Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 01:15 am GMT

PDB ID	:	2XKB
Title	:	Crystal structure of GDP-form protofilaments of Bacillus thuringiensis serovar israelensis TubZ
Authors	:	Aylett, C.H.S.; Lowe, J.
Deposited on	:	2010-07-07
Resolution	:	3.00 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 ⓘ symbol.

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

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

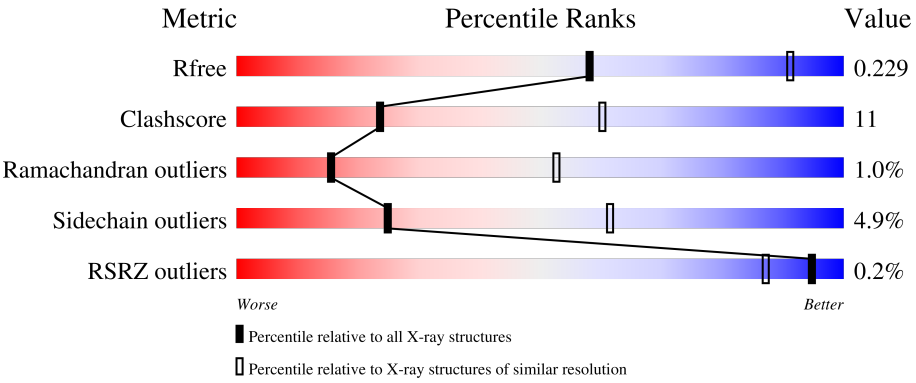
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.00 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))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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% 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	427	% 62% 27% • 8%
1	B	427	71% 22% • 5%
1	C	427	68% 22% • 9%
1	D	427	70% 20% • 8%
1	E	427	71% 19% • 7%

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Mol	Chain	Length	Quality of chain
1	F	427	68% 21% • 8%
1	G	427	70% 22% • 5%
1	H	427	68% 22% • 8%
1	I	427	67% 24% • 5%
1	J	427	68% 22% • 8%
1	K	427	69% 22% • 6%
1	L	427	66% 22% • 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 37877 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 FTSZ/TUBULIN-RELATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3095	1952	526	604	13			
1	B	405	Total	C	N	O	S	0	0	0
			3209	2022	544	630	13			
1	C	389	Total	C	N	O	S	0	0	0
			3095	1949	532	601	13			
1	D	391	Total	C	N	O	S	0	0	0
			3094	1949	528	604	13			
1	E	395	Total	C	N	O	S	0	0	0
			3137	1976	534	614	13			
1	F	391	Total	C	N	O	S	0	0	0
			3095	1949	529	605	12			
1	G	404	Total	C	N	O	S	0	0	0
			3198	2016	543	626	13			
1	H	394	Total	C	N	O	S	0	0	0
			3143	1983	533	614	13			
1	I	404	Total	C	N	O	S	0	0	0
			3202	2018	543	628	13			
1	J	393	Total	C	N	O	S	0	0	0
			3114	1963	531	608	12			
1	K	400	Total	C	N	O	S	0	0	0
			3182	2003	545	622	12			
1	L	379	Total	C	N	O	S	0	0	0
			3001	1897	507	585	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	HIS	-	expression tag	UNP Q8KNP3
A	423	HIS	-	expression tag	UNP Q8KNP3
A	424	HIS	-	expression tag	UNP Q8KNP3
A	425	HIS	-	expression tag	UNP Q8KNP3
A	426	HIS	-	expression tag	UNP Q8KNP3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	427	HIS	-	expression tag	UNP Q8KNP3
A	2	VAL	LEU	engineered mutation	UNP Q8KNP3
B	422	HIS	-	expression tag	UNP Q8KNP3
B	423	HIS	-	expression tag	UNP Q8KNP3
B	424	HIS	-	expression tag	UNP Q8KNP3
B	425	HIS	-	expression tag	UNP Q8KNP3
B	426	HIS	-	expression tag	UNP Q8KNP3
B	427	HIS	-	expression tag	UNP Q8KNP3
B	2	VAL	LEU	engineered mutation	UNP Q8KNP3
C	422	HIS	-	expression tag	UNP Q8KNP3
C	423	HIS	-	expression tag	UNP Q8KNP3
C	424	HIS	-	expression tag	UNP Q8KNP3
C	425	HIS	-	expression tag	UNP Q8KNP3
C	426	HIS	-	expression tag	UNP Q8KNP3
C	427	HIS	-	expression tag	UNP Q8KNP3
C	2	VAL	LEU	engineered mutation	UNP Q8KNP3
D	422	HIS	-	expression tag	UNP Q8KNP3
D	423	HIS	-	expression tag	UNP Q8KNP3
D	424	HIS	-	expression tag	UNP Q8KNP3
D	425	HIS	-	expression tag	UNP Q8KNP3
D	426	HIS	-	expression tag	UNP Q8KNP3
D	427	HIS	-	expression tag	UNP Q8KNP3
D	2	VAL	LEU	engineered mutation	UNP Q8KNP3
E	422	HIS	-	expression tag	UNP Q8KNP3
E	423	HIS	-	expression tag	UNP Q8KNP3
E	424	HIS	-	expression tag	UNP Q8KNP3
E	425	HIS	-	expression tag	UNP Q8KNP3
E	426	HIS	-	expression tag	UNP Q8KNP3
E	427	HIS	-	expression tag	UNP Q8KNP3
E	2	VAL	LEU	engineered mutation	UNP Q8KNP3
F	422	HIS	-	expression tag	UNP Q8KNP3
F	423	HIS	-	expression tag	UNP Q8KNP3
F	424	HIS	-	expression tag	UNP Q8KNP3
F	425	HIS	-	expression tag	UNP Q8KNP3
F	426	HIS	-	expression tag	UNP Q8KNP3
F	427	HIS	-	expression tag	UNP Q8KNP3
F	2	VAL	LEU	engineered mutation	UNP Q8KNP3
G	422	HIS	-	expression tag	UNP Q8KNP3
G	423	HIS	-	expression tag	UNP Q8KNP3
G	424	HIS	-	expression tag	UNP Q8KNP3
G	425	HIS	-	expression tag	UNP Q8KNP3
G	426	HIS	-	expression tag	UNP Q8KNP3

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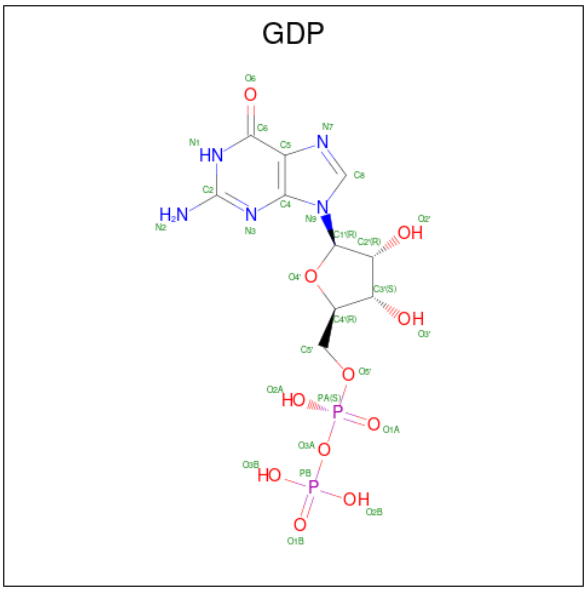
Chain	Residue	Modelled	Actual	Comment	Reference
G	427	HIS	-	expression tag	UNP Q8KNP3
G	2	VAL	LEU	engineered mutation	UNP Q8KNP3
H	422	HIS	-	expression tag	UNP Q8KNP3
H	423	HIS	-	expression tag	UNP Q8KNP3
H	424	HIS	-	expression tag	UNP Q8KNP3
H	425	HIS	-	expression tag	UNP Q8KNP3
H	426	HIS	-	expression tag	UNP Q8KNP3
H	427	HIS	-	expression tag	UNP Q8KNP3
H	2	VAL	LEU	engineered mutation	UNP Q8KNP3
I	422	HIS	-	expression tag	UNP Q8KNP3
I	423	HIS	-	expression tag	UNP Q8KNP3
I	424	HIS	-	expression tag	UNP Q8KNP3
I	425	HIS	-	expression tag	UNP Q8KNP3
I	426	HIS	-	expression tag	UNP Q8KNP3
I	427	HIS	-	expression tag	UNP Q8KNP3
I	2	VAL	LEU	engineered mutation	UNP Q8KNP3
J	422	HIS	-	expression tag	UNP Q8KNP3
J	423	HIS	-	expression tag	UNP Q8KNP3
J	424	HIS	-	expression tag	UNP Q8KNP3
J	425	HIS	-	expression tag	UNP Q8KNP3
J	426	HIS	-	expression tag	UNP Q8KNP3
J	427	HIS	-	expression tag	UNP Q8KNP3
J	2	VAL	LEU	engineered mutation	UNP Q8KNP3
K	422	HIS	-	expression tag	UNP Q8KNP3
K	423	HIS	-	expression tag	UNP Q8KNP3
K	424	HIS	-	expression tag	UNP Q8KNP3
K	425	HIS	-	expression tag	UNP Q8KNP3
K	426	HIS	-	expression tag	UNP Q8KNP3
K	427	HIS	-	expression tag	UNP Q8KNP3
K	2	VAL	LEU	engineered mutation	UNP Q8KNP3
L	422	HIS	-	expression tag	UNP Q8KNP3
L	423	HIS	-	expression tag	UNP Q8KNP3
L	424	HIS	-	expression tag	UNP Q8KNP3
L	425	HIS	-	expression tag	UNP Q8KNP3
L	426	HIS	-	expression tag	UNP Q8KNP3
L	427	HIS	-	expression tag	UNP Q8KNP3
L	2	VAL	LEU	engineered mutation	UNP Q8KNP3

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	E	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	F	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	G	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	I	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	J	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	K	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	L	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

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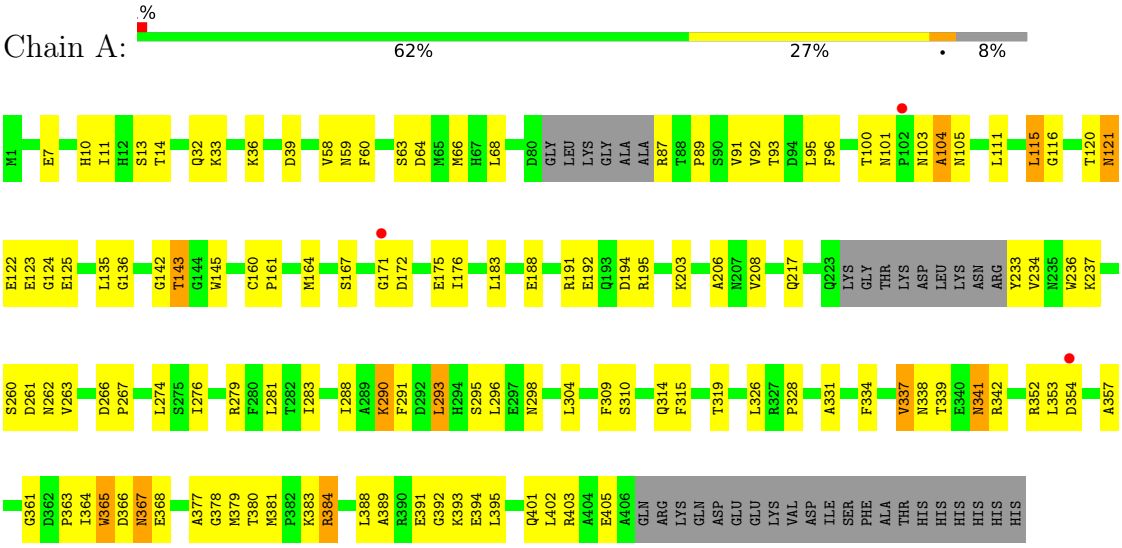
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

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

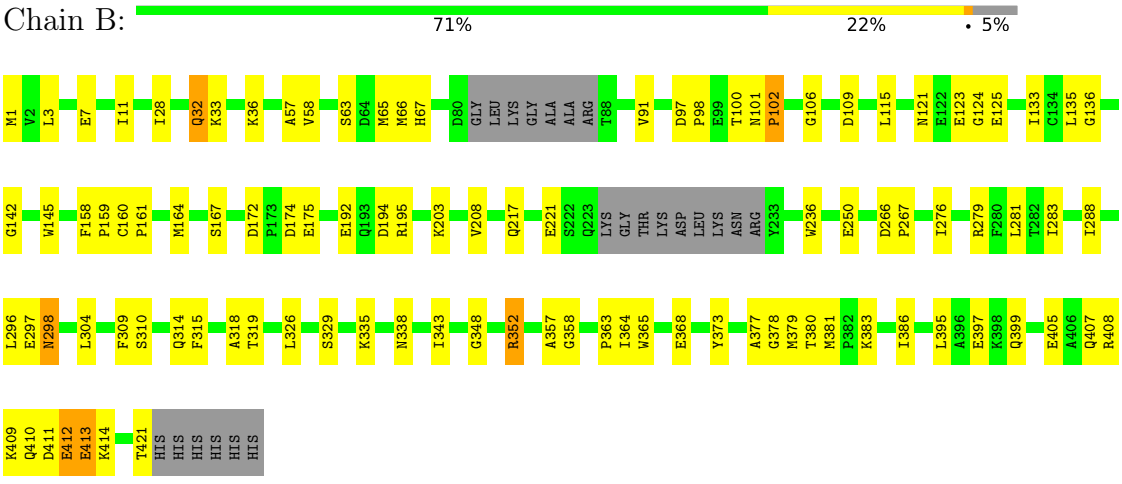
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain A:



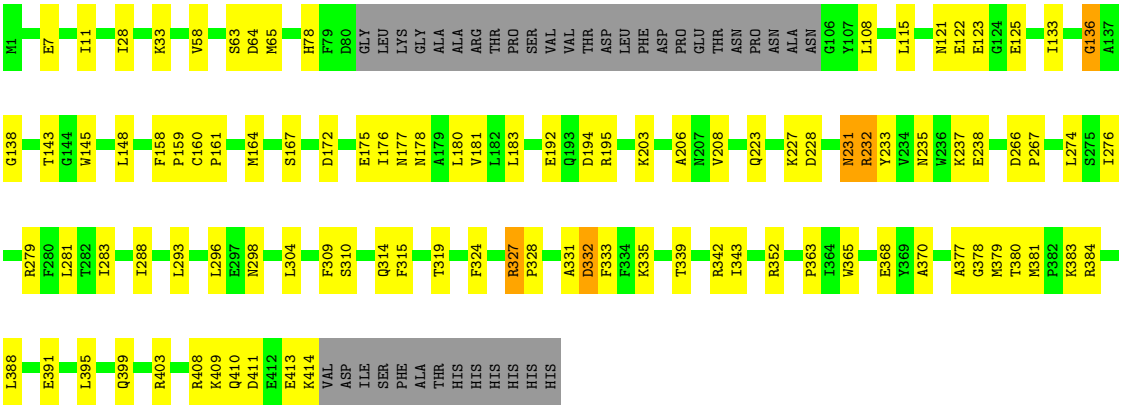
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain B:



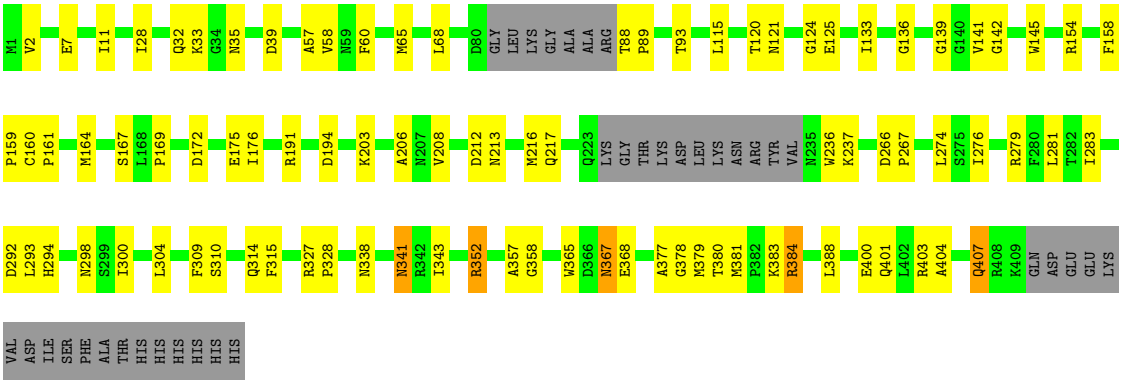
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain C:



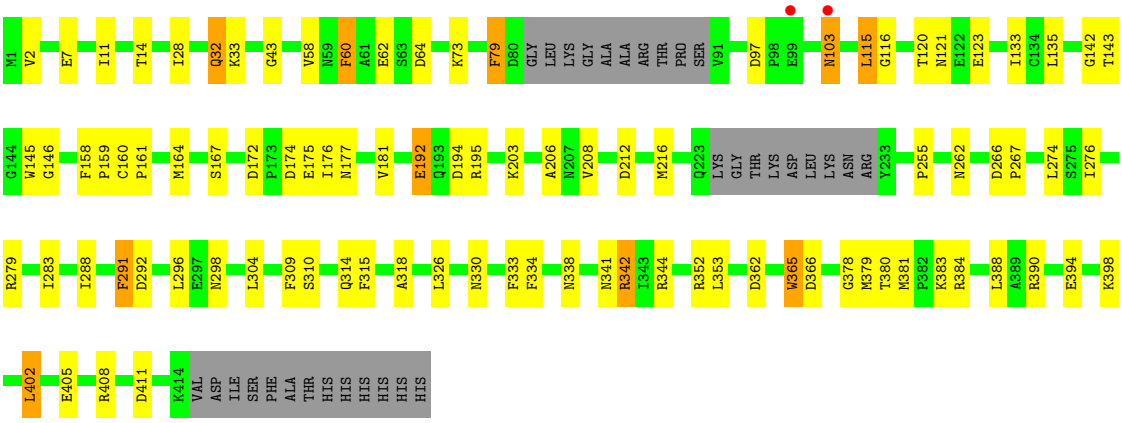
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain D:



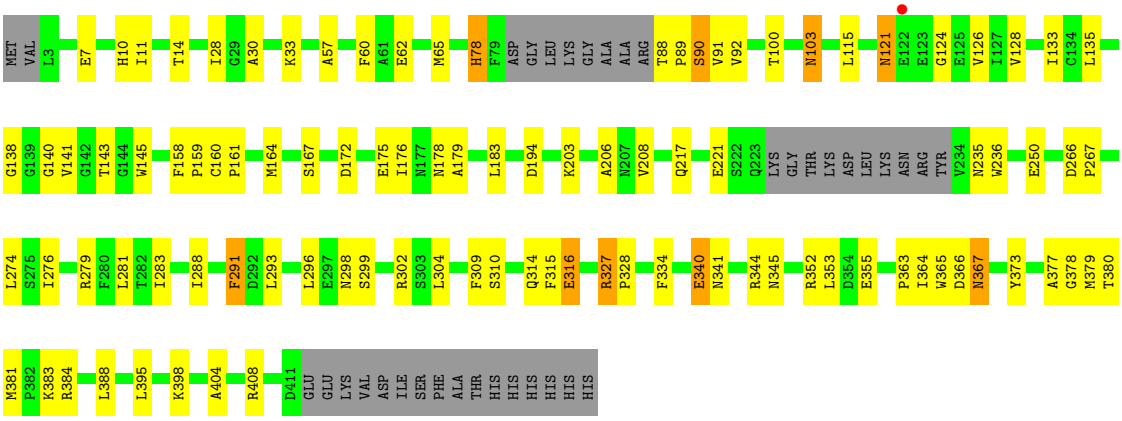
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain E:



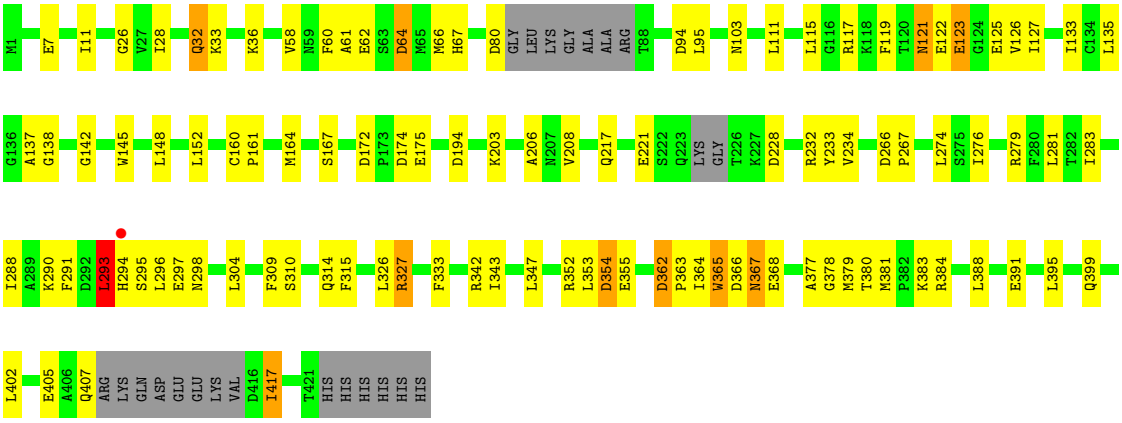
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain F:



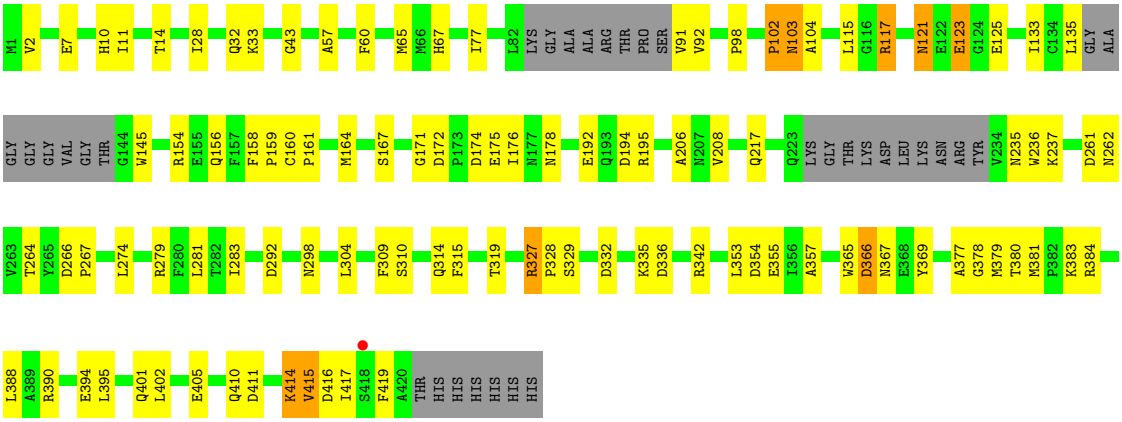
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain G:



