Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2024 – 09:29 PM JST

PDB ID	:	8XGA
Title	:	Crystal structure of human Golgi resident glutaminyl cyclase in complex with (Z)-3-((1H-benzo[d]imidazol-5-yl)methylene)-4-((tetrahydro-2H-pyran-4-yl)oxy)indolin-2-one
Authors	:	Li, G.-B.; Wang, X.-Y.
Deposited on	:	2023-12-15
Resolution	:	3.54 Å(reported)

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

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

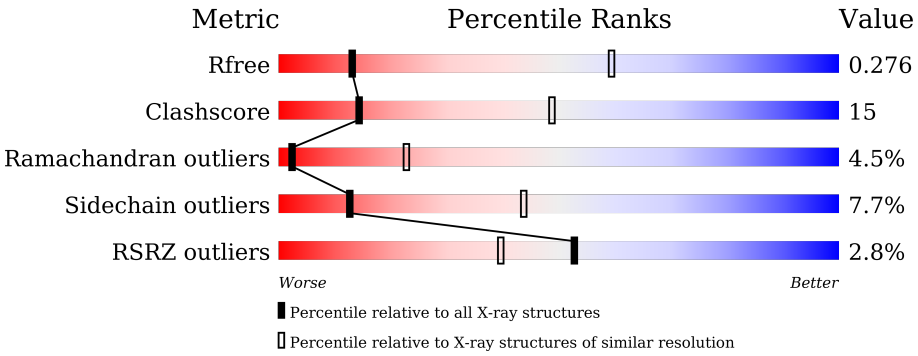
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.54 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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	313	71% 24% • •
1	B	313	65% 29% 5%
1	C	313	64% 31% 5% •
1	D	313	73% 21% 5% •
1	E	313	59% 34% 6% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	313	2% 67% 28% 5%
1	G	313	% 61% 30% 8%
1	H	313	6% 64% 31%
1	I	313	71% 26%
1	J	313	4% 64% 28% 7%
1	K	313	11% 62% 33% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	H	401	-	-	-	X
2	ZN	K	401	-	-	-	X
3	A1D47	A	402	-	-	-	X
3	A1D47	B	402	-	-	-	X
3	A1D47	C	402	-	-	-	X
3	A1D47	D	402	-	-	-	X
3	A1D47	E	402	-	-	-	X
3	A1D47	F	402	-	-	-	X
3	A1D47	G	402	-	-	-	X
3	A1D47	H	402	-	-	-	X
3	A1D47	I	402	-	-	-	X
3	A1D47	J	402	-	-	-	X
3	A1D47	K	402	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27526 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 Glutaminyl-peptide cyclotransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	B	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	C	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	D	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	E	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	F	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	G	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	H	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	I	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	J	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			
1	K	313	Total	C	N	O	S	8	0	0
			2474	1601	436	431	6			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

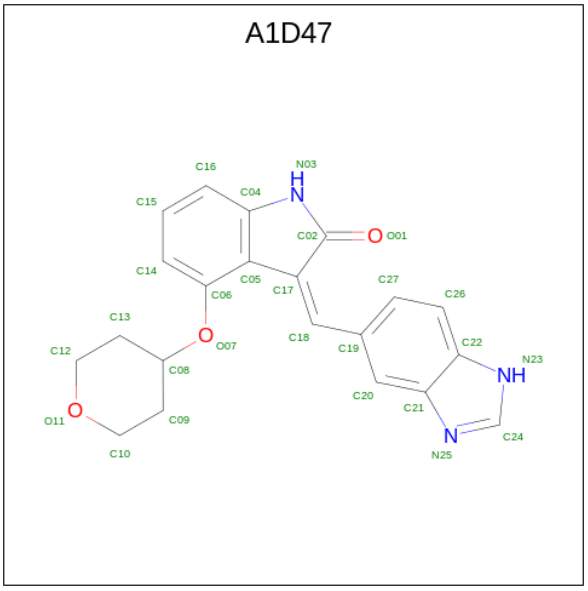
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	K	1	Total Zn 1 1	0	0

- Molecule 3 is (3 {Z})-3-(1 {H}-benzimidazol-5-ylmethylidene)-4-(oxan-4-yloxy)-1 {H}-indol-2-one (three-letter code: A1D47) (formula: $C_{21}H_{19}N_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 27 21 3 3	0	0
3	B	1	Total C N O 27 21 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			27	21	3	3		
3	D	1	Total	C	N	O	0	0
			27	21	3	3		
3	E	1	Total	C	N	O	0	0
			27	21	3	3		
3	F	1	Total	C	N	O	0	0
			27	21	3	3		
3	G	1	Total	C	N	O	0	0
			27	21	3	3		
3	H	1	Total	C	N	O	0	0
			27	21	3	3		
3	I	1	Total	C	N	O	0	0
			27	21	3	3		
3	J	1	Total	C	N	O	0	0
			27	21	3	3		
3	K	1	Total	C	N	O	0	0
			27	21	3	3		

- Molecule 4 is water.

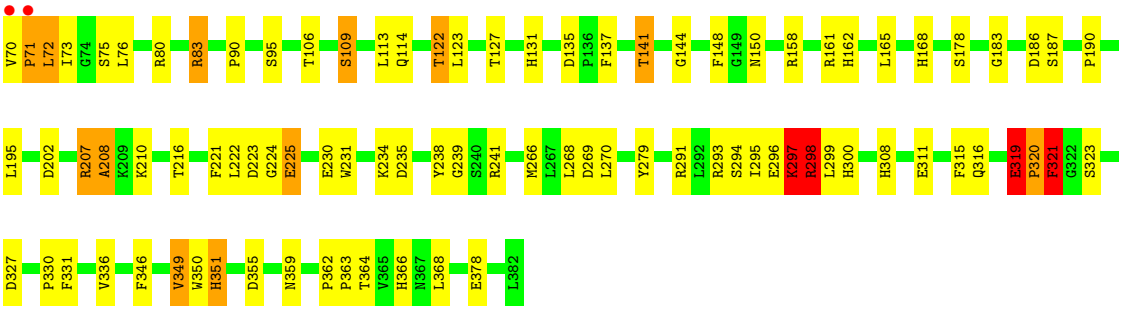
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	C	2	Total	O	0	0
			2	2		
4	E	1	Total	O	0	0
			1	1		

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.

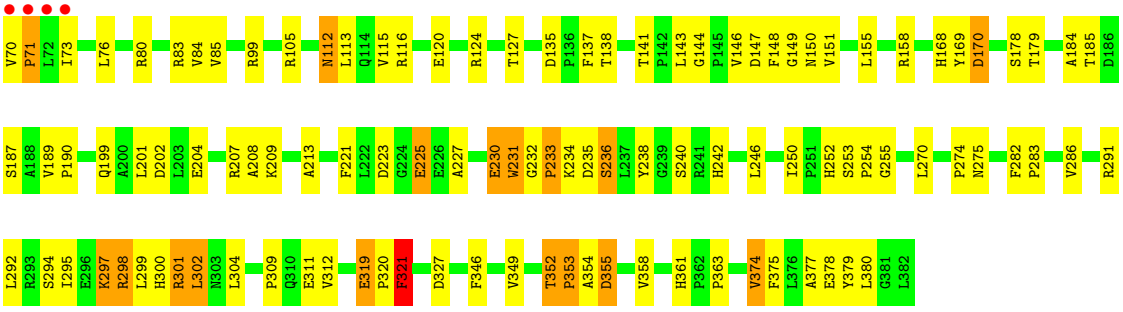
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain A:



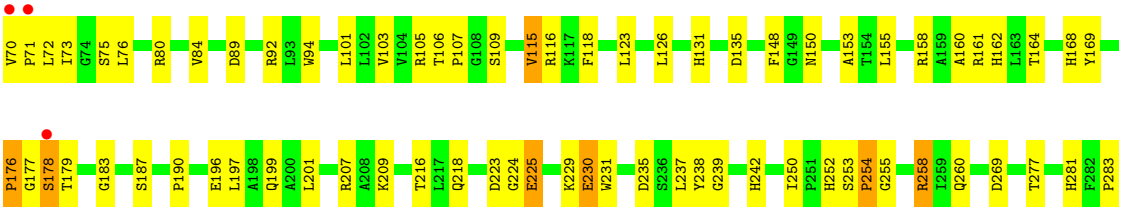
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

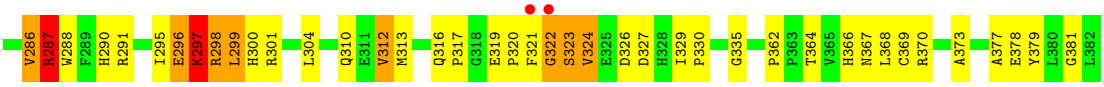
Chain B:



• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

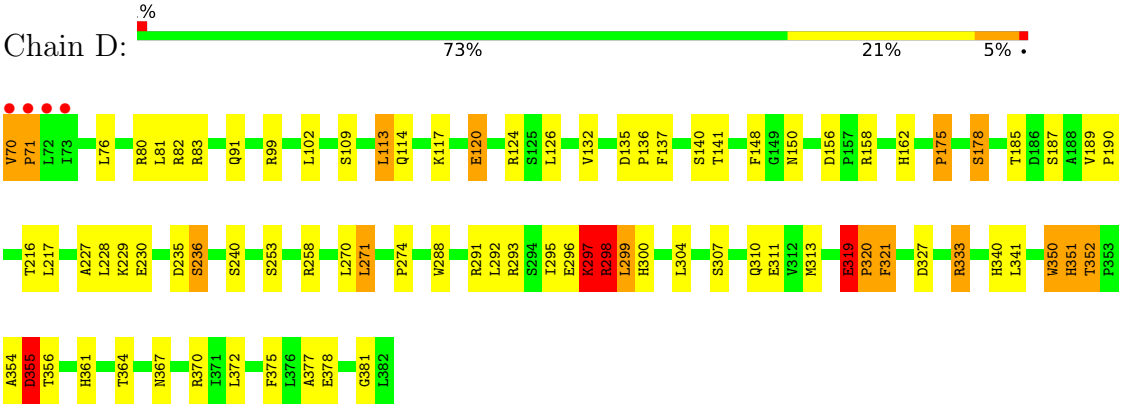
Chain C:





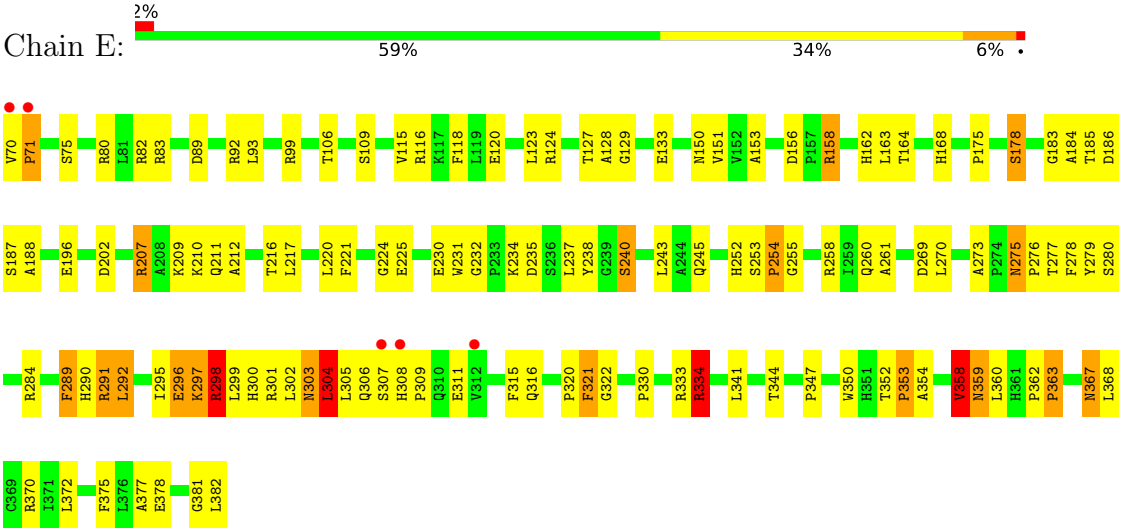
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain D:



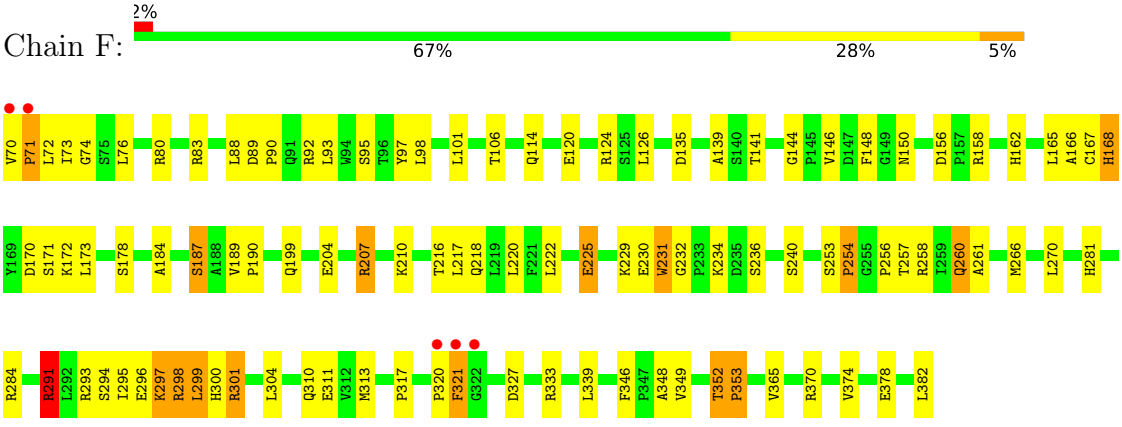
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain E:



