Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 02:31 am GMT

PDB ID	:	6GK9
Title	:	Inhibited structure of IMPDH from Pseudomonas aeruginosa
Authors	:	Labesse, G.; Alexandre, T.; Haouz, A.; Munier-Lehmann, H.
Deposited on	:	2018-05-18
Resolution	:	2.54 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

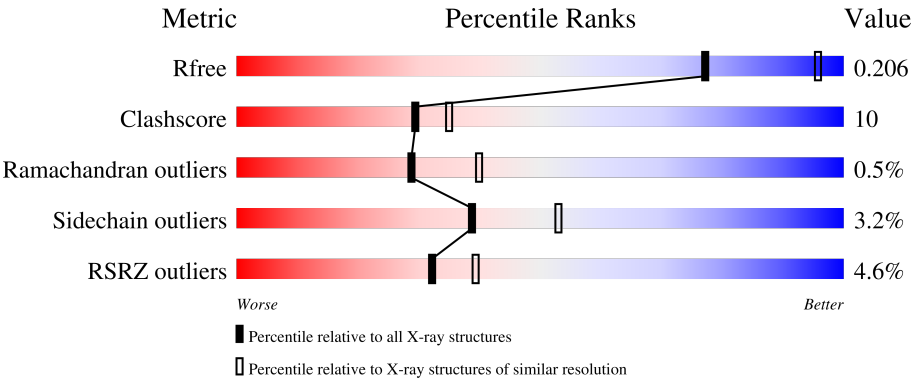
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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

Mol	Chain	Length	Quality of chain
1	A	509	67% 15% • 17%
1	B	509	% 70% 13% • 17%
1	C	509	8% 60% 13% • 25%
1	D	509	2% 65% 17% • 17%
1	E	509	4% 70% 13% • 17%

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Mol	Chain	Length	Quality of chain
1	F	509	55% 7% 38%
1	G	509	% 51% 13% 35%
1	H	509	12% 62% 19% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 24276 atoms, of which 18 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	3	0	0
			3136	1978	550	591	17			
1	B	424	Total	C	N	O	S	6	0	0
			3145	1985	551	592	17			
1	C	381	Total	C	N	O	S	2	0	0
			2816	1775	493	531	17			
1	D	424	Total	C	N	O	S	5	1	0
			3161	1992	555	597	17			
1	E	424	Total	C	N	O	S	6	1	0
			3158	1991	555	595	17			
1	F	317	Total	C	N	O	S	3	0	0
			2314	1451	413	437	13			
1	G	329	Total	C	N	O	S	4	0	0
			2390	1499	425	453	13			
1	H	419	Total	C	N	O	S	2	0	0
			3107	1958	547	585	17			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q9HXM5
A	-18	GLY	-	expression tag	UNP Q9HXM5
A	-17	SER	-	expression tag	UNP Q9HXM5
A	-16	SER	-	expression tag	UNP Q9HXM5
A	-15	HIS	-	expression tag	UNP Q9HXM5
A	-14	HIS	-	expression tag	UNP Q9HXM5
A	-13	HIS	-	expression tag	UNP Q9HXM5
A	-12	HIS	-	expression tag	UNP Q9HXM5
A	-11	HIS	-	expression tag	UNP Q9HXM5
A	-10	HIS	-	expression tag	UNP Q9HXM5
A	-9	SER	-	expression tag	UNP Q9HXM5
A	-8	SER	-	expression tag	UNP Q9HXM5
A	-7	GLY	-	expression tag	UNP Q9HXM5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP Q9HXM5
A	-5	VAL	-	expression tag	UNP Q9HXM5
A	-4	PRO	-	expression tag	UNP Q9HXM5
A	-3	ARG	-	expression tag	UNP Q9HXM5
A	-2	GLY	-	expression tag	UNP Q9HXM5
A	-1	SER	-	expression tag	UNP Q9HXM5
A	0	HIS	-	expression tag	UNP Q9HXM5
B	-19	MET	-	initiating methionine	UNP Q9HXM5
B	-18	GLY	-	expression tag	UNP Q9HXM5
B	-17	SER	-	expression tag	UNP Q9HXM5
B	-16	SER	-	expression tag	UNP Q9HXM5
B	-15	HIS	-	expression tag	UNP Q9HXM5
B	-14	HIS	-	expression tag	UNP Q9HXM5
B	-13	HIS	-	expression tag	UNP Q9HXM5
B	-12	HIS	-	expression tag	UNP Q9HXM5
B	-11	HIS	-	expression tag	UNP Q9HXM5
B	-10	HIS	-	expression tag	UNP Q9HXM5
B	-9	SER	-	expression tag	UNP Q9HXM5
B	-8	SER	-	expression tag	UNP Q9HXM5
B	-7	GLY	-	expression tag	UNP Q9HXM5
B	-6	LEU	-	expression tag	UNP Q9HXM5
B	-5	VAL	-	expression tag	UNP Q9HXM5
B	-4	PRO	-	expression tag	UNP Q9HXM5
B	-3	ARG	-	expression tag	UNP Q9HXM5
B	-2	GLY	-	expression tag	UNP Q9HXM5
B	-1	SER	-	expression tag	UNP Q9HXM5
B	0	HIS	-	expression tag	UNP Q9HXM5
C	-19	MET	-	initiating methionine	UNP Q9HXM5
C	-18	GLY	-	expression tag	UNP Q9HXM5
C	-17	SER	-	expression tag	UNP Q9HXM5
C	-16	SER	-	expression tag	UNP Q9HXM5
C	-15	HIS	-	expression tag	UNP Q9HXM5
C	-14	HIS	-	expression tag	UNP Q9HXM5
C	-13	HIS	-	expression tag	UNP Q9HXM5
C	-12	HIS	-	expression tag	UNP Q9HXM5
C	-11	HIS	-	expression tag	UNP Q9HXM5
C	-10	HIS	-	expression tag	UNP Q9HXM5
C	-9	SER	-	expression tag	UNP Q9HXM5
C	-8	SER	-	expression tag	UNP Q9HXM5
C	-7	GLY	-	expression tag	UNP Q9HXM5
C	-6	LEU	-	expression tag	UNP Q9HXM5
C	-5	VAL	-	expression tag	UNP Q9HXM5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP Q9HXM5
C	-3	ARG	-	expression tag	UNP Q9HXM5
C	-2	GLY	-	expression tag	UNP Q9HXM5
C	-1	SER	-	expression tag	UNP Q9HXM5
C	0	HIS	-	expression tag	UNP Q9HXM5
D	-19	MET	-	initiating methionine	UNP Q9HXM5
D	-18	GLY	-	expression tag	UNP Q9HXM5
D	-17	SER	-	expression tag	UNP Q9HXM5
D	-16	SER	-	expression tag	UNP Q9HXM5
D	-15	HIS	-	expression tag	UNP Q9HXM5
D	-14	HIS	-	expression tag	UNP Q9HXM5
D	-13	HIS	-	expression tag	UNP Q9HXM5
D	-12	HIS	-	expression tag	UNP Q9HXM5
D	-11	HIS	-	expression tag	UNP Q9HXM5
D	-10	HIS	-	expression tag	UNP Q9HXM5
D	-9	SER	-	expression tag	UNP Q9HXM5
D	-8	SER	-	expression tag	UNP Q9HXM5
D	-7	GLY	-	expression tag	UNP Q9HXM5
D	-6	LEU	-	expression tag	UNP Q9HXM5
D	-5	VAL	-	expression tag	UNP Q9HXM5
D	-4	PRO	-	expression tag	UNP Q9HXM5
D	-3	ARG	-	expression tag	UNP Q9HXM5
D	-2	GLY	-	expression tag	UNP Q9HXM5
D	-1	SER	-	expression tag	UNP Q9HXM5
D	0	HIS	-	expression tag	UNP Q9HXM5
E	-19	MET	-	initiating methionine	UNP Q9HXM5
E	-18	GLY	-	expression tag	UNP Q9HXM5
E	-17	SER	-	expression tag	UNP Q9HXM5
E	-16	SER	-	expression tag	UNP Q9HXM5
E	-15	HIS	-	expression tag	UNP Q9HXM5
E	-14	HIS	-	expression tag	UNP Q9HXM5
E	-13	HIS	-	expression tag	UNP Q9HXM5
E	-12	HIS	-	expression tag	UNP Q9HXM5
E	-11	HIS	-	expression tag	UNP Q9HXM5
E	-10	HIS	-	expression tag	UNP Q9HXM5
E	-9	SER	-	expression tag	UNP Q9HXM5
E	-8	SER	-	expression tag	UNP Q9HXM5
E	-7	GLY	-	expression tag	UNP Q9HXM5
E	-6	LEU	-	expression tag	UNP Q9HXM5
E	-5	VAL	-	expression tag	UNP Q9HXM5
E	-4	PRO	-	expression tag	UNP Q9HXM5
E	-3	ARG	-	expression tag	UNP Q9HXM5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q9HXM5
E	-1	SER	-	expression tag	UNP Q9HXM5
E	0	HIS	-	expression tag	UNP Q9HXM5
F	-19	MET	-	initiating methionine	UNP Q9HXM5
F	-18	GLY	-	expression tag	UNP Q9HXM5
F	-17	SER	-	expression tag	UNP Q9HXM5
F	-16	SER	-	expression tag	UNP Q9HXM5
F	-15	HIS	-	expression tag	UNP Q9HXM5
F	-14	HIS	-	expression tag	UNP Q9HXM5
F	-13	HIS	-	expression tag	UNP Q9HXM5
F	-12	HIS	-	expression tag	UNP Q9HXM5
F	-11	HIS	-	expression tag	UNP Q9HXM5
F	-10	HIS	-	expression tag	UNP Q9HXM5
F	-9	SER	-	expression tag	UNP Q9HXM5
F	-8	SER	-	expression tag	UNP Q9HXM5
F	-7	GLY	-	expression tag	UNP Q9HXM5
F	-6	LEU	-	expression tag	UNP Q9HXM5
F	-5	VAL	-	expression tag	UNP Q9HXM5
F	-4	PRO	-	expression tag	UNP Q9HXM5
F	-3	ARG	-	expression tag	UNP Q9HXM5
F	-2	GLY	-	expression tag	UNP Q9HXM5
F	-1	SER	-	expression tag	UNP Q9HXM5
F	0	HIS	-	expression tag	UNP Q9HXM5
G	-19	MET	-	initiating methionine	UNP Q9HXM5
G	-18	GLY	-	expression tag	UNP Q9HXM5
G	-17	SER	-	expression tag	UNP Q9HXM5
G	-16	SER	-	expression tag	UNP Q9HXM5
G	-15	HIS	-	expression tag	UNP Q9HXM5
G	-14	HIS	-	expression tag	UNP Q9HXM5
G	-13	HIS	-	expression tag	UNP Q9HXM5
G	-12	HIS	-	expression tag	UNP Q9HXM5
G	-11	HIS	-	expression tag	UNP Q9HXM5
G	-10	HIS	-	expression tag	UNP Q9HXM5
G	-9	SER	-	expression tag	UNP Q9HXM5
G	-8	SER	-	expression tag	UNP Q9HXM5
G	-7	GLY	-	expression tag	UNP Q9HXM5
G	-6	LEU	-	expression tag	UNP Q9HXM5
G	-5	VAL	-	expression tag	UNP Q9HXM5
G	-4	PRO	-	expression tag	UNP Q9HXM5
G	-3	ARG	-	expression tag	UNP Q9HXM5
G	-2	GLY	-	expression tag	UNP Q9HXM5
G	-1	SER	-	expression tag	UNP Q9HXM5