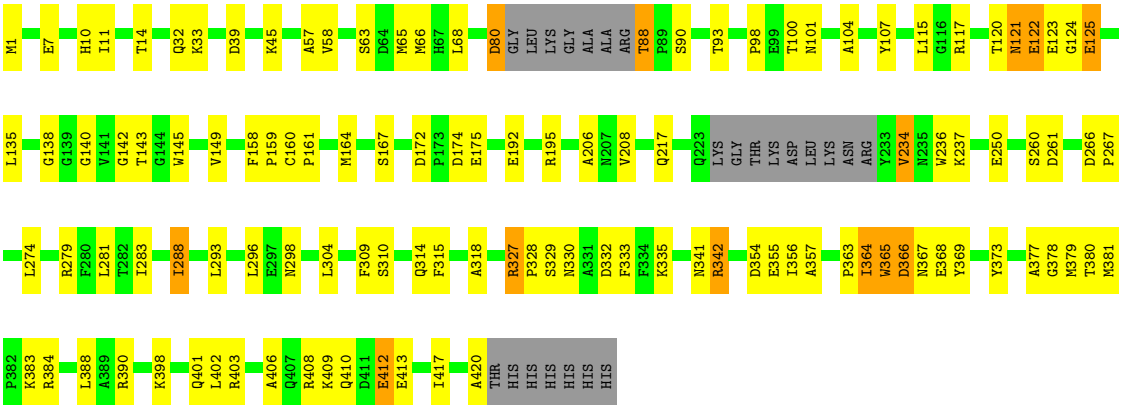
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain H:



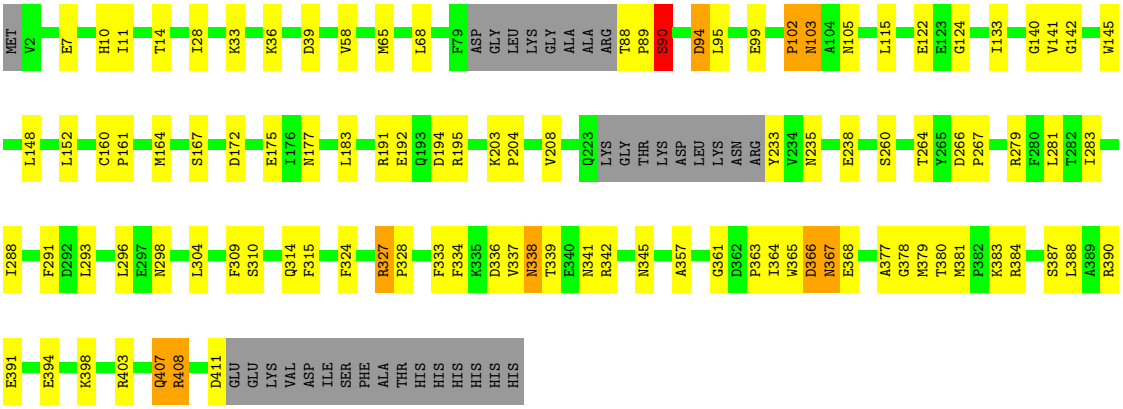
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain I:



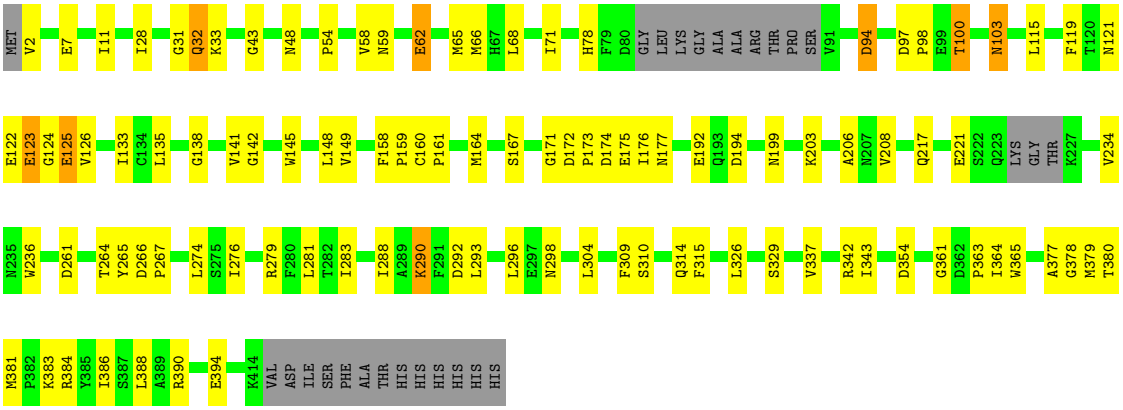
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain J:



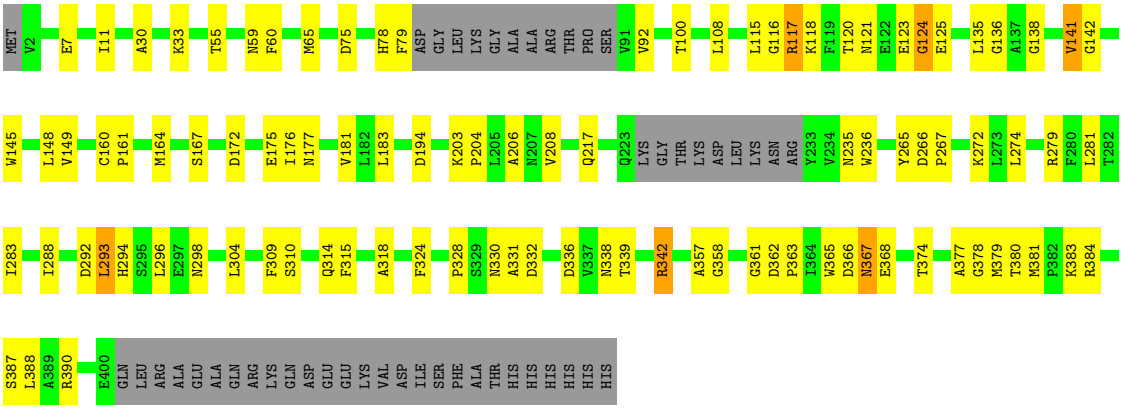
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain K:



• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain L:


MET V2 E7 I11 A30 K33 T55 N59 F60 M65 D75 H78 F79 ASP GLY LEU LYS GLY ALA ALA ARG THR PRO SER V91 V92 T100 L108 L115 G116 R117 K118 F119 T120 N121 E122 E123 G124 E125 L135 G136 A137 G138 V141 G142
W145 L148 V149 C160 P161 M164 S167 D172 E175 I176 N177 V181 L182 L183 D194 K203 P204 L205 A206 N207 V208 Q217 Q223 LYS GLY THR LYS ASP LEU LYS ASN ARG Y233 V234 N235 W236 Y265 D266 P267 K272 L273 L274 R279 F280 L281 T282
I283 I288 D292 L293 H294 S295 L296 E297 N298 L304 F309 S310 Q314 F315 A318 F324 P328 S329 N330 A331 D332 D336 V337 N338 T339 R342 A357 G358 G361 D362 P363 I364 W365 D366 N367 E368 T374 A377 G378 M379 T380 M381 P382 K383 R384
S387 L388 A389 R390 E400 GLN LEU ARG ALA GLU ALA GLN ARG LYS GLN ASP GLU GLU LYS VAL ASP ILE SER PHE ALA THR HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.95Å 541.10Å 86.13Å 90.00° 92.51° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 77.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.9 (50.00-3.00) 92.9 (77.66-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.294 0.231 , 0.229	Depositor DCC
R_{free} test set	4465 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	59.4	Xtriage
Anisotropy	0.870	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	37877	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: GDP, 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	0.49	0/3155	0.60	1/4268 (0.0%)
1	B	0.50	0/3270	0.60	0/4422
1	C	0.52	0/3152	0.61	1/4252 (0.0%)
1	D	0.57	3/3153 (0.1%)	0.72	5/4263 (0.1%)
1	E	0.48	0/3196	0.58	1/4319 (0.0%)
1	F	0.50	0/3154	0.64	2/4265 (0.0%)
1	G	0.53	0/3258	0.59	0/4405
1	H	0.52	0/3201	0.62	0/4325
1	I	0.50	0/3263	0.61	0/4412
1	J	0.52	0/3174	0.60	0/4293
1	K	0.50	0/3241	0.59	0/4378
1	L	0.50	0/3060	0.60	0/4140
All	All	0.51	3/38277 (0.0%)	0.61	10/51742 (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	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	154	ARG	CZ-NH1	11.48	1.48	1.33
1	D	154	ARG	NE-CZ	9.18	1.45	1.33
1	D	154	ARG	CD-NE	7.03	1.58	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	154	ARG	NE-CZ-NH1	-17.22	111.69	120.30
1	D	154	ARG	NH1-CZ-NH2	11.91	132.50	119.40
1	D	154	ARG	NE-CZ-NH2	-10.45	115.08	120.30
1	D	154	ARG	CD-NE-CZ	-10.31	109.17	123.60
1	F	316	GLU	CA-CB-CG	9.45	134.18	113.40
1	F	316	GLU	CB-CA-C	-7.62	95.16	110.40
1	A	115	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	C	136	GLY	N-CA-C	-5.72	98.79	113.10
1	E	115	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	D	154	ARG	CG-CD-NE	-5.20	100.88	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	223	GLN	Peptide

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	3095	0	3006	92	0
1	B	3209	0	3114	72	0
1	C	3095	0	3026	68	1
1	D	3094	0	3009	63	0
1	E	3137	0	3045	60	1
1	F	3095	0	3005	67	0
1	G	3198	0	3108	77	0
1	H	3143	0	3056	74	0
1	I	3202	0	3107	88	1
1	J	3114	0	3023	77	0
1	K	3182	0	3093	78	1
1	L	3001	0	2910	75	0
2	A	28	0	12	2	0
2	B	28	0	12	1	0
2	C	28	0	12	0	0
2	D	28	0	12	3	0
2	E	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	28	0	12	0	0
2	G	28	0	12	0	0
2	I	28	0	12	1	0
2	J	28	0	12	0	0
2	K	28	0	12	0	0
2	L	28	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
All	All	37877	0	36634	836	2