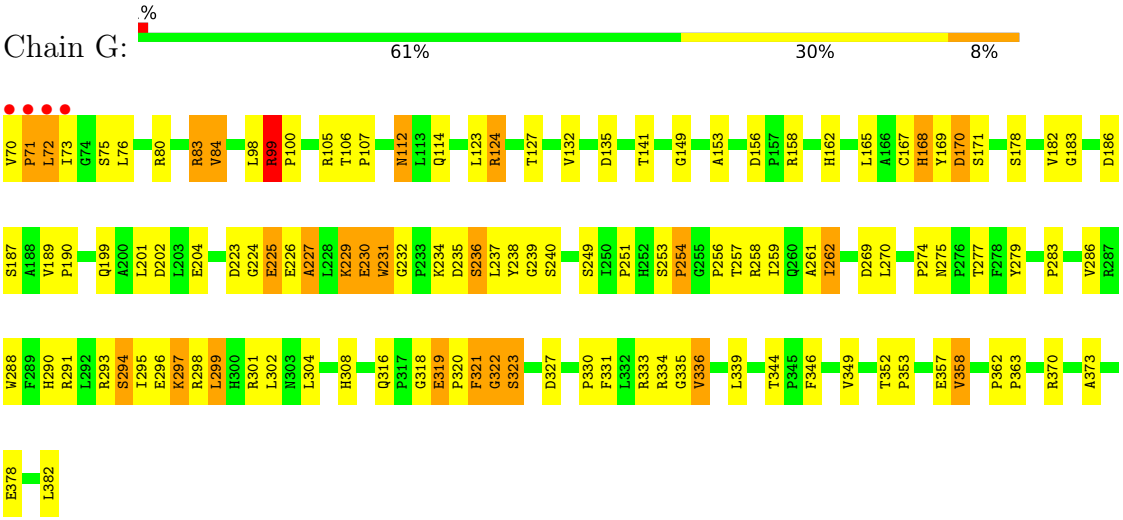
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain F:



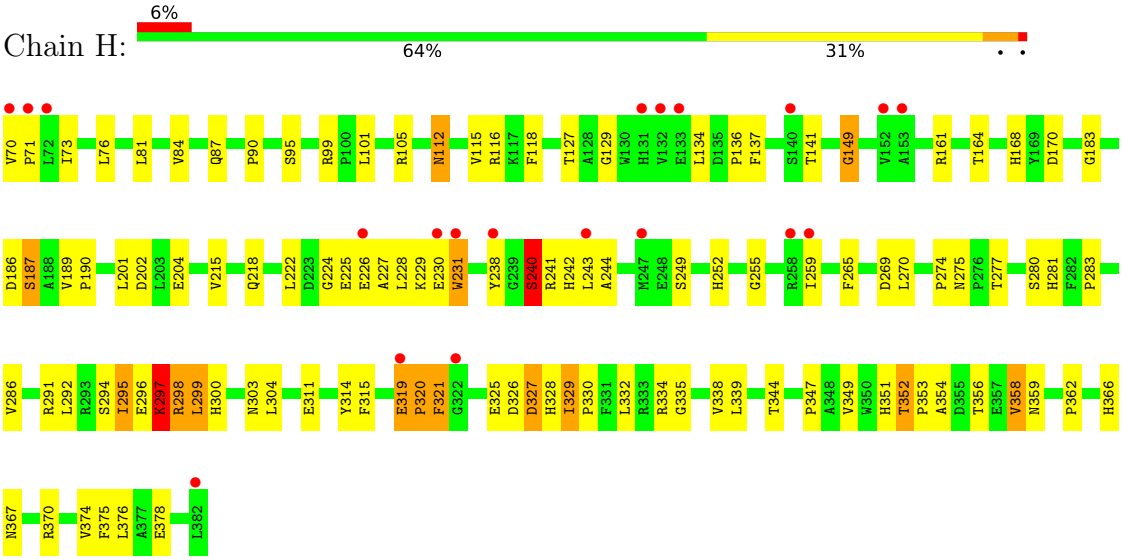
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain G:



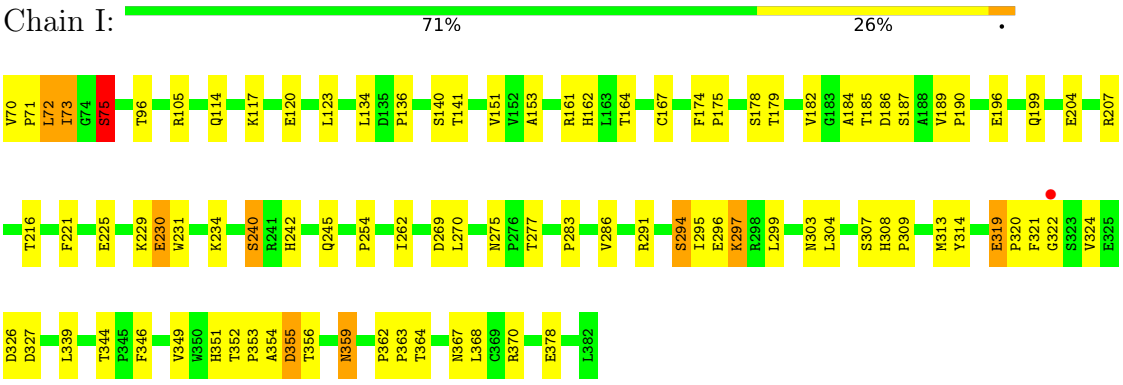
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain H:



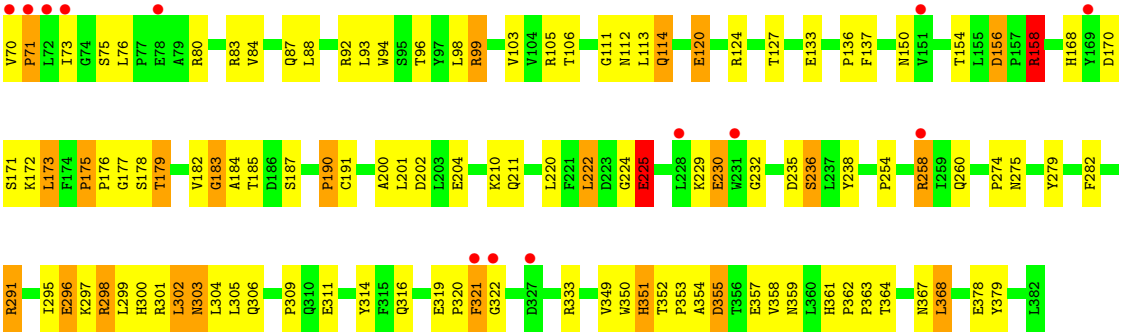
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain I:



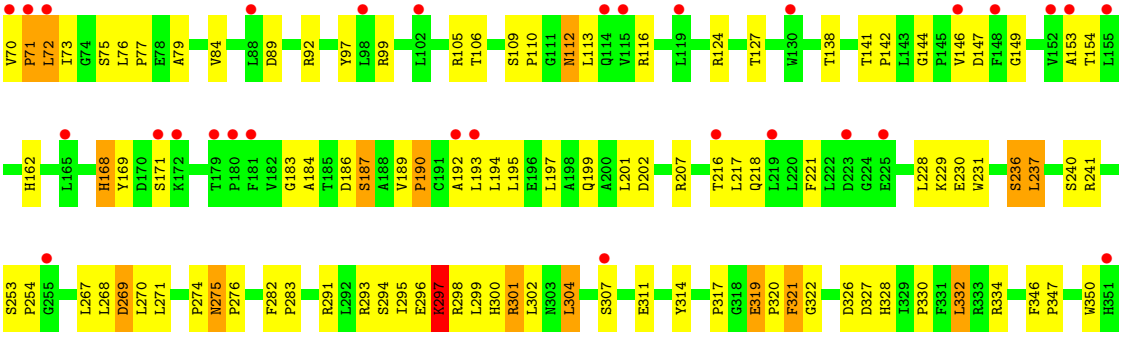
• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain J:



• Molecule 1: Glutaminyl-peptide cyclotransferase-like protein

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	125.69Å 108.01Å 159.82Å 90.00° 104.59° 90.00°	Depositor
Resolution (Å)	74.28 – 3.54 74.28 – 3.54	Depositor EDS
% Data completeness (in resolution range)	96.0 (74.28-3.54) 96.0 (74.28-3.54)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.199 , 0.280 0.202 , 0.276	Depositor DCC
R_{free} test set	1998 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å^2)	73.7	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 76.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	27526	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: ZN, A1D47