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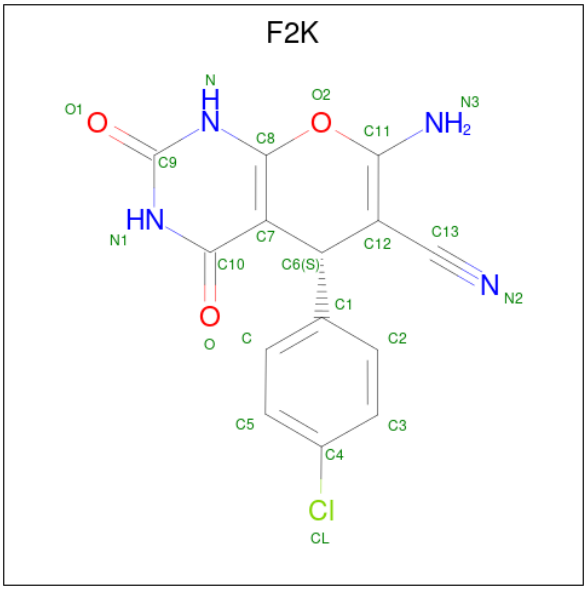
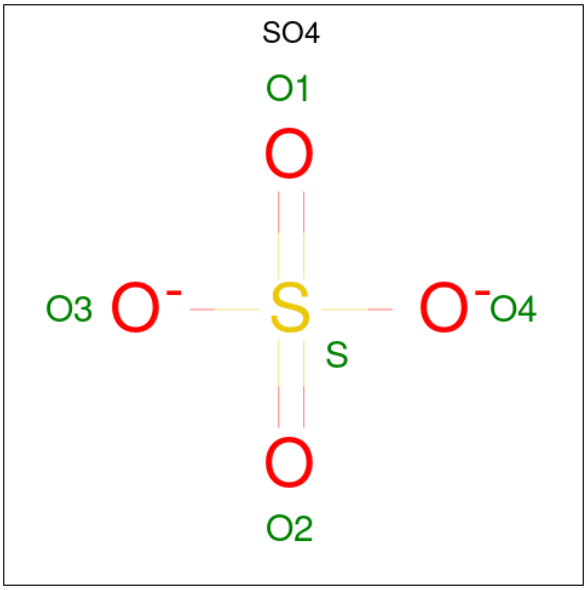
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q9HXM5
H	-19	MET	-	initiating methionine	UNP Q9HXM5
H	-18	GLY	-	expression tag	UNP Q9HXM5
H	-17	SER	-	expression tag	UNP Q9HXM5
H	-16	SER	-	expression tag	UNP Q9HXM5
H	-15	HIS	-	expression tag	UNP Q9HXM5
H	-14	HIS	-	expression tag	UNP Q9HXM5
H	-13	HIS	-	expression tag	UNP Q9HXM5
H	-12	HIS	-	expression tag	UNP Q9HXM5
H	-11	HIS	-	expression tag	UNP Q9HXM5
H	-10	HIS	-	expression tag	UNP Q9HXM5
H	-9	SER	-	expression tag	UNP Q9HXM5
H	-8	SER	-	expression tag	UNP Q9HXM5
H	-7	GLY	-	expression tag	UNP Q9HXM5
H	-6	LEU	-	expression tag	UNP Q9HXM5
H	-5	VAL	-	expression tag	UNP Q9HXM5
H	-4	PRO	-	expression tag	UNP Q9HXM5
H	-3	ARG	-	expression tag	UNP Q9HXM5
H	-2	GLY	-	expression tag	UNP Q9HXM5
H	-1	SER	-	expression tag	UNP Q9HXM5
H	0	HIS	-	expression tag	UNP Q9HXM5

- Molecule 2 is (5 {S})-7-azanyl-5-(4-chlorophenyl)-2,4-bis(oxidanylidene)-1,5-dihydropyrano[2,3-d]pyrimidine-6-carbonitrile (three-letter code: F2K) (formula: $C_{14}H_9ClN_4O_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	H	N	O	0	0
			31	14	1	9	4	3		
2	D	1	Total	C	Cl	H	N	O	0	0
			31	14	1	9	4	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O	0	0
			155	155		
4	B	164	Total	O	0	0
			164	164		
4	C	154	Total	O	0	0
			154	154		
4	D	123	Total	O	0	0
			123	123		
4	E	123	Total	O	0	0
			123	123		
4	F	133	Total	O	0	0
			133	133		
4	G	72	Total	O	0	0
			72	72		

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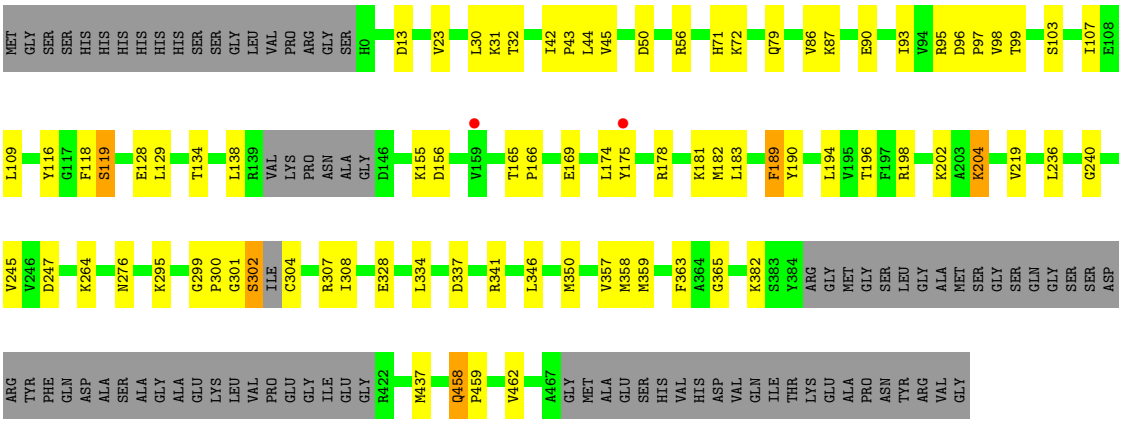
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	58	Total	O	0	0
			58	58		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

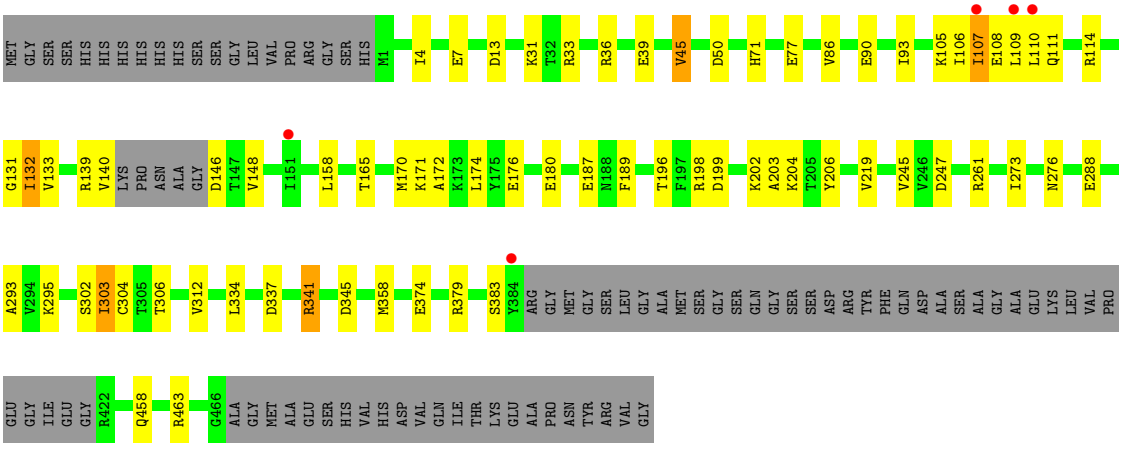
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain A:



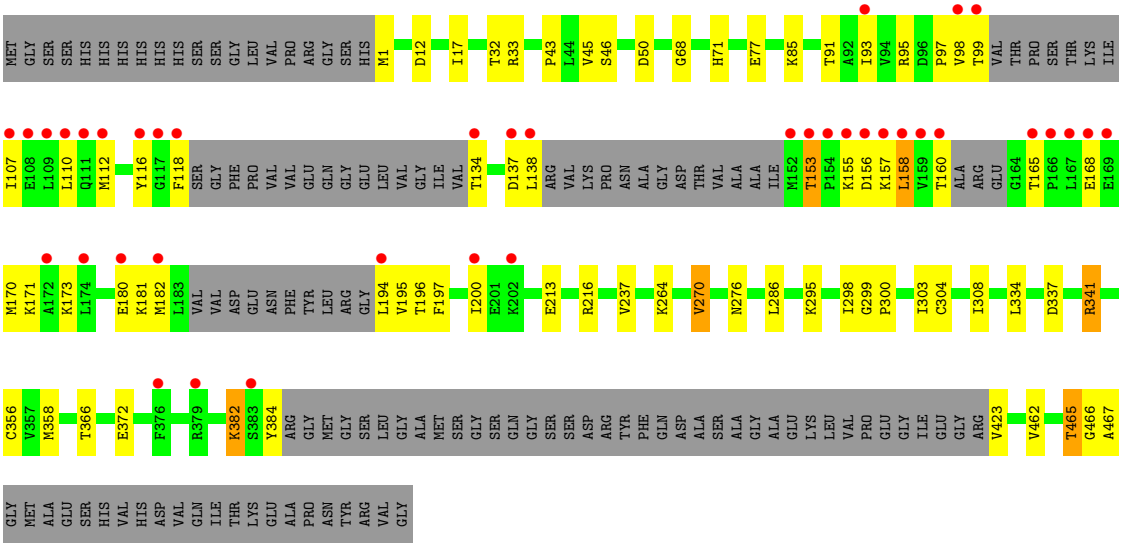
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain B:



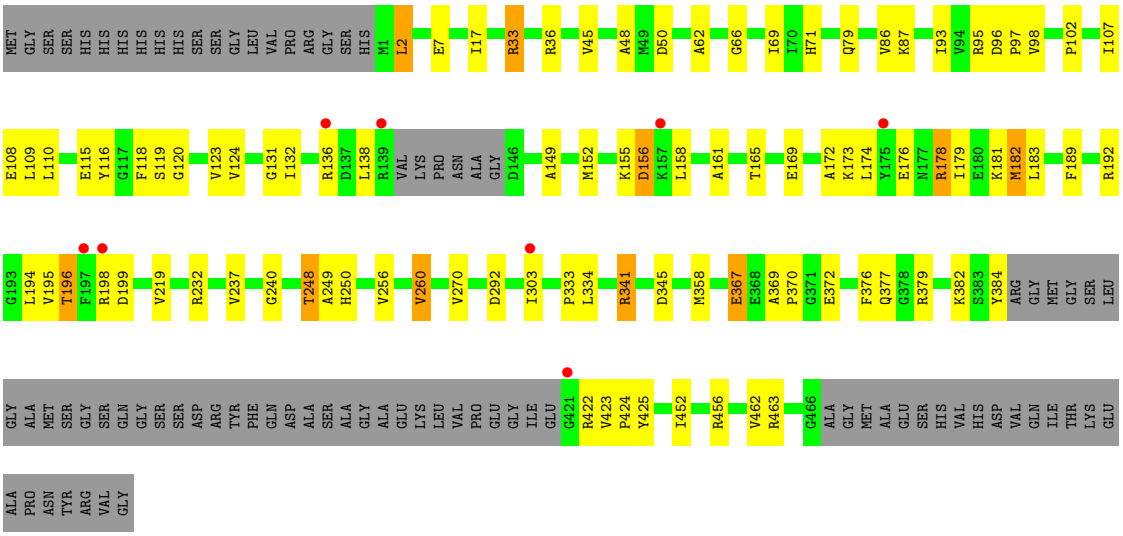
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain C:



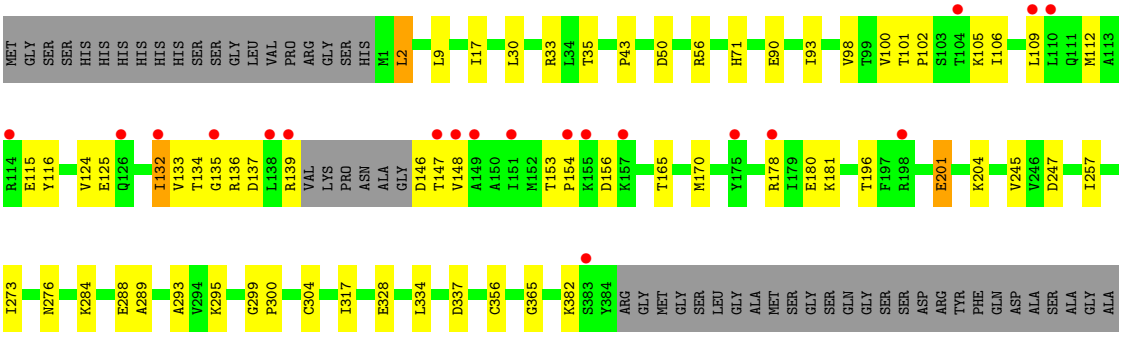
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