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 (836) 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:L:117:ARG:HH11	1:L:117:ARG:HG2	1.04	1.12
1:H:117:ARG:HG2	1:H:117:ARG:HH11	1.14	1.10
1:D:176:ILE:HD12	1:D:388:LEU:HD11	1.34	1.09
1:D:141:VAL:O	1:D:145:TRP:HD1	1.37	1.07
1:H:10:HIS:HB3	1:H:367:ASN:ND2	1.70	1.05
1:F:141:VAL:HG12	1:F:145:TRP:HE1	0.91	1.01
1:G:288:ILE:HD12	1:G:296:LEU:HD12	1.43	1.01
1:H:174:ASP:OD1	1:I:357:ALA:HB2	1.62	0.99
1:D:169:PRO:HG2	1:D:176:ILE:HD13	1.43	0.98
1:F:141:VAL:HG12	1:F:145:TRP:NE1	1.76	0.98
1:F:141:VAL:CG1	1:F:145:TRP:HE1	1.76	0.98
1:L:367:ASN:HD22	1:L:368:GLU:N	1.61	0.97
1:G:288:ILE:CD1	1:G:296:LEU:HD12	1.95	0.97
1:J:367:ASN:HD22	1:J:368:GLU:N	1.64	0.96
1:A:367:ASN:HD22	1:A:368:GLU:N	1.62	0.96
1:I:174:ASP:OD1	1:J:357:ALA:HB2	1.66	0.94
1:K:33:LYS:HE3	1:K:167:SER:HB2	1.51	0.93
1:A:367:ASN:ND2	1:A:368:GLU:H	1.66	0.92
1:B:315:PHE:HA	1:B:379:MET:HE2	1.51	0.92
1:E:390:ARG:O	1:E:394:GLU:HG2	1.70	0.92
1:J:315:PHE:HA	1:J:379:MET:HE2	1.51	0.91
1:A:315:PHE:HA	1:A:379:MET:HE2	1.53	0.91
1:L:315:PHE:HA	1:L:379:MET:HE2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LYS:HE3	1:B:167:SER:HB2	1.52	0.91
1:L:117:ARG:HG2	1:L:117:ARG:NH1	1.82	0.91
1:K:315:PHE:HA	1:K:379:MET:HE1	1.53	0.91
1:I:33:LYS:HE3	1:I:167:SER:HB2	1.54	0.90
1:L:33:LYS:HE3	1:L:167:SER:HB2	1.52	0.90
1:D:33:LYS:HE3	1:D:167:SER:HB2	1.51	0.90
1:K:288:ILE:HD13	1:K:296:LEU:HD12	1.52	0.90
1:L:367:ASN:HD22	1:L:368:GLU:H	1.15	0.90
1:C:33:LYS:HE3	1:C:167:SER:HB2	1.54	0.90
1:J:367:ASN:HD22	1:J:368:GLU:H	1.14	0.90
1:A:33:LYS:HE3	1:A:167:SER:HB2	1.52	0.89
1:J:367:ASN:ND2	1:J:368:GLU:H	1.69	0.89
1:H:33:LYS:HE3	1:H:167:SER:HB2	1.52	0.89
1:B:121:ASN:HD22	1:B:125:GLU:HG3	1.36	0.88
1:F:315:PHE:HA	1:F:379:MET:HE2	1.54	0.88
1:I:315:PHE:HA	1:I:379:MET:HE2	1.56	0.88
1:E:33:LYS:HE3	1:E:167:SER:HB2	1.54	0.86
1:E:315:PHE:HA	1:E:379:MET:HE2	1.57	0.86
1:D:141:VAL:O	1:D:145:TRP:CD1	2.27	0.86
1:L:145:TRP:CZ3	1:L:148:LEU:HD23	2.11	0.86
1:H:315:PHE:HA	1:H:379:MET:HE2	1.58	0.85
1:J:33:LYS:HE3	1:J:167:SER:HB2	1.56	0.85
1:G:33:LYS:HE3	1:G:167:SER:HB2	1.59	0.85
1:C:315:PHE:HA	1:C:379:MET:HE2	1.59	0.84
1:F:33:LYS:HE3	1:F:167:SER:HB2	1.57	0.83
1:G:293:LEU:HD12	1:G:342:ARG:HH11	1.43	0.83
1:G:315:PHE:HA	1:G:379:MET:HE2	1.59	0.83
1:A:58:VAL:HG11	1:A:145:TRP:CZ2	2.14	0.82
1:I:117:ARG:HG2	1:I:117:ARG:HH11	1.44	0.82
1:D:315:PHE:HA	1:D:379:MET:HE2	1.62	0.81
1:F:141:VAL:O	1:F:145:TRP:CD1	2.33	0.81
1:A:121:ASN:HD22	1:A:125:GLU:HB3	1.46	0.81
1:A:288:ILE:HD13	1:A:296:LEU:HD12	1.63	0.81
1:I:260:SER:HB2	1:I:363:PRO:HA	1.64	0.80
1:D:139:GLY:H	2:D:900:GDP:H5"	1.45	0.80
1:H:117:ARG:HH11	1:H:117:ARG:CG	1.94	0.79
1:H:117:ARG:HG2	1:H:117:ARG:NH1	1.92	0.79
1:H:174:ASP:OD1	1:I:357:ALA:CB	2.30	0.79
1:H:10:HIS:HB3	1:H:367:ASN:HD21	1.48	0.77
1:E:103:ASN:H	1:E:103:ASN:HD22	1.31	0.77
1:I:32:GLN:HE22	1:J:264:THR:H	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:HD22	1:B:142:GLY:O	1.86	0.76
1:J:88:THR:HB	1:J:89:PRO:CD	2.15	0.75
1:K:288:ILE:CD1	1:K:296:LEU:HD12	2.15	0.75
1:L:116:GLY:O	1:L:120:THR:OG1	2.02	0.75
1:A:14:THR:HG21	1:A:366:ASP:CG	2.06	0.75
1:A:288:ILE:HD13	1:A:296:LEU:CD1	2.17	0.75
1:I:63:SER:HA	1:I:66:MET:HG2	1.69	0.75
1:K:121:ASN:HB2	1:K:125:GLU:O	1.86	0.75
1:G:288:ILE:HD12	1:G:296:LEU:CD1	2.17	0.74
1:J:103:ASN:ND2	1:J:103:ASN:H	1.83	0.74
1:J:88:THR:HB	1:J:89:PRO:HD3	1.70	0.74
1:E:58:VAL:HG11	1:E:145:TRP:CZ2	2.22	0.73
1:L:328:PRO:HB3	1:L:367:ASN:O	1.88	0.73
1:B:58:VAL:HG11	1:B:145:TRP:CZ2	2.23	0.73
1:I:288:ILE:HD13	1:I:296:LEU:HD12	1.71	0.73
1:L:75:ASP:OD1	1:L:117:ARG:NH2	2.22	0.73
1:C:121:ASN:HB3	1:C:123:GLU:H	1.54	0.72
1:D:176:ILE:HD12	1:D:388:LEU:CD1	2.15	0.72
1:A:262:ASN:O	1:B:36:LYS:NZ	2.21	0.71
1:C:121:ASN:HB2	1:C:125:GLU:H	1.54	0.71
1:K:160:CYS:HB2	1:K:161:PRO:CD	2.21	0.71
1:B:386:ILE:HD11	1:C:410:GLN:NE2	2.06	0.71
1:I:314:GLN:HG2	1:I:383:LYS:HE3	1.73	0.71
1:L:367:ASN:ND2	1:L:368:GLU:H	1.87	0.71
1:D:121:ASN:HB2	1:D:125:GLU:H	1.56	0.70
1:G:121:ASN:HD22	1:G:125:GLU:HB3	1.54	0.70
1:F:217:GLN:O	1:F:221:GLU:HG2	1.92	0.70
1:C:328:PRO:HD3	1:C:370:ALA:HB2	1.72	0.69
1:K:172:ASP:OD2	1:L:357:ALA:HA	1.93	0.69
1:J:334:PHE:HA	1:J:339:THR:HG21	1.74	0.69
1:K:135:LEU:HD22	1:K:142:GLY:O	1.92	0.69
1:I:174:ASP:OD1	1:J:357:ALA:CB	2.39	0.69
1:A:160:CYS:HB2	1:A:161:PRO:CD	2.22	0.69
1:E:344:ARG:HG3	1:E:353:LEU:HD12	1.75	0.69
1:C:328:PRO:HB2	1:C:331:ALA:HB2	1.74	0.68
1:K:62:GLU:HB3	1:K:78:HIS:HB2	1.75	0.68
1:L:160:CYS:HB2	1:L:161:PRO:HD2	1.74	0.68
1:I:135:LEU:HD22	1:I:142:GLY:O	1.93	0.68
1:K:121:ASN:HD22	1:K:123:GLU:HG2	1.58	0.68
1:D:176:ILE:CD1	1:D:388:LEU:HD11	2.18	0.68
1:E:338:ASN:HA	1:E:341:ASN:ND2	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:THR:HG21	1:F:178:ASN:HB3	1.76	0.68
1:G:121:ASN:HB2	1:G:125:GLU:H	1.58	0.68
1:B:121:ASN:HD22	1:B:125:GLU:CG	2.07	0.68
1:K:160:CYS:HB2	1:K:161:PRO:HD2	1.76	0.67
1:A:384:ARG:NH1	1:A:391:GLU:OE2	2.28	0.67
1:A:288:ILE:CD1	1:A:296:LEU:HD12	2.23	0.67
1:E:338:ASN:HA	1:E:341:ASN:HD22	1.59	0.67
1:A:160:CYS:HB2	1:A:161:PRO:HD2	1.77	0.67
1:E:135:LEU:HD22	1:E:142:GLY:O	1.95	0.67
1:I:122:GLU:CD	1:I:122:GLU:H	1.98	0.67
1:D:213:ASN:HD21	2:D:900:GDP:H1'	1.60	0.67
1:K:386:ILE:CG2	1:K:390:ARG:NH1	2.58	0.66
1:L:160:CYS:HB2	1:L:161:PRO:CD	2.25	0.66
1:F:314:GLN:HG2	1:F:383:LYS:HE3	1.76	0.66
1:A:192:GLU:HG2	1:A:195:ARG:HH22	1.61	0.66
1:G:293:LEU:HD12	1:G:342:ARG:NH1	2.11	0.66
1:D:314:GLN:HG2	1:D:383:LYS:HE3	1.77	0.66
1:B:357:ALA:HA	1:C:172:ASP:OD2	1.95	0.66
1:E:160:CYS:HB2	1:E:161:PRO:HD2	1.76	0.66
1:J:314:GLN:HG2	1:J:383:LYS:HE3	1.78	0.66
1:L:315:PHE:HA	1:L:379:MET:CE	2.25	0.65
1:F:10:HIS:HB3	1:F:367:ASN:OD1	1.95	0.65
1:B:160:CYS:HB2	1:B:161:PRO:HD2	1.79	0.65
1:D:160:CYS:HB2	1:D:161:PRO:HD2	1.79	0.65
1:C:58:VAL:HG11	1:C:145:TRP:CZ2	2.32	0.65
1:C:314:GLN:HG2	1:C:383:LYS:HE3	1.78	0.65
1:H:172:ASP:OD2	1:I:357:ALA:HA	1.96	0.65
1:A:367:ASN:HD22	1:A:368:GLU:H	0.81	0.65
1:G:32:GLN:HE22	1:H:264:THR:H	1.44	0.65
1:I:117:ARG:HG2	1:I:117:ARG:NH1	2.12	0.65
1:A:314:GLN:HG2	1:A:383:LYS:HE3	1.79	0.65
1:G:228:ASP:O	1:G:232:ARG:N	2.27	0.64
1:G:233:TYR:HB3	1:H:336:ASP:HB2	1.77	0.64
1:I:138:GLY:O	1:I:175:GLU:HG2	1.96	0.64
1:J:327:ARG:HH11	1:J:364:ILE:HG13	1.62	0.64
1:I:398:LYS:HA	1:I:401:GLN:HE21	1.62	0.64
1:H:14:THR:HG21	1:H:366:ASP:HB2	1.80	0.64
1:K:390:ARG:O	1:K:394:GLU:HG2	1.96	0.64
1:B:160:CYS:HB2	1:B:161:PRO:CD	2.27	0.64
1:E:160:CYS:HB2	1:E:161:PRO:CD	2.27	0.64
1:I:293:LEU:O	1:I:296:LEU:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:160:CYS:HB2	1:J:161:PRO:CD	2.27	0.64
1:G:160:CYS:HB2	1:G:161:PRO:HD2	1.79	0.64
1:K:141:VAL:HG12	1:K:145:TRP:CD1	2.33	0.64
1:I:329:SER:HA	1:I:364:ILE:CG2	2.28	0.64
1:H:121:ASN:HB3	1:H:123:GLU:H	1.62	0.64
1:J:315:PHE:HA	1:J:379:MET:CE	2.26	0.64
1:L:145:TRP:CE3	1:L:148:LEU:HD23	2.33	0.64
1:G:315:PHE:HA	1:G:379:MET:CE	2.28	0.63
1:A:290:LYS:HD2	1:A:295:SER:HB2	1.80	0.63
1:J:103:ASN:H	1:J:103:ASN:HD22	1.44	0.63
1:E:14:THR:HG21	1:E:366:ASP:OD2	1.98	0.63
1:G:314:GLN:HG2	1:G:383:LYS:HE3	1.80	0.63
1:K:103:ASN:OD1	1:K:103:ASN:N	2.31	0.63
1:F:160:CYS:HB2	1:F:161:PRO:HD2	1.81	0.63
1:H:314:GLN:HG2	1:H:383:LYS:HE3	1.81	0.63
1:K:288:ILE:HD13	1:K:296:LEU:CD1	2.27	0.63
1:A:10:HIS:NE2	1:A:366:ASP:OD1	2.32	0.63
1:K:314:GLN:HG2	1:K:383:LYS:HE3	1.80	0.63
1:B:314:GLN:HG2	1:B:383:LYS:HE3	1.79	0.62
1:C:160:CYS:HB2	1:C:161:PRO:CD	2.29	0.62
1:K:62:GLU:HB3	1:K:78:HIS:CG	2.33	0.62
1:J:160:CYS:HB2	1:J:161:PRO:HD2	1.82	0.62
1:L:121:ASN:HB3	1:L:123:GLU:H	1.63	0.62
1:E:121:ASN:HB3	1:E:123:GLU:H	1.63	0.62
1:H:121:ASN:ND2	1:H:125:GLU:HB2	2.15	0.62
1:D:160:CYS:HB2	1:D:161:PRO:CD	2.30	0.61
1:D:367:ASN:HD22	1:D:368:GLU:H	1.48	0.61
1:F:160:CYS:HB2	1:F:161:PRO:CD	2.30	0.61
1:G:160:CYS:HB2	1:G:161:PRO:CD	2.30	0.61
1:K:296:LEU:HD21	1:K:343:ILE:HG13	1.81	0.61
1:G:288:ILE:HD13	1:G:296:LEU:HA	1.82	0.61
1:A:357:ALA:HB2	1:B:174:ASP:OD1	2.01	0.61
1:E:116:GLY:O	1:E:120:THR:OG1	2.15	0.61
1:A:164:MET:HB2	1:A:208:VAL:HG22	1.82	0.61
1:H:67:HIS:CG	1:I:261:ASP:HA	2.35	0.61
1:H:160:CYS:HB2	1:H:161:PRO:HD2	1.82	0.61
1:C:332:ASP:OD1	1:C:332:ASP:N	2.32	0.60
1:I:410:GLN:NE2	1:J:191:ARG:HH11	1.99	0.60
1:L:314:GLN:HG2	1:L:383:LYS:HE3	1.82	0.60
1:B:121:ASN:HB2	1:B:125:GLU:O	2.01	0.60
1:H:160:CYS:HB2	1:H:161:PRO:CD	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ASN:HD22	1:C:237:LYS:H	1.48	0.60
1:A:233:TYR:OH	1:G:122:GLU:HB2	2.01	0.60
1:A:331:ALA:HB1	1:A:334:PHE:HD1	1.65	0.60
1:D:217:GLN:HG2	1:D:236:TRP:CD2	2.37	0.60
1:D:357:ALA:HA	1:E:172:ASP:OD2	2.02	0.60
1:I:410:GLN:HB3	1:J:191:ARG:NH1	2.17	0.60
1:C:160:CYS:HB2	1:C:161:PRO:HD2	1.81	0.60
1:K:33:LYS:HE3	1:K:167:SER:CB	2.30	0.60
1:B:91:VAL:HG12	1:B:91:VAL:O	2.02	0.59
1:B:315:PHE:HA	1:B:379:MET:CE	2.27	0.59
1:C:296:LEU:HD21	1:C:343:ILE:HG13	1.85	0.59
1:E:123:GLU:CD	1:L:342:ARG:HH22	2.06	0.59
1:H:315:PHE:HA	1:H:379:MET:CE	2.32	0.59
1:A:135:LEU:HD22	1:A:142:GLY:O	2.03	0.59
1:A:188:GLU:O	1:A:192:GLU:HG3	2.02	0.59
1:A:293:LEU:HB3	1:A:342:ARG:NH2	2.18	0.59
1:B:412:GLU:O	1:B:414:LYS:N	2.29	0.59
1:I:10:HIS:CE1	1:I:367:ASN:HB2	2.38	0.59
1:L:117:ARG:HH11	1:L:117:ARG:CG	1.95	0.59
1:A:121:ASN:HD22	1:A:125:GLU:CB	2.14	0.58
1:G:111:LEU:CD1	1:G:145:TRP:HH2	2.17	0.58
1:G:119:PHE:O	1:G:127:ILE:HG12	2.04	0.58
1:B:288:ILE:HD13	1:B:296:LEU:HD12	1.85	0.58
1:I:98:PRO:HA	1:I:104:ALA:HB3	1.85	0.58
1:J:338:ASN:HA	1:J:341:ASN:HB2	1.85	0.58
1:B:358:GLY:N	1:C:172:ASP:OD2	2.34	0.58
1:E:314:GLN:HG2	1:E:383:LYS:HE3	1.85	0.58
1:F:288:ILE:HD13	1:F:296:LEU:CD1	2.34	0.58
1:I:160:CYS:HB2	1:I:161:PRO:CD	2.34	0.58
1:B:33:LYS:HE3	1:B:167:SER:CB	2.32	0.58
1:B:405:GLU:O	1:B:409:LYS:HB2	2.04	0.57
1:D:236:TRP:CZ2	1:D:237:LYS:HE3	2.38	0.57
1:I:410:GLN:CD	1:J:191:ARG:HH11	2.07	0.57
1:A:13:SER:HA	1:G:103:ASN:ND2	2.19	0.57
1:G:290:LYS:HB2	1:G:295:SER:OG	2.03	0.57
1:F:404:ALA:O	1:F:408:ARG:HB2	2.04	0.57
1:G:125:GLU:HG2	1:G:126:VAL:H	1.69	0.57
1:H:60:PHE:HZ	1:H:92:VAL:HG22	1.69	0.57
1:I:288:ILE:HD13	1:I:296:LEU:CD1	2.34	0.57
1:C:315:PHE:HA	1:C:379:MET:CE	2.33	0.57
1:I:327:ARG:HH11	1:I:364:ILE:HG12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:315:PHE:HA	1:K:379:MET:CE	2.29	0.57
1:F:315:PHE:HA	1:F:379:MET:CE	2.32	0.57
1:I:160:CYS:HB2	1:I:161:PRO:HD2	1.87	0.57
1:B:386:ILE:HD11	1:C:410:GLN:HE22	1.69	0.57
1:G:58:VAL:HG11	1:G:145:TRP:CZ2	2.39	0.57
1:H:417:ILE:HD11	1:I:390:ARG:NH1	2.20	0.57
1:D:380:THR:HG22	1:D:381:MET:N	2.21	0.56
1:C:228:ASP:O	1:C:232:ARG:HG3	2.06	0.56
1:I:315:PHE:HA	1:I:379:MET:CE	2.32	0.56
1:J:14:THR:HG21	1:J:366:ASP:CG	2.26	0.56
1:A:334:PHE:HA	1:A:339:THR:HG21	1.88	0.56
1:B:338:ASN:H	1:B:338:ASN:HD22	1.51	0.56
1:I:122:GLU:CD	1:I:122:GLU:N	2.58	0.56
1:I:1:MET:HG2	1:I:45:LYS:HB2	1.88	0.56
1:L:145:TRP:HZ3	1:L:148:LEU:HD23	1.68	0.56
1:D:57:ALA:HB1	1:D:65:MET:HE3	1.88	0.56
1:G:125:GLU:HG2	1:G:126:VAL:N	2.21	0.56
1:H:414:LYS:C	1:H:416:ASP:H	2.08	0.56
1:K:94:ASP:HB3	1:K:100:THR:HG21	1.87	0.56
1:D:57:ALA:CB	1:D:65:MET:HE3	2.36	0.56
1:D:315:PHE:HA	1:D:379:MET:CE	2.32	0.56
1:E:177:ASN:O	1:E:181:VAL:HG13	2.05	0.56
1:J:10:HIS:CG	1:J:367:ASN:OD1	2.59	0.56
1:K:121:ASN:CG	1:K:122:GLU:H	2.10	0.56
1:E:380:THR:HG22	1:E:381:MET:N	2.21	0.56
1:F:367:ASN:N	1:F:367:ASN:HD22	2.04	0.55
1:G:61:ALA:O	1:G:64:ASP:HB2	2.06	0.55
1:B:66:MET:HG3	1:B:67:HIS:CD2	2.41	0.55
1:K:59:ASN:HB2	1:K:65:MET:HE3	1.88	0.55
1:L:145:TRP:CZ3	1:L:148:LEU:CD2	2.87	0.55
1:L:120:THR:HA	1:L:125:GLU:O	2.07	0.55
1:C:33:LYS:HE3	1:C:167:SER:CB	2.34	0.55
1:C:228:ASP:CG	1:C:231:ASN:HB2	2.27	0.55
1:C:235:ASN:HB3	1:C:238:GLU:HG3	1.88	0.55
1:C:143:THR:HG21	1:C:178:ASN:HB3	1.87	0.55
1:H:281:LEU:HD12	1:H:377:ALA:HB2	1.89	0.55
1:K:172:ASP:OD2	1:L:358:GLY:N	2.35	0.55
1:C:121:ASN:HD22	1:C:125:GLU:HB3	1.71	0.55
1:H:164:MET:HB2	1:H:208:VAL:HG22	1.88	0.55
1:H:261:ASP:OD1	1:H:335:LYS:HE3	2.06	0.55
1:C:136:GLY:HA2	1:C:167:SER:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:380:THR:HG22	1:J:381:MET:N	2.22	0.55
1:H:57:ALA:HB3	1:H:65:MET:HE1	1.89	0.55
1:I:7:GLU:O	1:I:11:ILE:HG13	2.07	0.54
1:L:380:THR:HG22	1:L:381:MET:N	2.22	0.54
1:B:288:ILE:HD13	1:B:296:LEU:CD1	2.38	0.54
1:B:380:THR:HG22	1:B:381:MET:N	2.22	0.54
1:K:173:PRO:HG2	1:L:357:ALA:HB2	1.89	0.54
1:A:191:ARG:NH1	1:B:410:GLN:HB3	2.22	0.54
1:G:164:MET:HB2	1:G:208:VAL:HG22	1.88	0.54
1:F:176:ILE:HG23	1:F:388:LEU:HG	1.90	0.54
1:F:288:ILE:HD13	1:F:296:LEU:HD12	1.90	0.54
1:G:36:LYS:HD3	1:H:261:ASP:O	2.07	0.54
1:I:409:LYS:O	1:I:413:GLU:HG3	2.08	0.54
1:A:380:THR:HG22	1:A:381:MET:N	2.23	0.54
1:I:327:ARG:O	1:I:365:TRP:HD1	1.90	0.54
1:K:164:MET:HB2	1:K:208:VAL:HG22	1.90	0.54
1:B:66:MET:HG3	1:B:67:HIS:HD2	1.72	0.54
1:C:293:LEU:HB3	1:C:342:ARG:NH2	2.22	0.54
1:G:32:GLN:NE2	1:H:264:THR:H	2.06	0.54
1:G:111:LEU:HD13	1:G:145:TRP:HH2	1.73	0.53
1:L:266:ASP:HB2	1:L:267:PRO:HD2	1.90	0.53
1:I:328:PRO:C	1:I:330:ASN:H	2.12	0.53
1:G:174:ASP:OD1	1:H:357:ALA:HB2	2.09	0.53
1:A:32:GLN:HG2	1:A:36:LYS:HE2	1.90	0.53
1:B:164:MET:HB2	1:B:208:VAL:HG22	1.91	0.53
1:D:33:LYS:HE3	1:D:167:SER:CB	2.32	0.53
1:E:315:PHE:HA	1:E:379:MET:CE	2.33	0.53
1:L:164:MET:HB2	1:L:208:VAL:HG22	1.90	0.53
1:C:235:ASN:ND2	1:C:237:LYS:HG3	2.23	0.53
1:D:164:MET:HB2	1:D:208:VAL:HG22	1.91	0.53
1:H:67:HIS:CD2	1:I:261:ASP:HA	2.43	0.53
1:A:121:ASN:ND2	1:A:125:GLU:HB3	2.21	0.53
1:E:398:LYS:O	1:E:402:LEU:HD12	2.07	0.53
1:K:304:LEU:O	1:K:310:SER:HB3	2.08	0.53
1:G:279:ARG:HB2	1:G:378:GLY:HA2	1.90	0.53
1:B:1:MET:HG3	1:B:3:LEU:HD11	1.90	0.53
1:E:7:GLU:O	1:E:11:ILE:HG13	2.09	0.53
1:G:353:LEU:O	1:G:355:GLU:N	2.42	0.53
1:G:7:GLU:O	1:G:11:ILE:HG13	2.09	0.52
1:L:304:LEU:O	1:L:310:SER:HB3	2.09	0.52
1:B:7:GLU:O	1:B:11:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:ALA:HB3	1:D:65:MET:CE	2.39	0.52
1:K:380:THR:HG22	1:K:381:MET:N	2.24	0.52
1:G:137:ALA:HB3	1:G:167:SER:O	2.09	0.52
1:I:120:THR:HB	1:I:125:GLU:O	2.10	0.52
1:J:281:LEU:HD12	1:J:377:ALA:HB2	1.92	0.52
1:H:57:ALA:HB1	1:H:65:MET:CE	2.40	0.52
1:K:7:GLU:O	1:K:11:ILE:HG13	2.10	0.52
1:K:62:GLU:HB3	1:K:78:HIS:CB	2.38	0.52
1:G:327:ARG:HE	1:G:364:ILE:HG12	1.74	0.52
1:I:327:ARG:HE	1:I:364:ILE:HG12	1.74	0.52
1:K:145:TRP:CE3	1:K:148:LEU:HD23	2.44	0.52
1:F:14:THR:HG21	1:F:366:ASP:HB2	1.91	0.52
1:I:121:ASN:ND2	1:I:125:GLU:HB2	2.24	0.52
1:B:296:LEU:HD21	1:B:343:ILE:HG13	1.91	0.52
1:F:340:GLU:O	1:F:344:ARG:HB3	2.09	0.52
1:H:266:ASP:HB2	1:H:267:PRO:HD2	1.92	0.52
1:J:288:ILE:HD11	1:J:296:LEU:HD12	1.92	0.52
1:A:7:GLU:O	1:A:11:ILE:HG13	2.10	0.52
1:H:7:GLU:O	1:H:11:ILE:HG13	2.09	0.52
1:K:145:TRP:CZ3	1:K:148:LEU:HD23	2.45	0.52
1:A:191:ARG:HH11	1:B:410:GLN:HB3	1.74	0.52
1:H:172:ASP:OD2	1:I:356:ILE:O	2.28	0.52
1:H:172:ASP:HB3	1:H:175:GLU:HB2	1.92	0.52
1:L:30:ALA:HB1	1:L:145:TRP:CD1	2.45	0.51
1:E:33:LYS:HE3	1:E:167:SER:CB	2.34	0.51
1:G:326:LEU:HG	1:G:365:TRP:CD1	2.45	0.51
1:J:304:LEU:O	1:J:310:SER:HB3	2.10	0.51
1:A:136:GLY:HA2	1:A:167:SER:HB3	1.92	0.51
1:B:335:LYS:O	1:C:233:TYR:HA	2.10	0.51
1:C:380:THR:HG22	1:C:381:MET:N	2.25	0.51
1:E:172:ASP:HB3	1:E:175:GLU:HB2	1.91	0.51
1:I:329:SER:HA	1:I:364:ILE:HG21	1.91	0.51
1:B:407:GLN:O	1:B:411:ASP:HB2	2.11	0.51
1:I:32:GLN:HE22	1:J:264:THR:N	2.04	0.51
1:D:266:ASP:HB2	1:D:267:PRO:HD2	1.93	0.51
1:G:172:ASP:HB3	1:G:175:GLU:HB2	1.92	0.51
1:D:292:ASP:O	1:D:294:HIS:N	2.43	0.51
1:H:57:ALA:CB	1:H:65:MET:CE	2.89	0.51
1:I:88:THR:HG1	1:I:90:SER:HG	1.59	0.51
1:J:33:LYS:HE3	1:J:167:SER:CB	2.37	0.51
1:K:171:GLY:HA2	1:K:176:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLN:HG3	1:B:36:LYS:HE2	1.91	0.51
1:F:172:ASP:HB3	1:F:175:GLU:HB2	1.93	0.51
1:J:367:ASN:ND2	1:J:368:GLU:N	2.36	0.51
1:D:39:ASP:HB2	1:D:68:LEU:HD22	1.93	0.51
1:E:279:ARG:HB2	1:E:378:GLY:HA2	1.93	0.51
1:I:384:ARG:O	1:I:388:LEU:HB2	2.11	0.51
1:B:217:GLN:HG2	1:B:236:TRP:CD2	2.46	0.51
1:J:288:ILE:CD1	1:J:296:LEU:HD12	2.40	0.51
1:K:121:ASN:HB2	1:K:125:GLU:HB2	1.93	0.51
1:E:288:ILE:HD13	1:E:296:LEU:HD12	1.93	0.51
1:F:164:MET:HB2	1:F:208:VAL:HG22	1.92	0.51
1:F:341:ASN:O	1:F:345:ASN:N	2.43	0.51
1:F:380:THR:HG22	1:F:381:MET:N	2.26	0.51
1:K:290:LYS:HG3	1:K:292:ASP:OD2	2.11	0.51
1:L:324:PHE:HB2	1:L:363:PRO:HD2	1.92	0.50
1:D:401:GLN:O	1:D:404:ALA:HB3	2.11	0.50
1:K:386:ILE:HG22	1:K:390:ARG:NH1	2.26	0.50
1:B:283:ILE:O	1:B:309:PHE:HB2	2.12	0.50
1:B:338:ASN:H	1:B:338:ASN:ND2	2.10	0.50
1:C:164:MET:HB2	1:C:208:VAL:HG22	1.92	0.50
1:I:408:ARG:O	1:I:412:GLU:HG2	2.11	0.50
1:C:281:LEU:HD12	1:C:377:ALA:HB2	1.92	0.50
1:F:304:LEU:O	1:F:310:SER:HB3	2.11	0.50
1:C:172:ASP:HB3	1:C:175:GLU:HB2	1.93	0.50
1:C:304:LEU:O	1:C:310:SER:HB3	2.12	0.50
1:F:33:LYS:HE3	1:F:167:SER:CB	2.37	0.50
1:G:293:LEU:N	1:G:333:PHE:HZ	2.10	0.50
1:K:141:VAL:CG1	1:K:145:TRP:CD1	2.95	0.50
1:B:32:GLN:HB3	2:B:900:GDP:O2A	2.12	0.49
1:G:203:LYS:HD3	1:G:276:ILE:O	2.12	0.49
1:I:281:LEU:HD12	1:I:377:ALA:HB2	1.94	0.49
1:I:342:ARG:NH2	1:I:342:ARG:HB2	2.27	0.49
1:J:88:THR:C	1:J:140:GLY:HA2	2.33	0.49
1:B:348:GLY:HA2	1:B:352:ARG:HA	1.94	0.49
1:C:408:ARG:O	1:C:411:ASP:HB2	2.12	0.49
1:B:172:ASP:HB3	1:B:175:GLU:HB2	1.94	0.49
1:C:235:ASN:HD22	1:C:237:LYS:N	2.10	0.49
1:D:7:GLU:O	1:D:11:ILE:HG13	2.12	0.49
1:G:343:ILE:O	1:G:347:LEU:HG	2.13	0.49
1:G:352:ARG:NH2	1:G:352:ARG:HB3	2.27	0.49
1:J:380:THR:CG2	1:J:381:MET:N	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:SER:HA	1:G:103:ASN:HD22	1.77	0.49
1:C:332:ASP:HA	1:C:335:LYS:HE2	1.94	0.49
1:I:172:ASP:HB3	1:I:175:GLU:HB2	1.94	0.49
1:L:283:ILE:O	1:L:309:PHE:HB2	2.12	0.49
1:E:283:ILE:O	1:E:309:PHE:HB2	2.12	0.49
1:A:304:LEU:O	1:A:310:SER:HB3	2.13	0.49
1:D:203:LYS:HD3	1:D:276:ILE:O	2.13	0.49
1:E:262:ASN:HB3	1:E:362:ASP:OD2	2.12	0.49
1:L:172:ASP:HB3	1:L:175:GLU:HB2	1.95	0.49
1:D:58:VAL:HG11	1:D:145:TRP:CH2	2.48	0.49
1:G:304:LEU:O	1:G:310:SER:HB3	2.13	0.49
1:I:304:LEU:O	1:I:310:SER:HB3	2.12	0.49
1:J:164:MET:HB2	1:J:208:VAL:HG22	1.95	0.49
1:D:281:LEU:HD12	1:D:377:ALA:HB2	1.94	0.49
1:J:58:VAL:HG11	1:J:145:TRP:CZ2	2.48	0.49
1:K:279:ARG:HB2	1:K:378:GLY:HA2	1.95	0.49
1:H:327:ARG:HH22	1:H:335:LYS:CD	2.26	0.48
1:K:172:ASP:HB3	1:K:175:GLU:HB2	1.95	0.48
1:L:281:LEU:HD12	1:L:377:ALA:HB2	1.95	0.48
1:D:400:GLU:O	1:D:403:ARG:HB3	2.13	0.48
1:F:328:PRO:HG3	1:F:367:ASN:O	2.12	0.48
