:OG1	1:B:124:THR:HG22	2.08	0.54
1:B:176:LYS:HE2	1:B:196:HIS:O	2.08	0.54
1:A:63:LYS:HE3	5:A:710:HOH:O	2.07	0.54
1:D:147:ILE:HG12	1:D:153:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:HIS:HD2	1:D:167:THR:CG2	2.21	0.53
1:A:3:ILE:CG2	1:A:167:THR:HG21	2.38	0.53
1:A:139:HIS:HD2	1:A:167:THR:CB	2.20	0.53
1:B:147:ILE:HB	1:B:175:ILE:HG12	1.89	0.53
1:C:196:HIS:HE1	5:C:630:HOH:O	1.91	0.53
1:C:139:HIS:CD2	1:C:167:THR:HB	2.26	0.53
1:B:89:HIS:HD2	1:B:92:ARG:HH21	1.57	0.52
1:D:139:HIS:HD2	1:D:167:THR:HB	1.75	0.52
1:C:88:LYS:HE3	1:C:92:ARG:HH12	1.74	0.52
1:D:47:ASN:O	1:D:51:LYS:HG2	2.10	0.52
1:D:62:LYS:HZ1	1:D:94:HIS:CD2	2.28	0.52
1:C:172:CYS:O	1:C:189:VAL:HA	2.10	0.51
1:A:84:THR:HG21	1:B:84:THR:HG23	1.91	0.51
1:B:3:ILE:HG21	1:B:167:THR:HG21	1.91	0.51
1:A:84:THR:HG21	1:B:84:THR:CG2	2.40	0.51
1:D:35:HIS:CD2	1:D:35:HIS:H	2.27	0.51
1:D:62:LYS:HZ1	1:D:94:HIS:HD2	1.59	0.51
1:A:139:HIS:CD2	1:A:167:THR:HB	2.37	0.51
1:A:201:TYR:O	1:A:202:SER:HB2	2.11	0.51
1:C:41:THR:HG22	1:C:219:ASN:CB	2.37	0.51
1:D:113:VAL:CG1	1:D:125:LEU:HD11	2.41	0.51
1:B:68:GLU:HG2	5:B:733:HOH:O	2.10	0.50
1:D:47:ASN:HD21	1:D:51:LYS:HZ2	1.58	0.50
1:D:71:HIS:HD2	1:D:109:HIS:CE1	2.27	0.50
1:D:99:VAL:HG13	1:D:100:GLU:N	2.26	0.50
1:A:62:LYS:HZ2	1:A:94:HIS:HD2	1.58	0.50
1:D:137:GLY:C	1:D:166:LYS:HB2	2.32	0.50
1:B:154:VAL:HG12	1:B:155:LYS:N	2.26	0.50
1:D:73:LEU:CD2	1:D:111:VAL:HG23	2.42	0.50
1:B:73:LEU:HD21	1:B:111:VAL:CG2	2.42	0.49
1:B:74:CYS:HB2	1:B:83:PHE:CE1	2.47	0.49
1:B:62:LYS:HZ3	1:B:94:HIS:HD2	1.58	0.49
1:D:115:SER:HB3	1:D:125:LEU:HD12	1.94	0.49
1:C:50:ILE:O	1:C:54:ILE:HG13	2.13	0.49
1:A:72:ILE:HG23	1:A:143:VAL:CG2	2.44	0.48
1:C:74:CYS:HB2	1:C:83:PHE:CE1	2.49	0.48
1:D:172:CYS:O	1:D:189:VAL:HA	2.14	0.48
1:B:26:ASP:OD2	5:B:903:HOH:O	2.20	0.48
1:D:139:HIS:CD2	1:D:167:THR:CG2	2.97	0.48
1:D:196:HIS:HE1	5:D:884:HOH:O	1.96	0.48
1:A:154:VAL:HG13	1:A:155:LYS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:HIS:CE1	5:B:674:HOH:O	2.67	0.47
1:C:175:ILE:HG22	1:C:192:SER:HA	1.96	0.47
1:A:99:VAL:HG13	1:A:100:GLU:N	2.29	0.47
1:C:99:VAL:HG13	1:C:101:THR:H	1.79	0.47
1:D:140:VAL:HG13	1:D:165:ILE:HG21	1.96	0.47
1:A:72:ILE:HG23	1:A:143:VAL:HG23	1.96	0.47