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.37	0/2550	0.61	1/3488 (0.0%)
1	B	0.36	0/2550	0.58	0/3488
1	C	0.35	0/2550	0.56	0/3488
1	D	0.35	0/2550	0.55	0/3488
1	E	0.36	0/2550	0.57	2/3488 (0.1%)
1	F	0.35	0/2550	0.58	1/3488 (0.0%)
1	G	0.35	0/2550	0.54	0/3488
1	H	0.31	0/2550	0.56	0/3488
1	I	0.37	0/2550	0.57	0/3488
1	J	0.35	0/2550	0.57	2/3488 (0.1%)
1	K	0.33	0/2550	0.54	0/3488
All	All	0.35	0/28050	0.57	6/38368 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	319	GLU	C-N-CD	-10.41	97.70	120.60
1	J	158	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	E	334	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	F	291	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	E	334	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	J	158	ARG	NE-CZ-NH2	-5.34	117.63	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2474	0	2499	54	0
1	B	2474	0	2499	81	0
1	C	2474	0	2499	79	0
1	D	2474	0	2499	60	0
1	E	2474	0	2499	95	0
1	F	2474	0	2499	73	0
1	G	2474	0	2499	95	0
1	H	2474	0	2499	101	0
1	I	2474	0	2499	62	0
1	J	2474	0	2499	99	0
1	K	2474	0	2499	79	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
3	A	27	0	0	0	0
3	B	27	0	0	0	0
3	C	27	0	0	0	0
3	D	27	0	0	0	0
3	E	27	0	0	1	0
3	F	27	0	0	1	0
3	G	27	0	0	1	0
3	H	27	0	0	1	0
3	I	27	0	0	1	0
3	J	27	0	0	0	0
3	K	27	0	0	0	0
4	A	1	0	0	1	0
4	C	2	0	0	1	0
4	E	1	0	0	0	0
All	All	27526	0	27489	849	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (849) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:THR:O	1:A:109:SER:OG	1.74	1.05
1:J:99:ARG:NH1	1:J:357:GLU:OE2	1.95	0.98
1:A:291:ARG:NH2	1:A:378:GLU:OE1	1.98	0.96
1:D:291:ARG:NH2	1:D:378:GLU:OE1	2.01	0.94
1:C:286:VAL:O	1:C:288:TRP:N	2.02	0.93
1:C:291:ARG:NH2	1:C:378:GLU:OE1	2.02	0.91
1:F:120:GLU:OE1	1:F:124:ARG:NH1	2.06	0.88
1:C:161:ARG:NH1	1:C:260:GLN:O	2.07	0.88
1:K:291:ARG:NH2	1:K:378:GLU:OE1	2.07	0.87
1:H:352:THR:O	1:H:354:ALA:N	2.10	0.85
1:E:168:HIS:NE2	1:E:187:SER:OG	2.10	0.84
1:I:184:ALA:N	1:I:355:ASP:OD1	2.11	0.83
1:K:304:LEU:O	1:K:370:ARG:NH1	2.11	0.83
1:D:175:PRO:O	1:D:178:SER:OG	1.98	0.82
1:D:297:LYS:N	1:D:298:ARG:O	2.12	0.82
1:C:176:PRO:O	1:C:178:SER:N	2.13	0.82
1:J:120:GLU:OE1	1:J:124:ARG:NH1	2.12	0.81
1:E:354:ALA:O	1:E:359:ASN:ND2	2.13	0.81
1:F:291:ARG:NH2	1:F:378:GLU:OE1	2.13	0.81
1:F:298:ARG:O	1:F:300:HIS:N	2.13	0.81
1:J:184:ALA:N	1:J:355:ASP:OD1	2.14	0.80
1:B:120:GLU:OE1	1:B:124:ARG:NH1	2.15	0.80
1:F:168:HIS:ND1	1:F:170:ASP:OD1	2.13	0.80
1:E:175:PRO:O	1:E:178:SER:OG	2.00	0.79
1:C:106:THR:O	1:C:109:SER:OG	1.99	0.79
1:K:240:SER:OG	1:K:327:ASP:OD1	2.01	0.79
1:E:120:GLU:OE1	1:E:124:ARG:NH1	2.15	0.79
1:G:124:ARG:NH2	1:G:132:VAL:O	2.15	0.78
1:K:76:LEU:O	1:K:298:ARG:NH2	2.14	0.78
1:G:304:LEU:O	1:G:370:ARG:NH1	2.16	0.78
1:E:245:GLN:HA	1:E:334:ARG:HH22	1.49	0.77
1:G:235:ASP:OD1	1:G:238:TYR:OH	2.04	0.76
1:K:301:ARG:NH2	1:K:311:GLU:OE1	2.19	0.76
1:G:99:ARG:NH1	1:G:357:GLU:OE2	2.20	0.75
1:B:204:GLU:N	1:B:204:GLU:OE1	2.19	0.74
1:H:299:LEU:O	1:H:303:ASN:N	2.21	0.74
1:I:269:ASP:OD2	3:I:402:A1D47:N23	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LYS:N	1:A:298:ARG:O	2.22	0.72
1:G:223:ASP:OD1	1:G:224:GLY:N	2.22	0.72
1:I:70:VAL:O	1:I:294:SER:OG	2.06	0.72
1:H:354:ALA:O	1:H:359:ASN:ND2	2.24	0.71
1:H:298:ARG:O	1:H:300:HIS:N	2.24	0.71
1:I:275:ASN:OD1	1:J:260:GLN:NE2	2.24	0.71
1:I:174:PHE:HE2	1:J:321:PHE:CD2	2.07	0.70
1:H:224:GLY:O	1:H:238:TYR:N	2.24	0.70
1:I:291:ARG:NH2	1:I:378:GLU:OE1	2.25	0.69
1:H:277:THR:OG1	1:H:344:THR:O	2.10	0.69
1:B:232:GLY:O	1:B:234:LYS:N	2.27	0.68
1:F:297:LYS:N	1:F:298:ARG:O	2.26	0.68
1:G:70:VAL:HG11	1:G:298:ARG:HG3	1.76	0.67
1:I:204:GLU:OE1	1:I:204:GLU:N	2.28	0.67
1:B:298:ARG:O	1:B:300:HIS:N	2.27	0.67
1:H:304:LEU:O	1:H:370:ARG:NH1	2.27	0.67
1:J:176:PRO:O	1:J:178:SER:N	2.28	0.67
1:G:319:GLU:HB3	1:G:320:PRO:CD	2.25	0.67
1:A:300:HIS:CD2	1:A:311:GLU:HA	2.31	0.66
1:E:352:THR:O	1:E:354:ALA:N	2.29	0.66
1:G:75:SER:OG	1:G:76:LEU:N	2.29	0.66
1:H:291:ARG:NH2	1:H:378:GLU:OE1	2.29	0.65
1:I:320:PRO:HB2	1:I:321:PHE:C	2.16	0.65
1:E:106:THR:O	1:E:109:SER:OG	2.14	0.65
1:A:223:ASP:OD1	1:A:224:GLY:N	2.30	0.65
1:F:297:LYS:CA	1:F:298:ARG:O	2.45	0.65
1:E:292:LEU:HD23	1:E:375:PHE:CD2	2.31	0.64
1:I:291:ARG:O	1:I:295:ILE:HG13	1.97	0.64
1:I:174:PHE:CE2	1:J:321:PHE:CD2	2.87	0.63
1:A:207:ARG:O	1:A:210:LYS:N	2.31	0.63
1:K:105:ARG:NE	1:K:169:TYR:O	2.31	0.63
1:E:127:THR:OG1	1:E:202:ASP:OD2	2.16	0.63
1:C:298:ARG:O	1:C:301:ARG:N	2.32	0.63
1:G:291:ARG:O	1:G:294:SER:OG	2.17	0.62
1:I:354:ALA:O	1:I:356:THR:N	2.32	0.62
1:B:291:ARG:NH2	1:B:378:GLU:OE1	2.25	0.62
1:G:295:ILE:O	1:G:299:LEU:HD12	1.99	0.62
1:B:374:VAL:O	1:B:377:ALA:N	2.32	0.62
1:E:292:LEU:HD12	1:E:315:PHE:CE1	2.34	0.62
1:H:127:THR:OG1	1:H:202:ASP:OD2	2.17	0.62
1:A:295:ILE:O	1:A:299:LEU:HD12	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLY:O	1:B:235:ASP:N	2.32	0.61
1:G:290:HIS:O	1:G:294:SER:OG	2.18	0.61
1:E:185:THR:O	1:E:187:SER:HA	2.01	0.61
1:I:277:THR:OG1	1:I:344:THR:O	2.18	0.61
1:K:330:PRO:O	1:K:334:ARG:NH1	2.32	0.61
1:D:291:ARG:O	1:D:295:ILE:HG12	2.01	0.61
1:B:240:SER:OG	1:B:327:ASP:OD1	2.18	0.61
1:G:298:ARG:O	1:G:301:ARG:N	2.33	0.61
1:G:319:GLU:HB3	1:G:320:PRO:HD3	1.81	0.61
1:D:240:SER:OG	1:D:327:ASP:OD1	2.19	0.61
1:C:164:THR:OG1	1:C:218:GLN:OE1	2.17	0.61
1:I:351:HIS:HB3	1:J:321:PHE:HZ	1.66	0.60
1:J:298:ARG:CG	1:J:302:LEU:HD21	2.31	0.60
1:F:156:ASP:OD1	1:F:158:ARG:NE	2.34	0.60
1:H:328:HIS:O	1:H:329:ILE:HG12	2.02	0.60
1:D:320:PRO:HB2	1:D:321:PHE:C	2.23	0.60
1:G:288:TRP:CE3	1:G:291:ARG:HD2	2.36	0.60
1:A:319:GLU:O	1:A:320:PRO:O	2.20	0.60
1:B:112:ASN:OD1	1:B:113:LEU:N	2.35	0.59
1:J:185:THR:N	1:J:355:ASP:OD1	2.34	0.59
1:B:80:ARG:O	1:B:83:ARG:N	2.35	0.59
1:E:278:PHE:HD2	1:E:315:PHE:CE1	2.21	0.59
1:J:298:ARG:O	1:J:301:ARG:N	2.36	0.59
1:G:277:THR:OG1	1:G:344:THR:O	2.19	0.59
1:F:162:HIS:N	1:F:261:ALA:O	2.36	0.59
1:H:362:PRO:O	1:H:366:HIS:ND1	2.36	0.59
1:K:377:ALA:O	1:K:381:GLY:N	2.35	0.59
1:B:291:ARG:O	1:B:295:ILE:HD12	2.03	0.58
1:B:300:HIS:ND1	1:B:311:GLU:HA	2.18	0.58
1:I:351:HIS:C	1:J:321:PHE:CE2	2.77	0.58
1:J:158:ARG:HG2	1:J:158:ARG:HH11	1.67	0.58
1:K:72:LEU:HD21	1:K:294:SER:HB3	1.85	0.58
1:I:105:ARG:NH1	1:I:182:VAL:O	2.30	0.58
1:I:229:LYS:O	1:I:230:GLU:HB2	2.03	0.58
1:C:297:LYS:HA	1:C:298:ARG:C	2.24	0.58
1:C:320:PRO:HA	1:C:321:PHE:HB2	1.83	0.58
1:F:281:HIS:HA	1:F:320:PRO:HG2	1.86	0.58
1:K:84:VAL:HG13	1:K:201:LEU:HD21	1.84	0.58
1:D:76:LEU:O	1:D:298:ARG:NH2	2.36	0.58
1:E:304:LEU:O	1:E:370:ARG:NH1	2.36	0.58
1:E:245:GLN:HA	1:E:334:ARG:NH2	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:291:ARG:NH2	1:J:378:GLU:OE1	2.36	0.58
1:A:296:GLU:O	1:A:297:LYS:HG3	2.04	0.58
1:G:83:ARG:NH2	1:G:204:GLU:OE2	2.37	0.58
1:G:232:GLY:O	1:G:236:SER:OG	2.21	0.58
1:G:298:ARG:HB3	1:G:302:LEU:HG	1.85	0.58
1:H:332:LEU:O	1:H:335:GLY:N	2.30	0.58
1:A:141:THR:O	1:A:144:GLY:N	2.37	0.58
1:H:240:SER:OG	1:H:327:ASP:OD1	2.09	0.58
1:I:242:HIS:O	1:I:245:GLN:N	2.36	0.58
1:D:156:ASP:OD1	1:D:158:ARG:NE	2.34	0.57
1:D:300:HIS:ND1	1:D:311:GLU:HA	2.19	0.57
1:H:101:LEU:O	1:H:105:ARG:NH1	2.36	0.57
1:H:296:GLU:O	1:H:297:LYS:CG	2.52	0.57
1:H:87:GLN:NE2	1:H:204:GLU:OE2	2.36	0.57
1:A:72:LEU:HD11	1:A:294:SER:CB	2.35	0.57
1:G:240:SER:OG	1:G:327:ASP:OD1	2.23	0.57
1:I:320:PRO:HA	1:I:321:PHE:HB2	1.85	0.57
1:G:169:TYR:N	1:G:225:GLU:OE2	2.37	0.57
1:D:162:HIS:HB3	1:D:216:THR:HG22	1.87	0.57
1:C:115:VAL:O	1:C:118:PHE:N	2.37	0.57
1:C:295:ILE:O	1:C:297:LYS:N	2.37	0.57
1:F:297:LYS:HA	1:F:298:ARG:O	2.04	0.57
1:G:168:HIS:ND1	1:G:225:GLU:HB3	2.20	0.57
1:H:320:PRO:HA	1:H:321:PHE:HB2	1.86	0.57
1:F:374:VAL:HG13	1:F:378:GLU:OE2	2.05	0.57
1:K:189:VAL:O	1:K:192:ALA:N	2.36	0.57
1:E:300:HIS:NE2	1:E:308:HIS:O	2.38	0.56
1:G:73:ILE:HG23	1:G:291:ARG:NH2	2.20	0.56
1:H:296:GLU:O	1:H:297:LYS:HG2	2.05	0.56
1:E:320:PRO:HA	1:E:321:PHE:HB2	1.87	0.56
1:F:300:HIS:ND1	1:F:311:GLU:HA	2.20	0.56
1:J:232:GLY:O	1:J:236:SER:OG	2.16	0.56
1:B:320:PRO:HA	1:B:321:PHE:CB	2.36	0.56
1:C:135:ASP:OD2	1:C:242:HIS:ND1	2.33	0.56
1:G:72:LEU:HD12	1:G:291:ARG:HE	1.70	0.56
1:G:105:ARG:NH1	1:G:182:VAL:O	2.37	0.56
1:G:291:ARG:O	1:G:294:SER:N	2.38	0.56
1:K:347:PRO:O	1:K:350:TRP:N	2.38	0.56
1:B:135:ASP:HB3	1:B:150:ASN:HB2	1.87	0.56
1:H:189:VAL:HB	1:H:190:PRO:HD3	1.87	0.56
1:C:72:LEU:HD11	1:C:291:ARG:HA	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:THR:C	1:E:354:ALA:H	2.08	0.56
1:C:323:SER:OG	1:C:324:VAL:N	2.36	0.56
1:F:168:HIS:CD2	1:F:187:SER:OG	2.59	0.56
1:H:240:SER:O	1:H:242:HIS:N	2.39	0.56
1:K:149:GLY:O	1:K:169:TYR:OH	2.12	0.56
1:K:142:PRO:HB2	1:K:229:LYS:HD2	1.88	0.56
1:A:319:GLU:HB3	1:A:320:PRO:HD3	1.87	0.56
1:B:105:ARG:NE	1:B:169:TYR:O	2.38	0.55
1:J:305:LEU:HA	1:J:367:ASN:OD1	2.06	0.55
1:B:70:VAL:N	1:B:71:PRO:CD	2.69	0.55
1:E:302:LEU:CD2	1:E:304:LEU:HD12	2.36	0.55
1:H:328:HIS:O	1:H:330:PRO:HD3	2.06	0.55
1:A:127:THR:OG1	1:A:202:ASP:OD2	2.22	0.55
1:J:302:LEU:HD23	1:J:302:LEU:N	2.22	0.55
1:G:331:PHE:HB3	1:G:336:VAL:HG21	1.89	0.55
1:K:71:PRO:C	1:K:72:LEU:HD23	2.26	0.55
1:G:187:SER:HB3	1:G:190:PRO:HG2	1.89	0.55
1:G:199:GLN:O	1:G:202:ASP:N	2.36	0.55
1:G:237:LEU:HD22	1:G:327:ASP:HA	1.89	0.54
1:H:204:GLU:OE1	1:H:204:GLU:N	2.37	0.54
1:H:332:LEU:C	1:H:332:LEU:HD23	2.27	0.54
1:B:151:VAL:HB	1:B:221:PHE:HB2	1.89	0.54
1:G:251:PRO:HA	1:G:257:THR:HA	1.89	0.54
1:H:186:ASP:HB2	1:H:270:LEU:CD2	2.38	0.54
1:E:162:HIS:HB3	1:E:216:THR:HG22	1.88	0.54
1:F:216:THR:OG1	1:F:217:LEU:N	2.40	0.54
1:K:199:GLN:O	1:K:202:ASP:N	2.34	0.54
1:C:105:ARG:NE	1:C:169:TYR:O	2.39	0.54
1:E:151:VAL:HB	1:E:221:PHE:HB2	1.89	0.54
1:K:89:ASP:HB3	1:K:92:ARG:HB3	1.89	0.54
1:G:70:VAL:N	1:G:71:PRO:HD2	2.23	0.54
1:G:229:LYS:O	1:G:230:GLU:HB2	2.08	0.54
1:B:127:THR:OG1	1:B:202:ASP:OD2	2.24	0.54
1:H:326:ASP:OD1	1:H:327:ASP:N	2.37	0.54
1:I:70:VAL:HB	1:I:71:PRO:CD	2.37	0.54
1:K:142:PRO:HB2	1:K:229:LYS:CD	2.38	0.54
1:G:107:PRO:HA	1:G:112:ASN:OD1	2.08	0.54
1:A:270:LEU:HD12	1:A:346:PHE:CD1	2.43	0.53
1:F:165:LEU:HD23	1:F:266:MET:HB3	1.89	0.53
1:C:287:ARG:O	1:C:291:ARG:N	2.40	0.53
1:D:76:LEU:HG	1:D:378:GLU:HG3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:ASP:HA	1:G:238:TYR:OH	2.08	0.53
1:H:294:SER:O	1:H:296:GLU:N	2.41	0.53
1:J:168:HIS:CD2	1:J:225:GLU:HG3	2.42	0.53
1:C:281:HIS:HA	1:C:320:PRO:HG3	1.91	0.53
1:I:70:VAL:O	1:I:294:SER:CB	2.57	0.53
1:I:71:PRO:HB2	1:I:75:SER:OG	2.09	0.53
1:J:105:ARG:NH1	1:J:171:SER:OG	2.42	0.53
1:F:162:HIS:HB3	1:F:216:THR:HG23	1.90	0.53
1:D:350:TRP:O	1:D:352:THR:OG1	2.18	0.53
1:I:189:VAL:HB	1:I:190:PRO:HD3	1.89	0.53
1:J:156:ASP:OD1	1:J:158:ARG:NE	2.42	0.53
1:C:367:ASN:O	1:C:370:ARG:N	2.42	0.53
1:C:103:VAL:O	1:C:105:ARG:HG2	2.09	0.53
1:C:297:LYS:HE2	1:C:312:VAL:HG23	1.90	0.53
1:A:76:LEU:HG	1:A:378:GLU:HG3	1.90	0.52
1:H:300:HIS:ND1	1:H:311:GLU:HA	2.24	0.52
1:I:319:GLU:CG	1:I:320:PRO:HD2	2.39	0.52
1:C:223:ASP:OD1	1:C:224:GLY:N	2.42	0.52
1:H:297:LYS:N	1:H:298:ARG:O	2.41	0.52
1:I:240:SER:OG	1:I:327:ASP:OD1	2.25	0.52
1:B:184:ALA:N	1:B:355:ASP:OD1	2.41	0.52
1:E:163:LEU:HD12	1:E:164:THR:H	1.74	0.52
1:F:304:LEU:O	1:F:370:ARG:NH1	2.43	0.52
1:G:349:VAL:O	1:G:352:THR:OG1	2.26	0.52
1:A:293:ARG:HG3	1:A:315:PHE:O	2.09	0.52
1:K:319:GLU:HG2	1:K:320:PRO:O	2.09	0.52
1:B:189:VAL:HB	1:B:190:PRO:HD3	1.91	0.52
1:G:168:HIS:CD2	1:G:187:SER:HG	2.28	0.52
1:I:70:VAL:HG12	1:I:71:PRO:HD3	1.91	0.52
1:A:296:GLU:OE2	1:A:308:HIS:NE2	2.43	0.52
1:C:225:GLU:HG2	1:C:237:LEU:HD23	1.91	0.52
1:J:298:ARG:HG3	1:J:302:LEU:HD21	1.90	0.52
1:K:72:LEU:HD21	1:K:294:SER:CB	2.40	0.52
1:H:352:THR:C	1:H:354:ALA:H	2.12	0.52
1:I:72:LEU:HG	1:I:291:ARG:NH1	2.24	0.52
1:A:70:VAL:N	1:A:71:PRO:CD	2.73	0.52
1:B:199:GLN:O	1:B:202:ASP:HB2	2.10	0.52
1:E:289:PHE:HE1	1:E:315:PHE:HB3	1.74	0.52
1:J:105:ARG:CZ	1:J:171:SER:OG	2.58	0.52
1:E:115:VAL:O	1:E:118:PHE:N	2.43	0.52
1:C:250:ILE:HG21	1:C:258:ARG:HD2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:352:THR:HG21	1:J:282:PHE:CD1	2.45	0.51
1:A:297:LYS:CA	1:A:298:ARG:O	2.57	0.51
1:C:162:HIS:HB3	1:C:216:THR:HG22	1.92	0.51
1:C:176:PRO:O	1:C:178:SER:OG	2.28	0.51
1:B:116:ARG:HD3	1:B:149:GLY:O	2.11	0.51
1:C:70:VAL:N	1:C:71:PRO:CD	2.73	0.51
1:H:170:ASP:OD2	1:H:225:GLU:N	2.38	0.51
1:J:298:ARG:HB2	1:J:302:LEU:CD2	2.41	0.51
1:E:224:GLY:O	1:E:238:TYR:N	2.44	0.51
1:F:70:VAL:HG13	1:F:298:ARG:HD3	1.92	0.51
1:B:292:LEU:HA	1:B:295:ILE:HD12	1.92	0.51
1:F:257:THR:OG1	1:F:260:GLN:NE2	2.31	0.51
1:C:286:VAL:HG22	1:C:287:ARG:H	1.75	0.51
1:H:325:GLU:HB2	3:H:402:A1D47:C10	2.41	0.51
1:E:320:PRO:HB2	1:E:321:PHE:C	2.31	0.51
1:F:291:ARG:NH2	1:F:378:GLU:CD	2.64	0.51
1:G:259:ILE:O	1:G:262:ILE:HG13	2.11	0.51
1:I:283:PRO:O	1:I:286:VAL:HG12	2.10	0.51
1:C:101:LEU:O	1:C:105:ARG:NH1	2.43	0.51
1:K:320:PRO:HA	1:K:321:PHE:HB3	1.93	0.51
1:A:135:ASP:HB3	1:A:150:ASN:HB2	1.93	0.50
1:J:364:THR:O	1:J:368:LEU:N	2.44	0.50
1:G:162:HIS:CE1	1:G:262:ILE:HG12	2.46	0.50
1:I:297:LYS:HG2	1:I:297:LYS:O	2.10	0.50