1:G:26:GLY:HA3	1:G:119:PHE:HE2	1.77	0.48
1:I:33:LYS:HE3	1:I:167:SER:CB	2.35	0.48
1:A:266:ASP:HB2	1:A:267:PRO:HD2	1.95	0.48
1:E:326:LEU:HG	1:E:365:TRP:CD1	2.48	0.48
1:H:192:GLU:OE2	1:H:195:ARG:NH2	2.41	0.48
1:H:304:LEU:O	1:H:310:SER:HB3	2.12	0.48
1:H:380:THR:HG22	1:H:381:MET:N	2.28	0.48
1:A:183:LEU:HB3	1:A:381:MET:HE1	1.94	0.48
1:A:192:GLU:HG2	1:A:195:ARG:NH2	2.28	0.48
1:G:283:ILE:O	1:G:309:PHE:HB2	2.13	0.48
1:G:354:ASP:OD1	1:G:355:GLU:HG3	2.13	0.48
1:G:391:GLU:O	1:G:395:LEU:HG	2.12	0.48
1:I:80:ASP:HB2	1:I:107:TYR:OH	2.14	0.48
1:A:337:VAL:O	1:A:341:ASN:HB2	2.14	0.48
1:F:283:ILE:O	1:F:309:PHE:HB2	2.14	0.48
1:F:221:GLU:OE1	1:F:221:GLU:HA	2.13	0.48
1:I:121:ASN:HB3	1:I:123:GLU:H	1.79	0.48
1:I:380:THR:HG22	1:I:381:MET:N	2.28	0.48
1:E:380:THR:CG2	1:E:381:MET:N	2.76	0.48
1:H:206:ALA:HB1	1:H:274:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:266:ASP:HB2	1:I:267:PRO:HD2	1.94	0.48
1:L:92:VAL:HG21	1:L:141:VAL:HA	1.94	0.48
1:A:136:GLY:O	2:A:900:GDP:H5"	2.14	0.48
1:B:409:LYS:O	1:B:413:GLU:HB2	2.13	0.48
1:H:57:ALA:CB	1:H:65:MET:HE1	2.44	0.48
1:K:293:LEU:O	1:K:296:LEU:HB3	2.13	0.48
1:H:414:LYS:C	1:H:416:ASP:N	2.66	0.48
1:K:176:ILE:HG23	1:K:388:LEU:HG	1.96	0.48
1:K:384:ARG:O	1:K:388:LEU:HB2	2.14	0.48
1:A:116:GLY:HA2	1:A:120:THR:HG23	1.96	0.47
1:B:297:GLU:HG2	1:B:298:ASN:HD22	1.78	0.47
1:C:283:ILE:O	1:C:309:PHE:HB2	2.14	0.47
1:D:142:GLY:O	1:D:145:TRP:N	2.47	0.47
1:J:7:GLU:O	1:J:11:ILE:HG13	2.14	0.47
1:J:333:PHE:O	1:J:339:THR:OG1	2.24	0.47
1:A:122:GLU:C	1:A:124:GLY:H	2.16	0.47
1:E:164:MET:HB2	1:E:208:VAL:HG22	1.95	0.47
1:G:380:THR:HG22	1:G:381:MET:N	2.29	0.47
1:I:420:ALA:HB2	1:J:177:ASN:HD22	1.79	0.47
1:L:217:GLN:HG2	1:L:236:TRP:CD2	2.49	0.47
1:D:212:ASP:O	1:D:216:MET:HG3	2.13	0.47
1:E:266:ASP:HB2	1:E:267:PRO:HD2	1.95	0.47
1:E:304:LEU:O	1:E:310:SER:HB3	2.14	0.47
1:G:206:ALA:HB1	1:G:274:LEU:O	2.14	0.47
1:A:63:SER:HA	1:A:66:MET:CE	2.44	0.47
1:B:136:GLY:HA2	1:B:167:SER:HB3	1.96	0.47
1:D:380:THR:CG2	1:D:381:MET:N	2.77	0.47
1:H:33:LYS:HE3	1:H:167:SER:CB	2.36	0.47
1:D:136:GLY:HA3	2:D:900:GDP:H5'	1.96	0.47
1:F:183:LEU:HB3	1:F:381:MET:HE1	1.97	0.47
1:L:380:THR:CG2	1:L:381:MET:N	2.77	0.47
1:A:380:THR:CG2	1:A:381:MET:N	2.77	0.47
1:F:7:GLU:O	1:F:11:ILE:HG13	2.15	0.47
1:F:62:GLU:HG3	1:F:78:HIS:HB2	1.96	0.47
1:J:103:ASN:ND2	1:J:103:ASN:N	2.58	0.47
1:J:293:LEU:HD23	1:J:333:PHE:HE1	1.78	0.47
1:K:281:LEU:HD12	1:K:377:ALA:HB2	1.97	0.47
1:L:7:GLU:O	1:L:11:ILE:HG13	2.15	0.47
1:A:92:VAL:O	1:A:96:PHE:HD1	1.98	0.47
1:C:138:GLY:N	1:C:143:THR:OG1	2.39	0.47
1:C:399:GLN:HE21	1:C:403:ARG:HH11	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:ALA:CB	1:D:65:MET:CE	2.93	0.47
1:G:402:LEU:HA	1:G:405:GLU:HB3	1.97	0.47
1:I:342:ARG:HB2	1:I:342:ARG:HH21	1.80	0.47
1:J:260:SER:HB2	1:J:363:PRO:HA	1.97	0.47
1:K:2:VAL:HG21	1:K:43:GLY:HA3	1.96	0.47
1:L:318:ALA:HB2	1:L:379:MET:HE3	1.97	0.47
1:A:33:LYS:HE3	1:A:167:SER:CB	2.35	0.47
1:C:288:ILE:HD13	1:C:296:LEU:HD12	1.96	0.47
1:C:324:PHE:HB2	1:C:363:PRO:HD2	1.97	0.47
1:H:402:LEU:HA	1:H:405:GLU:HG3	1.97	0.47
1:J:103:ASN:HD22	1:J:103:ASN:N	2.11	0.47
1:B:250:GLU:OE2	1:B:373:TYR:OH	2.27	0.47
1:F:88:THR:N	1:F:140:GLY:HA2	2.29	0.47
1:B:57:ALA:CB	1:B:65:MET:CE	2.92	0.46
1:G:281:LEU:HD12	1:G:377:ALA:HB2	1.97	0.46
1:G:353:LEU:C	1:G:355:GLU:H	2.19	0.46
1:I:236:TRP:HB3	1:J:337:VAL:HG23	1.97	0.46
1:J:90:SER:O	1:J:94:ASP:HB2	2.15	0.46
1:K:177:ASN:ND2	1:K:177:ASN:O	2.48	0.46
1:L:367:ASN:ND2	1:L:368:GLU:N	2.44	0.46
1:C:145:TRP:CE3	1:C:148:LEU:HD23	2.50	0.46
1:L:55:THR:H	1:L:118:LYS:HE2	1.80	0.46
1:L:141:VAL:HG12	1:L:145:TRP:CD1	2.50	0.46
1:A:122:GLU:O	1:A:124:GLY:N	2.49	0.46
1:B:380:THR:CG2	1:B:381:MET:N	2.79	0.46
1:C:183:LEU:HD13	1:C:381:MET:HE1	1.97	0.46
1:D:352:ARG:CZ	1:D:352:ARG:HB3	2.45	0.46
1:H:279:ARG:HB2	1:H:378:GLY:HA2	1.97	0.46
1:K:380:THR:CG2	1:K:381:MET:N	2.78	0.46
1:L:293:LEU:O	1:L:296:LEU:HB3	2.16	0.46
1:A:291:PHE:CE2	1:A:334:PHE:HE1	2.33	0.46
1:B:281:LEU:HD12	1:B:377:ALA:HB2	1.98	0.46
1:D:120:THR:HB	1:D:124:GLY:HA2	1.98	0.46
1:D:283:ILE:O	1:D:309:PHE:HB2	2.15	0.46
1:E:326:LEU:HG	1:E:365:TRP:CG	2.50	0.46
1:F:380:THR:CG2	1:F:381:MET:N	2.79	0.46
1:H:395:LEU:HD11	1:I:355:GLU:HA	1.97	0.46
1:J:10:HIS:NE2	1:J:367:ASN:HB2	2.30	0.46
1:A:91:VAL:O	1:A:95:LEU:HG	2.16	0.46
1:A:206:ALA:HB1	1:A:274:LEU:O	2.15	0.46
1:E:405:GLU:OE1	1:E:408:ARG:NH2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:GLN:NE2	1:J:264:THR:H	2.06	0.46
1:I:58:VAL:HG11	1:I:145:TRP:CH2	2.50	0.46
1:A:315:PHE:HA	1:A:379:MET:CE	2.35	0.46
1:D:292:ASP:C	1:D:294:HIS:H	2.19	0.46
1:D:304:LEU:O	1:D:310:SER:HB3	2.15	0.46
1:F:89:PRO:HB3	1:F:143:THR:CG2	2.45	0.46
1:H:384:ARG:O	1:H:388:LEU:HB2	2.16	0.46
1:L:177:ASN:O	1:L:181:VAL:HG13	2.16	0.46
1:A:172:ASP:O	1:A:176:ILE:HD12	2.15	0.46
1:B:192:GLU:HA	1:B:195:ARG:NH2	2.31	0.46
1:B:304:LEU:O	1:B:310:SER:HB3	2.14	0.46
1:E:384:ARG:O	1:E:388:LEU:HB2	2.16	0.46
1:F:135:LEU:CD2	1:F:145:TRP:HB2	2.46	0.46
1:F:266:ASP:HB2	1:F:267:PRO:HD2	1.96	0.46
1:L:33:LYS:HE3	1:L:167:SER:CB	2.35	0.46
1:L:292:ASP:O	1:L:293:LEU:C	2.54	0.46
1:A:281:LEU:HD12	1:A:377:ALA:HB2	1.98	0.46
1:B:121:ASN:HB3	1:B:124:GLY:H	1.81	0.46
1:F:206:ALA:HB1	1:F:274:LEU:O	2.16	0.46
1:F:352:ARG:HB3	1:F:352:ARG:NH2	2.31	0.46
1:H:415:VAL:HG12	1:H:415:VAL:O	2.15	0.46
1:I:283:ILE:O	1:I:309:PHE:HB2	2.16	0.46
1:C:409:LYS:O	1:C:413:GLU:HG2	2.16	0.46
1:H:176:ILE:HG23	1:H:388:LEU:HG	1.98	0.46
1:J:283:ILE:O	1:J:309:PHE:HB2	2.15	0.46
1:J:328:PRO:HB3	1:J:367:ASN:O	2.16	0.46
1:K:138:GLY:O	1:K:175:GLU:HG2	2.16	0.46
1:L:265:TYR:HB2	1:L:361:GLY:HA3	1.97	0.46
1:A:279:ARG:HB2	1:A:378:GLY:HA2	1.98	0.46
1:H:353:LEU:C	1:H:355:GLU:H	2.19	0.46
1:D:172:ASP:HB3	1:D:175:GLU:HB2	1.98	0.45
1:E:103:ASN:HD22	1:E:103:ASN:N	2.06	0.45
1:J:39:ASP:HB2	1:J:68:LEU:HD22	1.98	0.45
1:A:290:LYS:CD	1:A:295:SER:HB2	2.45	0.45
1:F:30:ALA:HB1	1:F:145:TRP:CD1	2.52	0.45
1:F:281:LEU:HD12	1:F:377:ALA:HB2	1.98	0.45
1:G:138:GLY:O	1:G:175:GLU:HG2	2.17	0.45
1:I:328:PRO:HA	1:I:365:TRP:O	2.16	0.45
1:K:121:ASN:CB	1:K:125:GLU:HB2	2.46	0.45
1:K:288:ILE:CD1	1:K:296:LEU:CD1	2.91	0.45
1:B:266:ASP:HB2	1:B:267:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:LEU:HD22	1:G:142:GLY:O	2.17	0.45
1:J:65:MET:HB3	1:J:68:LEU:HD12	1.97	0.45
1:K:283:ILE:O	1:K:309:PHE:HB2	2.16	0.45
1:A:283:ILE:O	1:A:309:PHE:HB2	2.16	0.45
1:F:90:SER:C	1:F:92:VAL:H	2.20	0.45
1:H:279:ARG:HH12	1:H:319:THR:HG21	1.82	0.45
1:H:327:ARG:HH22	1:H:335:LYS:HD2	1.81	0.45
1:I:57:ALA:CB	1:I:65:MET:HE1	2.47	0.45
1:J:384:ARG:O	1:J:388:LEU:HB2	2.16	0.45
1:A:260:SER:HA	1:A:364:ILE:HD12	1.99	0.45
1:G:266:ASP:HB2	1:G:267:PRO:HD2	1.98	0.45
1:H:217:GLN:HG2	1:H:236:TRP:CD2	2.52	0.45
1:I:164:MET:HB2	1:I:208:VAL:HG22	1.98	0.45
1:L:78:HIS:CG	1:L:79:PHE:N	2.84	0.45
1:A:192:GLU:HA	1:A:195:ARG:NH2	2.32	0.45
1:B:106:GLY:O	1:B:109:ASP:HB2	2.16	0.45
1:B:121:ASN:N	1:B:125:GLU:O	2.50	0.45
1:F:384:ARG:O	1:F:388:LEU:HB2	2.17	0.45
1:I:57:ALA:HB3	1:I:65:MET:HE1	1.99	0.45
1:J:266:ASP:HB2	1:J:267:PRO:HD2	1.99	0.45
1:K:265:TYR:HB2	1:K:361:GLY:HA3	1.98	0.45
1:L:293:LEU:HD13	1:L:342:ARG:NH2	2.32	0.45
1:A:388:LEU:O	1:A:391:GLU:HB2	2.17	0.45
1:F:279:ARG:HB2	1:F:378:GLY:HA2	1.98	0.45
1:C:206:ALA:HB1	1:C:274:LEU:O	2.16	0.45
1:C:235:ASN:ND2	1:C:237:LYS:H	2.13	0.45
1:G:294:HIS:O	1:G:297:GLU:HB3	2.16	0.45
1:J:172:ASP:HB3	1:J:175:GLU:HB2	1.99	0.45
1:A:89:PRO:HG3	1:A:143:THR:HB	1.98	0.45
1:C:333:PHE:O	1:C:339:THR:OG1	2.12	0.45
1:D:158:PHE:HA	1:D:159:PRO:HD3	1.89	0.45
1:D:384:ARG:O	1:D:388:LEU:HB2	2.16	0.45
1:J:279:ARG:HB2	1:J:378:GLY:HA2	1.99	0.45
1:A:260:SER:HB2	1:A:363:PRO:HA	1.99	0.45
1:B:386:ILE:CD1	1:C:410:GLN:HE22	2.30	0.45
1:G:62:GLU:C	1:G:64:ASP:H	2.20	0.45
1:J:390:ARG:HG2	1:J:394:GLU:OE2	2.17	0.45
1:K:326:LEU:CD1	1:K:363:PRO:HB2	2.47	0.45
1:D:191:ARG:NH1	1:E:411:ASP:OD1	2.50	0.44
1:D:367:ASN:ND2	1:D:368:GLU:H	2.12	0.44
1:E:192:GLU:HA	1:E:195:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:ASN:H	1:F:103:ASN:ND2	2.15	0.44
1:A:338:ASN:HD22	1:A:338:ASN:H	1.64	0.44
1:E:291:PHE:CE1	1:E:334:PHE:HE1	2.35	0.44
1:C:279:ARG:HH12	1:C:319:THR:HG21	1.82	0.44
1:H:175:GLU:HA	1:H:178:ASN:HD22	1.82	0.44
1:A:101:ASN:HB3	1:A:104:ALA:HB2	1.99	0.44
1:B:326:LEU:CD1	1:B:363:PRO:HB2	2.47	0.44
1:I:380:THR:CG2	1:I:381:MET:N	2.81	0.44
1:K:206:ALA:HB1	1:K:274:LEU:O	2.17	0.44
1:L:387:SER:O	1:L:390:ARG:HB3	2.18	0.44
1:L:176:ILE:HG23	1:L:388:LEU:HG	2.00	0.44
1:A:87:ARG:O	1:A:87:ARG:HG2	2.18	0.44
1:A:384:ARG:O	1:A:388:LEU:HB2	2.16	0.44
1:D:236:TRP:CE2	1:D:237:LYS:HG2	2.52	0.44
1:H:235:ASN:OD1	1:H:237:LYS:HB2	2.17	0.44
1:K:173:PRO:HD2	1:L:357:ALA:HA	1.99	0.44
1:L:145:TRP:O	1:L:149:VAL:HG23	2.18	0.44
1:C:7:GLU:O	1:C:11:ILE:HG13	2.17	0.44
1:K:123:GLU:HB2	1:K:124:GLY:H	1.41	0.44
1:K:217:GLN:HG2	1:K:236:TRP:CE3	2.52	0.44
1:I:250:GLU:OE2	1:I:373:TYR:OH	2.24	0.44
1:J:387:SER:O	1:J:391:GLU:HB2	2.18	0.44
1:G:217:GLN:O	1:G:221:GLU:HG3	2.18	0.44
1:K:58:VAL:CA	1:K:65:MET:HE1	2.48	0.44
1:K:141:VAL:O	1:K:145:TRP:HD1	2.01	0.44
1:K:266:ASP:HB2	1:K:267:PRO:HD2	1.99	0.44
1:B:279:ARG:NH2	1:C:403:ARG:CZ	2.81	0.43
1:C:63:SER:C	1:C:65:MET:H	2.21	0.43
1:K:217:GLN:O	1:K:221:GLU:HG3	2.18	0.43
1:A:328:PRO:HA	1:A:365:TRP:O	2.18	0.43
1:C:380:THR:CG2	1:C:381:MET:N	2.80	0.43
1:F:291:PHE:N	1:F:291:PHE:CD2	2.86	0.43
1:A:172:ASP:HB3	1:A:175:GLU:HB2	2.01	0.43
1:E:203:LYS:HD3	1:E:276:ILE:O	2.18	0.43
1:G:66:MET:HG3	1:G:67:HIS:CD2	2.53	0.43
1:H:192:GLU:HA	1:H:195:ARG:NH2	2.33	0.43
1:I:14:THR:HG21	1:I:366:ASP:OD2	2.18	0.43
1:I:158:PHE:HA	1:I:159:PRO:HD3	1.90	0.43
1:I:206:ALA:HB1	1:I:274:LEU:O	2.17	0.43
1:J:407:GLN:O	1:J:408:ARG:C	2.56	0.43
1:A:111:LEU:HD11	1:A:145:TRP:HH2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:GLU:O	1:A:395:LEU:HG	2.18	0.43
1:B:221:GLU:HA	1:B:221:GLU:OE1	2.18	0.43
1:C:266:ASP:HB2	1:C:267:PRO:HD2	2.00	0.43
1:A:352:ARG:NH1	1:A:354:ASP:HB2	2.34	0.43
1:K:141:VAL:O	1:K:145:TRP:HB2	2.18	0.43
1:A:59:ASN:ND2	1:A:64:ASP:HB2	2.34	0.43
1:D:357:ALA:CB	1:E:174:ASP:OD1	2.66	0.43
1:E:158:PHE:HA	1:E:159:PRO:HD3	1.92	0.43
1:I:121:ASN:HB3	1:I:123:GLU:N	2.33	0.43
1:A:290:LYS:H	1:A:290:LYS:HG2	1.60	0.43
1:C:121:ASN:ND2	1:C:125:GLU:HB3	2.33	0.43
1:C:203:LYS:HD3	1:C:276:ILE:O	2.19	0.43
1:C:391:GLU:O	1:C:395:LEU:HG	2.19	0.43
1:G:384:ARG:O	1:G:388:LEU:HB2	2.18	0.43
1:H:67:HIS:CD2	1:I:260:SER:O	2.72	0.43
1:J:28:ILE:O	1:J:133:ILE:HA	2.18	0.43
1:J:183:LEU:HB3	1:J:381:MET:HE1	1.99	0.43
1:L:206:ALA:HB1	1:L:274:LEU:O	2.19	0.43
1:A:95:LEU:HD22	1:A:101:ASN:HD22	1.83	0.43
1:D:176:ILE:HG23	1:D:388:LEU:HG	2.01	0.43
1:D:206:ALA:HB1	1:D:274:LEU:O	2.19	0.43
1:G:121:ASN:ND2	1:G:125:GLU:HB3	2.28	0.43
1:G:291:PHE:HD2	1:G:333:PHE:CD2	2.37	0.43
1:I:39:ASP:HB2	1:I:68:LEU:HD22	2.00	0.43
1:J:141:VAL:O	1:J:145:TRP:HD1	2.02	0.43
1:J:192:GLU:HA	1:J:195:ARG:NH2	2.34	0.43
1:A:389:ALA:O	1:A:392:GLY:N	2.52	0.43
1:D:279:ARG:HB2	1:D:378:GLY:HA2	2.01	0.43
1:E:123:GLU:O	1:L:338:ASN:ND2	2.52	0.43
1:E:318:ALA:HB2	1:E:379:MET:HE3	2.00	0.43
1:B:28:ILE:O	1:B:133:ILE:HA	2.19	0.43
1:F:178:ASN:O	1:F:179:ALA:C	2.57	0.43
1:L:384:ARG:O	1:L:388:LEU:HB2	2.19	0.43
1:A:326:LEU:HG	1:A:365:TRP:CD1	2.54	0.42
1:E:143:THR:O	1:E:146:GLY:N	2.52	0.42
1:H:283:ILE:O	1:H:309:PHE:HB2	2.19	0.42
1:C:192:GLU:HA	1:C:195:ARG:NH2	2.34	0.42
1:G:121:ASN:HB3	1:G:123:GLU:HG3	2.01	0.42
1:H:380:THR:CG2	1:H:381:MET:N	2.82	0.42
1:L:117:ARG:NH1	1:L:117:ARG:CG	2.65	0.42
1:L:342:ARG:HA	1:L:342:ARG:HD3	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLY:HA2	1:A:176:ILE:HD11	2.00	0.42
1:A:203:LYS:HD3	1:A:276:ILE:O	2.19	0.42
1:E:398:LYS:HG2	1:E:402:LEU:HD12	2.01	0.42
1:H:390:ARG:O	1:H:394:GLU:HG2	2.19	0.42
1:I:333:PHE:C	1:I:335:LYS:H	2.22	0.42
1:L:136:GLY:HA3	2:L:900:GDP:H5"	2.00	0.42
1:A:263:VAL:HG12	1:A:361:GLY:HA2	2.01	0.42
1:A:353:LEU:HA	1:A:353:LEU:HD23	1.79	0.42
1:F:138:GLY:N	1:F:143:THR:OG1	2.44	0.42
1:G:111:LEU:HD11	1:G:145:TRP:HH2	1.85	0.42
1:G:362:ASP:N	1:G:363:PRO:CD	2.82	0.42
1:J:293:LEU:HD23	1:J:333:PHE:CE1	2.54	0.42
1:K:58:VAL:C	1:K:65:MET:HE1	2.39	0.42
1:L:362:ASP:N	1:L:363:PRO:CD	2.82	0.42
1:B:326:LEU:HD12	1:B:363:PRO:HB2	2.01	0.42
1:C:121:ASN:C	1:C:123:GLU:N	2.73	0.42
1:G:36:LYS:NZ	1:H:262:ASN:O	2.40	0.42
1:H:2:VAL:HG23	1:H:43:GLY:HA3	2.01	0.42
1:A:261:ASP:O	1:B:36:LYS:HD3	2.19	0.42
1:C:176:ILE:O	1:C:180:LEU:HG	2.20	0.42
1:D:300:ILE:HD11	1:D:343:ILE:HD13	2.01	0.42
1:E:206:ALA:HB1	1:E:274:LEU:O	2.20	0.42
1:F:30:ALA:HB1	1:F:145:TRP:CG	2.55	0.42
1:F:203:LYS:HD3	1:F:276:ILE:O	2.19	0.42
1:H:28:ILE:O	1:H:133:ILE:HA	2.19	0.42
1:K:68:LEU:HD13	1:K:71:ILE:HD12	2.02	0.42
1:B:279:ARG:HH12	1:B:319:THR:HG21	1.84	0.42
1:C:177:ASN:O	1:C:181:VAL:HG13	2.20	0.42
1:E:62:GLU:C	1:E:64:ASP:H	2.23	0.42
1:E:342:ARG:HA	1:E:342:ARG:HD3	1.92	0.42
1:F:91:VAL:O	1:F:91:VAL:HG12	2.18	0.42
1:F:327:ARG:NH1	1:F:364:ILE:HD11	2.34	0.42
1:G:395:LEU:O	1:G:399:GLN:HG2	2.19	0.42
1:I:342:ARG:HH21	1:I:342:ARG:CB	2.32	0.42
1:A:279:ARG:HH12	1:A:319:THR:HG21	1.84	0.42
1:D:358:GLY:N	1:E:172:ASP:OD2	2.53	0.42
1:J:88:THR:CB	1:J:89:PRO:HD3	2.46	0.42
1:J:102:PRO:HB2	1:J:103:ASN:HD22	1.85	0.42
1:K:121:ASN:CG	1:K:122:GLU:N	2.72	0.42
1:L:138:GLY:HA2	1:L:175:GLU:O	2.20	0.42
1:A:217:GLN:HG2	1:A:236:TRP:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:327:ARG:HG3	1:F:363:PRO:O	2.19	0.42
1:H:171:GLY:O	1:I:354:ASP:O	2.37	0.42
1:J:291:PHE:HB3	1:J:333:PHE:CD2	2.54	0.42
1:L:30:ALA:HB1	1:L:145:TRP:CG	2.55	0.42
1:C:121:ASN:C	1:C:123:GLU:H	2.23	0.42
1:D:88:THR:HA	1:D:89:PRO:HD3	1.74	0.42
1:F:291:PHE:CE1	1:F:334:PHE:CE1	3.08	0.42
1:F:299:SER:HB3	1:F:302:ARG:NH2	2.35	0.42
1:I:237:LYS:HD3	2:I:900:GDP:C5	2.55	0.42
1:J:341:ASN:O	1:J:345:ASN:CG	2.57	0.42
1:K:31:GLY:O	1:K:32:GLN:C	2.58	0.42
1:K:124:GLY:O	1:K:126:VAL:N	2.53	0.42
1:L:55:THR:N	1:L:118:LYS:HE2	2.35	0.42
1:L:59:ASN:HB2	1:L:65:MET:HE3	2.02	0.42
1:B:318:ALA:HB2	1:B:379:MET:HE3	2.01	0.41
1:C:28:ILE:O	1:C:133:ILE:HA	2.20	0.41
1:C:158:PHE:HA	1:C:159:PRO:HD3	1.89	0.41
1:C:384:ARG:O	1:C:388:LEU:HB2	2.20	0.41
1:G:148:LEU:O	1:G:152:LEU:HG	2.20	0.41
1:G:367:ASN:HD22	1:G:368:GLU:H	1.68	0.41
1:G:380:THR:CG2	1:G:381:MET:N	2.83	0.41
1:I:332:ASP:HA	1:I:335:LYS:HB2	2.01	0.41
1:L:283:ILE:HA	1:L:374:THR:O	2.20	0.41
1:D:328:PRO:HB3	1:D:367:ASN:O	2.20	0.41
1:G:28:ILE:O	1:G:133:ILE:HA	2.20	0.41
1:G:384:ARG:NH1	1:G:391:GLU:OE1	2.48	0.41
1:K:174:ASP:CG	1:L:272:LYS:HZ1	2.21	0.41
1:L:279:ARG:HB2	1:L:378:GLY:HA2	2.01	0.41
1:E:28:ILE:O	1:E:133:ILE:HA	2.20	0.41
1:E:288:ILE:CD1	1:E:296:LEU:HD12	2.49	0.41
1:F:352:ARG:HB3	1:F:352:ARG:HH21	1.85	0.41
1:D:58:VAL:HG11	1:D:145:TRP:CZ2	2.55	0.41
1:F:57:ALA:HB1	1:F:65:MET:HE2	2.02	0.41
1:F:367:ASN:N	1:F:367:ASN:ND2	2.68	0.41
1:H:102:PRO:HB2	1:H:103:ASN:H	1.76	0.41
1:A:111:LEU:CD1	1:A:145:TRP:HH2	2.33	0.41
1:B:135:LEU:CD2	1:B:142:GLY:O	2.62	0.41
1:B:395:LEU:O	1:B:399:GLN:HB2	2.21	0.41
1:D:28:ILE:O	1:D:133:ILE:HA	2.19	0.41
1:D:35:ASN:HB3	1:D:68:LEU:HD21	2.01	0.41
1:F:90:SER:C	1:F:92:VAL:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:353:LEU:C	1:F:355:GLU:H	2.23	0.41
1:G:145:TRP:HA	1:G:148:LEU:HB3	2.00	0.41
1:G:327:ARG:NH2	1:G:362:ASP:OD2	2.53	0.41
1:H:117:ARG:CG	1:H:117:ARG:NH1	2.64	0.41
1:H:158:PHE:HA	1:H:159:PRO:HD3	1.90	0.41
1:I:145:TRP:O	1:I:149:VAL:HG23	2.21	0.41
1:K:97:ASP:HA	1:K:98:PRO:HD3	1.94	0.41
1:F:28:ILE:O	1:F:133:ILE:HA	2.20	0.41
1:G:60:PHE:HE1	1:G:95:LEU:HD22	1.85	0.41
1:H:353:LEU:C	1:H:355:GLU:N	2.73	0.41
1:J:203:LYS:HA	1:J:204:PRO:HD3	1.97	0.41
1:J:324:PHE:HA	1:J:361:GLY:O	2.21	0.41
1:L:135:LEU:HD22	1:L:142:GLY:O	2.19	0.41
1:C:235:ASN:HD21	1:C:237:LYS:HG3	1.86	0.41
1:C:327:ARG:H	1:C:327:ARG:HG3	1.71	0.41
1:E:176:ILE:O	1:E:177:ASN:C	2.59	0.41
1:F:250:GLU:OE2	1:F:373:TYR:OH	2.26	0.41
1:J:403:ARG:HD2	1:K:199:ASN:HD21	1.85	0.41
1:K:28:ILE:O	1:K:133:ILE:HA	2.21	0.41
1:G:26:GLY:CA	1:G:119:PHE:HE2	2.34	0.41
1:I:234:VAL:O	1:J:337:VAL:N	2.53	0.41
1:K:145:TRP:O	1:K:149:VAL:HG23	2.20	0.41
1:L:336:ASP:O	1:L:339:THR:HB	2.20	0.41
1:B:279:ARG:HB2	1:B:378:GLY:HA2	2.03	0.41
1:C:279:ARG:HB2	1:C:378:GLY:HA2	2.01	0.41
1:D:403:ARG:HH22	1:D:407:GLN:HG3	1.85	0.41
1:E:292:ASP:C	1:E:333:PHE:CZ	2.94	0.41
1:F:126:VAL:HG12	1:F:128:VAL:H	1.86	0.41
1:F:158:PHE:HA	1:F:159:PRO:HD3	1.88	0.41
1:H:98:PRO:HA	1:H:104:ALA:HB3	2.02	0.41
1:J:10:HIS:CD2	1:J:367:ASN:OD1	2.74	0.41
1:J:148:LEU:O	1:J:152:LEU:HG	2.21	0.41
1:L:203:LYS:HA	1:L:204:PRO:HD3	1.95	0.41
1:L:292:ASP:O	1:L:294:HIS:N	2.54	0.41
1:A:237:LYS:HB3	2:A:900:GDP:C6	2.56	0.41
1:E:291:PHE:CE1	1:E:334:PHE:CE1	3.09	0.41
1:F:217:GLN:HG2	1:F:236:TRP:CD2	2.56	0.41
1:H:135:LEU:CD2	1:H:145:TRP:HB2	2.51	0.41
1:I:403:ARG:O	1:I:406:ALA:HB3	2.21	0.41
1:K:158:PHE:HA	1:K:159:PRO:HD3	1.89	0.41
1:K:203:LYS:HD3	1:K:276:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASN:C	1:A:105:ASN:H	2.25	0.40
1:B:101:ASN:HA	1:B:102:PRO:HD3	1.89	0.40
1:B:288:ILE:CD1	1:B:296:LEU:HD12	2.50	0.40
1:I:217:GLN:HG2	1:I:236:TRP:CD2	2.56	0.40
1:I:318:ALA:HB2	1:I:379:MET:HE3	2.03	0.40
1:J:336:ASP:HB3	1:J:339:THR:OG1	2.20	0.40
1:K:54:PRO:HB2	1:K:119:PHE:CE2	2.55	0.40
1:K:290:LYS:HE2	1:K:290:LYS:HA	2.02	0.40
1:A:63:SER:HA	1:A:66:MET:HE2	2.03	0.40
1:B:158:PHE:HA	1:B:159:PRO:HD3	1.89	0.40
1:D:338:ASN:HA	1:D:341:ASN:HB3	2.03	0.40
1:E:79:PHE:CD2	1:E:79:PHE:N	2.88	0.40
1:J:36:LYS:HD3	1:K:261:ASP:O	2.21	0.40
1:K:290:LYS:HA	1:K:290:LYS:CE	2.50	0.40
1:E:2:VAL:CG2	1:E:43:GLY:HA3	2.52	0.40
1:H:154:ARG:C	1:H:156:GLN:H	2.24	0.40
1:I:279:ARG:HB2	1:I:378:GLY:HA2	2.03	0.40
1:J:235:ASN:O	1:J:238:GLU:HB3	2.21	0.40
1:L:121:ASN:HB2	1:L:124:GLY:H	1.86	0.40
1:A:39:ASP:HB2	1:A:68:LEU:HD22	2.03	0.40
1:A:59:ASN:OD1	1:A:60:PHE:N	2.52	0.40
1:B:97:ASP:HA	1:B:98:PRO:HD3	1.95	0.40
1:E:255:PRO:O	1:E:267:PRO:HD3	2.21	0.40
1:F:57:ALA:CB	1:F:65:MET:HE2	2.52	0.40
1:F:135:LEU:HD21	1:F:145:TRP:HB2	2.04	0.40
1:L:141:VAL:HG13	1:L:145:TRP:HE1	1.87	0.40
1:L:183:LEU:HB3	1:L:381:MET:HE1	2.03	0.40
1:A:290:LYS:HB2	1:A:295:SER:OG	2.21	0.40
1:B:203:LYS:HD3	1:B:276:ILE:O	2.21	0.40
1:E:212:ASP:O	1:E:216:MET:HG3	2.22	0.40
1:H:77:ILE:HD12	1:H:77:ILE:N	2.37	0.40
1:I:192:GLU:HA	1:I:195:ARG:NH2	2.36	0.40
1:J:183:LEU:HD13	1:J:381:MET:HE1	2.04	0.40
1:L:266:ASP:HB2	1:L:267:PRO:CD	2.51	0.40