1:A:66:ASN:HB3	1:A:67:ASN:H	1.54	0.47
1:C:89:HIS:HD2	1:C:92:ARG:NH2	2.13	0.47
1:D:139:HIS:CA	1:D:167:THR:HG22	2.43	0.47
1:D:122:THR:OG1	1:D:124:THR:HG22	2.15	0.47
1:C:208:ILE:O	1:C:209:PHE:HB2	2.15	0.47
1:C:62:LYS:NZ	1:C:94:HIS:CD2	2.76	0.47
1:A:110:TYR:OH	1:B:80:ARG:HG3	2.15	0.46
1:C:3:ILE:CG2	1:C:167:THR:HG21	2.45	0.46
1:D:167:THR:HG23	5:D:571:HOH:O	2.15	0.46
1:C:35:HIS:H	1:C:35:HIS:CD2	2.31	0.46
1:C:49:VAL:CG2	1:D:49:VAL:CG2	2.93	0.46
1:A:113:VAL:HG12	1:A:125:LEU:HD11	1.97	0.46
1:A:135:LEU:HB3	1:A:165:ILE:HG12	1.96	0.46
1:D:208:ILE:HG13	1:D:226:TYR:CD1	2.50	0.46
1:A:73:LEU:CD2	1:A:111:VAL:HG23	2.44	0.46
1:A:76:LEU:HD22	1:A:110:TYR:HB3	1.98	0.46
1:A:172:CYS:O	1:A:189:VAL:HA	2.16	0.46
1:A:175:ILE:HG22	1:A:192:SER:HA	1.97	0.46
1:B:89:HIS:CD2	1:B:92:ARG:HH21	2.33	0.46
1:D:113:VAL:HG22	1:D:127:ILE:HG12	1.97	0.46
1:A:63:LYS:HE2	5:A:510:HOH:O	2.16	0.46
1:C:159:TYR:O	1:C:162:LYS:HG3	2.15	0.46
1:B:159:TYR:O	1:B:162:LYS:HG3	2.15	0.46
1:D:76:LEU:HA	1:D:77:LYS:HA	1.59	0.45
1:A:136:LYS:HE3	1:A:164:GLU:HG3	1.98	0.45
1:A:154:VAL:CG1	1:A:155:LYS:N	2.79	0.45
1:B:89:HIS:CD2	1:B:92:ARG:NH2	2.84	0.45
1:A:119:ASP:HA	1:A:197:PHE:CE1	2.52	0.45
1:D:135:LEU:HB3	1:D:165:ILE:HG12	1.99	0.45
1:C:115:SER:HB3	1:C:125:LEU:HD12	1.99	0.45
1:C:154:VAL:HG12	1:C:155:LYS:N	2.31	0.45
1:D:140:VAL:HG13	1:D:165:ILE:CG2	2.47	0.45
1:D:63:LYS:HE2	5:D:589:HOH:O	2.16	0.44
1:A:118:ASN:HD22	1:A:206:ASN:ND2	2.06	0.44
1:A:136:LYS:HE3	1:A:164:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:619:HOH:O	1:B:77:LYS:HB2	2.17	0.44
1:B:117:CYS:O	1:B:118:ASN:HB2	2.18	0.44
1:B:140:VAL:HG13	1:B:165:ILE:CG2	2.47	0.44
1:C:117:CYS:O	1:C:118:ASN:HB2	2.18	0.44
1:D:117:CYS:O	1:D:118:ASN:HB2	2.18	0.44
1:B:69:GLU:OE2	1:B:71:HIS:CE1	2.69	0.44
1:C:3:ILE:HG22	1:C:167:THR:HG21	1.99	0.44
1:A:4:PRO:HD3	1:A:64:VAL:HG11	2.00	0.44
1:B:50:ILE:O	1:B:54:ILE:HG13	2.18	0.44
1:D:162:LYS:H	1:D:162:LYS:HG2	1.39	0.44
1:A:47:ASN:HD21	1:A:51:LYS:NZ	2.16	0.44
1:D:76:LEU:HD22	1:D:110:TYR:HB3	1.99	0.43
1:D:3:ILE:HG21	1:D:167:THR:HG21	1.99	0.43
1:D:167:THR:CG2	5:D:571:HOH:O	2.65	0.43
1:D:72:ILE:CG2	1:D:83:PHE:HE1	2.32	0.43
1:C:130:GLU:O	1:C:132:LEU:HG	2.19	0.43
1:A:159:TYR:O	1:A:162:LYS:HG3	2.18	0.43