1:C:253:SER:HA	1:C:254:PRO:C	2.32	0.50
1:D:293:ARG:O	1:D:296:GLU:O	2.29	0.50
1:D:296:GLU:O	1:D:297:LYS:HG3	2.12	0.50
1:F:295:ILE:O	1:F:299:LEU:HD12	2.11	0.50
1:G:70:VAL:O	1:G:71:PRO:C	2.50	0.50
1:J:103:VAL:C	1:J:182:VAL:HG12	2.32	0.50
1:E:178:SER:HA	1:K:321:PHE:CE1	2.46	0.50
1:G:298:ARG:O	1:G:302:LEU:N	2.35	0.50
1:H:295:ILE:O	1:H:295:ILE:HG22	2.11	0.50
1:B:250:ILE:HD13	1:D:140:SER:OG	2.11	0.50
1:D:298:ARG:O	1:D:299:LEU:HB2	2.12	0.50
1:K:237:LEU:HD11	1:K:326:ASP:O	2.11	0.50
1:C:89:ASP:HB3	1:C:92:ARG:HB3	1.93	0.50
1:E:245:GLN:CA	1:E:334:ARG:HH22	2.21	0.50
1:H:298:ARG:HB3	1:H:299:LEU:HD12	1.94	0.50
1:J:204:GLU:OE1	1:J:204:GLU:N	2.37	0.50
1:J:235:ASP:O	1:J:236:SER:HB3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:TYR:C	1:E:289:PHE:HE2	2.14	0.50
1:F:166:ALA:HB1	1:F:220:LEU:HB2	1.93	0.50
1:G:295:ILE:HG22	1:G:299:LEU:CD1	2.41	0.50
1:I:304:LEU:O	1:I:370:ARG:NH1	2.44	0.50
1:J:87:GLN:NE2	1:J:204:GLU:OE2	2.41	0.50
1:F:189:VAL:HB	1:F:190:PRO:HD3	1.94	0.49
1:G:291:ARG:O	1:G:295:ILE:HD12	2.12	0.49
1:I:151:VAL:HB	1:I:221:PHE:HB2	1.93	0.49
1:J:156:ASP:OD1	1:J:158:ARG:CZ	2.59	0.49
1:J:229:LYS:O	1:J:230:GLU:CB	2.60	0.49
1:B:138:THR:OG1	1:B:147:ASP:OD1	2.14	0.49
1:E:291:ARG:NH2	1:E:378:GLU:HB3	2.27	0.49
1:G:156:ASP:OD1	1:G:158:ARG:NE	2.45	0.49
1:H:76:LEU:HD12	1:H:374:VAL:HG13	1.93	0.49
1:H:329:ILE:HB	1:H:330:PRO:HD3	1.95	0.49
1:I:162:HIS:HB3	1:I:216:THR:HG22	1.94	0.49
1:A:319:GLU:CB	1:A:320:PRO:HD3	2.41	0.49
1:A:331:PHE:O	1:A:336:VAL:HG23	2.12	0.49
1:A:364:THR:O	1:A:368:LEU:HG	2.13	0.49
1:B:149:GLY:O	1:B:223:ASP:HB2	2.12	0.49
1:B:320:PRO:HB2	1:B:321:PHE:C	2.32	0.49
1:C:297:LYS:O	1:C:297:LYS:HG2	2.12	0.49
1:G:322:GLY:O	1:G:323:SER:CB	2.61	0.49
1:B:112:ASN:O	1:B:115:VAL:N	2.39	0.49
1:E:156:ASP:OD1	1:E:158:ARG:NE	2.44	0.49
1:E:278:PHE:CD2	1:E:315:PHE:CE1	3.01	0.49
1:J:156:ASP:OD1	1:J:158:ARG:HD3	2.12	0.49
1:E:304:LEU:HD23	1:E:370:ARG:NH1	2.28	0.49
1:H:244:ALA:C	1:H:334:ARG:NH1	2.66	0.49
1:H:358:VAL:HG22	1:H:358:VAL:O	2.13	0.49
1:H:294:SER:O	1:H:298:ARG:HB2	2.13	0.49
1:H:319:GLU:HG2	1:H:320:PRO:N	2.27	0.49
1:J:92:ARG:O	1:J:96:THR:HB	2.12	0.49
1:B:320:PRO:HA	1:B:321:PHE:HB2	1.95	0.48
1:D:297:LYS:CA	1:D:298:ARG:O	2.61	0.48
1:D:372:LEU:O	1:D:375:PHE:N	2.46	0.48
1:E:358:VAL:O	1:E:360:LEU:N	2.45	0.48
1:F:76:LEU:HG	1:F:378:GLU:CD	2.32	0.48
1:F:293:ARG:O	1:F:296:GLU:O	2.30	0.48
1:B:135:ASP:OD2	1:B:242:HIS:ND1	2.45	0.48
1:H:281:HIS:HA	1:H:320:PRO:CD	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:366:HIS:O	1:K:369:CYS:N	2.46	0.48
1:A:291:ARG:O	1:A:295:ILE:HG13	2.13	0.48
1:E:304:LEU:O	1:E:305:LEU:HD23	2.13	0.48
1:F:253:SER:HA	1:F:254:PRO:C	2.34	0.48
1:F:298:ARG:HA	1:F:301:ARG:HG3	1.95	0.48
1:G:327:ASP:O	1:G:330:PRO:HD2	2.14	0.48
1:B:319:GLU:HG2	1:B:320:PRO:HD2	1.96	0.48
1:D:228:LEU:O	1:D:229:LYS:HE2	2.13	0.48
1:F:270:LEU:HD12	1:F:346:PHE:CD1	2.48	0.48
1:J:279:TYR:CE1	1:J:316:GLN:HB2	2.48	0.48
1:J:306:GLN:N	1:J:367:ASN:HD21	2.11	0.48
1:K:113:LEU:HD11	1:K:116:ARG:CZ	2.43	0.48
1:H:295:ILE:O	1:H:299:LEU:CD1	2.61	0.48
1:B:227:ALA:HB2	1:B:235:ASP:O	2.14	0.48
1:D:113:LEU:HD11	1:D:117:LYS:HD3	1.96	0.48
1:E:162:HIS:N	1:E:261:ALA:O	2.43	0.48
1:E:296:GLU:O	1:E:297:LYS:HB3	2.14	0.48
1:E:253:SER:HA	1:E:254:PRO:C	2.34	0.48
1:A:76:LEU:HD22	1:A:80:ARG:HD2	1.96	0.48
1:B:358:VAL:HG22	1:B:358:VAL:O	2.14	0.48
1:C:72:LEU:HD13	1:C:291:ARG:CZ	2.43	0.48
1:E:231:TRP:CD1	1:E:232:GLY:N	2.82	0.48
1:H:265:PHE:HB3	1:H:338:VAL:HG22	1.95	0.48
1:A:279:TYR:CE1	1:A:316:GLN:HB2	2.49	0.48
1:A:319:GLU:HG2	1:A:320:PRO:N	2.29	0.47
1:E:184:ALA:O	1:E:188:ALA:HB3	2.14	0.47
1:G:127:THR:OG1	1:G:202:ASP:OD2	2.24	0.47
1:H:297:LYS:HA	1:H:298:ARG:O	2.14	0.47
1:J:168:HIS:HA	1:J:222:LEU:O	2.13	0.47
1:J:172:LYS:NZ	1:J:173:LEU:O	2.47	0.47
1:D:80:ARG:O	1:D:83:ARG:N	2.47	0.47
1:E:93:LEU:HG	1:E:196:GLU:HB2	1.97	0.47
1:H:295:ILE:O	1:H:299:LEU:HD13	2.14	0.47
1:K:142:PRO:CB	1:K:229:LYS:HD3	2.44	0.47
1:K:298:ARG:O	1:K:302:LEU:HG	2.14	0.47
1:B:187:SER:HB2	1:B:190:PRO:HG2	1.97	0.47
1:K:70:VAL:N	1:K:71:PRO:CD	2.77	0.47
1:H:168:HIS:CD2	1:H:225:GLU:OE1	2.68	0.47
1:J:300:HIS:O	1:J:303:ASN:N	2.44	0.47
1:G:72:LEU:CD1	1:G:291:ARG:HE	2.27	0.47
1:G:189:VAL:HB	1:G:190:PRO:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:295:ILE:CG2	1:H:299:LEU:HD11	2.45	0.47
1:H:351:HIS:O	1:H:352:THR:HG23	2.15	0.47
1:B:76:LEU:HG	1:B:378:GLU:HG3	1.97	0.47
1:C:286:VAL:HG13	1:C:287:ARG:N	2.30	0.47
1:C:298:ARG:O	1:C:299:LEU:C	2.52	0.47
1:E:82:ARG:CZ	1:E:302:LEU:HD21	2.45	0.47
1:E:277:THR:OG1	1:E:344:THR:O	2.31	0.47
1:G:72:LEU:HD21	1:G:378:GLU:CD	2.35	0.47
1:G:269:ASP:OD2	3:G:402:A1D47:N23	2.48	0.47
1:I:352:THR:HG21	1:J:282:PHE:CE1	2.50	0.47
1:J:158:ARG:HD3	1:J:158:ARG:H	1.80	0.47
1:J:235:ASP:OD1	1:J:238:TYR:OH	2.20	0.47
1:A:141:THR:HB	1:A:238:TYR:OH	2.15	0.47
1:A:223:ASP:O	1:A:239:GLY:HA3	2.14	0.47
1:E:297:LYS:HA	1:E:298:ARG:C	2.35	0.47
1:E:377:ALA:HA	1:E:382:LEU:HD12	1.97	0.47
1:J:354:ALA:O	1:J:359:ASN:ND2	2.47	0.47
1:K:217:LEU:HD13	1:K:380:LEU:HD11	1.97	0.47
1:K:236:SER:O	1:K:241:ARG:NE	2.47	0.47
1:C:319:GLU:HG3	1:C:320:PRO:CD	2.45	0.47
1:F:74:GLY:O	1:F:378:GLU:HG2	2.14	0.47
1:G:362:PRO:HB2	1:G:363:PRO:HD3	1.97	0.47
1:H:76:LEU:HG	1:H:378:GLU:CG	2.44	0.47
1:K:168:HIS:O	1:K:187:SER:HB2	2.15	0.47
1:D:70:VAL:HG22	1:D:298:ARG:HG2	1.97	0.47
1:H:164:THR:HA	1:H:218:GLN:O	2.15	0.47
1:I:270:LEU:CD1	1:I:346:PHE:CD1	2.98	0.47
1:I:320:PRO:HB2	1:I:322:GLY:N	2.30	0.47
1:J:300:HIS:ND1	1:J:311:GLU:HA	2.30	0.47
1:A:359:ASN:OD1	1:D:333:ARG:HA	2.14	0.46
1:E:367:ASN:O	1:E:370:ARG:N	2.47	0.46
1:I:189:VAL:HB	1:I:190:PRO:CD	2.45	0.46
1:J:302:LEU:HD23	1:J:302:LEU:H	1.80	0.46
1:C:319:GLU:HG3	1:C:320:PRO:HG2	1.97	0.46
1:D:350:TRP:O	1:D:352:THR:N	2.48	0.46
1:G:80:ARG:NH1	1:G:382:LEU:OXT	2.48	0.46
1:H:90:PRO:HB3	1:H:366:HIS:CD2	2.51	0.46
1:J:175:PRO:HB3	1:J:176:PRO:HD2	1.97	0.46
1:K:275:ASN:OD1	1:K:275:ASN:N	2.49	0.46
1:F:135:ASP:HB3	1:F:150:ASN:HB2	1.97	0.46
1:F:349:VAL:O	1:F:352:THR:HG23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:296:GLU:OE2	1:G:308:HIS:NE2	2.46	0.46
1:G:370:ARG:O	1:G:373:ALA:HB3	2.15	0.46
1:H:294:SER:O	1:H:298:ARG:HG2	2.15	0.46
1:H:328:HIS:O	1:H:329:ILE:CG1	2.64	0.46
1:H:328:HIS:CE1	1:H:329:ILE:HD13	2.50	0.46
1:A:137:PHE:CE1	1:A:148:PHE:HB2	2.49	0.46
1:C:321:PHE:O	1:F:353:PRO:HG2	2.15	0.46
1:D:126:LEU:O	1:I:117:LYS:NZ	2.44	0.46
1:D:135:ASP:HB3	1:D:150:ASN:HB2	1.97	0.46
1:F:139:ALA:HB3	1:F:148:PHE:HE2	1.79	0.46
1:G:168:HIS:HD2	1:G:168:HIS:O	1.99	0.46
1:H:296:GLU:O	1:H:297:LYS:CB	2.63	0.46
1:B:116:ARG:CD	1:B:169:TYR:OH	2.64	0.46
1:B:141:THR:O	1:B:144:GLY:N	2.47	0.46
1:B:208:ALA:HB1	1:B:213:ALA:HB2	1.96	0.46
1:D:189:VAL:HB	1:D:190:PRO:HD3	1.96	0.46
1:F:166:ALA:CB	1:F:220:LEU:HB2	2.45	0.46
1:J:75:SER:HA	1:J:291:ARG:HH22	1.81	0.46
1:C:107:PRO:HB3	1:C:148:PHE:CE2	2.50	0.46
1:C:115:VAL:O	1:C:116:ARG:C	2.54	0.46
1:E:292:LEU:CD1	1:E:315:PHE:CZ	2.99	0.46
1:E:330:PRO:O	1:E:334:ARG:HD3	2.15	0.46
1:F:88:LEU:O	1:F:90:PRO:HD3	2.15	0.46
1:G:283:PRO:O	1:G:286:VAL:HG12	2.15	0.46
1:H:292:LEU:HD13	1:H:315:PHE:CE1	2.50	0.46
1:E:70:VAL:N	1:E:71:PRO:CD	2.79	0.46
1:K:97:TYR:HB3	1:K:195:LEU:HD12	1.98	0.46
1:K:197:LEU:HD22	1:K:376:LEU:HD12	1.98	0.46
1:K:296:GLU:OE2	1:K:314:TYR:HB2	2.15	0.46
1:E:300:HIS:ND1	1:E:311:GLU:HA	2.31	0.46
1:J:80:ARG:HG2	1:J:83:ARG:NH1	2.30	0.46
1:K:109:SER:HB2	1:K:110:PRO:HD2	1.97	0.46
1:K:275:ASN:N	1:K:276:PRO:CD	2.79	0.46
1:H:81:LEU:HD13	1:H:298:ARG:NH2	2.31	0.46
1:B:352:THR:C	1:B:354:ALA:N	2.69	0.46
1:G:279:TYR:CE1	1:G:316:GLN:HB2	2.50	0.46
1:J:106:THR:CB	1:J:173:LEU:HD12	2.46	0.46
1:K:253:SER:HA	1:K:254:PRO:C	2.36	0.46
1:K:268:LEU:HD23	1:K:271:LEU:CD1	2.46	0.46
1:C:160:ALA:HB1	1:C:254:PRO:HD2	1.98	0.45
1:C:162:HIS:HB3	1:C:216:THR:CG2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:GLU:O	1:C:297:LYS:HB3	2.16	0.45
1:E:235:ASP:HA	1:E:238:TYR:OH	2.16	0.45
1:E:280:SER:HB2	1:E:289:PHE:CD2	2.51	0.45
1:F:83:ARG:NH2	1:F:204:GLU:OE2	2.49	0.45
1:G:294:SER:O	1:G:297:LYS:O	2.33	0.45
1:H:70:VAL:N	1:H:71:PRO:HD3	2.30	0.45
1:B:178:SER:O	1:B:179:THR:C	2.55	0.45
1:B:275:ASN:ND2	1:F:260:GLN:OE1	2.43	0.45
1:C:364:THR:O	1:C:368:LEU:HG	2.17	0.45
1:D:70:VAL:N	1:D:71:PRO:HD3	2.31	0.45
1:D:319:GLU:CB	1:D:320:PRO:CD	2.94	0.45
1:F:71:PRO:C	1:F:72:LEU:HD23	2.36	0.45
1:H:240:SER:O	1:H:243:LEU:N	2.49	0.45
1:I:73:ILE:HD12	1:I:73:ILE:H	1.80	0.45
1:K:270:LEU:HD12	1:K:346:PHE:CD1	2.51	0.45
1:B:113:LEU:O	1:B:113:LEU:HD12	2.17	0.45
1:E:240:SER:HB2	1:E:330:PRO:HG2	1.97	0.45
1:H:70:VAL:N	1:H:71:PRO:CD	2.78	0.45
1:J:76:LEU:HG	1:J:378:GLU:HG3	1.98	0.45
1:J:295:ILE:O	1:J:297:LYS:N	2.49	0.45
1:K:296:GLU:HB2	1:K:371:ILE:HD13	1.98	0.45
1:D:216:THR:HG23	1:D:217:LEU:N	2.31	0.45
1:D:291:ARG:C	1:D:295:ILE:HG12	2.35	0.45
1:E:297:LYS:HB2	1:E:300:HIS:CB	2.47	0.45
1:F:320:PRO:HB3	1:F:321:PHE:C	2.36	0.45
1:G:112:ASN:C	1:G:112:ASN:HD22	2.18	0.45
1:G:237:LEU:CD2	1:G:327:ASP:HA	2.45	0.45
1:H:84:VAL:HG13	1:H:201:LEU:HD21	1.97	0.45
1:H:280:SER:O	1:H:320:PRO:HD2	2.15	0.45
1:I:351:HIS:O	1:J:321:PHE:CZ	2.69	0.45
1:J:84:VAL:HG13	1:J:201:LEU:HD21	1.98	0.45
1:A:225:GLU:HG3	1:A:327:ASP:OD2	2.16	0.45
1:D:367:ASN:O	1:D:370:ARG:N	2.48	0.45
1:I:123:LEU:HD13	1:I:153:ALA:CB	2.47	0.45
1:I:185:THR:N	1:I:355:ASP:OD1	2.48	0.45
1:K:146:VAL:HG12	1:K:147:ASP:N	2.31	0.45
1:C:321:PHE:HA	1:F:178:SER:HA	1.98	0.45
1:D:291:ARG:O	1:D:295:ILE:N	2.50	0.45
1:G:331:PHE:O	1:G:336:VAL:HG22	2.17	0.45
1:I:359:ASN:ND2	1:J:333:ARG:HA	2.32	0.45
1:J:70:VAL:N	1:J:71:PRO:CD	2.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:350:TRP:O	1:J:351:HIS:C	2.55	0.45
1:K:106:THR:O	1:K:112:ASN:HB3	2.16	0.45
1:A:350:TRP:CD1	1:A:351:HIS:CD2	3.05	0.45
1:C:287:ARG:O	1:C:290:HIS:HB2	2.16	0.45
1:D:377:ALA:O	1:D:381:GLY:N	2.50	0.45
1:E:186:ASP:HB2	1:E:270:LEU:CD2	2.46	0.45
1:F:97:TYR:O	1:F:101:LEU:HD12	2.16	0.45
1:H:291:ARG:HH22	1:H:378:GLU:CB	2.30	0.45
1:B:137:PHE:CE1	1:B:148:PHE:HB2	2.52	0.45
1:B:155:LEU:O	1:B:209:LYS:HE3	2.17	0.45
1:C:76:LEU:HG	1:C:378:GLU:HG2	1.98	0.45
1:C:94:TRP:CH2	1:C:362:PRO:HG3	2.52	0.45
1:C:252:HIS:O	1:C:255:GLY:HA3	2.16	0.45
1:J:80:ARG:O	1:J:84:VAL:HG23	2.17	0.45
1:K:293:ARG:HH12	1:K:317:PRO:N	2.15	0.45
1:B:292:LEU:HG	1:B:375:PHE:CD2	2.51	0.45
1:E:299:LEU:HB2	1:E:305:LEU:HD11	1.98	0.45
1:B:309:PRO:HG2	1:F:256:PRO:HG3	1.99	0.45
1:D:350:TRP:O	1:D:351:HIS:C	2.55	0.45
1:E:168:HIS:CD2	1:E:187:SER:OG	2.69	0.45
1:E:320:PRO:HA	1:E:321:PHE:CB	2.46	0.45
1:G:253:SER:HA	1:G:254:PRO:C	2.37	0.45
1:I:174:PHE:HB3	1:I:175:PRO:CD	2.47	0.45
1:J:235:ASP:HA	1:J:238:TYR:OH	2.16	0.45
1:K:186:ASP:HB2	1:K:270:LEU:HD22	1.98	0.45
1:E:207:ARG:N	1:E:207:ARG:HD2	2.33	0.44
1:H:265:PHE:O	1:H:338:VAL:HA	2.17	0.44
1:H:292:LEU:HG	1:H:375:PHE:CD2	2.52	0.44
1:J:168:HIS:CG	1:J:225:GLU:HG3	2.52	0.44
1:K:153:ALA:O	1:K:218:GLN:HA	2.17	0.44
1:C:84:VAL:HG13	1:C:201:LEU:HD21	1.98	0.44
1:C:366:HIS:O	1:C:369:CYS:HB3	2.17	0.44
1:D:298:ARG:CG	1:D:298:ARG:HH11	2.31	0.44
1:E:353:PRO:CD	1:K:321:PHE:O	2.65	0.44
1:G:98:LEU:O	1:G:99:ARG:C	2.56	0.44
1:H:291:ARG:NH2	1:H:378:GLU:HB3	2.33	0.44
1:A:349:VAL:HG21	1:A:355:ASP:HA	1.98	0.44
1:B:168:HIS:ND1	1:B:187:SER:OG	2.47	0.44
1:E:158:ARG:NH2	1:E:209:LYS:O	2.50	0.44
1:E:216:THR:HG23	1:E:217:LEU:N	2.31	0.44
1:E:358:VAL:HG22	1:E:359:ASN:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:TRP:CE3	3:F:402:A1D47:O01	2.70	0.44
1:G:84:VAL:HG13	1:G:201:LEU:HD21	1.99	0.44
1:G:170:ASP:OD1	1:G:225:GLU:HG2	2.17	0.44
1:G:297:LYS:HA	1:G:298:ARG:C	2.37	0.44
1:H:81:LEU:HD13	1:H:298:ARG:HH21	1.82	0.44
1:J:70:VAL:HG22	1:J:298:ARG:HB3	1.98	0.44
1:E:278:PHE:CE2	1:E:341:LEU:HD11	2.52	0.44
1:G:168:HIS:CD2	1:G:168:HIS:O	2.71	0.44
1:I:326:ASP:OD1	1:I:327:ASP:N	2.46	0.44
1:J:296:GLU:OE2	1:J:314:TYR:N	2.38	0.44
1:K:327:ASP:O	1:K:330:PRO:HD2	2.18	0.44
1:B:349:VAL:O	1:B:352:THR:OG1	2.36	0.44
1:C:297:LYS:CE	1:C:312:VAL:HG23	2.47	0.44
1:C:320:PRO:CB	1:C:321:PHE:C	2.86	0.44
1:D:292:LEU:HG	1:D:375:PHE:CD2	2.52	0.44
1:E:115:VAL:O	1:E:116:ARG:C	2.56	0.44
1:F:291:ARG:O	1:F:295:ILE:HG13	2.18	0.44
1:G:70:VAL:N	1:G:71:PRO:CD	2.80	0.44
1:H:226:GLU:OE1	1:H:226:GLU:HA	2.17	0.44
1:H:244:ALA:HB1	1:H:334:ARG:HH11	1.83	0.44
1:I:134:LEU:O	1:I:136:PRO:HD3	2.18	0.44
1:J:350:TRP:O	1:J:352:THR:N	2.51	0.44
1:A:320:PRO:HB2	1:A:321:PHE:C	2.37	0.44
1:B:168:HIS:CE1	1:B:187:SER:HG	2.35	0.44
1:D:137:PHE:CZ	1:D:148:PHE:HB2	2.52	0.44
1:F:172:LYS:CG	1:F:173:LEU:N	2.80	0.44
1:K:267:LEU:HD23	1:K:328:HIS:HD2	1.82	0.44
1:A:80:ARG:O	1:A:83:ARG:N	2.51	0.44
1:B:253:SER:HA	1:B:254:PRO:C	2.38	0.44
1:B:374:VAL:HG12	1:B:378:GLU:OE2	2.18	0.44
1:D:80:ARG:O	1:D:81:LEU:C	2.55	0.44
1:D:354:ALA:O	1:D:356:THR:N	2.51	0.44
1:H:295:ILE:HA	1:H:298:ARG:HG3	1.99	0.44
1:H:297:LYS:CA	1:H:298:ARG:O	2.66	0.44
1:K:142:PRO:CB	1:K:229:LYS:CD	2.96	0.44
1:B:297:LYS:HE3	1:B:312:VAL:CG2	2.48	0.44
1:G:223:ASP:O	1:G:239:GLY:HA3	2.17	0.44