All (2) 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:E:73:LYS:NZ	1:K:48:ASN:O[1_655]	1.73	0.47
1:C:232:ARG:NH2	1:I:124:GLY:O[1_655]	2.09	0.11

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	385/427 (90%)	355 (92%)	24 (6%)	6 (2%)	9 40
1	B	399/427 (93%)	371 (93%)	25 (6%)	3 (1%)	19 57
1	C	385/427 (90%)	357 (93%)	26 (7%)	2 (0%)	29 68
1	D	385/427 (90%)	356 (92%)	28 (7%)	1 (0%)	41 76
1	E	389/427 (91%)	364 (94%)	22 (6%)	3 (1%)	19 57
1	F	385/427 (90%)	347 (90%)	33 (9%)	5 (1%)	12 45
1	G	396/427 (93%)	356 (90%)	35 (9%)	5 (1%)	12 45
1	H	386/427 (90%)	349 (90%)	32 (8%)	5 (1%)	12 45
1	I	398/427 (93%)	365 (92%)	30 (8%)	3 (1%)	19 57
1	J	387/427 (91%)	353 (91%)	28 (7%)	6 (2%)	9 40
1	K	394/427 (92%)	368 (93%)	24 (6%)	2 (0%)	29 68
1	L	373/427 (87%)	342 (92%)	26 (7%)	5 (1%)	12 45
All	All	4662/5124 (91%)	4283 (92%)	333 (7%)	46 (1%)	15 53

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	B	102	PRO
1	B	413	GLU
1	E	60	PHE
1	F	121	ASN
1	F	398	LYS
1	G	293	LEU
1	G	417	ILE
1	H	121	ASN
1	I	121	ASN
1	J	407	GLN
1	A	123	GLU

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Mol	Chain	Res	Type
1	C	64	ASP
1	D	293	LEU
1	G	354	ASP
1	H	102	PRO
1	H	415	VAL
1	I	125	GLU
1	I	140	GLY
1	J	408	ARG
1	K	125	GLU
1	L	60	PHE
1	L	124	GLY
1	A	290	LYS
1	H	419	PHE
1	J	90	SER
1	A	405	GLU
1	B	397	GLU
1	C	232	ARG
1	E	291	PHE
1	F	293	LEU
1	G	121	ASN
1	H	354	ASP
1	J	102	PRO
1	K	32	GLN
1	L	331	ALA
1	A	104	ALA
1	E	32	GLN
1	J	142	GLY
1	L	293	LEU
1	A	293	LEU
1	F	60	PHE
1	G	117	ARG
1	J	124	GLY
1	L	141	VAL
1	F	124	GLY

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	339/369 (92%)	322 (95%)	17 (5%)	24	60
1	B	352/369 (95%)	337 (96%)	15 (4%)	29	66
1	C	337/369 (91%)	323 (96%)	14 (4%)	30	66
1	D	339/369 (92%)	325 (96%)	14 (4%)	30	67
1	E	343/369 (93%)	329 (96%)	14 (4%)	30	67
1	F	339/369 (92%)	323 (95%)	16 (5%)	26	63
1	G	351/369 (95%)	334 (95%)	17 (5%)	25	62
1	H	346/369 (94%)	325 (94%)	21 (6%)	18	53
1	I	351/369 (95%)	329 (94%)	22 (6%)	18	51
1	J	341/369 (92%)	322 (94%)	19 (6%)	21	56
1	K	348/369 (94%)	329 (94%)	19 (6%)	21	57
1	L	329/369 (89%)	315 (96%)	14 (4%)	29	66
All	All	4115/4428 (93%)	3913 (95%)	202 (5%)	25	61

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	THR
1	A	100	THR
1	A	115	LEU
1	A	143	THR
1	A	194	ASP
1	A	234	VAL
1	A	298	ASN
1	A	337	VAL
1	A	341	ASN
1	A	365	TRP
1	A	367	ASN
1	A	384	ARG
1	A	393	LYS
1	A	394	GLU
1	A	401	GLN
1	A	402	LEU
1	A	403	ARG
1	B	32	GLN
1	B	63	SER
1	B	100	THR
1	B	115	LEU
1	B	123	GLU

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Mol	Chain	Res	Type
1	B	194	ASP
1	B	298	ASN
1	B	329	SER
1	B	352	ARG
1	B	364	ILE
1	B	365	TRP
1	B	368	GLU
1	B	408	ARG
1	B	412	GLU
1	B	421	THR
1	C	78	HIS
1	C	108	LEU
1	C	115	LEU
1	C	122	GLU
1	C	194	ASP
1	C	227	LYS
1	C	231	ASN
1	C	298	ASN
1	C	327	ARG
1	C	332	ASP
1	C	352	ARG
1	C	365	TRP
1	C	368	GLU
1	C	414	LYS
1	D	2	VAL
1	D	32	GLN
1	D	60	PHE
1	D	93	THR
1	D	115	LEU
1	D	194	ASP
1	D	298	ASN
1	D	327	ARG
1	D	341	ASN
1	D	352	ARG
1	D	365	TRP
1	D	367	ASN
1	D	384	ARG
1	D	407	GLN
1	E	32	GLN
1	E	60	PHE
1	E	79	PHE
1	E	97	ASP

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Mol	Chain	Res	Type
1	E	103	ASN
1	E	115	LEU
1	E	192	GLU
1	E	194	ASP
1	E	298	ASN
1	E	330	ASN
1	E	342	ARG
1	E	352	ARG
1	E	365	TRP
1	E	402	LEU
1	F	78	HIS
1	F	90	SER
1	F	100	THR
1	F	103	ASN
1	F	115	LEU
1	F	121	ASN
1	F	194	ASP
1	F	235	ASN
1	F	291	PHE
1	F	298	ASN
1	F	316	GLU
1	F	327	ARG
1	F	340	GLU
1	F	365	TRP
1	F	367	ASN
1	F	395	LEU
1	G	32	GLN
1	G	64	ASP
1	G	80	ASP
1	G	94	ASP
1	G	115	LEU
1	G	123	GLU
1	G	194	ASP
1	G	234	VAL
1	G	293	LEU
1	G	298	ASN
1	G	327	ARG
1	G	362	ASP
1	G	365	TRP
1	G	366	ASP
1	G	367	ASN
1	G	407	GLN

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Mol	Chain	Res	Type
1	G	417	ILE
1	H	32	GLN
1	H	91	VAL
1	H	103	ASN
1	H	115	LEU
1	H	117	ARG
1	H	123	GLU
1	H	194	ASP
1	H	292	ASP
1	H	298	ASN
1	H	327	ARG
1	H	328	PRO
1	H	329	SER
1	H	332	ASP
1	H	342	ARG
1	H	365	TRP
1	H	366	ASP
1	H	369	TYR
1	H	401	GLN
1	H	410	GLN
1	H	411	ASP
1	H	414	LYS
1	I	80	ASP
1	I	88	THR
1	I	93	THR
1	I	100	THR
1	I	101	ASN
1	I	115	LEU
1	I	122	GLU
1	I	143	THR
1	I	234	VAL
1	I	288	ILE
1	I	298	ASN
1	I	327	ARG
1	I	341	ASN
1	I	342	ARG
1	I	364	ILE
1	I	365	TRP
1	I	366	ASP
1	I	368	GLU
1	I	369	TYR
1	I	402	LEU

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Mol	Chain	Res	Type
1	I	412	GLU
1	I	417	ILE
1	J	90	SER
1	J	94	ASP
1	J	95	LEU
1	J	99	GLU
1	J	103	ASN
1	J	105	ASN
1	J	115	LEU
1	J	122	GLU
1	J	194	ASP
1	J	233	TYR
1	J	298	ASN
1	J	327	ARG
1	J	338	ASN
1	J	342	ARG
1	J	365	TRP
1	J	366	ASP
1	J	367	ASN
1	J	398	LYS
1	J	411	ASP
1	K	62	GLU
1	K	66	MET
1	K	94	ASP
1	K	100	THR
1	K	103	ASN
1	K	115	LEU
1	K	123	GLU
1	K	192	GLU
1	K	194	ASP
1	K	234	VAL
1	K	264	THR
1	K	290	LYS
1	K	298	ASN
1	K	329	SER
1	K	337	VAL
1	K	342	ARG
1	K	354	ASP
1	K	364	ILE
1	K	365	TRP
1	L	100	THR
1	L	108	LEU

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Mol	Chain	Res	Type
1	L	115	LEU
1	L	117	ARG
1	L	194	ASP
1	L	235	ASN
1	L	288	ILE
1	L	298	ASN
1	L	330	ASN
1	L	332	ASP
1	L	342	ARG
1	L	365	TRP
1	L	366	ASP
1	L	367	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	16	HIS
1	A	32	GLN
1	A	121	ASN
1	A	177	ASN
1	A	298	ASN
1	A	338	ASN
1	A	367	ASN
1	B	67	HIS
1	B	121	ASN
1	B	178	ASN
1	B	235	ASN
1	B	298	ASN
1	B	338	ASN
1	B	401	GLN
1	C	6	ASN
1	C	32	GLN
1	C	78	HIS
1	C	235	ASN
1	C	298	ASN
1	C	341	ASN
1	C	399	GLN
1	C	410	GLN
1	D	32	GLN
1	D	67	HIS
1	D	298	ASN

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Mol	Chain	Res	Type
1	D	341	ASN
1	D	367	ASN
1	D	401	GLN
1	D	407	GLN
1	E	6	ASN
1	E	32	GLN
1	E	103	ASN
1	E	235	ASN
1	E	298	ASN
1	F	70	ASN
1	F	103	ASN
1	F	121	ASN
1	F	298	ASN
1	F	410	GLN
1	G	6	ASN
1	G	32	GLN
1	G	67	HIS
1	G	70	ASN
1	G	78	HIS
1	G	103	ASN
1	G	121	ASN
1	G	298	ASN
1	G	367	ASN
1	G	399	GLN
1	H	177	ASN
1	H	178	ASN
1	H	298	ASN
1	H	341	ASN
1	H	367	ASN
1	H	410	GLN
1	I	32	GLN
1	I	298	ASN
1	I	341	ASN
1	I	401	GLN
1	J	6	ASN
1	J	67	HIS
1	J	103	ASN
1	J	298	ASN
1	J	341	ASN
1	K	6	ASN
1	K	121	ASN
1	K	199	ASN

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Mol	Chain	Res	Type
1	K	231	ASN
1	K	298	ASN
1	K	341	ASN
1	K	410	GLN
1	L	103	ASN
1	L	298	ASN
1	L	367	ASN
1	L	399	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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GDP	D	900	-	24,30,30	0.90	0	30,47,47	1.28	5 (16%)
2	GDP	A	900	3	24,30,30	1.03	1 (4%)	30,47,47	1.42	4 (13%)
2	GDP	E	900	-	24,30,30	1.09	2 (8%)	30,47,47	1.14	5 (16%)
2	GDP	J	900	-	24,30,30	0.93	1 (4%)	30,47,47	1.22	4 (13%)
2	GDP	C	900	-	24,30,30	1.04	1 (4%)	30,47,47	1.48	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GDP	F	900	-	24,30,30	0.89	0	30,47,47	1.10	3 (10%)
2	GDP	G	900	3	24,30,30	0.97	2 (8%)	30,47,47	1.23	5 (16%)
2	GDP	I	900	3	24,30,30	1.02	0	30,47,47	1.40	4 (13%)
2	GDP	K	900	-	24,30,30	0.97	1 (4%)	30,47,47	1.12	3 (10%)
2	GDP	B	900	3	24,30,30	1.12	2 (8%)	30,47,47	1.37	7 (23%)
2	GDP	L	900	-	24,30,30	1.01	2 (8%)	30,47,47	1.53	8 (26%)

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	GDP	D	900	-	-	2/12/32/32	0/3/3/3
2	GDP	A	900	3	-	6/12/32/32	0/3/3/3
2	GDP	E	900	-	-	2/12/32/32	0/3/3/3
2	GDP	J	900	-	-	4/12/32/32	0/3/3/3
2	GDP	C	900	-	-	7/12/32/32	0/3/3/3
2	GDP	F	900	-	-	4/12/32/32	0/3/3/3
2	GDP	G	900	3	-	4/12/32/32	0/3/3/3
2	GDP	I	900	3	-	4/12/32/32	0/3/3/3
2	GDP	K	900	-	-	2/12/32/32	0/3/3/3
2	GDP	B	900	3	-	2/12/32/32	0/3/3/3
2	GDP	L	900	-	-	5/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	GDP	C6-N1	-2.78	1.33	1.37
2	E	900	GDP	C6-N1	-2.49	1.34	1.37
2	C	900	GDP	C6-N1	-2.39	1.34	1.37
2	L	900	GDP	C5-C4	2.39	1.49	1.43
2	B	900	GDP	C6-N1	-2.35	1.34	1.37
2	E	900	GDP	O4'-C1'	2.27	1.44	1.41
2	B	900	GDP	C5-C4	2.21	1.48	1.43
2	J	900	GDP	O4'-C1'	2.12	1.44	1.41
2	G	900	GDP	C6-N1	-2.09	1.34	1.37
2	G	900	GDP	O4'-C1'	2.06	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	900	GDP	O4'-C1'	2.01	1.43	1.41
2	K	900	GDP	C5-C4	2.00	1.48	1.43