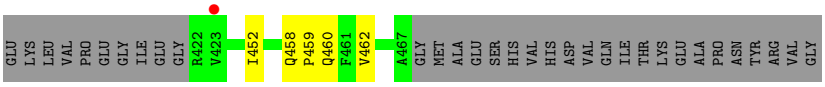
Chain D:



• Molecule 1: Inosine-5'-monophosphate dehydrogenase

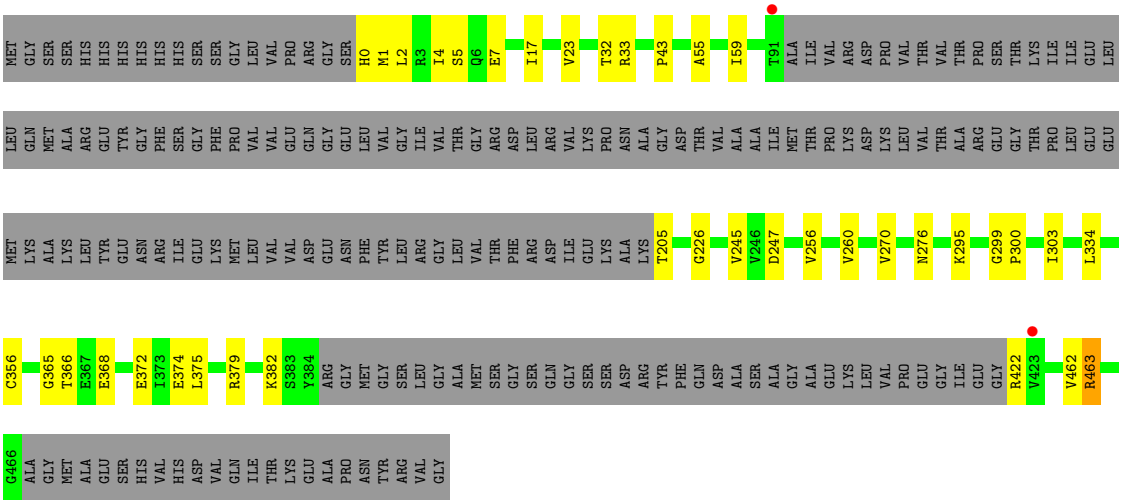
Chain E:





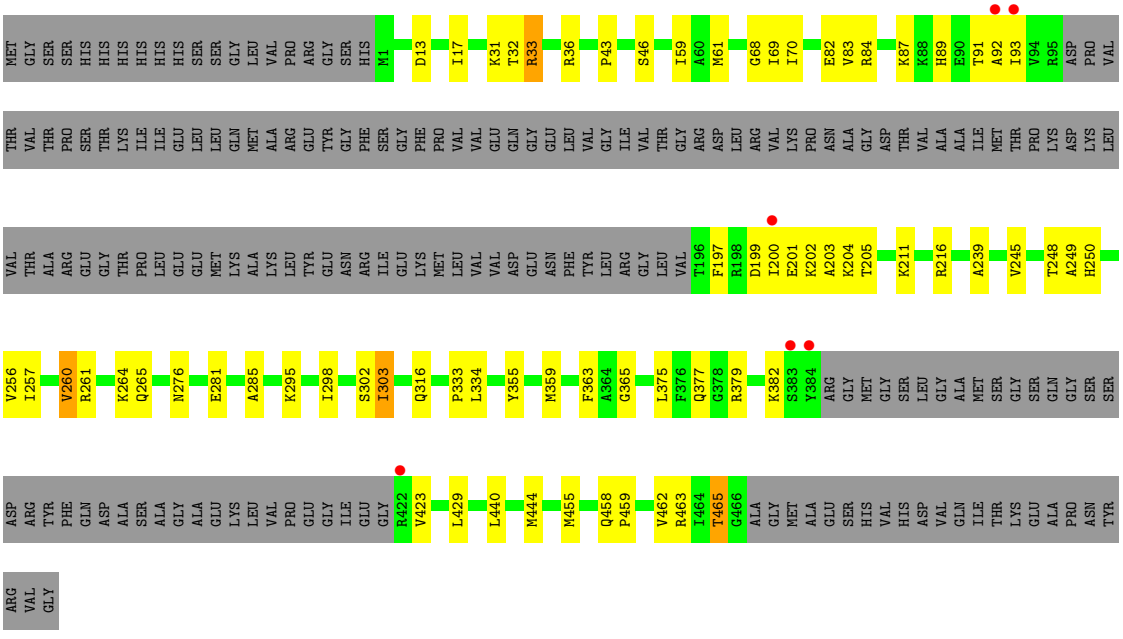
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain F:



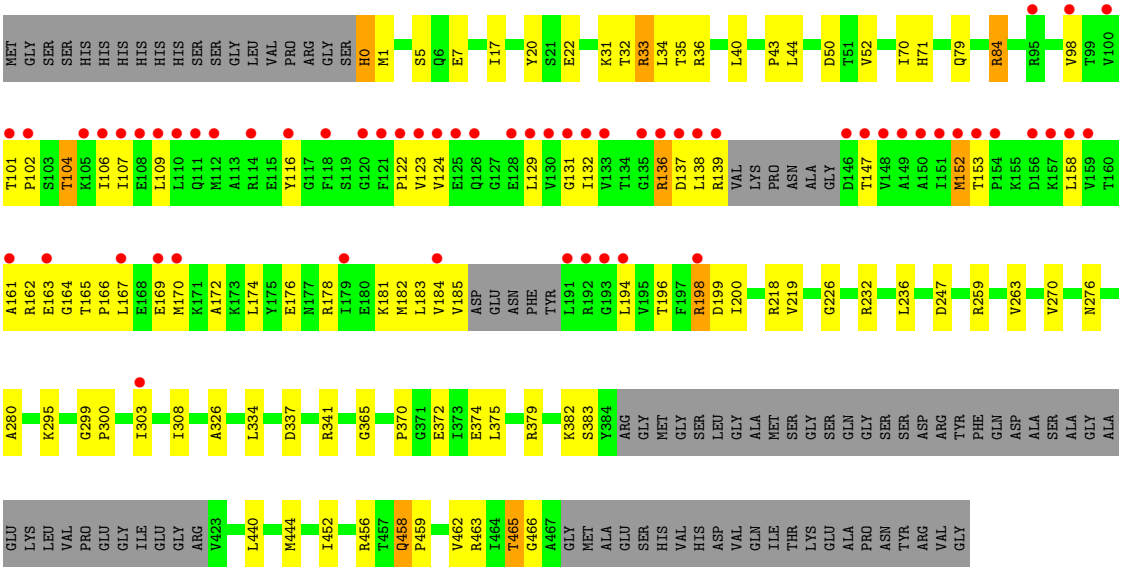
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain G:



• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain H:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER H0 M1 S5 Q6 E7 I17 Y20 S21 E22 K31 T32 R33 L34 T35 R36 L40 P43 L44 D50 T51 V52 I70 H71 Q79 R84 R95 V98 T99 V100
T101 P102 S103 T104 K105 I106 I107 E108 L109 L110 Q111 M112 A113 R114 E115 Y116 G117 F118 S119 G120 F121 P122 V123 V124 E125 Q126 G127 E128 L129 V130 G131 I132 V133 T134 G135 R136 D137 L138 R139 VAL LYS PRO ASN ALA GLY D146 T147 V148 A149 A150 I151 M152 T153 P154 K155 D156 K157 L158 V159 T160
A161 R162 E163 G164 T165 P166 L167 E168 E169 M170 K171 A172 K173 L174 Y175 E176 N177 R178 I179 E180 K181 M182 L183 V184 V185 ASP GLU ASN PHE TYR L191 R192 G193 L194 V195 T196 F197 R198 D199 I200 R218 V219 G226 R232 L236 D247 R259 V263 V270 N276
A280 K295 G299 P300 I303 I308 A326 L334 D337 R341 G365 P370 G371 E372 I373 E374 L375 R379 K382 S383 Y384 ARG GLY MET GLY SER LEU GLY ALA MET SER GLY SER GLN GLY SER SER ASP ARG TYR PHE GLN ASP ALA SER ALA GLY ALA
GLU LYS LEU VAL PRO GLU GLY ILE GLU GLY ARG V423 L440 M444 I452 R456 T457 Q458 P459 V462 R463 I464 T465 G466 A467 GLY MET ALA GLU SER HIS VAL HIS ASP VAL GLN ILE THR LYS GLU ALA PRO ASN TYR ARG VAL GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	115.64Å 196.96Å 123.63Å 90.00° 113.99° 90.00°	Depositor
Resolution (Å)	48.99 – 2.54 48.99 – 2.54	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.99-2.54) 100.0 (48.99-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 2.54Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.159 , 0.205 0.160 , 0.206	Depositor DCC
R_{free} test set	8272 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24276	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F2K, SO4

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	0.40	0/3176	0.61	1/4294 (0.0%)
1	B	0.40	0/3185	0.59	0/4306
1	C	0.40	1/2847 (0.0%)	0.59	0/3839
1	D	0.40	0/3204	0.61	0/4329
1	E	0.40	0/3202	0.60	0/4327
1	F	0.41	0/2341	0.60	0/3164
1	G	0.36	0/2416	0.56	0/3265
1	H	0.34	0/3145	0.55	0/4249
All	All	0.39	1/23516 (0.0%)	0.59	1/31773 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	356	CYS	CB-SG	-5.46	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	ARG	NE-CZ-NH2	-5.32	117.64	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3136	0	3227	68	1
1	B	3145	0	3246	47	0
1	C	2816	0	2903	69	0
1	D	3161	0	3265	72	1
1	E	3158	0	3261	53	0
1	F	2314	0	2375	22	0
1	G	2390	0	2446	46	0
1	H	3107	0	3218	90	0
2	A	22	9	0	0	0
2	D	22	9	0	1	0
3	E	5	0	0	0	0
4	A	155	0	0	3	0
4	B	164	0	0	2	0
4	C	154	0	0	2	0
4	D	123	0	0	0	0
4	E	123	0	0	1	0
4	F	133	0	0	2	0
4	G	72	0	0	5	0
4	H	58	0	0	1	0
All	All	24258	18	23941	449	1

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 10.