1:H:330:PRO:O	1:H:334:ARG:HD2	2.18	0.44
1:J:92:ARG:O	1:J:93:LEU:C	2.56	0.44
1:K:321:PHE:CD1	1:K:322:GLY:N	2.86	0.44
1:B:282:PHE:CD1	1:G:352:THR:HG21	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ILE:HG23	1:B:374:VAL:HG11	2.00	0.44
1:F:295:ILE:HG22	1:F:299:LEU:CD1	2.48	0.44
1:G:105:ARG:NE	1:G:169:TYR:O	2.46	0.44
1:H:328:HIS:CE1	1:H:329:ILE:CD1	3.01	0.44
1:K:77:PRO:O	1:K:79:ALA:N	2.51	0.44
1:K:138:THR:OG1	1:K:147:ASP:OD1	2.19	0.44
1:K:189:VAL:HB	1:K:190:PRO:CD	2.48	0.44
1:B:179:THR:HB	1:B:353:PRO:HB3	1.99	0.43
1:B:283:PRO:O	1:B:286:VAL:HG12	2.17	0.43
1:B:297:LYS:HA	1:B:298:ARG:C	2.37	0.43
1:I:70:VAL:HB	1:I:71:PRO:HD2	2.00	0.43
1:I:362:PRO:N	1:I:363:PRO:CD	2.81	0.43
1:J:362:PRO:N	1:J:363:PRO:CD	2.81	0.43
1:K:184:ALA:HB3	1:K:360:LEU:HD21	1.99	0.43
1:K:274:PRO:HB3	1:K:361:HIS:CG	2.53	0.43
1:D:274:PRO:HB3	1:D:361:HIS:HB2	1.99	0.43
1:D:297:LYS:HD2	1:D:297:LYS:O	2.18	0.43
1:H:115:VAL:O	1:H:118:PHE:N	2.51	0.43
1:A:70:VAL:HG22	1:A:298:ARG:HG2	2.01	0.43
1:A:168:HIS:HA	1:A:222:LEU:O	2.17	0.43
1:B:352:THR:C	1:B:354:ALA:H	2.20	0.43
1:C:70:VAL:N	1:C:71:PRO:HD3	2.32	0.43
1:C:298:ARG:O	1:C:300:HIS:N	2.51	0.43
1:D:70:VAL:N	1:D:71:PRO:CD	2.80	0.43
1:E:70:VAL:N	1:E:71:PRO:HD3	2.34	0.43
1:E:168:HIS:O	1:E:187:SER:HB2	2.19	0.43
1:E:292:LEU:HD23	1:E:375:PHE:HD2	1.79	0.43
1:H:300:HIS:C	1:H:300:HIS:CD2	2.90	0.43
1:B:274:PRO:HB3	1:B:361:HIS:HB2	1.99	0.43
1:C:304:LEU:O	1:C:370:ARG:NH1	2.49	0.43
1:C:316:GLN:HB3	1:C:317:PRO:HD2	2.00	0.43
1:D:70:VAL:HG13	1:D:71:PRO:HD3	2.00	0.43
1:D:113:LEU:HD12	1:D:113:LEU:O	2.18	0.43
1:D:235:ASP:O	1:D:236:SER:HB3	2.19	0.43
1:E:127:THR:O	1:E:129:GLY:N	2.51	0.43
1:F:225:GLU:HG3	1:F:327:ASP:OD2	2.19	0.43
1:F:298:ARG:NH2	1:F:378:GLU:OE1	2.51	0.43
1:H:300:HIS:CE1	1:H:311:GLU:HA	2.53	0.43
1:J:156:ASP:CG	1:J:158:ARG:CZ	2.87	0.43
1:A:122:THR:HG21	1:A:195:LEU:HD22	2.00	0.43
1:A:235:ASP:HA	1:A:238:TYR:OH	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:HIS:O	1:B:255:GLY:HA3	2.18	0.43
1:E:278:PHE:O	1:E:279:TYR:CD1	2.72	0.43
1:F:126:LEU:HD22	1:F:199:GLN:OE1	2.18	0.43
1:F:168:HIS:HA	1:F:222:LEU:H	1.83	0.43
1:G:298:ARG:HB3	1:G:302:LEU:CG	2.48	0.43
1:I:186:ASP:N	1:I:187:SER:HA	2.34	0.43
1:J:111:GLY:O	1:J:114:GLN:N	2.52	0.43
1:J:136:PRO:O	1:J:137:PHE:HB3	2.18	0.43
1:J:156:ASP:OD1	1:J:156:ASP:C	2.56	0.43
1:K:295:ILE:O	1:K:299:LEU:HB2	2.18	0.43
1:E:123:LEU:HD11	1:E:221:PHE:HE2	1.84	0.43
1:G:298:ARG:HA	1:G:301:ARG:HB2	2.00	0.43
1:H:240:SER:HB2	1:H:330:PRO:HG2	1.99	0.43
1:H:319:GLU:CB	1:H:320:PRO:HD2	2.48	0.43
1:A:320:PRO:HB2	1:A:321:PHE:CA	2.48	0.43
1:B:246:LEU:HG	1:B:250:ILE:HD11	2.00	0.43
1:D:120:GLU:OE1	1:D:124:ARG:NH1	2.45	0.43
1:D:187:SER:OG	1:D:190:PRO:HG2	2.19	0.43
1:F:320:PRO:HA	1:F:321:PHE:CB	2.49	0.43
1:H:76:LEU:HG	1:H:378:GLU:HG2	2.00	0.43
1:K:127:THR:N	1:K:202:ASP:OD2	2.47	0.43
1:C:197:LEU:HD22	1:C:373:ALA:HA	2.00	0.43
1:D:185:THR:HG23	1:D:355:ASP:OD1	2.18	0.43
1:F:167:CYS:O	1:F:222:LEU:HD12	2.18	0.43
1:H:252:HIS:O	1:H:255:GLY:HA3	2.19	0.43
1:I:364:THR:O	1:I:368:LEU:HG	2.18	0.43
1:J:358:VAL:O	1:J:358:VAL:HG22	2.18	0.43
1:B:301:ARG:NH2	1:B:311:GLU:OE1	2.52	0.43
1:B:379:TYR:HD1	1:B:380:LEU:HD23	1.82	0.43
1:D:296:GLU:O	1:D:297:LYS:C	2.57	0.43
1:E:220:LEU:HD13	1:E:243:LEU:CD2	2.49	0.43
1:E:279:TYR:CE1	1:E:316:GLN:HB2	2.54	0.43
1:E:304:LEU:O	1:E:304:LEU:HD23	2.19	0.43
1:K:268:LEU:O	1:K:269:ASP:HB2	2.18	0.43
1:B:230:GLU:O	1:B:231:TRP:O	2.37	0.43
1:E:297:LYS:HE3	1:E:301:ARG:NH1	2.34	0.43
1:F:296:GLU:O	1:F:297:LYS:HB3	2.19	0.43
1:G:99:ARG:HB3	1:G:100:PRO:CD	2.48	0.43
1:G:298:ARG:O	1:G:299:LEU:C	2.57	0.43
1:H:134:LEU:O	1:H:136:PRO:HD3	2.19	0.43
1:J:321:PHE:N	1:J:321:PHE:CD1	2.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:142:PRO:C	1:K:144:GLY:H	2.22	0.43
1:K:282:PHE:HE1	1:K:332:LEU:HD21	1.84	0.43
1:A:123:LEU:HD11	1:A:221:PHE:HE2	1.83	0.42
1:C:80:ARG:O	1:C:84:VAL:HG23	2.19	0.42
1:E:273:ALA:HB2	1:E:347:PRO:HB3	2.01	0.42
1:E:333:ARG:HG2	1:J:359:ASN:OD1	2.19	0.42
1:F:76:LEU:HG	1:F:378:GLU:HG3	2.01	0.42
1:F:187:SER:CB	1:F:190:PRO:HG2	2.48	0.42
1:G:162:HIS:CD2	1:G:261:ALA:HB1	2.53	0.42
1:H:229:LYS:O	1:H:230:GLU:HB2	2.19	0.42
1:I:367:ASN:O	1:I:370:ARG:N	2.51	0.42
1:J:298:ARG:O	1:J:300:HIS:N	2.51	0.42
1:K:362:PRO:N	1:K:363:PRO:CD	2.82	0.42
1:B:185:THR:O	1:B:270:LEU:HA	2.18	0.42
1:J:133:GLU:OE2	1:J:258:ARG:NH1	2.46	0.42
1:J:274:PRO:HB3	1:J:361:HIS:HB2	2.00	0.42
1:J:379:TYR:O	1:J:379:TYR:CD1	2.72	0.42
1:K:72:LEU:HD23	1:K:72:LEU:N	2.35	0.42
1:K:162:HIS:NE2	1:K:218:GLN:OE1	2.51	0.42
1:K:297:LYS:O	1:K:297:LYS:HG3	2.18	0.42
1:C:377:ALA:O	1:C:381:GLY:N	2.52	0.42
1:E:362:PRO:N	1:E:363:PRO:CD	2.82	0.42
1:G:274:PRO:O	1:G:275:ASN:C	2.58	0.42
1:H:201:LEU:HD12	1:H:376:LEU:HD12	2.01	0.42
1:C:126:LEU:HD22	1:C:199:GLN:OE1	2.19	0.42
1:E:252:HIS:O	1:E:255:GLY:HA3	2.19	0.42
1:E:295:ILE:O	1:E:297:LYS:N	2.52	0.42
1:G:123:LEU:HD13	1:G:153:ALA:CB	2.49	0.42
1:G:249:SER:O	1:G:251:PRO:HD3	2.19	0.42
1:I:196:GLU:O	1:I:199:GLN:N	2.53	0.42
1:J:156:ASP:OD1	1:J:158:ARG:CD	2.67	0.42
1:J:296:GLU:O	1:J:297:LYS:CB	2.67	0.42
1:B:116:ARG:CG	1:B:169:TYR:CZ	3.03	0.42
1:B:235:ASP:HA	1:B:238:TYR:OH	2.20	0.42
1:B:292:LEU:HG	1:B:375:PHE:CE2	2.55	0.42
1:B:320:PRO:CA	1:B:321:PHE:CB	2.97	0.42
1:D:81:LEU:HD23	1:D:82:ARG:N	2.34	0.42
1:H:367:ASN:O	1:H:370:ARG:N	2.53	0.42
1:I:164:THR:OG1	1:I:262:ILE:HG23	2.19	0.42
1:I:296:GLU:OE1	1:I:314:TYR:HB2	2.19	0.42
1:J:352:THR:HB	1:J:353:PRO:HD2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ASP:O	1:C:239:GLY:HA3	2.20	0.42
1:D:361:HIS:HB3	1:D:364:THR:HB	2.01	0.42
1:A:187:SER:OG	1:A:190:PRO:HG2	2.20	0.42
1:C:135:ASP:HB3	1:C:150:ASN:HB2	2.01	0.42
1:E:123:LEU:HD13	1:E:153:ALA:HB2	2.01	0.42
1:E:368:LEU:O	1:E:372:LEU:HG	2.20	0.42
1:F:349:VAL:O	1:F:349:VAL:HG23	2.19	0.42
1:I:295:ILE:HG22	1:I:299:LEU:HD12	2.02	0.42
1:J:224:GLY:O	1:J:225:GLU:C	2.58	0.42
1:K:162:HIS:HD2	1:K:218:GLN:HB3	1.85	0.42
1:A:150:ASN:OD1	1:A:223:ASP:N	2.45	0.42
1:B:374:VAL:CG1	1:B:378:GLU:OE2	2.67	0.42
1:C:187:SER:HB3	1:C:190:PRO:HG2	2.01	0.42
1:C:281:HIS:HA	1:C:320:PRO:CG	2.50	0.42
1:D:99:ARG:HA	1:D:102:LEU:HD12	2.01	0.42
1:D:288:TRP:CZ3	1:D:291:ARG:HD3	2.54	0.42
1:E:89:ASP:HB3	1:E:92:ARG:CB	2.50	0.42
1:E:225:GLU:HG2	1:E:237:LEU:HD23	2.02	0.42
1:G:73:ILE:HG23	1:G:291:ARG:HH22	1.84	0.42
1:G:320:PRO:CB	1:G:321:PHE:C	2.88	0.42
1:H:227:ALA:HB2	1:H:231:TRP:HA	2.01	0.42
1:J:106:THR:O	1:J:112:ASN:HB2	2.19	0.42
1:J:320:PRO:O	1:J:321:PHE:HB2	2.20	0.42
1:K:112:ASN:OD1	1:K:113:LEU:HD12	2.19	0.42
1:A:268:LEU:HD12	1:A:268:LEU:N	2.34	0.42
1:F:89:ASP:HB3	1:F:92:ARG:HB3	2.02	0.42
1:G:168:HIS:HD1	1:G:225:GLU:HB3	1.85	0.42
1:G:170:ASP:CG	1:G:225:GLU:CG	2.88	0.42
1:I:353:PRO:HG3	1:J:322:GLY:HA3	2.01	0.42
1:J:178:SER:O	1:J:179:THR:C	2.58	0.42
1:A:186:ASP:N	1:A:187:SER:HA	2.35	0.42
1:D:124:ARG:NH2	1:D:132:VAL:O	2.53	0.42
1:F:291:ARG:HH22	1:F:298:ARG:NH2	2.18	0.42
1:F:295:ILE:HG23	1:F:299:LEU:HD11	2.02	0.42
1:H:274:PRO:O	1:H:275:ASN:C	2.57	0.42
1:H:297:LYS:CG	1:H:297:LYS:O	2.67	0.42
1:I:352:THR:HB	1:I:353:PRO:HD2	2.02	0.42
1:K:168:HIS:ND1	1:K:168:HIS:N	2.68	0.42
1:A:207:ARG:O	1:A:208:ALA:C	2.59	0.41
1:A:241:ARG:HG2	1:A:330:PRO:HG3	2.01	0.41
1:B:116:ARG:CG	1:B:169:TYR:OH	2.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ASP:OD1	1:C:327:ASP:N	2.47	0.41
1:E:260:GLN:NE2	1:J:275:ASN:OD1	2.53	0.41
1:H:329:ILE:HD13	1:H:329:ILE:N	2.34	0.41
1:K:76:LEU:HG	1:K:378:GLU:HG3	2.02	0.41
1:F:98:LEU:O	1:F:101:LEU:HB2	2.20	0.41
1:F:162:HIS:CD2	1:F:218:GLN:HB2	2.55	0.41
1:K:297:LYS:HA	1:K:298:ARG:C	2.41	0.41
1:G:293:ARG:HH12	1:G:316:GLN:C	2.24	0.41
1:H:295:ILE:HD12	1:H:375:PHE:HB2	2.02	0.41
1:K:320:PRO:CB	1:K:321:PHE:C	2.88	0.41
1:A:162:HIS:HB3	1:A:216:THR:HG22	2.03	0.41
1:A:178:SER:HB3	1:D:321:PHE:HA	2.03	0.41
1:B:298:ARG:O	1:B:301:ARG:N	2.53	0.41
1:D:113:LEU:CD1	1:D:117:LYS:HD3	2.50	0.41
1:E:350:TRP:CE3	1:K:283:PRO:HB2	2.55	0.41
1:F:165:LEU:HD21	1:F:266:MET:SD	2.61	0.41
1:F:310:GLN:HB2	1:F:313:MET:HG3	2.02	0.41
1:G:358:VAL:O	1:G:358:VAL:CG2	2.68	0.41
1:H:303:ASN:O	1:H:304:LEU:HD23	2.19	0.41
1:I:319:GLU:HG2	1:I:320:PRO:HD2	2.02	0.41
1:I:351:HIS:HB3	1:J:321:PHE:CZ	2.50	0.41
1:C:196:GLU:OE1	1:C:196:GLU:HA	2.20	0.41
1:E:275:ASN:N	1:E:275:ASN:OD1	2.52	0.41
1:H:222:LEU:HD13	1:H:327:ASP:CG	2.40	0.41
1:J:94:TRP:CD2	1:J:98:LEU:HD23	2.55	0.41
1:J:150:ASN:OD1	1:J:222:LEU:HA	2.21	0.41
1:C:235:ASP:HA	1:C:238:TYR:OH	2.21	0.41
1:F:291:ARG:HH21	1:F:378:GLU:CB	2.33	0.41
1:J:297:LYS:O	1:J:297:LYS:CG	2.68	0.41
1:K:142:PRO:HD2	1:K:228:LEU:HD12	2.02	0.41
1:K:236:SER:O	1:K:241:ARG:NH2	2.52	0.41
1:K:269:ASP:OD1	1:K:270:LEU:HD23	2.21	0.41
1:A:362:PRO:N	1:A:363:PRO:CD	2.83	0.41
1:B:302:LEU:N	1:B:302:LEU:HD23	2.35	0.41
1:B:374:VAL:O	1:B:375:PHE:C	2.59	0.41
1:C:73:ILE:HG23	1:C:73:ILE:O	2.20	0.41
1:C:288:TRP:CH2	1:C:379:TYR:CD2	3.09	0.41
1:C:310:GLN:HB2	1:C:313:MET:HG3	2.01	0.41
1:E:296:GLU:OE1	1:E:315:PHE:HD2	2.03	0.41
1:F:293:ARG:HH12	1:F:317:PRO:N	2.18	0.41
1:B:232:GLY:O	1:B:233:PRO:C	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:VAL:HG21	1:C:301:ARG:HD2	2.02	0.41
1:D:270:LEU:C	1:D:271:LEU:HD23	2.40	0.41
1:E:322:GLY:HA3	1:J:353:PRO:HG3	2.01	0.41
1:G:106:THR:O	1:G:112:ASN:HB2	2.21	0.41
1:G:318:GLY:O	1:G:319:GLU:HG2	2.21	0.41
1:H:186:ASP:HA	1:H:187:SER:OG	2.21	0.41
1:H:283:PRO:HA	1:H:286:VAL:HB	2.02	0.41
1:I:70:VAL:C	1:I:294:SER:HG	2.13	0.41
1:J:235:ASP:O	1:J:236:SER:CB	2.69	0.41
1:K:162:HIS:HB3	1:K:216:THR:HG22	2.02	0.41
1:B:291:ARG:HG2	1:B:291:ARG:HH11	1.86	0.41
1:C:131:HIS:HB3	4:C:502:HOH:O	2.20	0.41
1:C:155:LEU:O	1:C:209:LYS:HE3	2.20	0.41
1:C:168:HIS:CD2	1:C:187:SER:HG	2.32	0.41
1:C:283:PRO:O	1:C:286:VAL:HG12	2.20	0.41
1:C:329:ILE:HB	1:C:330:PRO:HD3	2.03	0.41
1:C:335:GLY:O	1:F:348:ALA:HB2	2.21	0.41
1:D:299:LEU:O	1:D:304:LEU:N	2.52	0.41
1:E:133:GLU:OE2	1:E:258:ARG:NH2	2.53	0.41
1:E:270:LEU:HD21	3:E:402:A1D47:C24	2.51	0.41
1:F:80:ARG:NH1	1:F:382:LEU:OXT	2.53	0.41
1:F:144:GLY:O	1:F:146:VAL:HG23	2.21	0.41
1:H:105:ARG:HB2	1:H:112:ASN:HA	2.03	0.41
1:H:116:ARG:CZ	1:H:149:GLY:HA3	2.51	0.41
1:H:259:ILE:HG21	1:H:334:ARG:HB3	2.03	0.41
1:H:303:ASN:C	1:H:304:LEU:HD23	2.41	0.41
1:I:174:PHE:HB3	1:I:175:PRO:HD2	2.03	0.41
1:I:309:PRO:HD2	1:I:313:MET:SD	2.61	0.41
1:J:106:THR:HB	1:J:173:LEU:HD12	2.03	0.41
1:J:182:VAL:O	1:J:183:GLY:C	2.59	0.41
1:J:298:ARG:O	1:J:299:LEU:C	2.60	0.41
1:K:113:LEU:HD11	1:K:116:ARG:NH1	2.36	0.41
1:F:70:VAL:N	1:F:71:PRO:CD	2.84	0.41
1:G:135:ASP:O	1:G:149:GLY:HA2	2.20	0.41
1:H:332:LEU:O	1:H:332:LEU:HD23	2.21	0.41
1:J:304:LEU:O	1:J:305:LEU:HD23	2.21	0.41
1:E:80:ARG:HG2	1:E:83:ARG:NH1	2.36	0.40
1:E:210:LYS:C	1:E:212:ALA:H	2.24	0.40
1:F:184:ALA:O	1:F:189:VAL:HG23	2.21	0.40
1:J:70:VAL:N	1:J:71:PRO:HD3	2.36	0.40
1:J:127:THR:OG1	1:J:202:ASP:OD2	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PRO:HB3	1:A:366:HIS:NE2	2.36	0.40
1:A:131:HIS:HB3	4:A:501:HOH:O	2.21	0.40
1:B:168:HIS:CD2	1:B:225:GLU:HB3	2.56	0.40
1:B:375:PHE:C	1:B:375:PHE:CD1	2.95	0.40
1:E:277:THR:HG1	1:E:344:THR:C	2.22	0.40
1:E:301:ARG:C	1:E:303:ASN:H	2.25	0.40
1:G:186:ASP:HA	1:G:187:SER:OG	2.21	0.40
1:H:161:ARG:O	1:H:215:VAL:HA	2.22	0.40
1:K:194:LEU:HB2	1:K:221:PHE:CZ	2.56	0.40
1:C:123:LEU:HD13	1:C:153:ALA:HB2	2.03	0.40
1:G:72:LEU:O	1:G:75:SER:N	2.54	0.40
1:G:227:ALA:HB1	1:G:235:ASP:OD2	2.22	0.40
1:H:299:LEU:HD12	1:H:299:LEU:N	2.36	0.40
1:J:298:ARG:O	1:J:302:LEU:HD23	2.21	0.40
1:A:165:LEU:HD23	1:A:266:MET:HB3	2.03	0.40
1:B:168:HIS:HD2	1:B:170:ASP:OD1	2.04	0.40
1:C:322:GLY:O	1:C:323:SER:CB	2.69	0.40
1:F:232:GLY:O	1:F:236:SER:OG	2.29	0.40
1:F:291:ARG:HH21	1:F:378:GLU:CD	2.24	0.40
1:G:80:ARG:O	1:G:84:VAL:HG23	2.22	0.40
1:G:170:ASP:CG	1:G:225:GLU:HG2	2.41	0.40
1:G:270:LEU:HD12	1:G:346:PHE:CD1	2.57	0.40
1:H:136:PRO:O	1:H:137:PHE:HB3	2.21	0.40
1:H:295:ILE:HG22	1:H:299:LEU:HD11	2.03	0.40
1:J:172:LYS:CG	1:J:173:LEU:N	2.84	0.40
1:B:321:PHE:HA	1:G:178:SER:HB3	2.04	0.40
1:B:346:PHE:O	1:F:284:ARG:NH1	2.54	0.40
1:D:310:GLN:HB2	1:D:313:MET:HG3	2.04	0.40
1:E:89:ASP:HB3	1:E:92:ARG:HB2	2.03	0.40
1:I:184:ALA:CA	1:I:355:ASP:OD1	2.68	0.40
1:J:88:LEU:HD23	1:J:200:ALA:CB	2.51	0.40
1:J:190:PRO:O	1:J:191:CYS:C	2.60	0.40
1:K:193:LEU:O	1:K:197:LEU:HD12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	311/313 (99%)	257 (83%)	42 (14%)	12 (4%)	3	26
1	B	311/313 (99%)	248 (80%)	48 (15%)	15 (5%)	2	22
1	C	311/313 (99%)	251 (81%)	44 (14%)	16 (5%)	2	20
1	D	311/313 (99%)	260 (84%)	38 (12%)	13 (4%)	3	24
1	E	311/313 (99%)	239 (77%)	50 (16%)	22 (7%)	1	14
1	F	311/313 (99%)	260 (84%)	42 (14%)	9 (3%)	4	33
1	G	311/313 (99%)	236 (76%)	58 (19%)	17 (6%)	2	19
1	H	311/313 (99%)	244 (78%)	50 (16%)	17 (6%)	2	19
1	I	311/313 (99%)	264 (85%)	38 (12%)	9 (3%)	4	33
1	J	311/313 (99%)	246 (79%)	49 (16%)	16 (5%)	2	20
1	K	311/313 (99%)	252 (81%)	52 (17%)	7 (2%)	6	38
All	All	3421/3443 (99%)	2757 (81%)	511 (15%)	153 (4%)	2	23