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	GDP	PA-O3A-PB	-3.55	120.64	132.83
2	I	900	GDP	PA-O3A-PB	-3.34	121.36	132.83
2	I	900	GDP	O2B-PB-O3A	3.33	115.80	104.64
2	J	900	GDP	PA-O3A-PB	-3.30	121.52	132.83
2	C	900	GDP	C5-C6-N1	3.25	119.69	113.95
2	B	900	GDP	O4'-C1'-C2'	-3.17	102.29	106.93
2	C	900	GDP	C3'-C2'-C1'	3.13	105.69	100.98
2	B	900	GDP	C5-C6-N1	3.11	119.44	113.95
2	L	900	GDP	C3'-C2'-C1'	3.09	105.64	100.98
2	B	900	GDP	PA-O3A-PB	-3.05	122.37	132.83
2	L	900	GDP	N2-C2-N1	3.02	123.15	116.71
2	G	900	GDP	PA-O3A-PB	-3.02	122.46	132.83
2	A	900	GDP	C5-C6-N1	3.01	119.27	113.95
2	D	900	GDP	PA-O3A-PB	-2.95	122.71	132.83
2	L	900	GDP	PA-O3A-PB	-2.92	122.79	132.83
2	K	900	GDP	PA-O3A-PB	-2.84	123.08	132.83
2	C	900	GDP	PA-O3A-PB	-2.83	123.11	132.83
2	A	900	GDP	O6-C6-C5	-2.79	118.92	124.37
2	C	900	GDP	O3'-C3'-C4'	-2.76	103.06	111.05
2	L	900	GDP	C5-C6-N1	2.73	118.77	113.95
2	A	900	GDP	C3'-C2'-C1'	2.69	105.03	100.98
2	E	900	GDP	C8-N7-C5	2.53	107.81	102.99
2	G	900	GDP	C5-C6-N1	2.53	118.41	113.95
2	I	900	GDP	C8-N7-C5	2.47	107.70	102.99
2	F	900	GDP	C5-C6-N1	2.46	118.29	113.95
2	F	900	GDP	C8-N7-C5	2.41	107.58	102.99
2	J	900	GDP	C5-C6-N1	2.40	118.18	113.95
2	C	900	GDP	C2'-C3'-C4'	2.39	107.29	102.64
2	B	900	GDP	O6-C6-C5	-2.38	119.72	124.37
2	D	900	GDP	C5-C6-N1	2.37	118.14	113.95
2	L	900	GDP	O6-C6-C5	-2.35	119.78	124.37
2	B	900	GDP	C8-N7-C5	2.33	107.43	102.99
2	L	900	GDP	C8-N7-C5	2.32	107.42	102.99
2	K	900	GDP	C5-C6-N1	2.32	118.05	113.95
2	D	900	GDP	C3'-C2'-C1'	2.31	104.45	100.98
2	L	900	GDP	N2-C2-N3	-2.30	115.26	119.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	900	GDP	O2B-PB-O3A	2.29	112.33	104.64
2	G	900	GDP	O4'-C1'-C2'	-2.29	103.58	106.93
2	J	900	GDP	C8-N7-C5	2.28	107.33	102.99
2	K	900	GDP	C8-N7-C5	2.25	107.28	102.99
2	E	900	GDP	C5-C6-N1	2.23	117.89	113.95
2	D	900	GDP	C8-N7-C5	2.23	107.23	102.99
2	J	900	GDP	O6-C6-C5	-2.18	120.11	124.37
2	E	900	GDP	C3'-C2'-C1'	2.18	104.26	100.98
2	D	900	GDP	C2'-C3'-C4'	2.17	106.85	102.64
2	G	900	GDP	O6-C6-C5	-2.15	120.17	124.37
2	L	900	GDP	C2'-C3'-C4'	2.15	106.82	102.64
2	E	900	GDP	PA-O3A-PB	-2.13	125.50	132.83
2	B	900	GDP	C2-N1-C6	-2.12	121.19	125.10
2	E	900	GDP	O3'-C3'-C4'	-2.12	104.93	111.05
2	C	900	GDP	C8-N7-C5	2.08	106.96	102.99
2	G	900	GDP	C8-N7-C5	2.08	106.95	102.99
2	F	900	GDP	C3'-C2'-C1'	2.07	104.09	100.98
2	I	900	GDP	C5-C6-N1	2.00	117.49	113.95

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	GDP	PA-O3A-PB-O3B
2	A	900	GDP	C5'-O5'-PA-O3A
2	A	900	GDP	O4'-C4'-C5'-O5'
2	B	900	GDP	C5'-O5'-PA-O3A
2	C	900	GDP	PA-O3A-PB-O2B
2	C	900	GDP	PA-O3A-PB-O3B
2	C	900	GDP	C5'-O5'-PA-O1A
2	C	900	GDP	C5'-O5'-PA-O2A
2	C	900	GDP	O4'-C4'-C5'-O5'
2	D	900	GDP	PA-O3A-PB-O3B
2	G	900	GDP	C5'-O5'-PA-O3A
2	I	900	GDP	PA-O3A-PB-O2B
2	I	900	GDP	C5'-O5'-PA-O3A
2	I	900	GDP	C5'-O5'-PA-O1A
2	I	900	GDP	C5'-O5'-PA-O2A
2	L	900	GDP	C5'-O5'-PA-O1A
2	C	900	GDP	C3'-C4'-C5'-O5'
2	L	900	GDP	O4'-C4'-C5'-O5'
2	A	900	GDP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	J	900	GDP	O4'-C4'-C5'-O5'
2	L	900	GDP	C3'-C4'-C5'-O5'
2	F	900	GDP	O4'-C4'-C5'-O5'
2	G	900	GDP	PA-O3A-PB-O3B
2	C	900	GDP	C5'-O5'-PA-O3A
2	K	900	GDP	PB-O3A-PA-O2A
2	A	900	GDP	C5'-O5'-PA-O1A
2	G	900	GDP	C5'-O5'-PA-O1A
2	G	900	GDP	C5'-O5'-PA-O2A
2	J	900	GDP	C3'-C4'-C5'-O5'
2	F	900	GDP	PB-O3A-PA-O2A
2	F	900	GDP	C3'-C4'-C5'-O5'
2	E	900	GDP	PA-O3A-PB-O1B
2	L	900	GDP	C4'-C5'-O5'-PA
2	A	900	GDP	PA-O3A-PB-O2B
2	E	900	GDP	PA-O3A-PB-O2B
2	L	900	GDP	C5'-O5'-PA-O3A
2	F	900	GDP	PB-O3A-PA-O1A
2	J	900	GDP	PB-O3A-PA-O1A
2	J	900	GDP	PB-O3A-PA-O2A
2	K	900	GDP	PB-O3A-PA-O1A
2	B	900	GDP	C5'-O5'-PA-O2A
2	D	900	GDP	PA-O3A-PB-O1B

There are no ring outliers.

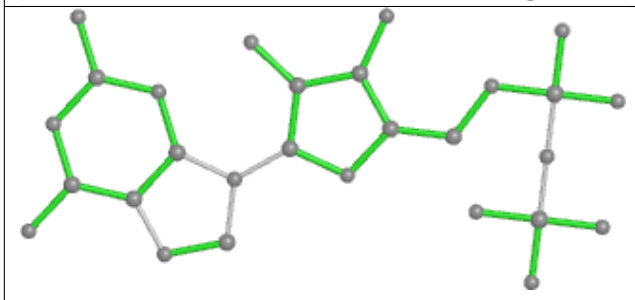
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	900	GDP	3	0
2	A	900	GDP	2	0
2	I	900	GDP	1	0
2	B	900	GDP	1	0
2	L	900	GDP	1	0

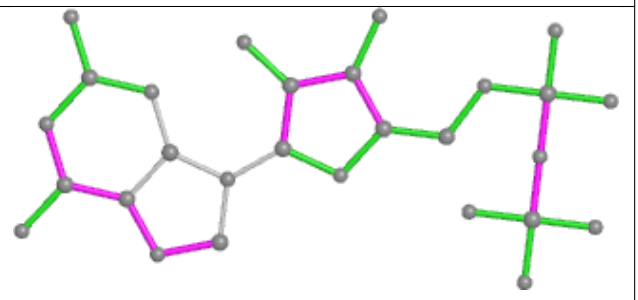
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

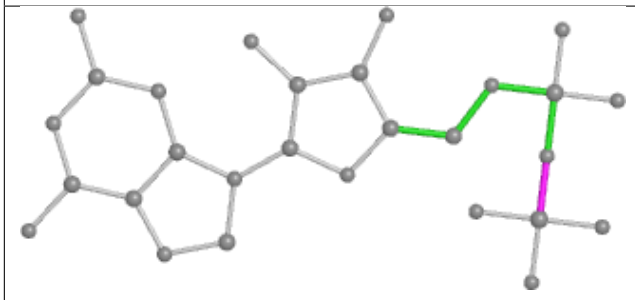
Ligand GDP D 900



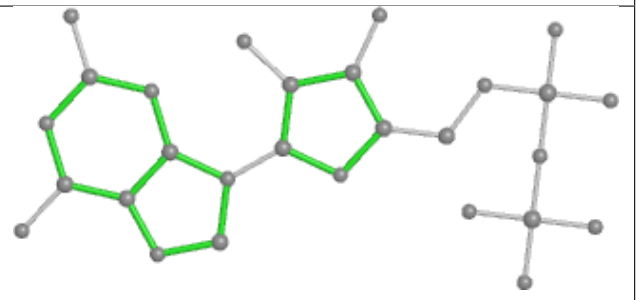
Bond lengths



Bond angles

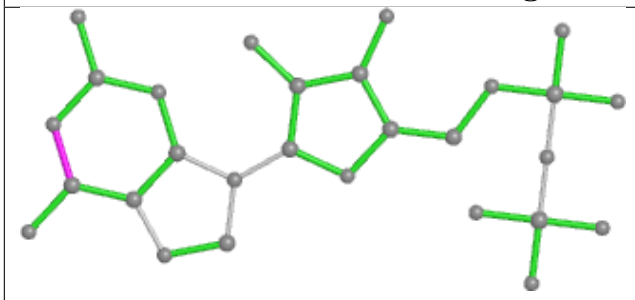


Torsions

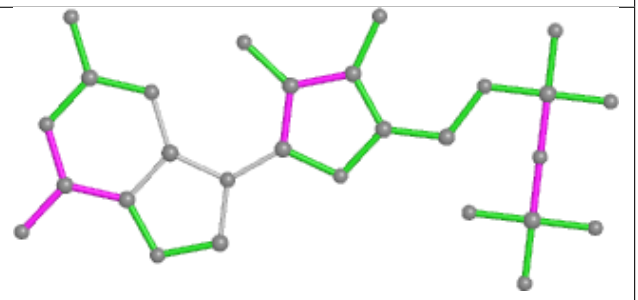


Rings

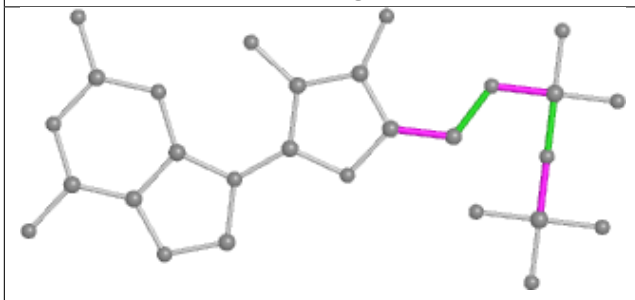
Ligand GDP A 900



Bond lengths



Bond angles



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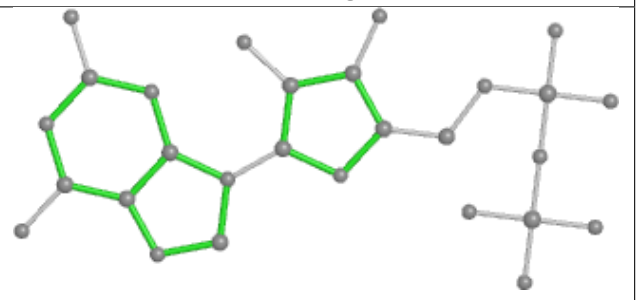
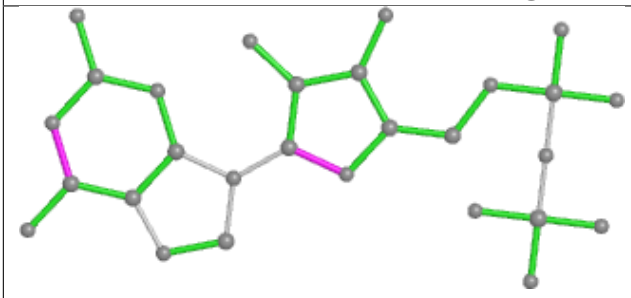


Rings

Ligand GDP E 900



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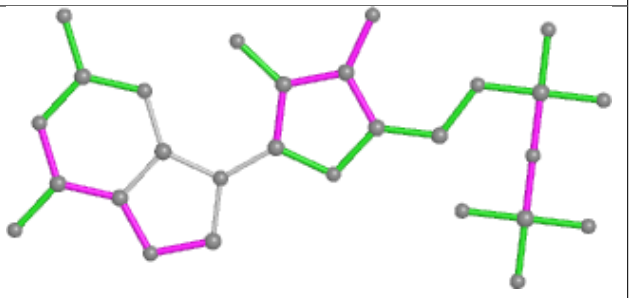
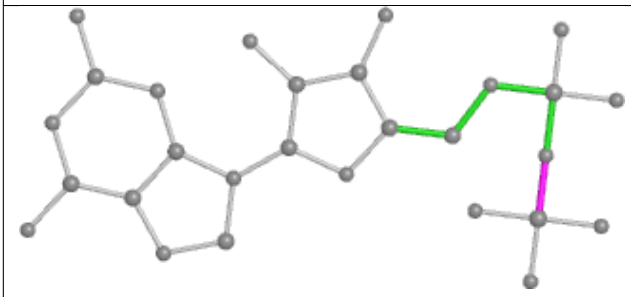


Bond angles



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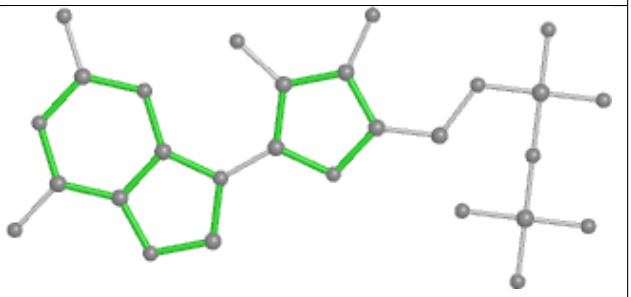
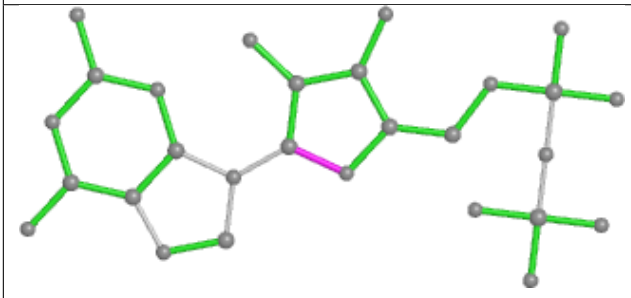
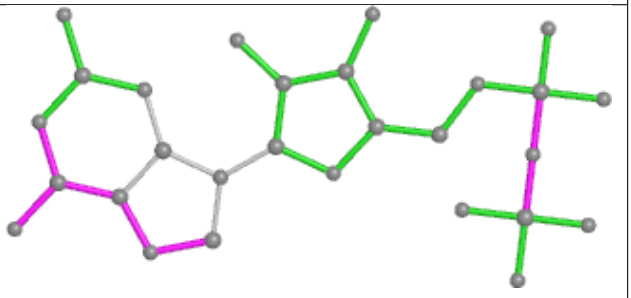


Rings

Ligand GDP J 900



Bond lengths



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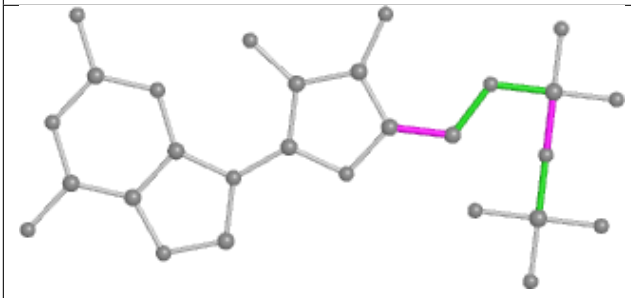
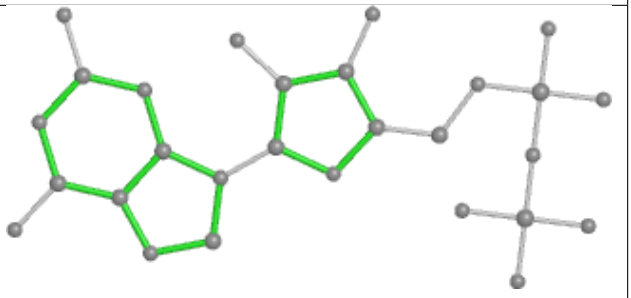
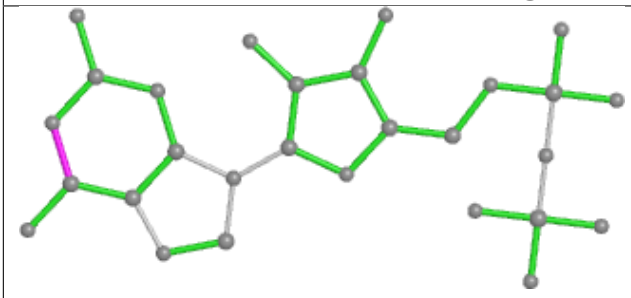