1:C:200:GLY:HA2	1:C:212:LEU:HB3	2.01	0.43
1:C:113:VAL:HG13	1:C:125:LEU:CD1	2.47	0.43
1:C:167:THR:CG2	5:C:519:HOH:O	2.59	0.42
1:B:76:LEU:HA	1:B:77:LYS:HA	1.70	0.42
1:B:167:THR:HG22	5:B:506:HOH:O	2.18	0.42
1:A:51:LYS:HZ2	1:A:51:LYS:HG3	1.63	0.42
1:B:136:LYS:HE2	1:B:164:GLU:OE2	2.19	0.42
1:A:109:HIS:HD2	1:A:130:GLU:OE2	2.02	0.42
1:C:130:GLU:O	1:C:132:LEU:N	2.52	0.42
1:D:111:VAL:HG22	1:D:129:SER:CB	2.46	0.42
1:D:139:HIS:HD2	1:D:167:THR:CB	2.32	0.42
1:B:196:HIS:HE1	5:B:683:HOH:O	2.01	0.42
1:C:162:LYS:H	1:C:162:LYS:HG2	1.56	0.42
1:D:175:ILE:O	1:D:175:ILE:CG2	2.68	0.42
1:B:17:VAL:HB	1:B:191:PHE:CD2	2.54	0.42
1:C:4:PRO:HD3	1:C:64:VAL:HG11	2.02	0.41
1:A:99:VAL:HG13	1:A:101:THR:H	1.84	0.41
1:B:3:ILE:CG2	1:B:167:THR:HG21	2.50	0.41
1:B:3:ILE:HD11	1:B:68:GLU:HG2	2.02	0.41
1:D:119:ASP:HA	1:D:197:PHE:CE1	2.55	0.41
1:A:208:ILE:O	1:A:209:PHE:HB2	2.21	0.41
1:C:76:LEU:HD22	1:C:110:TYR:HB3	2.03	0.41
1:D:41:THR:HG22	1:D:219:ASN:CB	2.47	0.41
1:D:73:LEU:HD21	1:D:111:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:CE1	1:A:138:LYS:HD2	2.55	0.41
1:D:47:ASN:ND2	5:D:888:HOH:O	2.44	0.41
1:D:147:ILE:CG1	1:D:153:LEU:HD12	2.50	0.41
1:A:99:VAL:CG1	1:A:101:THR:H	2.34	0.41
1:B:115:SER:HB3	1:B:125:LEU:HD12	2.03	0.41
1:C:89:HIS:CD2	1:C:92:ARG:NH2	2.89	0.41
1:C:111:VAL:HG11	1:C:156:PHE:CE1	2.55	0.41
1:C:204:ASP:HB3	1:C:210:ARG:HG2	2.03	0.41
1:B:74:CYS:HB2	1:B:83:PHE:CD1	2.56	0.40
1:A:65:TYR:O	1:A:68:GLU:HB2	2.21	0.40
1:D:99:VAL:CG1	1:D:100:GLU:N	2.84	0.40
1:A:139:HIS:HD2	1:A:167:THR:CG2	2.34	0.40
1:D:131:ASP:OD1	1:D:133:SER:HB3	2.20	0.40
1:D:142:ILE:HD12	1:D:170:ILE:HD13	2.02	0.40
1:D:205:TYR:CE2	1:D:223:LYS:HA	2.56	0.40
1:A:132:LEU:HD12	1:A:159:TYR:HE2	1.85	0.40
1:C:111:VAL:HG12	1:C:113:VAL:HG23	2.03	0.40
1:D:99:VAL:CG1	1:D:101:THR:H	2.35	0.40
1:B:172:CYS:O	1:B:189:VAL:HA	2.22	0.40
1:C:90:LEU:HD23	1:C:90:LEU:HA	1.96	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	226/231 (98%)	217 (96%)	9 (4%)	0	100	100
1	B	226/231 (98%)	218 (96%)	8 (4%)	0	100	100
1	C	228/231 (99%)	219 (96%)	8 (4%)	1 (0%)	34	30
1	D	226/231 (98%)	216 (96%)	10 (4%)	0	100	100
All	All	906/924 (98%)	870 (96%)	35 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	131	ASP