All (153) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	TRP
1	A	298	ARG
1	A	319	GLU
1	A	320	PRO
1	B	230	GLU
1	B	231	TRP
1	B	233	PRO
1	B	299	LEU
1	C	176	PRO
1	C	177	GLY
1	C	230	GLU
1	C	231	TRP
1	C	254	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	286	VAL
1	C	323	SER
1	D	351	HIS
1	D	355	ASP
1	E	298	ARG
1	F	298	ARG
1	G	71	PRO
1	G	231	TRP
1	G	236	SER
1	G	254	PRO
1	G	323	SER
1	H	297	LYS
1	H	298	ARG
1	H	299	LEU
1	H	329	ILE
1	H	353	PRO
1	I	254	PRO
1	I	355	ASP
1	J	230	GLU
1	J	236	SER
1	J	296	GLU
1	J	319	GLU
1	J	351	HIS
1	A	230	GLU
1	A	297	LYS
1	A	321	PHE
1	B	85	VAL
1	B	201	LEU
1	C	75	SER
1	C	178	SER
1	C	287	ARG
1	C	296	GLU
1	C	299	LEU
1	D	297	LYS
1	D	298	ARG
1	D	350	TRP
1	E	307	SER
1	E	359	ASN
1	F	299	LEU
1	G	227	ALA
1	H	183	GLY
1	H	231	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	240	SER
1	I	231	TRP
1	J	177	GLY
1	J	225	GLU
1	J	303	ASN
1	A	207	ARG
1	B	112	ASN
1	B	236	SER
1	B	321	PHE
1	B	355	ASP
1	C	322	GLY
1	D	178	SER
1	E	353	PRO
1	F	230	GLU
1	F	231	TRP
1	H	241	ARG
1	H	295	ILE
1	H	314	TYR
1	H	320	PRO
1	I	75	SER
1	I	230	GLU
1	J	321	PHE
1	K	75	SER
1	K	230	GLU
1	K	269	ASP
1	A	72	LEU
1	A	208	ALA
1	B	71	PRO
1	B	84	VAL
1	D	236	SER
1	E	254	PRO
1	E	296	GLU
1	E	304	LEU
1	E	306	GLN
1	F	207	ARG
1	F	254	PRO
1	G	167	CYS
1	G	256	PRO
1	G	297	LYS
1	H	347	PRO
1	I	303	ASN
1	J	71	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	175	PRO
1	J	183	GLY
1	J	254	PRO
1	K	297	LYS
1	C	297	LYS
1	D	227	ALA
1	D	299	LEU
1	E	75	SER
1	E	128	ALA
1	E	211	GLN
1	E	230	GLU
1	E	297	LYS
1	E	309	PRO
1	E	358	VAL
1	E	367	ASN
1	E	381	GLY
1	F	365	VAL
1	G	230	GLU
1	G	319	GLU
1	G	353	PRO
1	I	167	CYS
1	J	190	PRO
1	K	71	PRO
1	A	71	PRO
1	B	363	PRO
1	B	374	VAL
1	D	230	GLU
1	E	178	SER
1	E	363	PRO
1	F	353	PRO
1	I	73	ILE
1	E	183	GLY
1	G	335	GLY
1	K	183	GLY
1	K	190	PRO
1	C	115	VAL
1	D	136	PRO
1	G	183	GLY
1	G	322	GLY
1	H	349	VAL
1	A	183	GLY
1	C	183	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	71	PRO
1	G	84	VAL
1	H	129	GLY
1	I	349	VAL
1	J	309	PRO
1	B	353	PRO
1	D	319	GLU
1	E	71	PRO
1	F	71	PRO
1	H	149	GLY
1	E	276	PRO
1	G	99	ARG
1	H	358	VAL
1	J	156	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	271/271 (100%)	251 (93%)	20 (7%)	13 45
1	B	271/271 (100%)	253 (93%)	18 (7%)	16 50
1	C	271/271 (100%)	257 (95%)	14 (5%)	23 58
1	D	271/271 (100%)	249 (92%)	22 (8%)	11 42
1	E	271/271 (100%)	252 (93%)	19 (7%)	15 47
1	F	271/271 (100%)	246 (91%)	25 (9%)	9 38
1	G	271/271 (100%)	245 (90%)	26 (10%)	8 36
1	H	271/271 (100%)	254 (94%)	17 (6%)	18 52
1	I	271/271 (100%)	249 (92%)	22 (8%)	11 42
1	J	271/271 (100%)	248 (92%)	23 (8%)	10 40
1	K	271/271 (100%)	246 (91%)	25 (9%)	9 38
All	All	2981/2981 (100%)	2750 (92%)	231 (8%)	13 44