Torsions

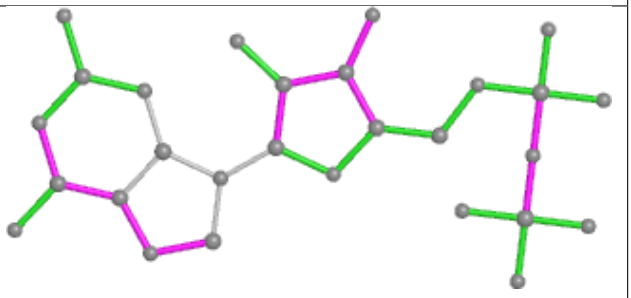


Rings

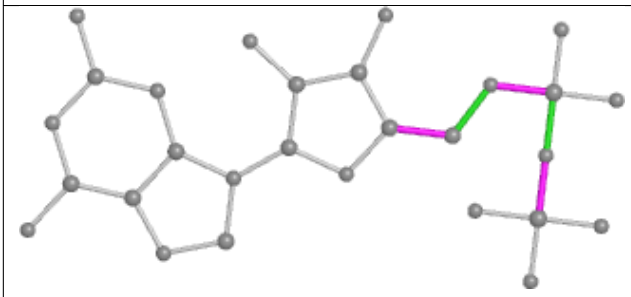
Ligand GDP C 900



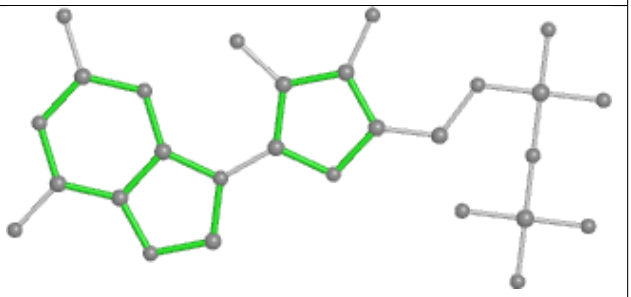
Bond lengths



Bond angles

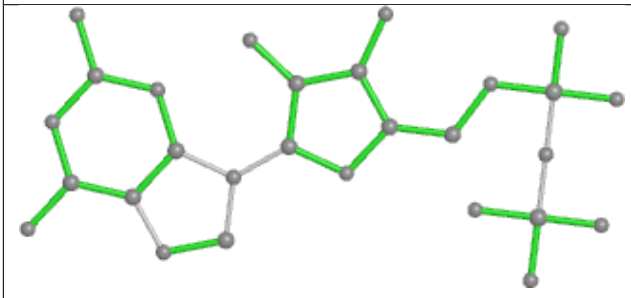


Torsions

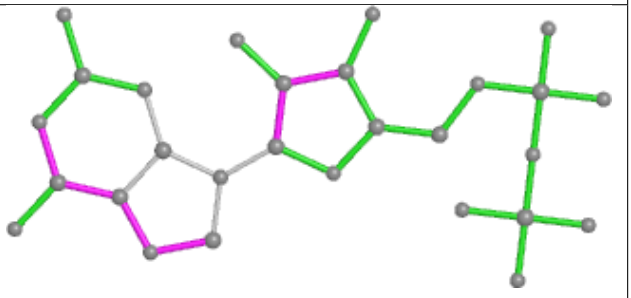


Rings

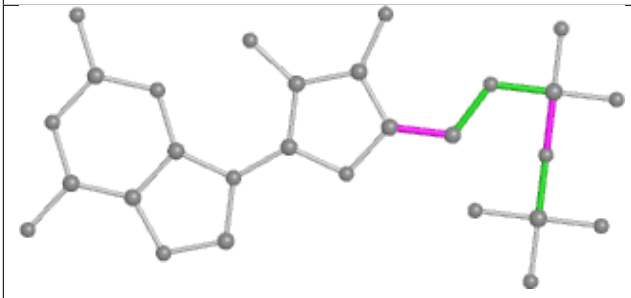
Ligand GDP F 900



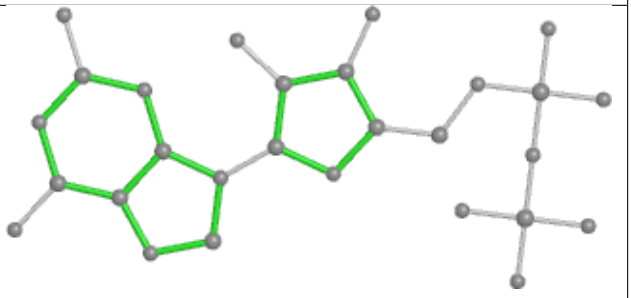
Bond lengths



Bond angles

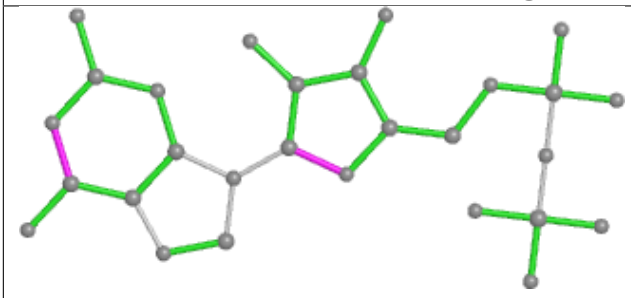


Torsions

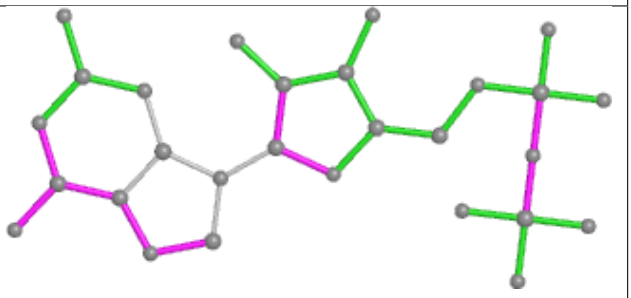


Rings

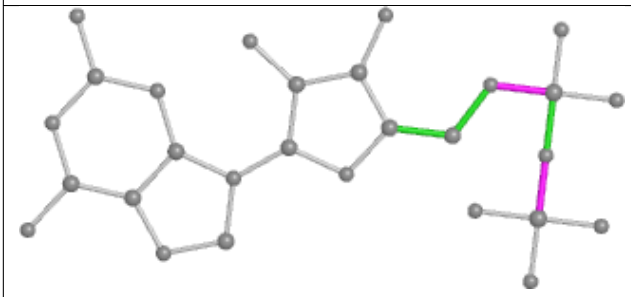
Ligand GDP G 900



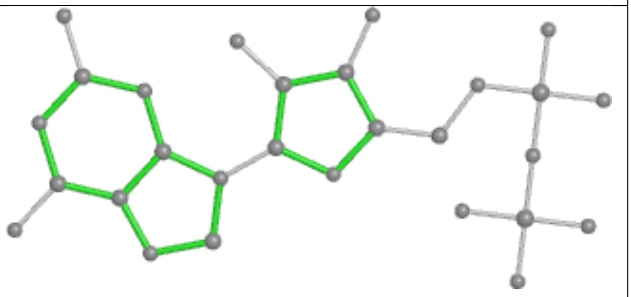
Bond lengths



Bond angles

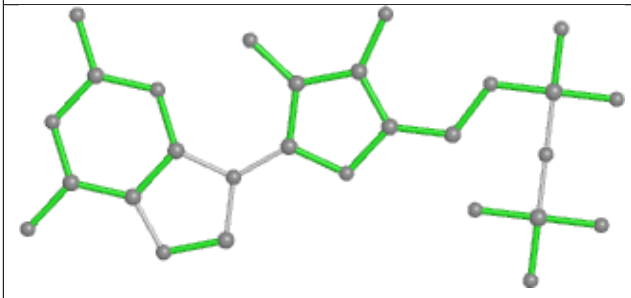


Torsions

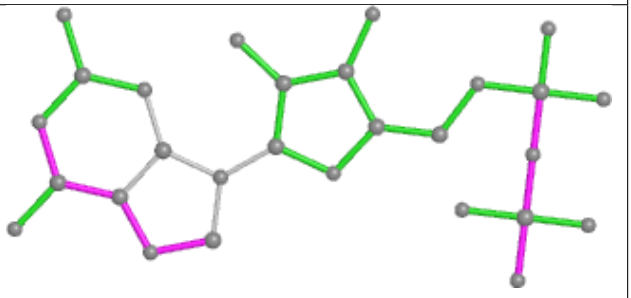


Rings

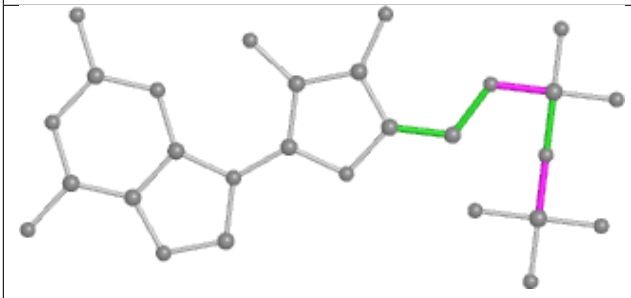
Ligand GDP I 900



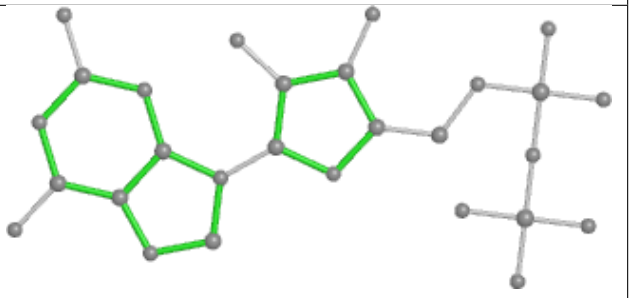
Bond lengths



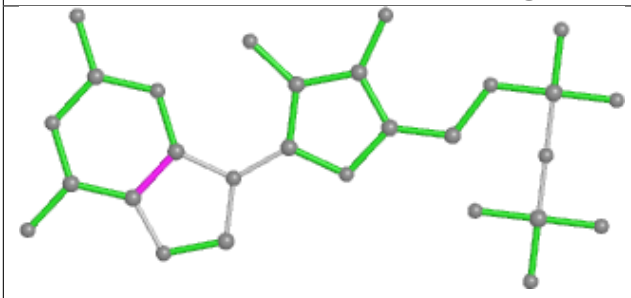
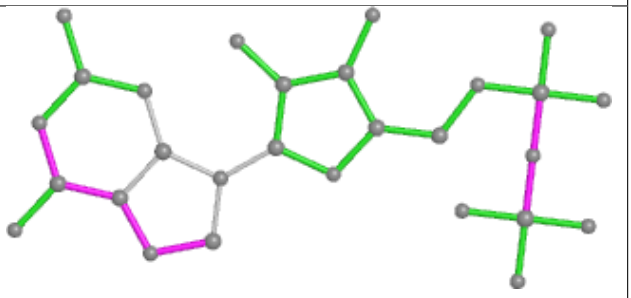
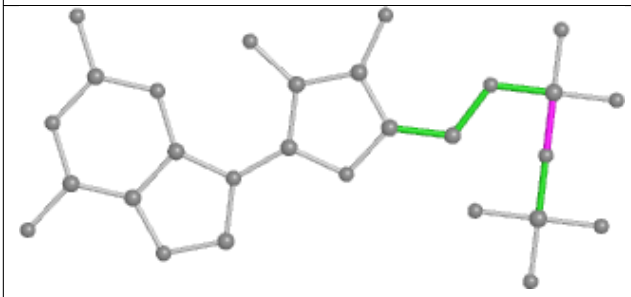
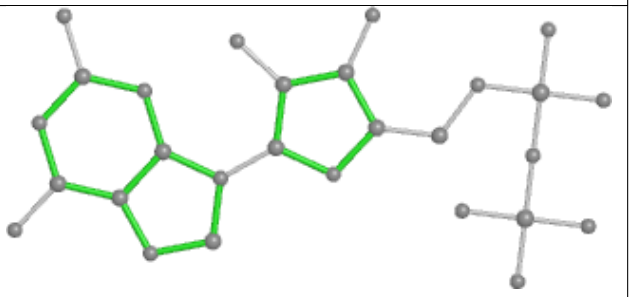
Bond angles

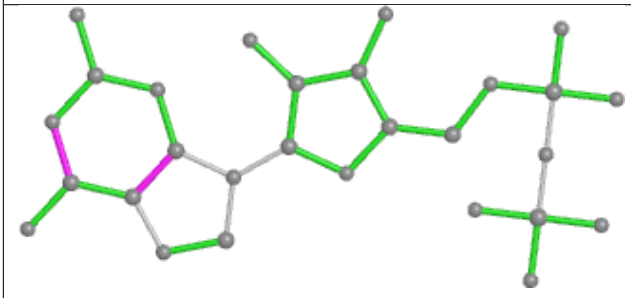
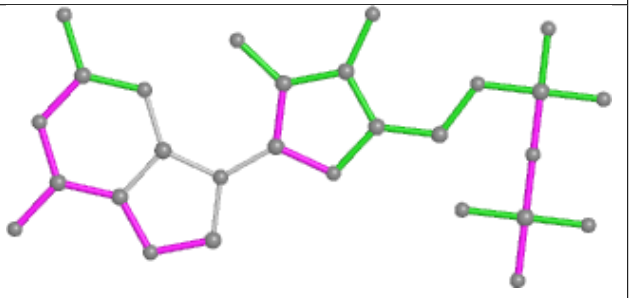
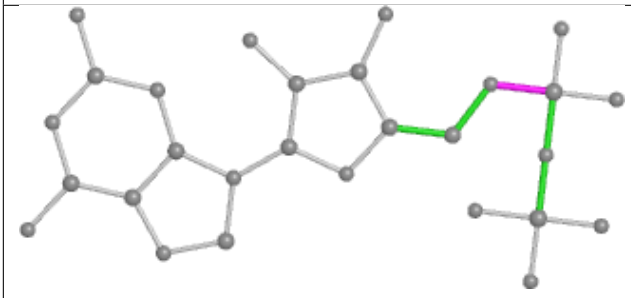
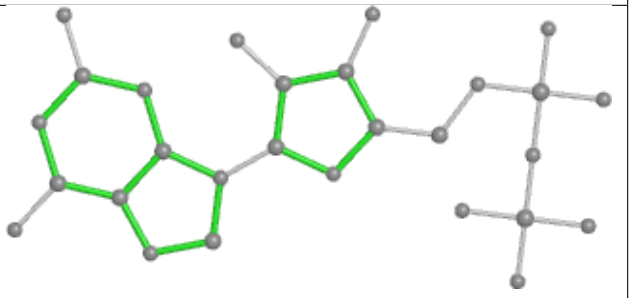


Torsions

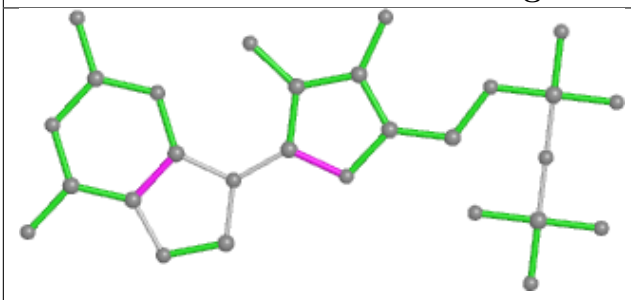


Rings

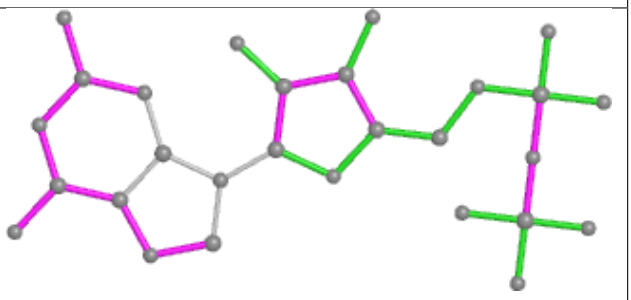
Ligand GDP K 900	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP B 900	
 Bond lengths	 Bond angles
 Torsions	 Rings

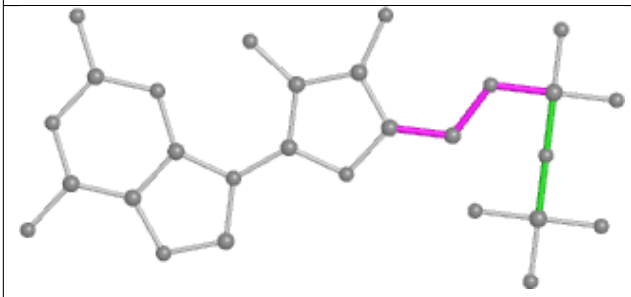
Ligand GDP L 900



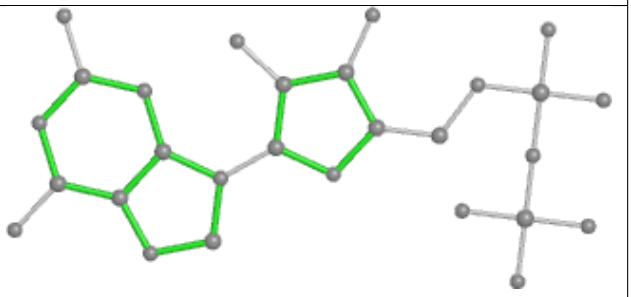
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	391/427 (91%)	-0.25	3 (0%) 86 65	35, 54, 77, 83	0
1	B	405/427 (94%)	-0.26	0 100 100	18, 53, 84, 92	0
1	C	389/427 (91%)	-0.30	0 100 100	35, 54, 68, 85	0
1	D	391/427 (91%)	-0.26	0 100 100	35, 56, 87, 95	0
1	E	395/427 (92%)	-0.26	2 (0%) 91 75	35, 54, 72, 103	0
1	F	391/427 (91%)	-0.25	1 (0%) 94 84	35, 55, 78, 87	0
1	G	404/427 (94%)	-0.09	1 (0%) 95 87	35, 56, 82, 88	0
1	H	394/427 (92%)	-0.25	1 (0%) 94 84	35, 53, 71, 82	0
1	I	404/427 (94%)	-0.23	0 100 100	35, 55, 91, 105	0
1	J	393/427 (92%)	-0.33	0 100 100	35, 55, 79, 108	0
1	K	400/427 (93%)	-0.32	0 100 100	35, 55, 75, 115	0
1	L	379/427 (88%)	-0.23	0 100 100	35, 55, 78, 104	0
All	All	4736/5124 (92%)	-0.25	8 (0%) 95 87	18, 55, 79, 115	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	418	SER	3.5
1	E	99	GLU	3.1
1	F	122	GLU	3.0
1	A	171	GLY	2.2
1	E	103	ASN	2.1
1	G	294	HIS	2.1
1	A	354	ASP	2.0
1	A	102	PRO	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)

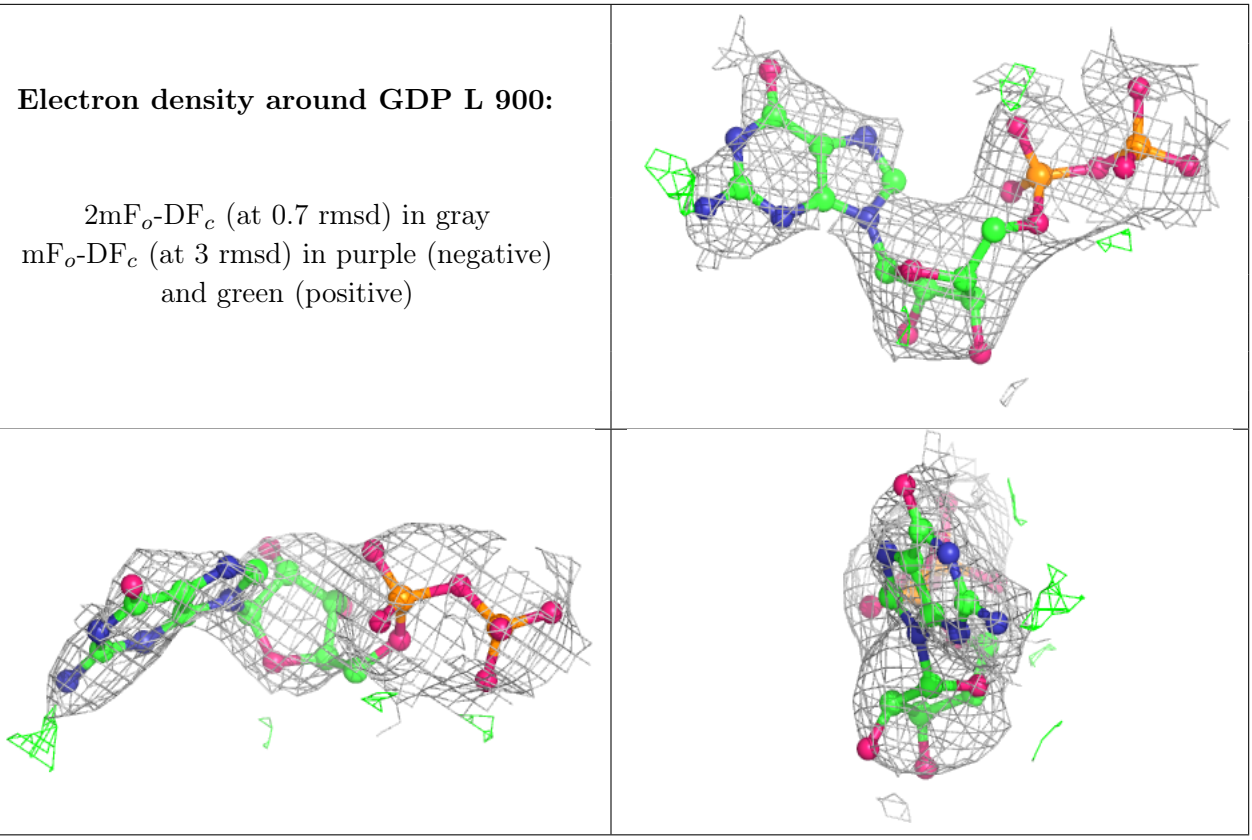
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GDP	L	900	28/28	0.84	0.23	110,112,115,115	0
2	GDP	F	900	28/28	0.90	0.27	107,107,110,110	0
2	GDP	J	900	28/28	0.90	0.19	89,91,92,93	0
2	GDP	D	900	28/28	0.90	0.26	107,110,111,111	0
3	MG	A	999	1/1	0.93	0.20	12,12,12,12	0
3	MG	G	999	1/1	0.93	0.18	17,17,17,17	0
2	GDP	K	900	28/28	0.94	0.18	67,70,70,70	0
3	MG	B	999	1/1	0.95	0.17	13,13,13,13	0
2	GDP	C	900	28/28	0.95	0.16	37,42,43,43	0
2	GDP	E	900	28/28	0.96	0.13	36,45,52,52	0
2	GDP	B	900	28/28	0.96	0.14	36,37,39,40	0
2	GDP	A	900	28/28	0.97	0.14	47,49,50,51	0
2	GDP	G	900	28/28	0.97	0.14	35,39,44,44	0
2	GDP	I	900	28/28	0.97	0.14	26,30,34,34	0
3	MG	I	999	1/1	0.99	0.28	17,17,17,17	0

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

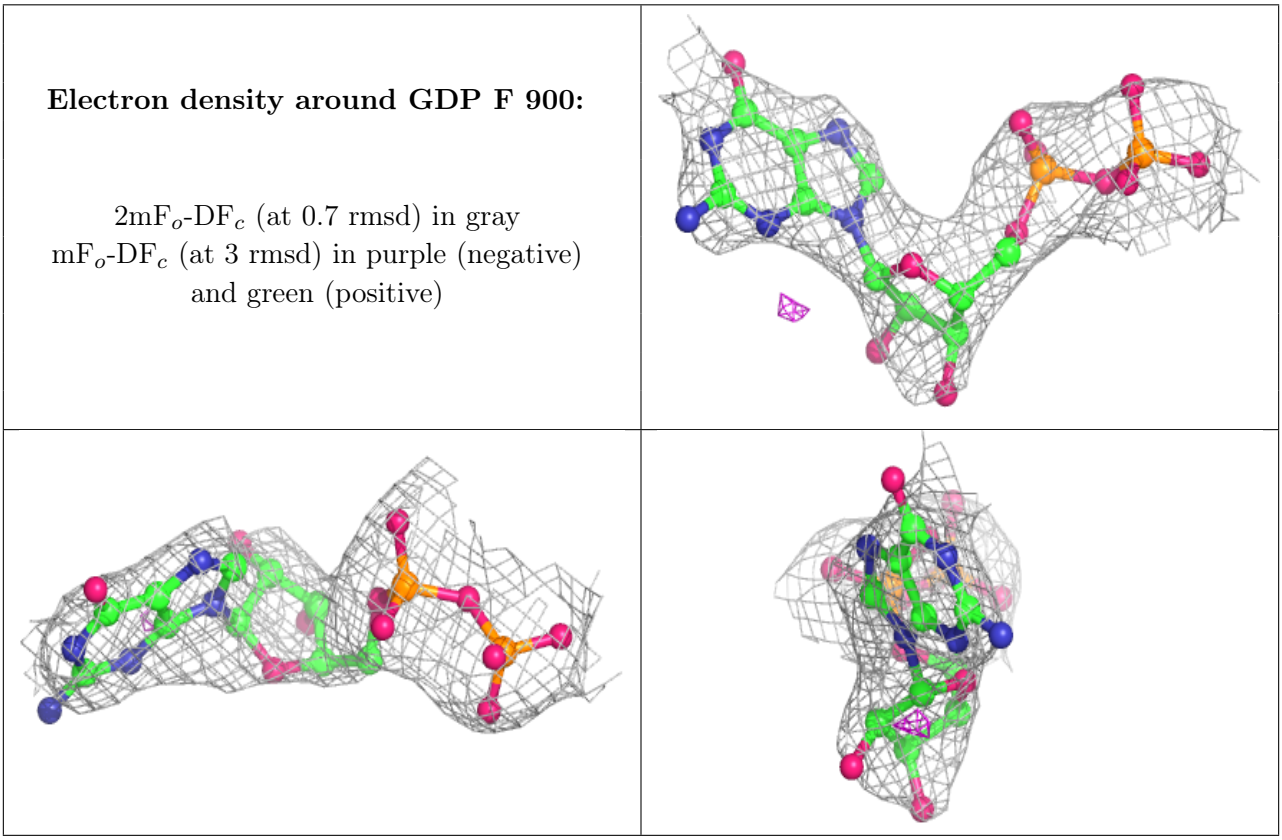
Electron density around GDP L 900:

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



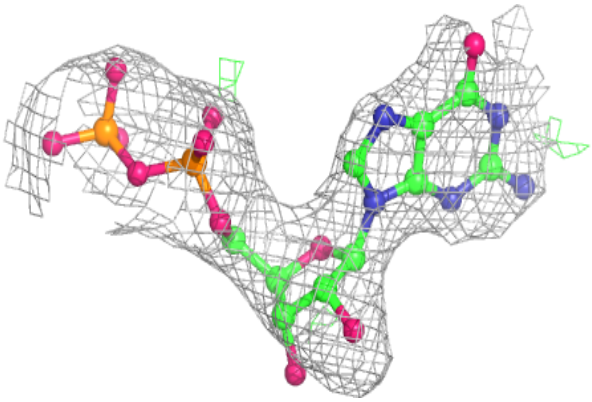
Electron density around GDP F 900:

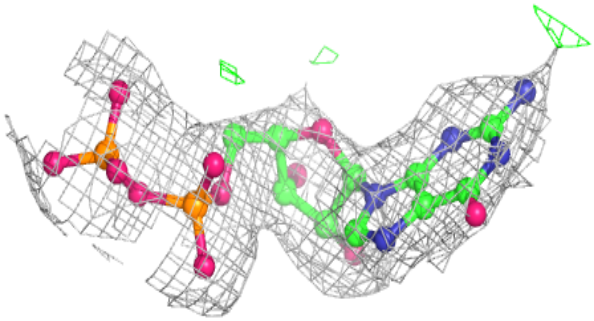
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