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	202/207 (98%)	183 (91%)	19 (9%)	8 5
1	B	202/207 (98%)	181 (90%)	21 (10%)	7 4
1	C	205/207 (99%)	183 (89%)	22 (11%)	6 3
1	D	202/207 (98%)	177 (88%)	25 (12%)	4 2
All	All	811/828 (98%)	724 (89%)	87 (11%)	6 3

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	41	THR
1	A	57	LEU
1	A	63	LYS
1	A	68	GLU
1	A	73	LEU
1	A	76	LEU
1	A	96	TYR
1	A	99	VAL
1	A	112	ARG
1	A	126	GLU
1	A	135	LEU
1	A	136	LYS
1	A	141	LEU
1	A	162	LYS
1	A	167	THR
1	A	175	ILE
1	A	218	VAL
1	A	221	GLU

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Mol	Chain	Res	Type
1	B	6	ASN
1	B	41	THR
1	B	57	LEU
1	B	63	LYS
1	B	75	LEU
1	B	77	LYS
1	B	84	THR
1	B	99	VAL
1	B	103	LYS
1	B	112	ARG
1	B	135	LEU
1	B	136	LYS
1	B	140	VAL
1	B	141	LEU
1	B	154	VAL
1	B	162	LYS
1	B	167	THR
1	B	175	ILE
1	B	178	THR
1	B	218	VAL
1	B	221	GLU
1	C	6	ASN
1	C	41	THR
1	C	57	LEU
1	C	73	LEU
1	C	75	LEU
1	C	76	LEU
1	C	99	VAL
1	C	112	ARG
1	C	129	SER
1	C	130	GLU
1	C	135	LEU
1	C	136	LYS
1	C	140	VAL
1	C	141	LEU
1	C	154	VAL
1	C	162	LYS
1	C	167	THR
1	C	175	ILE
1	C	218	VAL
1	C	221	GLU
1	C	227	LYS

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Mol	Chain	Res	Type
1	C	230	SER
1	D	6	ASN
1	D	41	THR
1	D	57	LEU
1	D	69	GLU
1	D	73	LEU
1	D	75	LEU
1	D	76	LEU
1	D	77	LYS
1	D	96	TYR
1	D	99	VAL
1	D	112	ARG
1	D	124	THR
1	D	130	GLU
1	D	135	LEU
1	D	136	LYS
1	D	140	VAL
1	D	141	LEU
1	D	154	VAL
1	D	162	LYS
1	D	167	THR
1	D	175	ILE
1	D	178	THR
1	D	202	SER
1	D	218	VAL
1	D	221	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	20	ASN
1	A	35	HIS
1	A	47	ASN
1	A	71	HIS
1	A	89	HIS
1	A	94	HIS
1	A	109	HIS
1	A	118	ASN
1	A	139	HIS
1	A	196	HIS
1	A	214	HIS

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Mol	Chain	Res	Type
1	B	6	ASN
1	B	20	ASN
1	B	35	HIS
1	B	47	ASN
1	B	71	HIS
1	B	89	HIS
1	B	94	HIS
1	B	109	HIS
1	B	118	ASN
1	B	139	HIS
1	B	196	HIS
1	B	214	HIS
1	C	6	ASN
1	C	20	ASN
1	C	35	HIS
1	C	47	ASN
1	C	52	ASN
1	C	71	HIS
1	C	89	HIS
1	C	94	HIS
1	C	109	HIS
1	C	118	ASN
1	C	139	HIS
1	C	196	HIS
1	C	214	HIS
1	D	6	ASN
1	D	20	ASN
1	D	35	HIS
1	D	47	ASN
1	D	52	ASN
1	D	71	HIS
1	D	94	HIS
1	D	109	HIS
1	D	118	ASN
1	D	139	HIS
1	D	214	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
4	POP	B	400	2	6,8,8	1.42	1 (16%)	13,13,13	0.97	2 (15%)
4	POP	D	400	2	6,8,8	1.37	0	13,13,13	0.88	1 (7%)
3	IRP	B	300	2	23,25,25	2.44	8 (34%)	20,38,38	2.20	6 (30%)
4	POP	A	400	2	6,8,8	1.38	0	13,13,13	0.93	1 (7%)
3	IRP	A	300	2	23,25,25	2.32	8 (34%)	20,38,38	2.18	6 (30%)
4	POP	C	400	2	6,8,8	1.46	1 (16%)	13,13,13	0.89	1 (7%)
3	IRP	C	300	2	23,25,25	2.37	8 (34%)	20,38,38	2.16	5 (25%)
3	IRP	D	300	2	23,25,25	2.39	9 (39%)	20,38,38	2.18	6 (30%)