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ILE
1	A	75	SER
1	A	83	ARG
1	A	95	SER
1	A	109	SER
1	A	113	LEU
1	A	114	GLN
1	A	122	THR
1	A	141	THR
1	A	158	ARG
1	A	161	ARG
1	A	225	GLU
1	A	234	LYS
1	A	269	ASP
1	A	297	LYS
1	A	298	ARG
1	A	321	PHE
1	A	323	SER
1	A	349	VAL
1	A	351	HIS
1	B	73	ILE
1	B	99	ARG
1	B	143	LEU
1	B	146	VAL
1	B	158	ARG
1	B	170	ASP
1	B	207	ARG
1	B	225	GLU
1	B	236	SER
1	B	294	SER
1	B	297	LYS
1	B	298	ARG
1	B	301	ARG
1	B	302	LEU
1	B	304	LEU
1	B	319	GLU
1	B	321	PHE
1	B	352	THR
1	C	158	ARG
1	C	179	THR
1	C	207	ARG
1	C	225	GLU
1	C	229	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	230	GLU
1	C	258	ARG
1	C	269	ASP
1	C	277	THR
1	C	287	ARG
1	C	297	LYS
1	C	298	ARG
1	C	312	VAL
1	C	324	VAL
1	D	70	VAL
1	D	91	GLN
1	D	109	SER
1	D	113	LEU
1	D	114	GLN
1	D	120	GLU
1	D	141	THR
1	D	175	PRO
1	D	253	SER
1	D	258	ARG
1	D	271	LEU
1	D	297	LYS
1	D	298	ARG
1	D	307	SER
1	D	319	GLU
1	D	320	PRO
1	D	321	PHE
1	D	333	ARG
1	D	340	HIS
1	D	341	LEU
1	D	352	THR
1	D	355	ASP
1	E	99	ARG
1	E	150	ASN
1	E	158	ARG
1	E	207	ARG
1	E	234	LYS
1	E	240	SER
1	E	269	ASP
1	E	275	ASN
1	E	284	ARG
1	E	289	PHE
1	E	290	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	291	ARG
1	E	292	LEU
1	E	298	ARG
1	E	303	ASN
1	E	304	LEU
1	E	321	PHE
1	E	334	ARG
1	E	358	VAL
1	F	73	ILE
1	F	93	LEU
1	F	95	SER
1	F	106	THR
1	F	114	GLN
1	F	141	THR
1	F	168	HIS
1	F	171	SER
1	F	187	SER
1	F	207	ARG
1	F	210	LYS
1	F	225	GLU
1	F	229	LYS
1	F	234	LYS
1	F	240	SER
1	F	258	ARG
1	F	260	GLN
1	F	291	ARG
1	F	294	SER
1	F	297	LYS
1	F	301	ARG
1	F	321	PHE
1	F	333	ARG
1	F	339	LEU
1	F	352	THR
1	G	72	LEU
1	G	83	ARG
1	G	99	ARG
1	G	112	ASN
1	G	114	GLN
1	G	124	ARG
1	G	141	THR
1	G	165	LEU
1	G	168	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	170	ASP
1	G	171	SER
1	G	225	GLU
1	G	226	GLU
1	G	229	LYS
1	G	231	TRP
1	G	234	LYS
1	G	258	ARG
1	G	262	ILE
1	G	294	SER
1	G	299	LEU
1	G	321	PHE
1	G	333	ARG
1	G	334	ARG
1	G	336	VAL
1	G	339	LEU
1	G	358	VAL
1	H	73	ILE
1	H	95	SER
1	H	99	ARG
1	H	112	ASN
1	H	141	THR
1	H	187	SER
1	H	228	LEU
1	H	240	SER
1	H	249	SER
1	H	269	ASP
1	H	297	LYS
1	H	319	GLU
1	H	321	PHE
1	H	327	ASP
1	H	339	LEU
1	H	352	THR
1	H	356	THR
1	I	72	LEU
1	I	75	SER
1	I	96	THR
1	I	114	GLN
1	I	120	GLU
1	I	140	SER
1	I	141	THR
1	I	161	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	178	SER
1	I	179	THR
1	I	207	ARG
1	I	225	GLU
1	I	234	LYS
1	I	240	SER
1	I	294	SER
1	I	297	LYS
1	I	307	SER
1	I	308	HIS
1	I	319	GLU
1	I	324	VAL
1	I	339	LEU
1	I	359	ASN
1	J	73	ILE
1	J	99	ARG
1	J	113	LEU
1	J	114	GLN
1	J	120	GLU
1	J	154	THR
1	J	158	ARG
1	J	170	ASP
1	J	173	LEU
1	J	179	THR
1	J	187	SER
1	J	210	LYS
1	J	211	GLN
1	J	220	LEU
1	J	222	LEU
1	J	225	GLU
1	J	258	ARG
1	J	291	ARG
1	J	298	ARG
1	J	302	LEU
1	J	349	VAL
1	J	355	ASP
1	J	368	LEU
1	K	72	LEU
1	K	73	ILE
1	K	99	ARG
1	K	112	ASN
1	K	124	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	141	THR
1	K	154	THR
1	K	168	HIS
1	K	171	SER
1	K	187	SER
1	K	207	ARG
1	K	231	TRP
1	K	236	SER
1	K	237	LEU
1	K	275	ASN
1	K	297	LYS
1	K	300	HIS
1	K	301	ARG
1	K	304	LEU
1	K	307	SER
1	K	319	GLU
1	K	321	PHE
1	K	332	LEU
1	K	352	THR
1	K	358	VAL