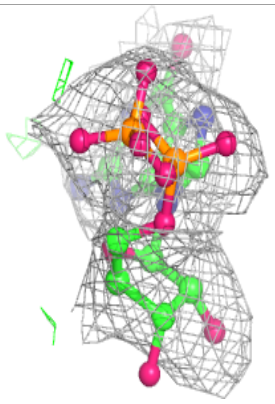


Electron density around GDP J 900:

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







Electron density around GDP D 900:

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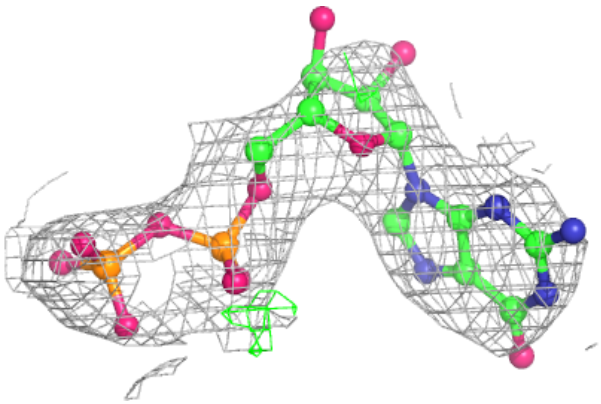
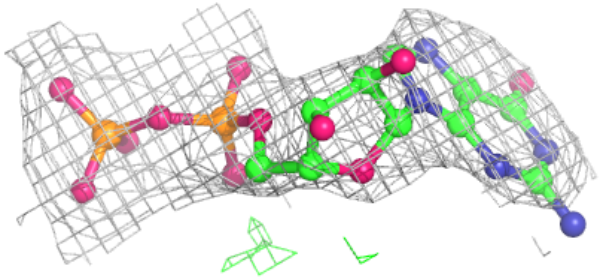
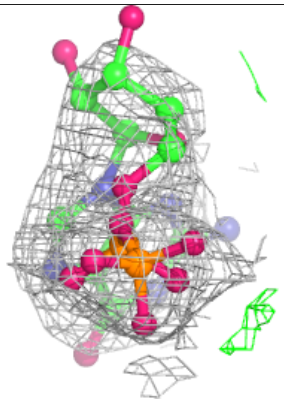
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

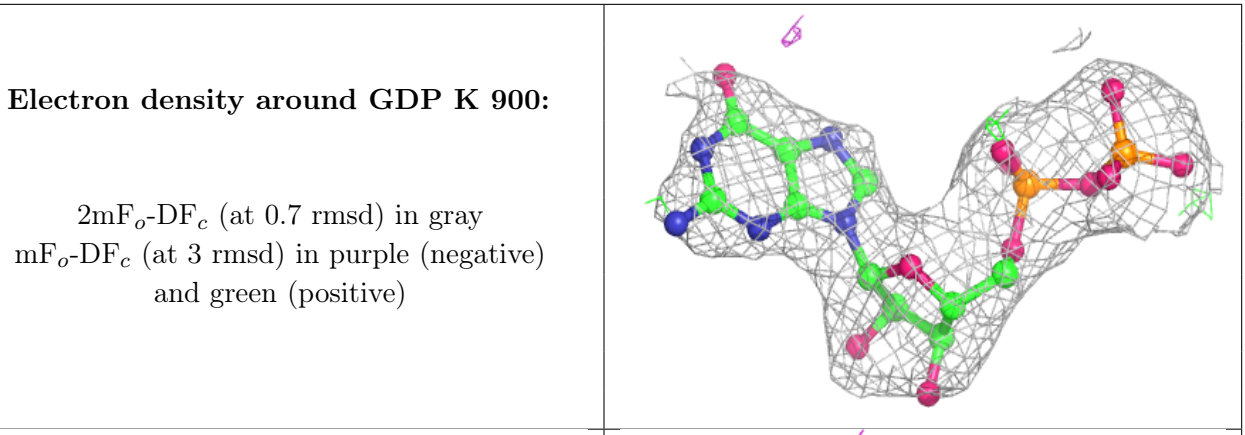


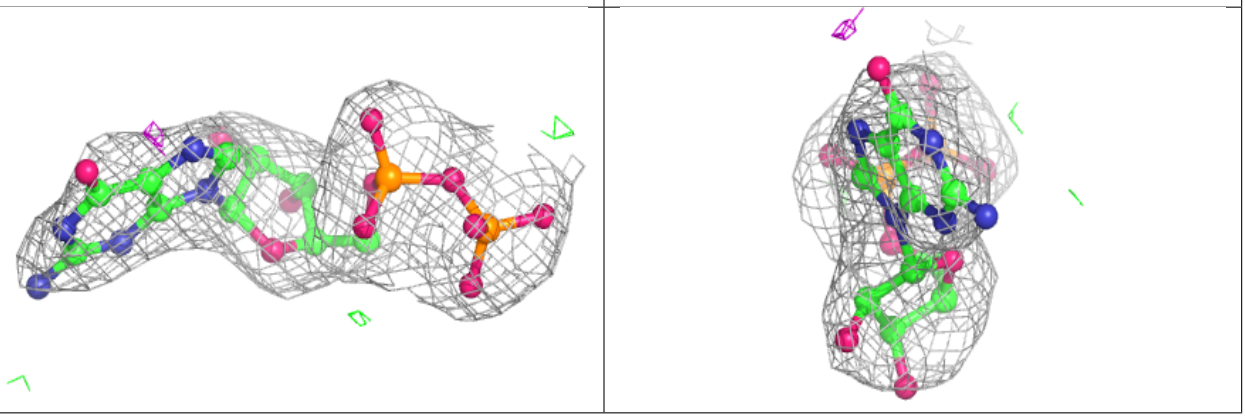




Electron density around GDP K 900:

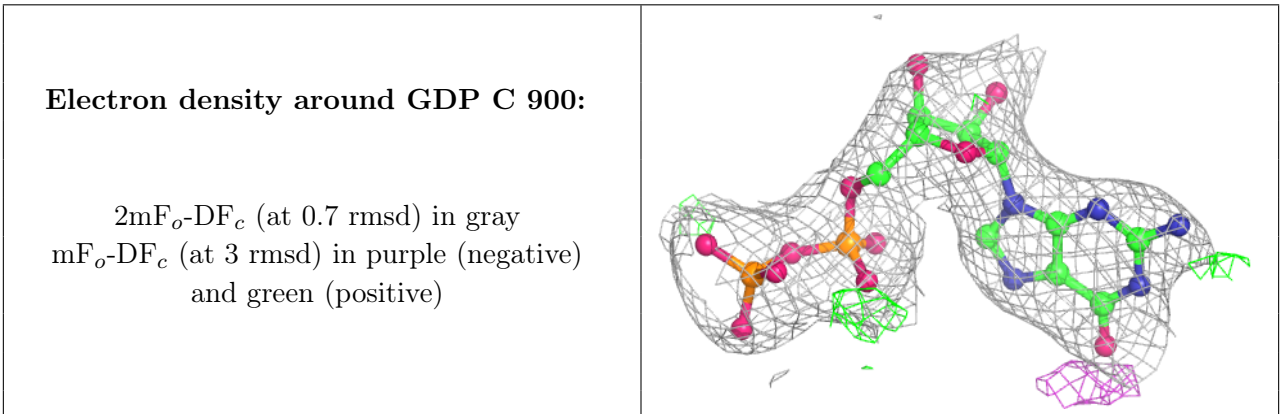
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

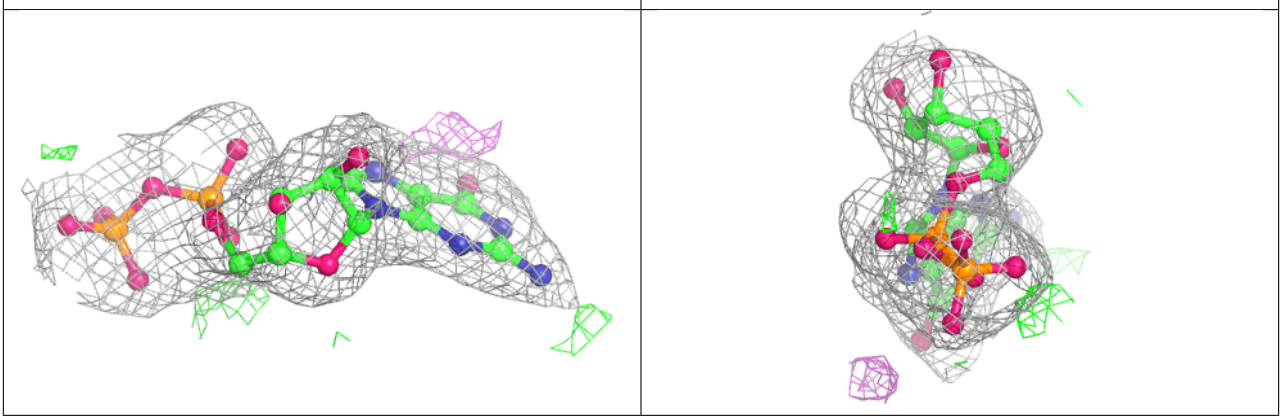




Electron density around GDP C 900:

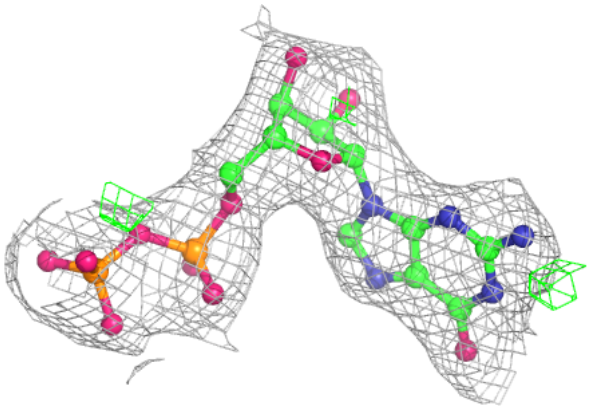
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

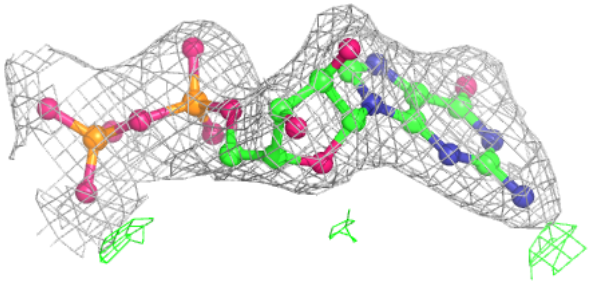


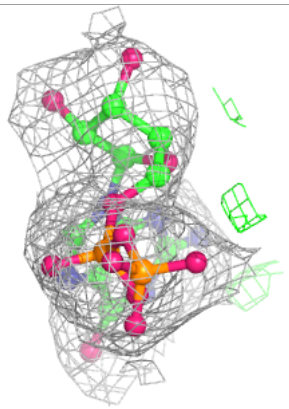


Electron density around GDP E 900:

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

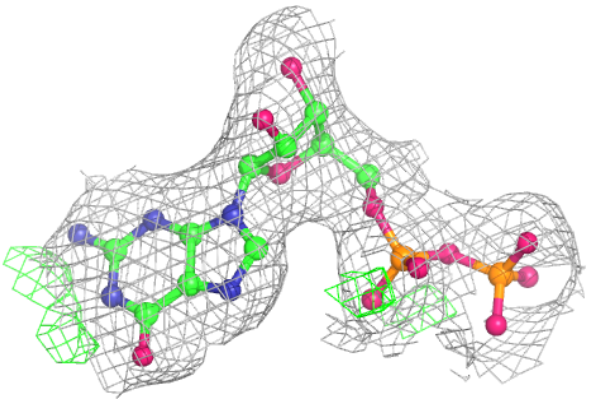


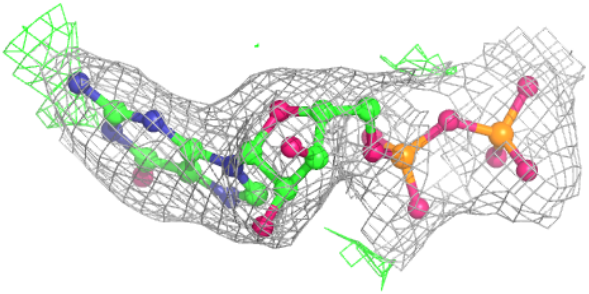


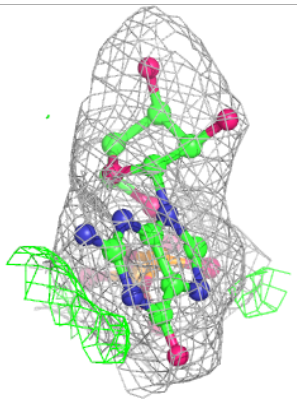


Electron density around GDP B 900:

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

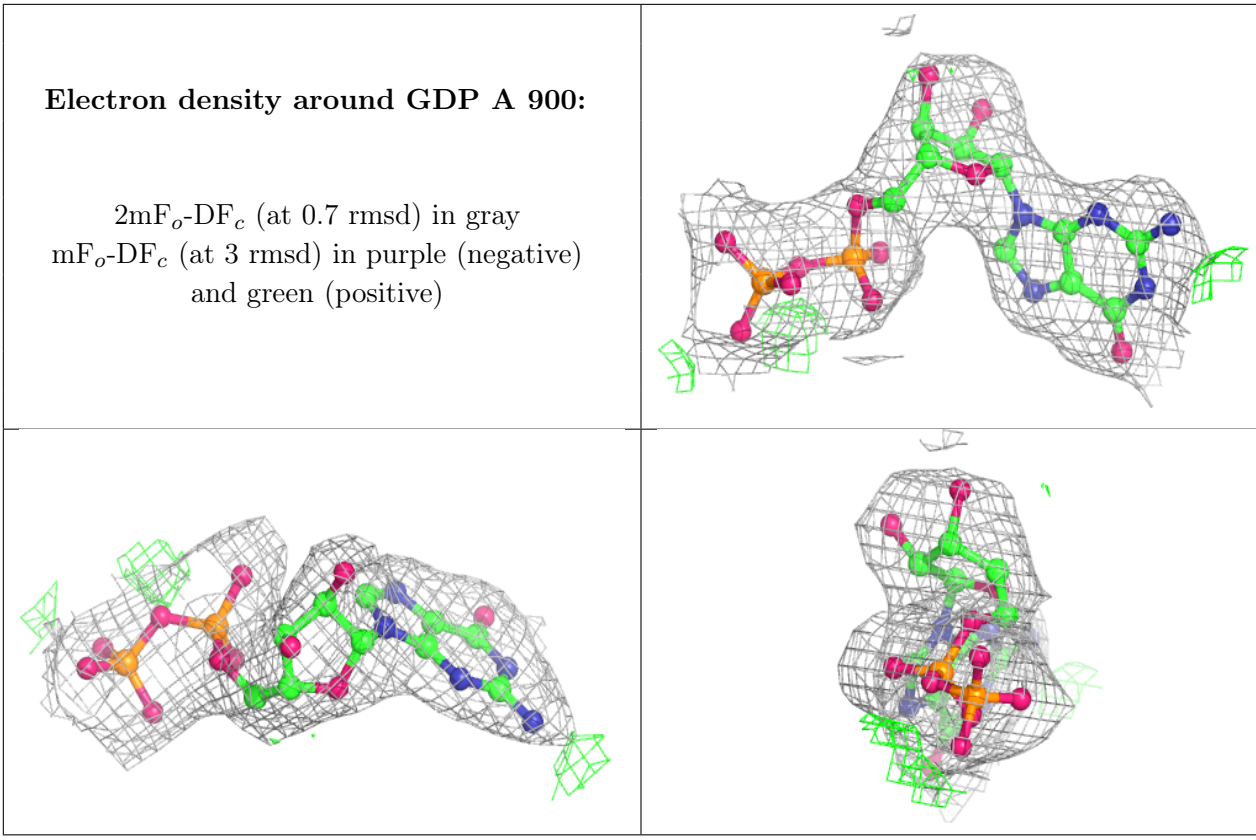






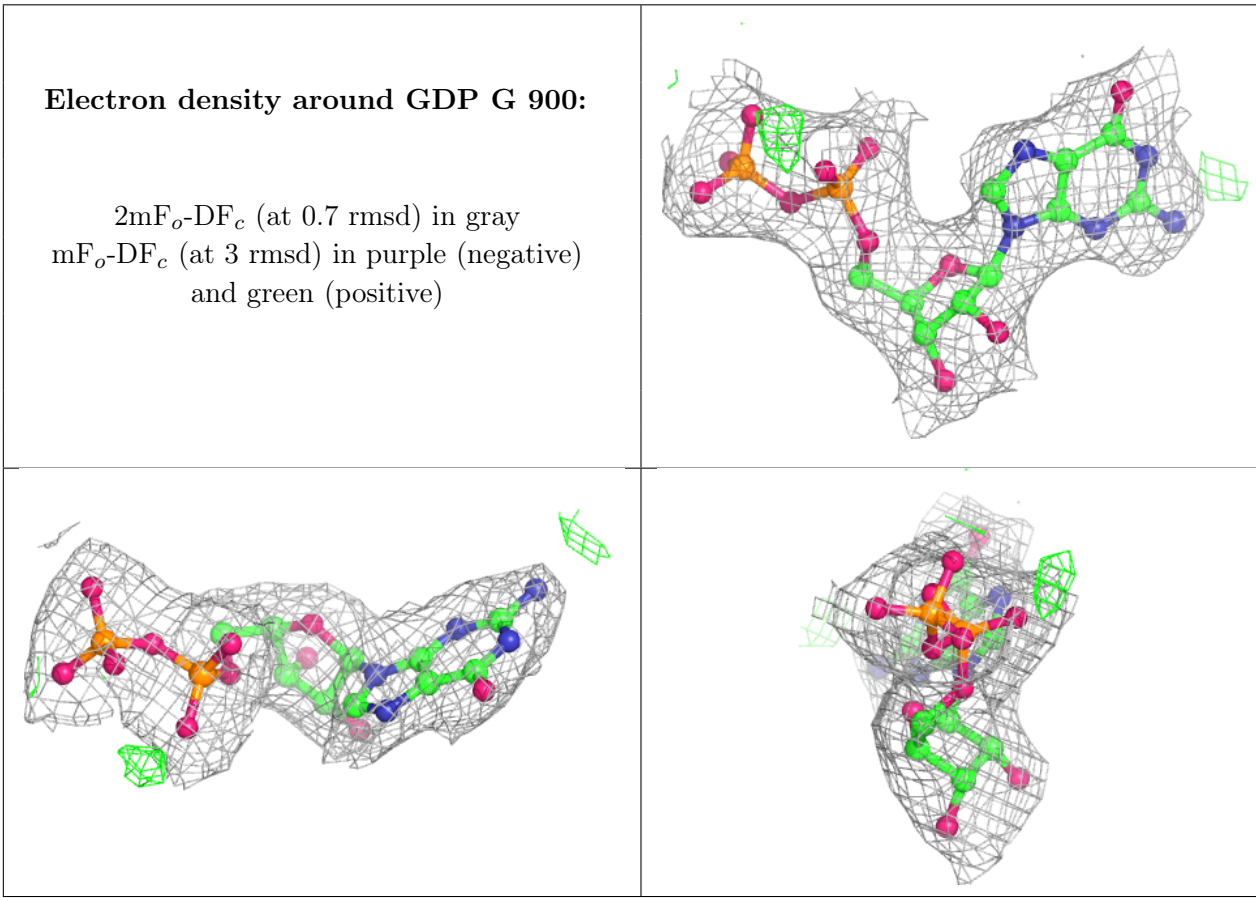
Electron density around GDP A 900:

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



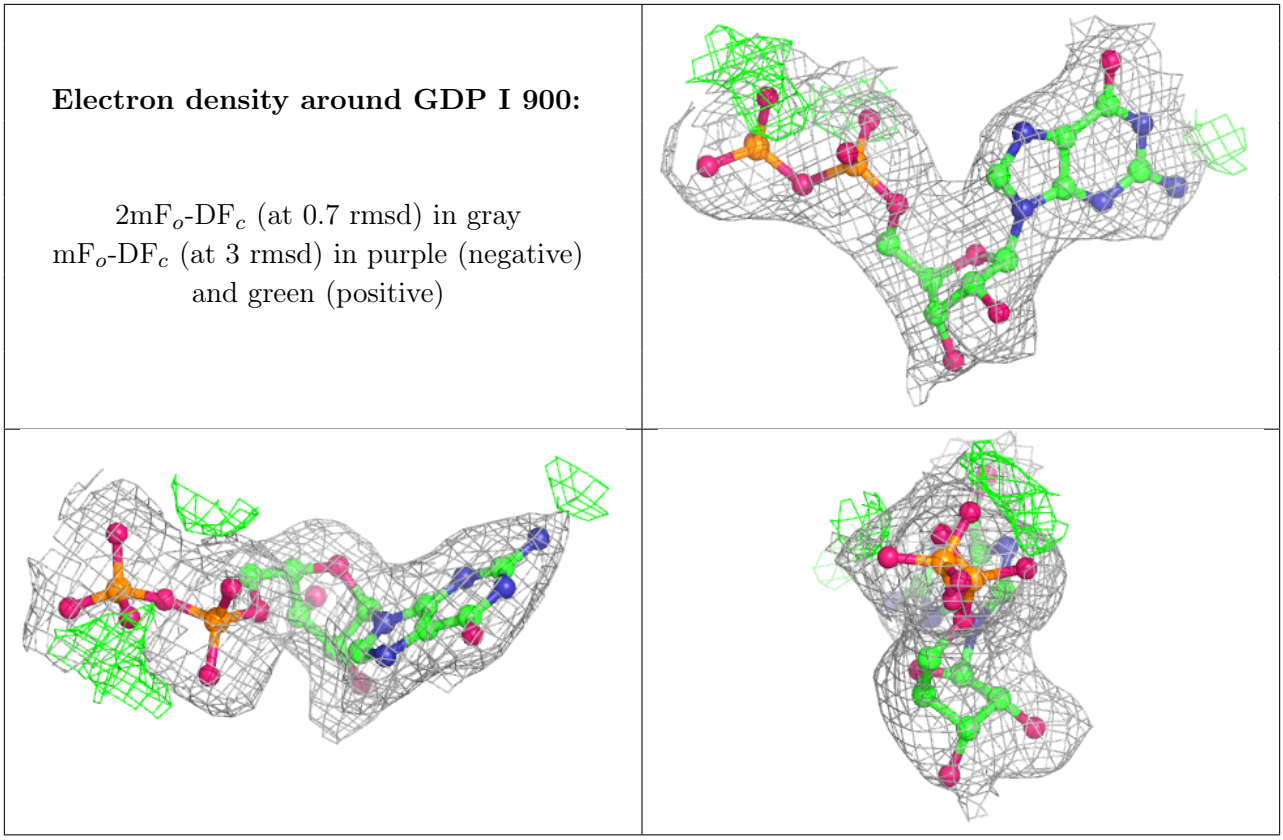
Electron density around GDP G 900:

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



Electron density around GDP I 900:

$2mF_o$-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.