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
4	POP	B	400	2	-	0/6/6/6	-
4	POP	D	400	2	-	0/6/6/6	-
3	IRP	B	300	2	-	3/6/26/26	0/3/3/3
4	POP	A	400	2	-	0/6/6/6	-
3	IRP	A	300	2	-	3/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POP	C	400	2	-	0/6/6/6	-
3	IRP	C	300	2	-	3/6/26/26	0/3/3/3
3	IRP	D	300	2	-	3/6/26/26	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	300	IRP	C3'-C4'	-5.18	1.48	1.53
3	C	300	IRP	C1'-N4'	-4.92	1.41	1.47
3	B	300	IRP	C6-N1	4.87	1.41	1.33
3	A	300	IRP	C6-N1	4.74	1.41	1.33
3	C	300	IRP	C6-N1	4.56	1.41	1.33
3	D	300	IRP	C1'-N4'	-4.54	1.42	1.47
3	A	300	IRP	C1'-N4'	-4.53	1.42	1.47
3	D	300	IRP	C6-N1	4.51	1.40	1.33
3	B	300	IRP	C2-N1	4.32	1.41	1.33
3	B	300	IRP	C1'-N4'	-4.15	1.42	1.47
3	D	300	IRP	C2-N1	4.04	1.41	1.33
3	C	300	IRP	C2-N1	3.98	1.41	1.33
3	D	300	IRP	C3'-C4'	-3.92	1.49	1.53
3	A	300	IRP	C2-N1	3.83	1.41	1.33
3	C	300	IRP	C4'-N4'	-3.71	1.42	1.48
3	A	300	IRP	C3'-C4'	-3.47	1.50	1.53
3	D	300	IRP	C4'-N4'	-3.41	1.43	1.48
3	C	300	IRP	C3'-C4'	-3.36	1.50	1.53
3	A	300	IRP	C4'-N4'	-3.35	1.43	1.48
3	C	300	IRP	C2-N3	3.30	1.37	1.32
3	D	300	IRP	C2-N3	3.29	1.37	1.32
3	B	300	IRP	C8-N7	-3.26	1.30	1.36
3	A	300	IRP	C8-N7	-3.24	1.30	1.36
3	A	300	IRP	C2-N3	3.23	1.37	1.32
3	B	300	IRP	C2-N3	3.22	1.37	1.32
3	D	300	IRP	C8-N7	-3.10	1.30	1.36
3	B	300	IRP	C4'-N4'	-3.04	1.43	1.48
3	C	300	IRP	C8-N7	-2.76	1.31	1.36
3	D	300	IRP	C4-N3	2.35	1.40	1.37
3	C	300	IRP	P-O2P	-2.34	1.45	1.54
3	D	300	IRP	P-O2P	-2.16	1.46	1.54
4	B	400	POP	P2-O5	-2.15	1.46	1.54
3	B	300	IRP	P-O2P	-2.14	1.46	1.54
3	A	300	IRP	P-O2P	-2.07	1.46	1.54
4	C	400	POP	P2-O5	-2.06	1.46	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	300	IRP	C2-N1-C6	5.34	124.82	115.88
3	C	300	IRP	C2-N1-C6	5.30	124.75	115.88
3	A	300	IRP	C2-N1-C6	5.24	124.66	115.88
3	B	300	IRP	C2-N1-C6	5.22	124.62	115.88
3	B	300	IRP	N3-C2-N1	-4.10	122.26	128.68
3	D	300	IRP	N3-C2-N1	-4.10	122.27	128.68
3	C	300	IRP	N3-C2-N1	-4.09	122.28	128.68
3	A	300	IRP	N3-C2-N1	-4.05	122.34	128.68
3	B	300	IRP	C9-C8-N7	3.71	115.86	108.79
3	A	300	IRP	P-O5'-C5'	3.57	128.12	118.30
3	C	300	IRP	P-O5'-C5'	3.57	128.12	118.30
3	D	300	IRP	C9-C8-N7	3.56	115.59	108.79
3	A	300	IRP	C9-C8-N7	3.43	115.33	108.79
3	C	300	IRP	C9-C8-N7	3.41	115.31	108.79
3	D	300	IRP	P-O5'-C5'	3.29	127.37	118.30
3	B	300	IRP	P-O5'-C5'	3.11	126.85	118.30
3	B	300	IRP	C5'-C4'-C3'	-2.83	108.78	113.75
3	B	300	IRP	O3'-C3'-C4'	-2.39	106.52	112.92
4	A	400	POP	O3-P1-O	2.39	112.64	104.64
3	A	300	IRP	O3'-C3'-C4'	-2.33	106.69	112.92
4	D	400	POP	O3-P1-O	2.32	112.41	104.64
3	D	300	IRP	C5'-C4'-C3'	-2.26	109.77	113.75
3	A	300	IRP	C5'-C4'-C3'	-2.25	109.79	113.75
3	C	300	IRP	O3'-C3'-C4'	-2.24	106.94	112.92
4	B	400	POP	O3-P1-O	2.20	112.01	104.64
3	D	300	IRP	O3'-C3'-C4'	-2.19	107.06	112.92
4	C	400	POP	O3-P1-O	2.17	111.93	104.64
4	B	400	POP	O5-P2-O	2.15	111.84	104.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	300	IRP	C5'-O5'-P-O1P
3	A	300	IRP	C5'-O5'-P-O2P
3	A	300	IRP	C5'-O5'-P-O3P
3	B	300	IRP	C5'-O5'-P-O2P
3	C	300	IRP	C5'-O5'-P-O1P
3	C	300	IRP	C5'-O5'-P-O2P
3	D	300	IRP	C5'-O5'-P-O2P
3	B	300	IRP	C5'-O5'-P-O3P