All (449) 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:A:43:PRO:HD2	1:A:437:MET:HE1	1.38	1.02
1:D:196:THR:HG22	1:D:199:ASP:H	1.23	1.01
1:B:13:ASP:OD1	1:G:465:THR:HG21	1.62	0.98
1:G:13:ASP:OD1	1:H:465:THR:HG21	1.62	0.97
1:A:13:ASP:OD1	1:C:465:THR:HG21	1.64	0.96
1:H:101:THR:HG23	1:H:104:THR:H	1.33	0.92
1:A:350:MET:CE	1:A:357:VAL:HG23	1.99	0.92
1:B:107:ILE:H	1:B:107:ILE:HD12	1.36	0.91
1:A:204:LYS:HE2	1:A:204:LYS:HA	1.52	0.91
1:G:248:THR:HG22	1:G:250:HIS:H	1.35	0.90
1:D:341:ARG:NH1	1:D:345:ASP:OD2	2.06	0.88
1:A:43:PRO:HD2	1:A:437:MET:CE	2.01	0.88
1:G:92:ALA:HB2	1:G:203:ALA:HB2	1.55	0.86
1:A:365:GLY:HA2	1:A:382:LYS:HG3	1.58	0.86
1:H:129:LEU:HD21	1:H:183:LEU:HD13	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:GLU:OE2	1:F:463:ARG:NH1	2.07	0.85
1:C:93:ILE:O	1:C:95:ARG:NH1	2.11	0.83
1:F:2:LEU:HD23	1:F:4:ILE:HD11	1.62	0.81
1:A:30:LEU:HD13	1:A:437:MET:CE	2.10	0.81
1:C:118:PHE:N	1:E:180:GLU:OE2	2.14	0.80
1:E:105:LYS:HG3	1:E:146:ASP:O	1.80	0.80
1:B:341:ARG:NH1	1:B:345:ASP:OD2	2.13	0.80
1:H:131:GLY:HA2	1:H:158:LEU:HD11	1.65	0.79
1:H:101:THR:HG22	1:H:104:THR:HG23	1.66	0.78
1:A:30:LEU:HD13	1:A:437:MET:HE2	1.65	0.78
1:A:183:LEU:HD23	1:A:194:LEU:HD13	1.66	0.78
1:A:42:ILE:HB	1:A:437:MET:HE1	1.65	0.77
1:D:248:THR:CG2	1:D:250:HIS:H	1.98	0.77
1:C:110:LEU:HD23	1:E:178:ARG:HH21	1.51	0.76
1:A:350:MET:HE3	1:A:357:VAL:HG23	1.67	0.76
1:D:123:VAL:HG11	1:D:152:MET:HE2	1.67	0.76
1:D:174:LEU:HD21	1:D:182:MET:HB3	1.68	0.75
1:E:247:ASP:OD1	1:E:295:LYS:NZ	2.18	0.75
1:G:70:ILE:HD13	1:G:82:GLU:HB3	1.68	0.75
1:C:276:ASN:OD1	1:C:295:LYS:HE2	1.87	0.75
1:C:181:LYS:HD3	1:C:194:LEU:HD11	1.69	0.74
1:E:98:VAL:HG21	1:E:116:TYR:CD2	2.22	0.74
1:G:281:GLU:OE1	1:G:281:GLU:N	2.14	0.74
1:D:248:THR:HG23	1:D:250:HIS:H	1.53	0.73
4:A:631:HOH:O	1:C:465:THR:HB	1.86	0.73
1:C:295:LYS:HE3	1:C:337:ASP:OD2	1.88	0.73
1:G:444:MET:HG3	4:G:543:HOH:O	1.87	0.73
1:E:276:ASN:OD1	1:E:295:LYS:HE2	1.90	0.71
1:B:295:LYS:HE3	1:B:337:ASP:OD2	1.89	0.71
1:E:98:VAL:HG21	1:E:116:TYR:CE2	2.25	0.71
1:E:100:VAL:HG12	1:E:112:MET:HE1	1.72	0.71
1:H:79:GLN:HG2	1:H:236:LEU:HD21	1.73	0.71
1:H:276:ASN:OD1	1:H:295:LYS:HE2	1.90	0.71
1:B:276:ASN:OD1	1:B:295:LYS:HE2	1.89	0.71
1:H:138:LEU:O	1:H:138:LEU:HD23	1.91	0.70
1:D:123:VAL:HG11	1:D:152:MET:CE	2.20	0.70
1:E:90:GLU:HB3	1:E:93:ILE:HD12	1.74	0.70
1:A:276:ASN:OD1	1:A:295:LYS:HE2	1.90	0.70
1:G:261:ARG:O	1:G:265:GLN:HG2	1.91	0.70
1:A:183:LEU:CD2	1:A:194:LEU:HD13	2.22	0.69
1:E:102:PRO:HA	1:E:148:VAL:CG2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:THR:O	1:A:138:LEU:HD12	1.91	0.69
1:A:43:PRO:CD	1:A:437:MET:HE1	2.18	0.69
1:C:98:VAL:HG21	1:C:116:TYR:HE2	1.57	0.69
1:E:328:GLU:OE1	1:H:0:HIS:N	2.26	0.69
1:A:299:GLY:N	1:A:300:PRO:HD3	2.08	0.68
1:H:295:LYS:HE3	1:H:337:ASP:OD2	1.93	0.68
1:C:91:THR:HG21	1:C:95:ARG:NH2	2.09	0.68
1:C:195:VAL:CG2	1:C:200:ILE:HD11	2.24	0.67
1:H:132:ILE:HG12	1:H:158:LEU:HD21	1.75	0.67
1:G:302:SER:HB3	1:G:303:ILE:HD12	1.76	0.67
1:H:374:GLU:HG3	1:H:383:SER:HB2	1.76	0.67
1:C:91:THR:HG21	1:C:95:ARG:HH22	1.59	0.67
1:B:172:ALA:O	1:B:176:GLU:HG3	1.95	0.66
1:F:7:GLU:CD	1:F:463:ARG:HH12	1.96	0.66
1:C:195:VAL:HG22	1:C:200:ILE:HD11	1.76	0.66
1:C:118:PHE:CE2	1:E:178:ARG:HG3	2.30	0.66
1:D:237:VAL:HG22	1:D:270:VAL:HG11	1.78	0.66
1:G:204:LYS:HE3	1:G:205:THR:O	1.96	0.66
1:C:98:VAL:HG21	1:C:116:TYR:CE2	2.31	0.65
1:F:2:LEU:CD2	1:F:4:ILE:HD11	2.27	0.65
1:H:172:ALA:O	1:H:176:GLU:HG2	1.98	0.64
1:D:131:GLY:HA2	1:D:158:LEU:HD11	1.80	0.64
1:G:256:VAL:O	1:G:260:VAL:HG13	1.96	0.64
1:A:107:ILE:HD12	1:A:107:ILE:H	1.63	0.63
1:H:101:THR:CG2	1:H:104:THR:HG23	2.28	0.63
1:C:366:THR:O	1:C:382:LYS:HE3	1.99	0.63
1:G:276:ASN:OD1	1:G:295:LYS:HE3	1.99	0.63
1:B:131:GLY:HA2	1:B:158:LEU:HD11	1.81	0.62
1:G:92:ALA:CB	1:G:203:ALA:HB2	2.29	0.62
1:C:85:LYS:NZ	4:C:501:HOH:O	2.31	0.62
1:E:181:LYS:HG2	1:E:196:THR:HG22	1.79	0.62
1:C:299:GLY:N	1:C:300:PRO:HD3	2.15	0.62
1:A:30:LEU:HD13	1:A:437:MET:HE3	1.82	0.61
1:A:129:LEU:HD23	1:A:189:PHE:HE1	1.66	0.61
1:D:178:ARG:N	1:D:178:ARG:HD2	2.15	0.61
1:H:247:ASP:OD1	1:H:295:LYS:NZ	2.33	0.61
1:A:174:LEU:HD21	1:A:182:MET:HB2	1.83	0.61
1:E:102:PRO:HA	1:E:148:VAL:HG22	1.81	0.61
1:B:245:VAL:HG12	1:B:247:ASP:HB2	1.84	0.60
1:E:106:ILE:HD11	1:E:147:THR:O	2.01	0.60
1:H:122:PRO:HA	1:H:132:ILE:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:LEU:HA	1:E:112:MET:HE2	1.81	0.60
1:E:295:LYS:HE3	1:E:337:ASP:OD2	2.02	0.60
1:D:376:PHE:CD2	1:D:377:GLN:HG2	2.37	0.60
1:A:119:SER:OG	1:B:198:ARG:NH2	2.35	0.60
1:E:201:GLU:OE1	1:E:201:GLU:HA	2.02	0.60
1:D:194:LEU:HD12	1:D:194:LEU:O	2.01	0.60
1:E:106:ILE:HD12	1:E:106:ILE:H	1.66	0.59
1:B:196:THR:HG22	1:B:199:ASP:H	1.68	0.59
1:F:375:LEU:HD12	1:F:379:ARG:O	2.02	0.59
1:A:204:LYS:HA	1:A:204:LYS:CE	2.29	0.59
1:C:91:THR:HG21	1:C:95:ARG:NH1	2.18	0.58
1:D:256:VAL:O	1:D:260:VAL:HG13	2.03	0.58
1:G:83:VAL:O	1:G:87:LYS:HG2	2.03	0.58
1:C:465:THR:CG2	1:C:467:ALA:H	2.16	0.58
1:A:23:VAL:HB	4:A:703:HOH:O	2.02	0.58
1:H:101:THR:HG23	1:H:104:THR:N	2.12	0.58
1:D:156:ASP:N	1:D:156:ASP:OD1	2.36	0.58
1:C:95:ARG:HD3	1:C:95:ARG:N	2.19	0.58
1:D:183:LEU:HD12	1:D:183:LEU:N	2.18	0.58
1:H:174:LEU:HD21	1:H:182:MET:HB2	1.84	0.58
1:C:180:GLU:OE2	1:C:197:PHE:HB3	2.04	0.58
1:F:276:ASN:OD1	1:F:295:LYS:HE2	2.04	0.57
1:H:132:ILE:HD12	4:H:554:HOH:O	2.04	0.57
1:B:90:GLU:HG2	1:B:93:ILE:HG23	1.86	0.57
1:H:365:GLY:HA2	1:H:382:LYS:HG3	1.87	0.57
1:E:458:GLN:HB2	1:E:459:PRO:HD3	1.87	0.57
1:G:17:ILE:HD11	1:G:462:VAL:HG13	1.86	0.57
1:E:204:LYS:HA	1:E:204:LYS:HE2	1.84	0.57
1:B:139:ARG:O	1:B:140:VAL:HG12	2.04	0.57
1:C:465:THR:HG22	1:C:467:ALA:N	2.20	0.57
1:A:96:ASP:N	1:A:97:PRO:HD3	2.20	0.57
1:G:455:MET:HE1	4:G:543:HOH:O	2.04	0.57
1:C:12:ASP:OD1	1:C:341:ARG:NH2	2.38	0.57
1:D:423:VAL:HG23	1:D:424:PRO:HD2	1.85	0.57
1:F:379:ARG:HD3	1:G:379:ARG:NH1	2.20	0.57
1:H:174:LEU:HD21	1:H:182:MET:CB	2.35	0.57
1:A:72:LYS:HG2	4:A:680:HOH:O	2.05	0.56
1:C:155:LYS:HA	1:C:158:LEU:HD12	1.87	0.56
1:H:218:ARG:HG2	1:H:218:ARG:HH21	1.69	0.56
1:A:295:LYS:HE3	1:A:337:ASP:OD2	2.05	0.56
1:G:455:MET:CE	4:G:543:HOH:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PHE:O	1:A:119:SER:CB	2.53	0.56
1:B:109:LEU:C	1:B:109:LEU:HD23	2.26	0.56
1:C:304:CYS:O	1:C:308:ILE:HD12	2.05	0.56
1:D:155:LYS:HE3	1:D:189:PHE:CE2	2.39	0.56
1:H:170:MET:HB3	1:H:182:MET:HE3	1.86	0.56
1:A:155:LYS:HE3	1:A:189:PHE:CD2	2.41	0.56
1:C:91:THR:HG21	1:C:95:ARG:HH12	1.71	0.56
1:C:181:LYS:CD	1:C:194:LEU:HD11	2.36	0.56
1:F:17:ILE:HD11	1:F:462:VAL:HG13	1.88	0.56
1:F:32:THR:HG21	1:F:43:PRO:HB3	1.87	0.56