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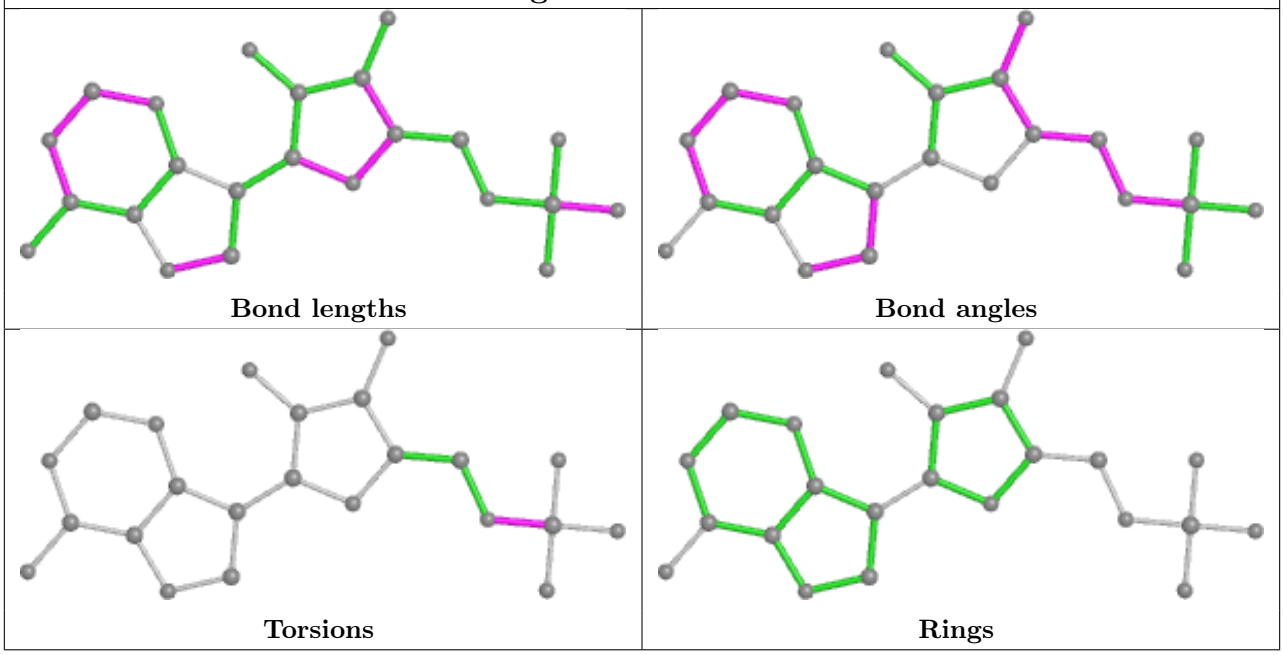
Mol	Chain	Res	Type	Atoms
3	C	300	IRP	C5'-O5'-P-O3P
3	D	300	IRP	C5'-O5'-P-O3P
3	B	300	IRP	C5'-O5'-P-O1P
3	D	300	IRP	C5'-O5'-P-O1P

There are no ring outliers.

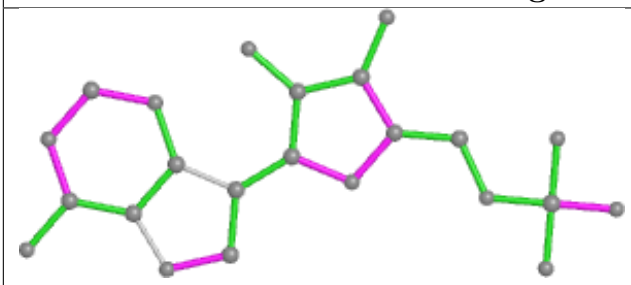
No monomer is involved in short contacts.

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.

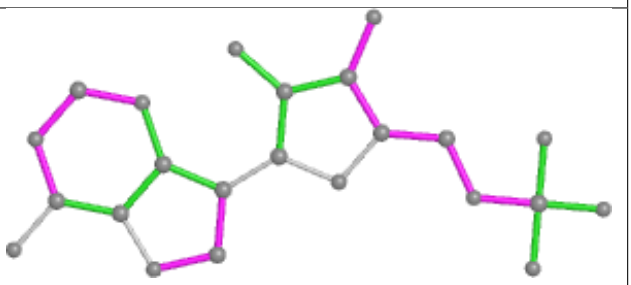
Ligand IRP B 300



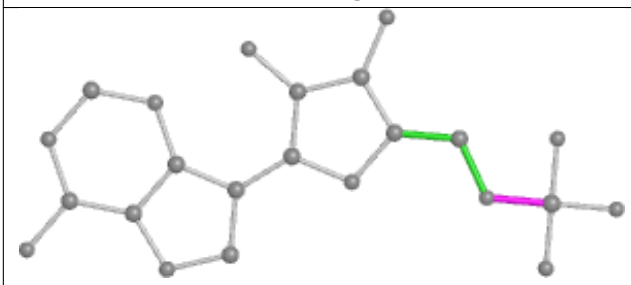
Ligand IRP A 300



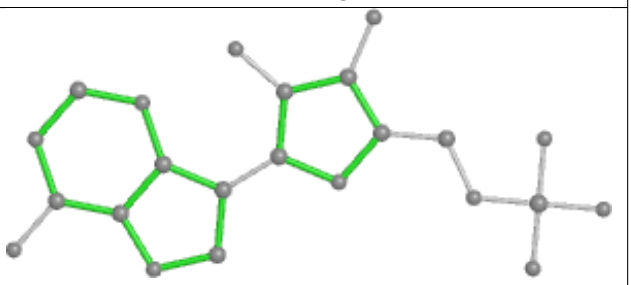
Bond lengths



Bond angles