1:C:95:ARG:O	1:C:97:PRO:HD3	2.06	0.55
1:B:109:LEU:HD11	1:B:133:VAL:HG11	1.89	0.55
1:C:196:THR:O	1:C:200:ILE:HD12	2.07	0.55
1:H:33:ARG:NH1	1:H:36:ARG:O	2.39	0.55
1:H:84:ARG:HG2	1:H:84:ARG:HH11	1.72	0.55
1:A:86:VAL:HG11	1:A:219:VAL:HB	1.89	0.55
1:C:110:LEU:CD2	1:E:178:ARG:HH21	2.20	0.55
1:C:195:VAL:HG22	1:C:200:ILE:CD1	2.37	0.55
1:D:87:LYS:HE2	1:D:240:GLY:O	2.07	0.55
1:D:95:ARG:NH1	1:D:192:ARG:O	2.40	0.54
1:H:132:ILE:CG2	1:H:183:LEU:HD11	2.38	0.54
1:A:165:THR:HG22	1:A:169:GLU:HB2	1.89	0.54
1:H:161:ALA:O	1:H:184:VAL:HA	2.08	0.54
1:H:163:GLU:HG3	1:H:164:GLY:H	1.71	0.54
1:C:91:THR:HG21	1:C:95:ARG:CZ	2.38	0.54
1:H:32:THR:HG21	1:H:43:PRO:HB3	1.90	0.54
1:G:69:ILE:HD12	1:G:245:VAL:HG21	1.89	0.53
1:G:204:LYS:HD2	1:G:205:THR:H	1.74	0.53
1:H:17:ILE:HD11	1:H:462:VAL:HG13	1.89	0.53
1:B:31:LYS:HE2	1:B:39:GLU:OE1	2.08	0.53
1:B:196:THR:HG22	1:B:198:ARG:N	2.23	0.53
1:H:162:ARG:HB2	1:H:185:VAL:C	2.29	0.53
1:A:107:ILE:HD12	1:A:107:ILE:N	2.23	0.53
1:D:196:THR:CG2	1:D:199:ASP:H	2.10	0.53
1:D:183:LEU:HD12	1:D:183:LEU:H	1.74	0.53
1:H:129:LEU:HD21	1:H:183:LEU:CD1	2.35	0.53
1:D:196:THR:HG22	1:D:199:ASP:N	2.08	0.53
1:E:33:ARG:HD2	1:E:35:THR:O	2.09	0.52
1:G:440:LEU:HD12	4:G:543:HOH:O	2.09	0.52
1:H:167:LEU:HD23	1:H:170:MET:CE	2.38	0.52
1:D:181:LYS:HE3	1:D:194:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:VAL:CG1	1:E:112:MET:HE1	2.38	0.52
1:B:180:GLU:OE2	1:B:196:THR:HG23	2.09	0.52
1:D:172:ALA:O	1:D:176:GLU:HG2	2.10	0.52
1:E:273:ILE:HG12	1:E:293:ALA:HB3	1.91	0.52
1:F:256:VAL:O	1:F:260:VAL:HG13	2.09	0.52
1:B:86:VAL:HG11	1:B:219:VAL:HB	1.92	0.52
1:D:69:ILE:N	1:D:69:ILE:HD12	2.24	0.52
1:H:163:GLU:OE1	1:H:163:GLU:HA	2.10	0.52
1:C:165:THR:O	1:C:170:MET:HE3	2.09	0.52
1:C:181:LYS:CG	1:C:194:LEU:HD11	2.40	0.52
1:C:181:LYS:NZ	1:C:194:LEU:HD21	2.24	0.52
1:H:102:PRO:HD3	1:H:124:VAL:O	2.10	0.52
1:H:132:ILE:HG12	1:H:158:LEU:CD2	2.40	0.52
1:H:458:GLN:HB2	1:H:459:PRO:HD3	1.91	0.52
1:C:17:ILE:HD11	1:C:462:VAL:HG13	1.92	0.51
1:D:96:ASP:N	1:D:97:PRO:HD3	2.25	0.51
1:A:87:LYS:HE2	1:A:240:GLY:O	2.09	0.51
1:D:367:GLU:HG3	1:D:425:TYR:OH	2.10	0.51
1:E:136:ARG:O	1:E:139:ARG:HG2	2.11	0.51
1:H:34:LEU:HG	1:H:35:THR:HG23	1.91	0.51
1:A:165:THR:HG23	1:A:169:GLU:OE1	2.10	0.51
1:H:166:PRO:HG2	1:H:169:GLU:OE2	2.10	0.51
1:E:134:THR:HG22	1:E:135:GLY:N	2.26	0.51
1:H:131:GLY:CA	1:H:158:LEU:HD11	2.39	0.51
1:A:181:LYS:HG3	1:A:196:THR:HG22	1.92	0.50
1:E:106:ILE:HD12	1:E:106:ILE:N	2.27	0.50
1:E:284:LYS:O	1:E:288:GLU:HG2	2.11	0.50
1:A:42:ILE:HB	1:A:437:MET:CE	2.38	0.50
1:E:101:THR:HA	1:E:124:VAL:O	2.12	0.50
1:E:299:GLY:N	1:E:300:PRO:HD3	2.26	0.50
1:G:84:ARG:HG3	1:G:239:ALA:HB1	1.94	0.50
1:H:174:LEU:CD2	1:H:182:MET:HB2	2.41	0.50
1:H:375:LEU:HD12	1:H:379:ARG:O	2.12	0.50
1:C:112:MET:O	1:C:116:TYR:HB2	2.11	0.50
1:D:33:ARG:NH1	1:D:36:ARG:O	2.44	0.50
1:G:375:LEU:HD12	1:G:379:ARG:O	2.12	0.50
1:D:119:SER:CB	1:H:198:ARG:HH12	2.25	0.50
1:E:165:THR:HB	1:E:170:MET:CE	2.41	0.50
1:F:299:GLY:N	1:F:300:PRO:HD3	2.26	0.50
1:B:303:ILE:HG13	1:B:303:ILE:O	2.11	0.50
1:C:134:THR:O	1:C:138:LEU:HD12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:PRO:HB2	1:F:356:CYS:HA	1.94	0.50
1:G:92:ALA:HB2	1:G:203:ALA:CB	2.35	0.50
1:D:93:ILE:HG12	1:D:195:VAL:CG1	2.41	0.50
1:H:106:ILE:HD11	1:H:147:THR:O	2.12	0.50
1:H:259:ARG:O	1:H:263:VAL:HG23	2.12	0.50
1:D:248:THR:HG23	1:D:249:ALA:N	2.26	0.49
1:C:110:LEU:HD12	1:C:110:LEU:N	2.28	0.49
1:H:166:PRO:HD2	1:H:169:GLU:CD	2.33	0.49
1:H:132:ILE:HG21	1:H:183:LEU:HD11	1.95	0.49
1:C:237:VAL:HG22	1:C:270:VAL:HG11	1.94	0.49
1:C:303:ILE:HG23	1:C:303:ILE:O	2.12	0.49
1:A:166:PRO:HD2	1:A:169:GLU:CD	2.33	0.49
1:H:98:VAL:HG11	1:H:116:TYR:CD2	2.47	0.49
1:H:196:THR:HG22	1:H:198:ARG:N	2.28	0.48
1:D:452:ILE:O	1:D:456:ARG:HG3	2.13	0.48
1:E:17:ILE:HG12	1:E:462:VAL:HG13	1.95	0.48
1:D:50:ASP:HA	1:D:71:HIS:CD2	2.48	0.48
1:E:115:GLU:O	1:E:115:GLU:HG2	2.13	0.48
1:G:202:LYS:HD3	1:G:202:LYS:C	2.33	0.48
1:D:102:PRO:HD3	1:D:124:VAL:O	2.13	0.48
1:E:165:THR:HB	1:E:170:MET:HE3	1.95	0.48
1:B:374:GLU:OE1	1:B:383:SER:HB3	2.13	0.48
1:B:202:LYS:HE3	1:B:202:LYS:HB2	1.51	0.48
1:E:9:LEU:O	1:E:317:ILE:HB	2.14	0.48
1:D:370:PRO:O	1:D:382:LYS:HE2	2.14	0.48
1:C:77:GLU:OE1	1:C:77:GLU:HA	2.13	0.47
1:H:34:LEU:HB2	1:H:40:LEU:HD11	1.96	0.47
1:H:107:ILE:HD12	1:H:107:ILE:H	1.79	0.47
1:A:79:GLN:HG2	1:A:236:LEU:HD21	1.96	0.47
1:A:109:LEU:HD23	1:A:109:LEU:C	2.35	0.47
1:B:187:GLU:CD	1:B:187:GLU:H	2.18	0.47
1:C:97:PRO:O	1:C:99:THR:HG23	2.14	0.47
1:D:149:ALA:HA	1:D:152:MET:HE3	1.97	0.47
1:C:93:ILE:HB	1:C:95:ARG:NH1	2.29	0.47
1:D:109:LEU:HD21	1:D:138:LEU:HD11	1.95	0.47
1:F:366:THR:O	1:F:382:LYS:NZ	2.47	0.47
1:H:163:GLU:HG3	1:H:164:GLY:N	2.29	0.47
1:C:264:LYS:HD2	1:C:264:LYS:HA	1.38	0.47
1:G:32:THR:HG21	1:G:43:PRO:HB3	1.96	0.47
1:H:79:GLN:OE1	1:H:232:ARG:HD3	2.14	0.47
1:H:123:VAL:HG11	1:H:152:MET:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LYS:NZ	1:B:108:GLU:HB2	2.29	0.47
1:F:303:ILE:O	1:F:303:ILE:HG22	2.15	0.47
1:H:374:GLU:OE1	1:H:383:SER:OG	2.21	0.47
1:D:194:LEU:HD12	1:D:194:LEU:C	2.35	0.47
1:D:423:VAL:CG2	1:D:424:PRO:HD2	2.45	0.47
1:D:132:ILE:HG12	1:D:158:LEU:HD21	1.96	0.47
1:F:55:ALA:O	1:F:59:ILE:HG13	2.14	0.47
1:A:264:LYS:HA	1:A:264:LYS:HE2	1.96	0.47
1:B:261:ARG:NH2	1:B:288:GLU:OE2	2.48	0.47
1:G:365:GLY:HA2	1:G:382:LYS:HG3	1.97	0.47
1:B:50:ASP:HA	1:B:71:HIS:CD2	2.50	0.46
1:C:372:GLU:HA	4:C:522:HOH:O	2.15	0.46
1:G:248:THR:HG22	1:G:249:ALA:N	2.29	0.46
1:C:181:LYS:HG3	1:C:196:THR:HG22	1.97	0.46
1:A:50:ASP:HA	1:A:71:HIS:CD2	2.50	0.46
1:A:198:ARG:O	1:A:202:LYS:HG2	2.15	0.46
1:H:194:LEU:HD12	1:H:194:LEU:C	2.35	0.46
1:D:136:ARG:HD2	1:H:136:ARG:HH22	1.81	0.46
1:H:50:ASP:HA	1:H:71:HIS:CD2	2.51	0.46
1:B:45:VAL:O	1:B:358:MET:HA	2.15	0.46
1:B:204:LYS:HD2	1:B:206:TYR:OH	2.15	0.46
1:H:372:GLU:OE1	1:H:372:GLU:HA	2.16	0.46
1:A:45:VAL:O	1:A:358:MET:HA	2.15	0.46
1:G:197:PHE:C	1:G:199:ASP:H	2.19	0.46
1:G:211:LYS:HA	1:G:216:ARG:O	2.16	0.46
1:B:165:THR:HB	1:B:170:MET:CE	2.46	0.46
1:H:7:GLU:OE1	1:H:463:ARG:NH2	2.40	0.46
1:D:248:THR:HG22	1:D:250:HIS:H	1.78	0.45
1:H:196:THR:HG22	1:H:199:ASP:H	1.81	0.45
1:H:452:ILE:O	1:H:456:ARG:HG3	2.16	0.45
1:B:306:THR:HG22	1:B:312:VAL:O	2.16	0.45
1:D:2:LEU:HD12	1:D:2:LEU:HA	1.76	0.45
1:F:0:HIS:CD2	4:F:567:HOH:O	2.68	0.45
1:F:245:VAL:HG12	1:F:247:ASP:HB2	1.97	0.45
1:H:196:THR:O	1:H:200:ILE:HG13	2.15	0.45
1:A:189:PHE:HD1	1:A:189:PHE:O	1.99	0.45
1:B:111:GLN:OE1	1:B:114:ARG:HD2	2.16	0.45
1:G:359:MET:HB2	1:G:363:PHE:CE2	2.51	0.45
1:A:350:MET:CE	1:A:357:VAL:CG2	2.85	0.45