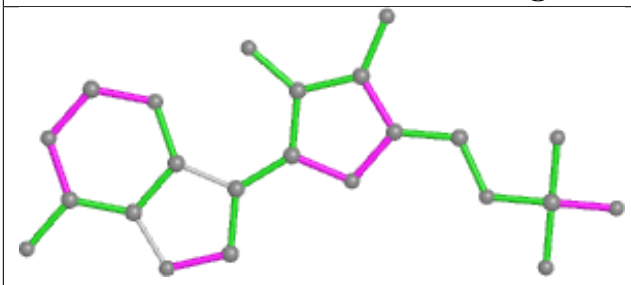


Torsions

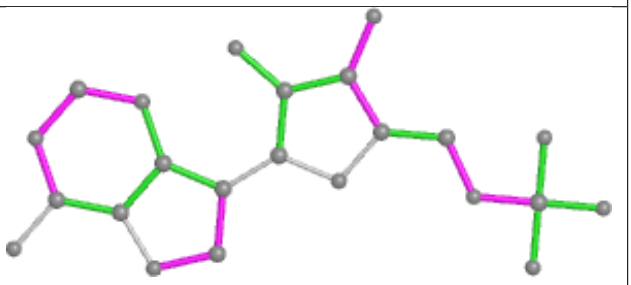


Rings

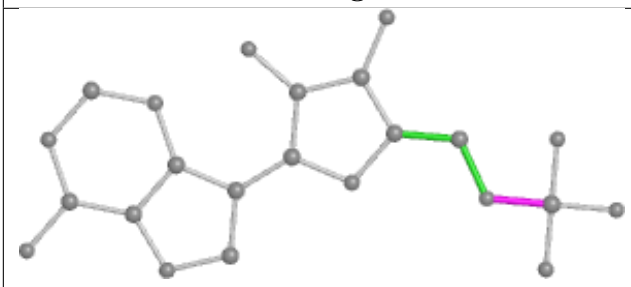
Ligand IRP C 300



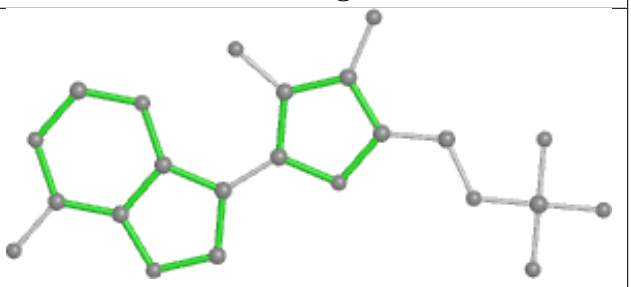
Bond lengths



Bond angles

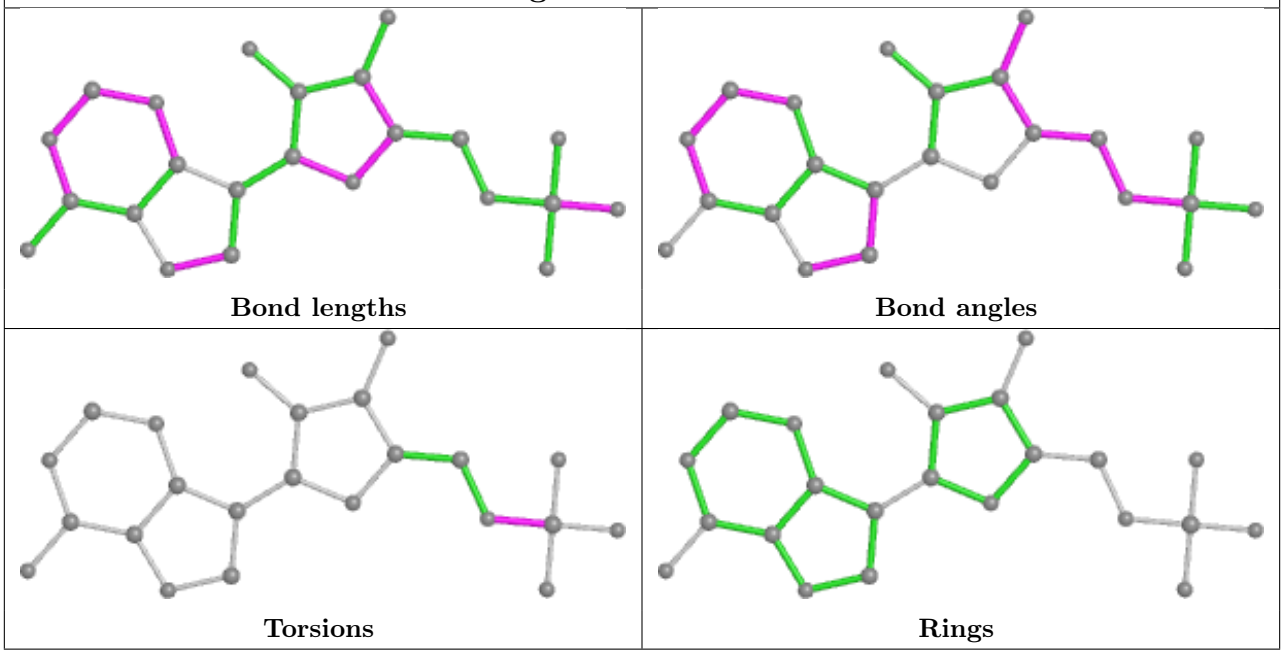


Torsions



Rings

Ligand IRP D 300



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.