1:C:465:THR:HG23	1:C:466:GLY:N	2.31	0.45
1:D:7:GLU:OE2	1:D:463:ARG:NH2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:GLU:HG3	1:E:125:GLU:O	2.15	0.45
1:G:33:ARG:NH1	1:G:36:ARG:O	2.49	0.45
1:G:333:PRO:HB3	1:G:355:TYR:CD2	2.52	0.45
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.88	0.45
1:B:105:LYS:HB3	1:B:107:ILE:CD1	2.46	0.45
1:D:178:ARG:O	1:H:139:ARG:NH1	2.49	0.45
1:C:107:ILE:HD12	1:C:107:ILE:N	2.31	0.45
1:D:422:ARG:HG3	1:D:422:ARG:NH1	2.31	0.45
1:F:374:GLU:OE2	1:F:422:ARG:HD3	2.16	0.45
1:G:17:ILE:CD1	1:G:462:VAL:HG13	2.46	0.45
1:G:302:SER:CB	1:G:303:ILE:HD12	2.44	0.45
1:G:316:GLN:HA	1:G:316:GLN:OE1	2.17	0.45
1:H:280:ALA:HB1	1:H:326:ALA:HB2	1.98	0.45
1:B:33:ARG:NH1	1:B:36:ARG:O	2.49	0.45
1:D:303:ILE:HD12	1:D:303:ILE:O	2.17	0.45
1:H:162:ARG:HB2	1:H:185:VAL:O	2.16	0.45
1:A:90:GLU:HG2	1:A:93:ILE:HB	1.99	0.45
1:A:107:ILE:H	1:A:107:ILE:CD1	2.30	0.45
1:C:91:THR:CG2	1:C:95:ARG:HH12	2.29	0.45
1:E:90:GLU:CB	1:E:93:ILE:HD12	2.45	0.45
1:D:17:ILE:HD11	1:D:462:VAL:HG13	1.98	0.44
1:C:157:LYS:HG3	1:C:157:LYS:O	2.18	0.44
1:D:161:ALA:HB2	1:D:182:MET:CE	2.48	0.44
1:G:200:ILE:HG13	1:G:201:GLU:N	2.32	0.44
1:D:45:VAL:O	1:D:358:MET:HA	2.18	0.44
1:D:183:LEU:HD11	2:D:501:F2K:C5	2.47	0.44
1:H:109:LEU:C	1:H:109:LEU:HD23	2.37	0.44
1:H:374:GLU:HG3	1:H:383:SER:CB	2.43	0.44
1:D:372:GLU:HA	1:D:372:GLU:OE1	2.18	0.44
1:E:134:THR:HG22	1:E:136:ARG:H	1.82	0.44
1:E:365:GLY:HA2	1:E:382:LYS:HD3	2.00	0.44
1:G:248:THR:CG2	1:G:249:ALA:N	2.80	0.44
1:G:257:ILE:CD1	1:G:285:ALA:HB1	2.46	0.44
1:B:302:SER:O	1:B:303:ILE:O	2.35	0.44
1:E:178:ARG:HD2	1:E:178:ARG:N	2.32	0.44
1:A:304:CYS:O	1:A:308:ILE:HG12	2.18	0.44
1:H:70:ILE:CD1	1:H:219:VAL:CG2	2.95	0.44
1:A:128:GLU:HB2	1:A:190:TYR:CE1	2.52	0.44
1:B:107:ILE:H	1:B:107:ILE:CD1	2.07	0.44
1:A:98:VAL:HG21	1:A:116:TYR:CE2	2.53	0.43
1:A:346:LEU:HG	1:A:357:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:ILE:HG23	1:E:289:ALA:HB2	2.00	0.43
1:F:368:GLU:OE1	1:F:368:GLU:N	2.51	0.43
1:G:440:LEU:CD1	4:G:543:HOH:O	2.65	0.43
1:A:359:MET:HB2	1:A:363:PHE:CE2	2.52	0.43
1:C:32:THR:HG21	1:C:43:PRO:HB3	1.99	0.43
1:D:79:GLN:OE1	1:D:232:ARG:HD3	2.18	0.43
1:C:12:ASP:CG	1:C:341:ARG:HH22	2.22	0.43
1:B:273:ILE:HG12	1:B:293:ALA:HB3	2.00	0.43
1:C:46:SER:OG	1:C:68:GLY:HA2	2.19	0.43
1:C:181:LYS:HG2	1:C:182:MET:N	2.34	0.43
1:D:384:TYR:OH	1:D:423:VAL:HG11	2.19	0.43
1:H:170:MET:HB3	1:H:182:MET:CE	2.48	0.43
1:H:374:GLU:CG	1:H:383:SER:HB2	2.46	0.43
1:C:195:VAL:HG21	1:C:200:ILE:HD11	2.01	0.43
1:D:86:VAL:HG11	1:D:219:VAL:HB	2.01	0.43
1:G:458:GLN:HB2	1:G:459:PRO:HD3	2.01	0.43
1:A:118:PHE:O	1:A:119:SER:HB3	2.17	0.43
1:A:155:LYS:HE3	1:A:189:PHE:CE2	2.53	0.43
1:B:171:LYS:HA	1:B:174:LEU:HD12	2.01	0.43
1:C:137:ASP:OD2	1:C:153:THR:HG23	2.18	0.43
1:D:379:ARG:NH1	1:H:379:ARG:HD3	2.34	0.43
1:E:50:ASP:HA	1:E:71:HIS:CD2	2.54	0.43
1:B:7:GLU:OE2	1:B:463:ARG:NH2	2.51	0.43
1:H:374:GLU:OE1	1:H:383:SER:CB	2.67	0.43
1:F:1:MET:HE3	1:F:1:MET:HA	2.00	0.42
1:F:365:GLY:HA2	1:F:382:LYS:HG3	2.00	0.42
1:G:91:THR:O	1:G:93:ILE:HD12	2.19	0.42
1:H:101:THR:HG22	1:H:104:THR:CG2	2.44	0.42
1:H:164:GLY:O	1:H:165:THR:C	2.57	0.42
1:E:460:GLN:OE1	1:H:5:SER:HB2	2.19	0.42
1:A:247:ASP:OD1	1:A:295:LYS:NZ	2.48	0.42
1:C:95:ARG:HH21	1:C:216:ARG:CG	2.32	0.42
1:D:173:LYS:HA	1:D:176:GLU:HG2	2.00	0.42
1:D:174:LEU:HD23	1:D:179:ILE:HG13	2.00	0.42
1:H:299:GLY:N	1:H:300:PRO:CD	2.82	0.42
1:B:165:THR:HB	1:B:170:MET:HE3	2.01	0.42
1:C:95:ARG:HH21	1:C:216:ARG:HD3	1.85	0.42
1:D:341:ARG:NH1	1:D:345:ASP:CG	2.70	0.42
1:B:139:ARG:C	1:B:140:VAL:HG12	2.39	0.42
1:D:98:VAL:HG21	1:D:116:TYR:CZ	2.54	0.42
1:E:245:VAL:HG12	1:E:247:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:ILE:HD13	1:G:89:HIS:CG	2.55	0.42
1:H:137:ASP:OD2	1:H:153:THR:OG1	2.33	0.42
1:A:183:LEU:HD23	1:A:194:LEU:CD1	2.43	0.42
1:D:123:VAL:HG11	1:D:152:MET:HE1	2.01	0.42
1:D:165:THR:HG22	1:D:169:GLU:HB2	2.00	0.42
1:A:175:TYR:CE2	1:B:114:ARG:HG2	2.54	0.42
1:H:44:LEU:HD23	1:H:44:LEU:HA	1.89	0.42
1:B:90:GLU:HG2	1:B:93:ILE:CG2	2.49	0.42
1:C:50:ASP:HA	1:C:71:HIS:CD2	2.54	0.42
1:D:48:ALA:HB2	1:D:69:ILE:HG22	2.02	0.42
1:F:422:ARG:N	4:F:506:HOH:O	2.52	0.42
1:H:20:TYR:CE2	1:H:22:GLU:HG3	2.55	0.42
1:A:32:THR:HG21	1:A:43:PRO:HB3	2.01	0.41
1:C:286:LEU:HD23	1:C:286:LEU:HA	1.76	0.41
1:E:43:PRO:HB2	1:E:356:CYS:HA	2.03	0.41
1:E:56:ARG:HD3	4:E:673:HOH:O	2.19	0.41
1:E:299:GLY:HA2	1:E:304:CYS:SG	2.60	0.41
1:H:465:THR:HG23	1:H:466:GLY:N	2.35	0.41
1:B:379:ARG:HB2	4:B:547:HOH:O	2.20	0.41
4:B:571:HOH:O	1:G:465:THR:HB	2.20	0.41
1:C:160:THR:O	1:C:173:LYS:HE2	2.20	0.41
1:C:168:GLU:OE1	1:C:171:LYS:HE2	2.20	0.41
1:C:423:VAL:O	1:C:423:VAL:HG13	2.21	0.41
1:D:62:ALA:HA	1:D:66:GLY:O	2.20	0.41
1:H:0:HIS:HB2	1:H:1:MET:H	1.40	0.41
1:H:440:LEU:O	1:H:444:MET:HG3	2.20	0.41
1:A:97:PRO:O	1:A:99:THR:HG23	2.19	0.41
1:A:42:ILE:CB	1:A:437:MET:HE1	2.42	0.41
1:A:245:VAL:HG12	1:A:247:ASP:HB2	2.02	0.41
1:D:87:LYS:HA	1:D:87:LYS:HD2	1.90	0.41
1:A:299:GLY:N	1:A:300:PRO:CD	2.82	0.41
1:C:465:THR:HG23	1:C:467:ALA:H	1.85	0.41
1:D:110:LEU:HD22	1:H:178:ARG:HH11	1.84	0.41
1:D:292:ASP:O	1:D:333:PRO:HD2	2.19	0.41
1:H:52:VAL:O	1:H:370:PRO:HD3	2.20	0.41
1:D:107:ILE:HG13	1:D:108:GLU:N	2.35	0.41
1:B:302:SER:O	1:B:303:ILE:HG12	2.20	0.41
1:E:137:ASP:OD2	1:E:153:THR:OG1	2.35	0.41
1:H:107:ILE:HD12	1:H:107:ILE:N	2.34	0.41
1:H:303:ILE:HD12	1:H:308:ILE:HD11	2.01	0.41
1:A:458:GLN:H	1:A:459:PRO:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:ARG:HG3	1:D:422:ARG:HH11	1.85	0.41
1:E:30:LEU:HA	1:E:452:ILE:HD11	2.03	0.41
1:H:70:ILE:HD11	1:H:219:VAL:HG21	2.01	0.41
1:B:106:ILE:HD12	1:B:106:ILE:H	1.85	0.41
1:C:45:VAL:O	1:C:358:MET:HA	2.21	0.41
1:H:136:ARG:C	1:H:138:LEU:H	2.24	0.41
1:A:30:LEU:CD1	1:A:437:MET:HE2	2.43	0.41
1:G:46:SER:OG	1:G:68:GLY:HA2	2.20	0.41
1:C:299:GLY:N	1:C:300:PRO:CD	2.83	0.40
1:E:2:LEU:HD12	1:E:2:LEU:HA	1.85	0.40
1:H:17:ILE:CD1	1:H:462:VAL:HG13	2.50	0.40
1:A:156:ASP:OD1	1:A:156:ASP:N	2.54	0.40
1:A:178:ARG:NH1	1:B:110:LEU:HD21	2.36	0.40
1:A:302:SER:H	1:A:307:ARG:HD2	1.86	0.40
1:A:341:ARG:HE	1:A:341:ARG:HB2	1.63	0.40
1:C:465:THR:CG2	1:C:466:GLY:N	2.84	0.40
1:E:153:THR:HA	1:E:154:PRO:HD3	1.95	0.40
1:D:369:ALA:O	1:D:382:LYS:NZ	2.49	0.40
1:D:69:ILE:N	1:D:69:ILE:CD1	2.84	0.40
1:D:118:PHE:O	1:D:120:GLY:N	2.54	0.40
1:E:132:ILE:HG13	1:E:133:VAL:N	2.36	0.40
1:B:106:ILE:HD12	1:B:106:ILE:N	2.37	0.40
1:B:132:ILE:HG13	1:B:133:VAL:N	2.37	0.40
1:G:61:MET:SD	1:G:429:LEU:HD21	2.62	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TYR:OH	1:D:108:GLU:OE2[1_656]	1.92	0.28

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	418/509 (82%)	400 (96%)	15 (4%)	3 (1%)	22	30
1	B	418/509 (82%)	402 (96%)	13 (3%)	3 (1%)	22	30
1	C	367/509 (72%)	353 (96%)	13 (4%)	1 (0%)	41	51
1	D	419/509 (82%)	401 (96%)	17 (4%)	1 (0%)	47	60
1	E	419/509 (82%)	403 (96%)	15 (4%)	1 (0%)	47	60
1	F	311/509 (61%)	299 (96%)	11 (4%)	1 (0%)	41	51
1	G	323/509 (64%)	308 (95%)	13 (4%)	2 (1%)	25	34
1	H	411/509 (81%)	389 (95%)	19 (5%)	3 (1%)	22	30
All	All	3086/4072 (76%)	2955 (96%)	116 (4%)	15 (0%)	29	40

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	LEU
1	G	377	GLN
1	H	152	MET
1	B	303	ILE
1	C	158	LEU
1	F	226	GLY
1	B	203	ALA
1	D	2	LEU
1	H	226	GLY
1	A	119	SER
1	H	458	GLN
1	A	301	GLY
1	B	458	GLN
1	G	303	ILE
1	A	458	GLN

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	321/390 (82%)	312 (97%)	9 (3%)	43	58
1	B	324/390 (83%)	313 (97%)	11 (3%)	37	50
1	C	288/390 (74%)	276 (96%)	12 (4%)	30	40
1	D	327/390 (84%)	315 (96%)	12 (4%)	34	46
1	E	326/390 (84%)	322 (99%)	4 (1%)	71	81
1	F	233/390 (60%)	225 (97%)	8 (3%)	37	50
1	G	238/390 (61%)	229 (96%)	9 (4%)	33	45
1	H	321/390 (82%)	309 (96%)	12 (4%)	34	46
All	All	2378/3120 (76%)	2301 (97%)	77 (3%)	39	53

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	95	ARG
1	A	103	SER
1	A	189	PHE
1	A	204	LYS
1	A	302	SER
1	A	328	GLU
1	A	334	LEU
1	A	462	VAL
1	B	4	ILE
1	B	45	VAL
1	B	77	GLU
1	B	107	ILE
1	B	132	ILE
1	B	146	ASP
1	B	148	VAL
1	B	189	PHE
1	B	304	CYS
1	B	334	LEU
1	B	341	ARG
1	C	1	MET
1	C	33	ARG
1	C	153	THR
1	C	156	ASP
1	C	213	GLU
1	C	270	VAL
1	C	298	ILE

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Mol	Chain	Res	Type
1	C	334	LEU
1	C	341	ARG
1	C	382	LYS
1	C	384	TYR
1	C	465	THR
1	D	33	ARG
1	D	115	GLU
1	D	156	ASP
1	D	178	ARG
1	D	182	MET
1	D	196	THR
1	D	198	ARG
1	D	248	THR
1	D	260	VAL
1	D	334	LEU
1	D	341	ARG
1	D	367	GLU
1	E	132	ILE
1	E	156	ASP
1	E	201	GLU
1	E	334	LEU
1	F	5	SER
1	F	23	VAL
1	F	33	ARG
1	F	205	THR
1	F	270	VAL
1	F	334	LEU
1	F	372	GLU
1	F	463	ARG
1	G	31	LYS
1	G	33	ARG
1	G	260	VAL
1	G	264	LYS
1	G	298	ILE
1	G	334	LEU
1	G	423	VAL
1	G	463	ARG
1	G	465	THR
1	H	0	HIS
1	H	31	LYS
1	H	33	ARG
1	H	84	ARG

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Mol	Chain	Res	Type
1	H	104	THR
1	H	136	ARG
1	H	181	LYS
1	H	198	ARG
1	H	270	VAL
1	H	334	LEU
1	H	341	ARG
1	H	465	THR

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

Mol	Chain	Res	Type
1	D	177	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	F2K	D	501	-	24,24,24	0.53	1 (4%)	30,35,35	0.64	1 (3%)
3	SO4	E	501	-	4,4,4	0.23	0	6,6,6	0.41	0
2	F2K	A	501	-	24,24,24	0.55	1 (4%)	30,35,35	0.63	1 (3%)

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	F2K	D	501	-	-	2/4/22/22	0/3/3/3
2	F2K	A	501	-	-	2/4/22/22	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	F2K	C8-N	2.50	1.41	1.37
2	D	501	F2K	C8-N	2.40	1.41	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	F2K	C6-C7-C10	2.30	122.42	119.50
2	A	501	F2K	C6-C7-C10	2.27	122.38	119.50

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	F2K	C-C1-C6-C7
2	A	501	F2K	C2-C1-C6-C7
2	D	501	F2K	C-C1-C6-C7
2	D	501	F2K	C2-C1-C6-C7

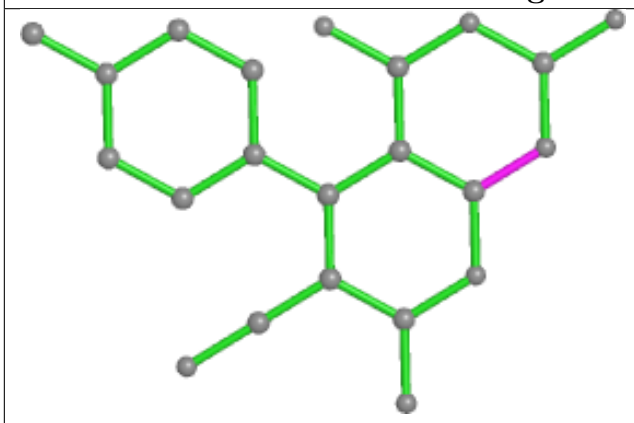
There are no ring outliers.

1 monomer is involved in 1 short contact:

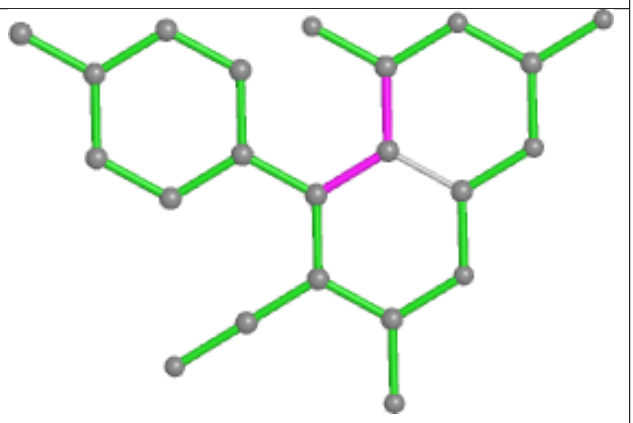
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	F2K	1	0

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

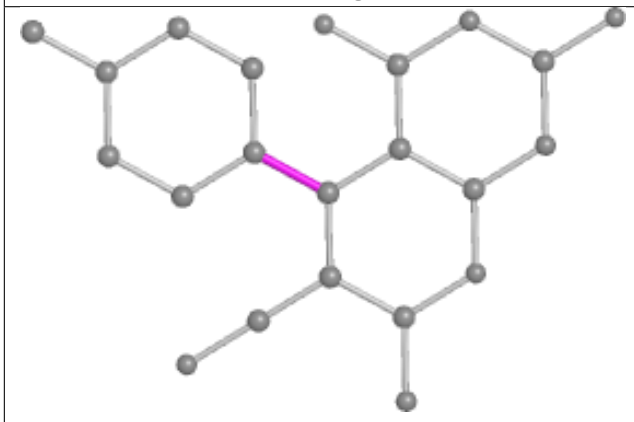
Ligand F2K D 501



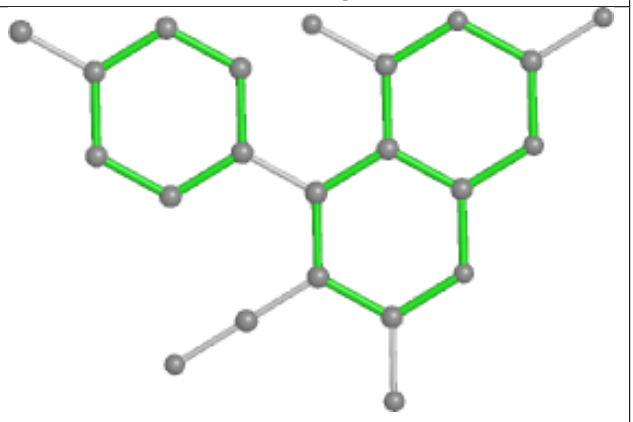
Bond lengths



Bond angles

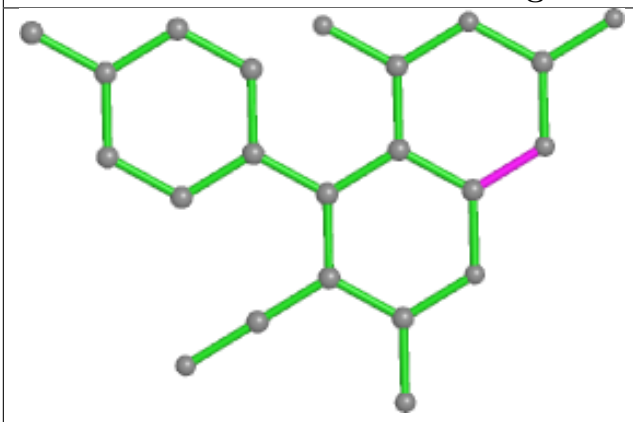


Torsions

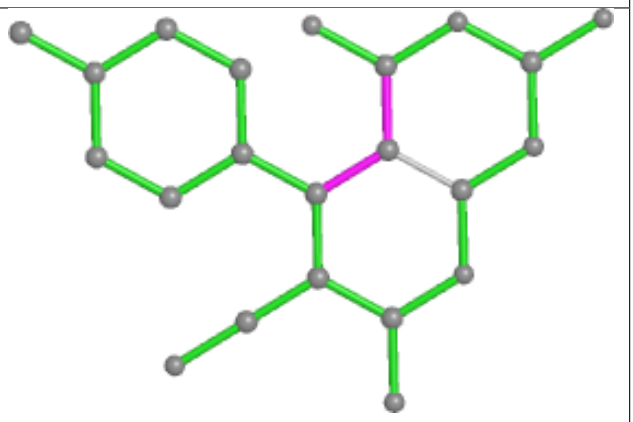


Rings

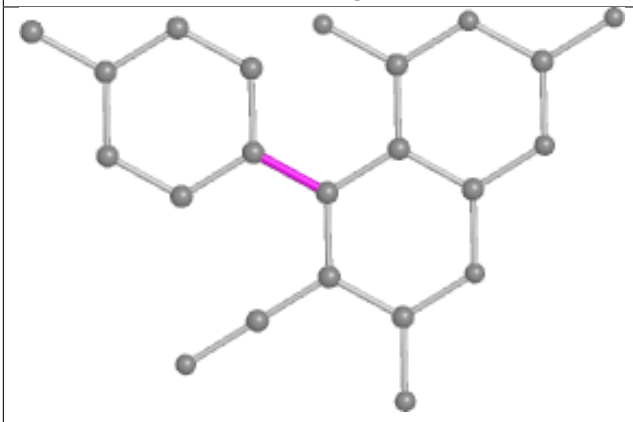
Ligand F2K A 501



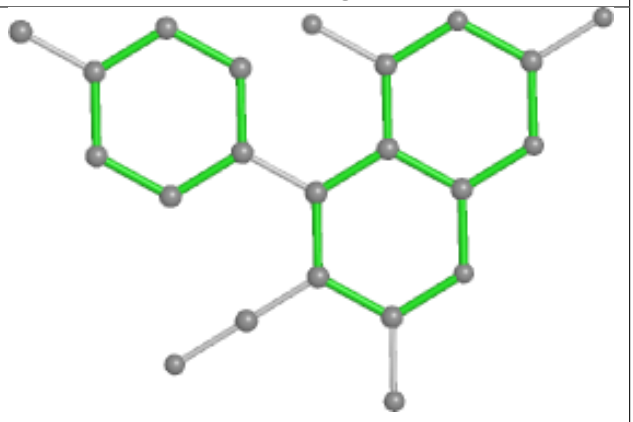
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	424/509 (83%)	-0.14	2 (0%) 91 94	24, 41, 82, 121	26 (6%)
1	B	424/509 (83%)	-0.06	5 (1%) 79 84	26, 41, 82, 99	25 (5%)
1	C	381/509 (74%)	0.29	39 (10%) 6 8	26, 40, 123, 158	23 (6%)
1	D	424/509 (83%)	-0.15	8 (1%) 66 73	26, 47, 90, 108	23 (5%)
1	E	424/509 (83%)	0.19	21 (4%) 28 34	26, 40, 110, 138	27 (6%)
1	F	317/509 (62%)	-0.10	2 (0%) 89 92	27, 41, 76, 109	17 (5%)
1	G	329/509 (64%)	0.02	6 (1%) 68 74	34, 51, 97, 132	18 (5%)
1	H	419/509 (82%)	0.40	60 (14%) 2 3	34, 56, 114, 163	25 (5%)
All	All	3142/4072 (77%)	0.06	143 (4%) 32 39	24, 45, 102, 163	184 (5%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	129	LEU	7.1
1	C	154	PRO	6.5
1	C	107	ILE	5.8
1	H	151	ILE	5.5
1	H	158	LEU	5.4
1	C	109	LEU	5.4
1	C	158	LEU	5.3
1	C	156	ASP	5.3
1	H	107	ILE	5.2
1	H	128	GLU	5.1
1	C	98	VAL	5.1
1	C	138	LEU	4.7
1	H	118	PHE	4.7
1	H	147	THR	4.7
1	C	169	GLU	4.6
1	H	159	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	H	157	LYS	4.5
1	F	91	THR	4.5
1	E	175	TYR	4.5
1	C	99	THR	4.4
1	C	172	ALA	4.2
1	C	159	VAL	4.1
1	H	191	LEU	4.1
1	G	200	ILE	4.0
1	C	108	GLU	3.9
1	H	106	ILE	3.9
1	E	135	GLY	3.9
1	E	154	PRO	3.8
1	C	153	THR	3.8
1	C	152	MET	3.8
1	E	178	ARG	3.8
1	H	124	VAL	3.7
1	H	303	ILE	3.7
1	H	123	VAL	3.7
1	C	110	LEU	3.6
1	G	422	ARG	3.6
1	H	130	VAL	3.6
1	C	112	MET	3.6
1	H	109	LEU	3.5
1	H	138	LEU	3.5
1	H	156	ASP	3.5
1	H	132	ILE	3.5
1	E	147	THR	3.4
1	H	154	PRO	3.4
1	C	182	MET	3.4
1	H	198	ARG	3.4
1	H	148	VAL	3.4
1	H	139	ARG	3.4
1	H	137	ASP	3.3
1	H	146	ASP	3.3
1	C	160	THR	3.3
1	C	174	LEU	3.2
1	D	198	ARG	3.2
1	C	157	LYS	3.2
1	D	139	ARG	3.2
1	H	184	VAL	3.2
1	H	133	VAL	3.1
1	E	138	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	167	LEU	3.1
1	E	423	VAL	3.1
1	H	136	ARG	3.0
1	C	155	LYS	3.0
1	H	163	GLU	3.0
1	H	194	LEU	3.0
1	G	93	ILE	3.0
1	C	116	TYR	3.0
1	H	121	PHE	2.9
1	H	111	GLN	2.9
1	C	194	LEU	2.9
1	H	125	GLU	2.8
1	D	175	TYR	2.8
1	C	134	THR	2.8
1	H	152	MET	2.8
1	H	100	VAL	2.7
1	E	104	THR	2.7
1	H	122	PRO	2.7
1	H	135	GLY	2.7
1	H	192	ARG	2.7
1	H	150	ALA	2.7
1	E	383	SER	2.6
1	H	101	THR	2.6
1	H	170	MET	2.6
1	B	110	LEU	2.6
1	H	116	TYR	2.6
1	G	383	SER	2.6
1	E	155	LYS	2.6
1	B	107	ILE	2.6
1	H	114	ARG	2.6
1	D	197	PHE	2.5
1	H	153	THR	2.5
1	E	114	ARG	2.5
1	H	131	GLY	2.5
1	H	108	GLU	2.5
1	G	384	TYR	2.5
1	B	151	ILE	2.5
1	B	109	LEU	2.4
1	E	110	LEU	2.4
1	C	379	ARG	2.4
1	E	148	VAL	2.4
1	H	110	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	112	MET	2.4
1	H	102	PRO	2.4
1	E	109	LEU	2.4
1	H	167	LEU	2.4
1	C	117	GLY	2.4
1	C	166	PRO	2.4
1	H	98	VAL	2.3
1	H	179	ILE	2.3
1	D	421	GLY	2.3
1	C	202	LYS	2.3
1	E	151	ILE	2.3
1	C	383	SER	2.3
1	H	193	GLY	2.3
1	C	200	ILE	2.3
1	E	157	LYS	2.3
1	F	423	VAL	2.3
1	E	149	ALA	2.3
1	D	136	ARG	2.2
1	C	168	GLU	2.2
1	C	165	THR	2.2
1	B	384	TYR	2.2
1	A	175	TYR	2.2
1	E	132	ILE	2.2
1	C	180	GLU	2.2
1	H	120	GLY	2.2
1	C	137	ASP	2.1
1	D	303	ILE	2.1
1	H	126	GLN	2.1
1	C	118	PHE	2.1
1	E	139	ARG	2.1
1	C	376	PHE	2.1
1	E	198	ARG	2.1
1	C	111	GLN	2.1
1	H	169	GLU	2.1
1	C	93	ILE	2.1
1	E	126	GLN	2.1
1	H	161	ALA	2.1
1	H	149	ALA	2.0
1	G	92	ALA	2.0
1	A	159	VAL	2.0
1	H	105	LYS	2.0
1	D	157	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	95	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

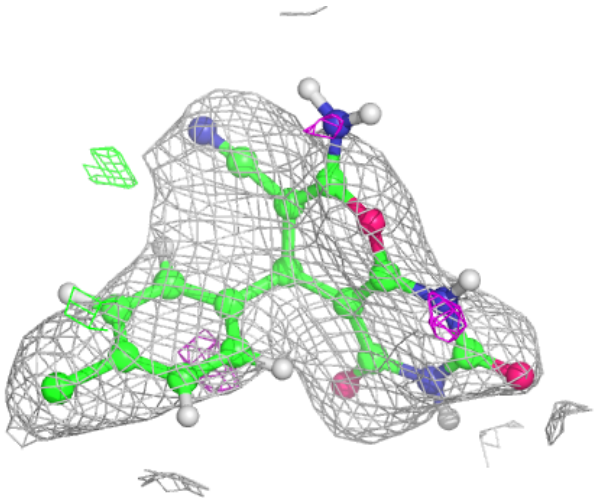
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

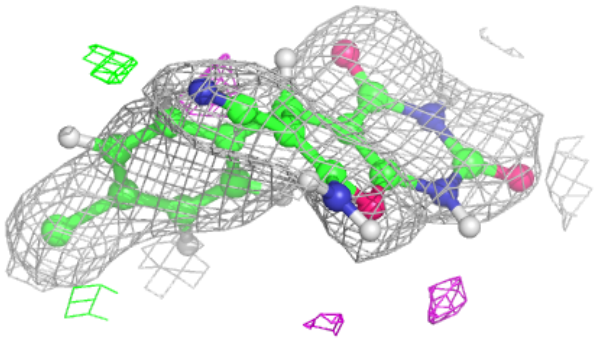
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	F2K	A	501	22/22	0.81	0.26	73,101,122,128	0
2	F2K	D	501	22/22	0.87	0.36	73,86,99,114	31
3	SO4	E	501	5/5	0.94	0.19	40,48,52,59	5

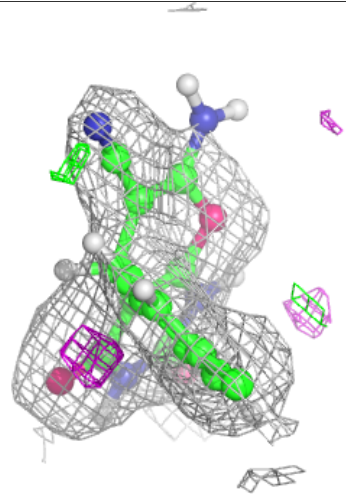
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around F2K A 501:

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

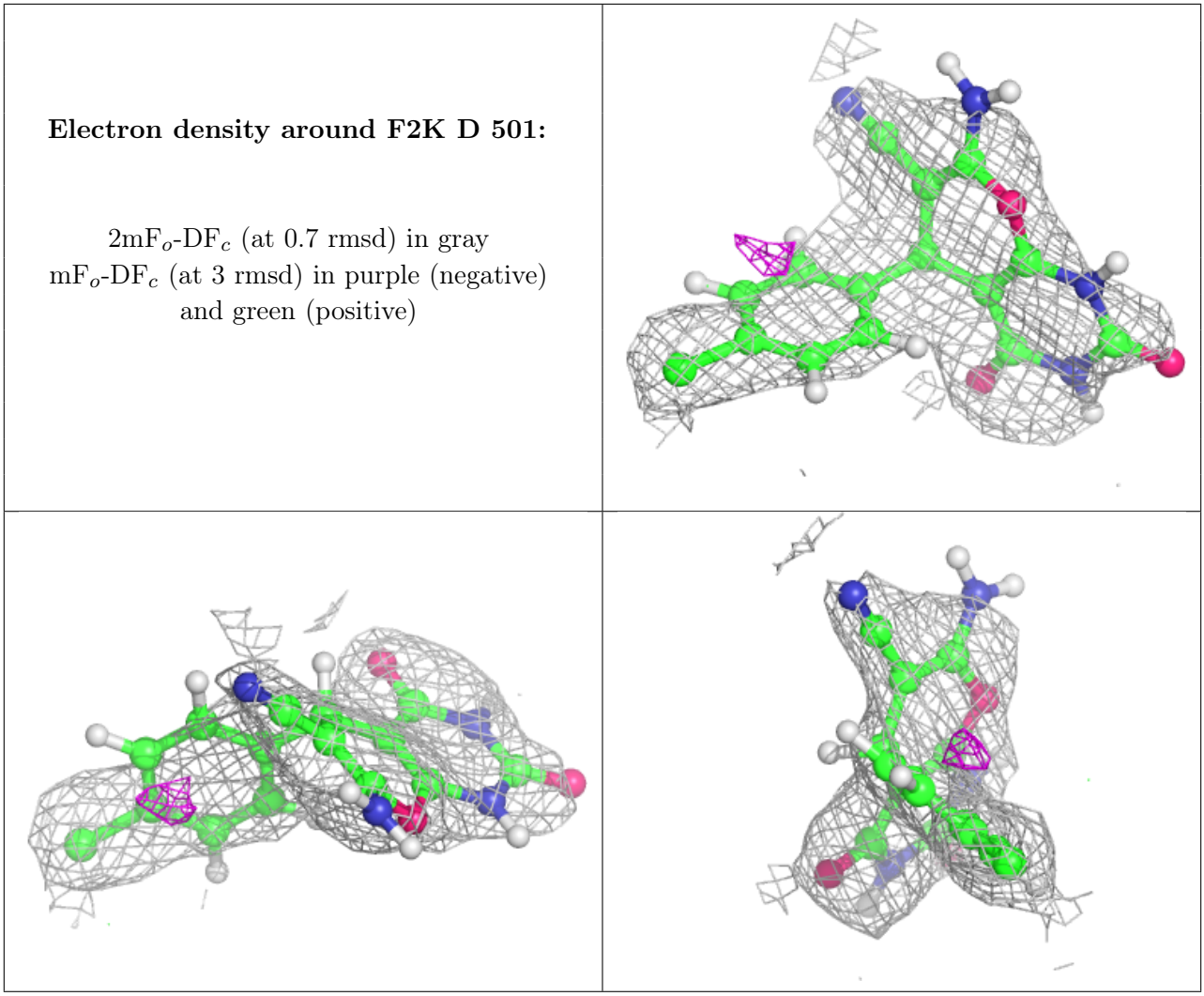






Electron density around F2K D 501:

$2mF_o$-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.