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

Mol	Chain	Res	Type
1	D	367	ASN

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 22 ligands modelled in this entry, 11 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	$\#\|Z\| > 2$
3	A1D47	C	402	2	29,31,31	2.55	6 (20%)	36,44,44	1.92	6 (16%)
3	A1D47	B	402	2	29,31,31	2.46	6 (20%)	36,44,44	2.01	8 (22%)
3	A1D47	E	402	2	29,31,31	2.58	5 (17%)	36,44,44	1.96	8 (22%)
3	A1D47	K	402	2	29,31,31	2.63	6 (20%)	36,44,44	1.69	6 (16%)
3	A1D47	G	402	2	29,31,31	2.62	6 (20%)	36,44,44	1.85	9 (25%)
3	A1D47	A	402	-	29,31,31	2.63	6 (20%)	36,44,44	1.57	6 (16%)
3	A1D47	J	402	2	29,31,31	2.57	6 (20%)	36,44,44	1.93	9 (25%)
3	A1D47	F	402	2	29,31,31	2.58	6 (20%)	36,44,44	1.70	7 (19%)
3	A1D47	H	402	2	29,31,31	2.63	6 (20%)	36,44,44	1.87	10 (27%)
3	A1D47	I	402	2	29,31,31	2.64	6 (20%)	36,44,44	2.13	11 (30%)
3	A1D47	D	402	2	29,31,31	2.52	6 (20%)	36,44,44	1.83	6 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1D47	C	402	2	-	2/8/28/28	0/5/5/5
3	A1D47	B	402	2	-	5/8/28/28	0/5/5/5
3	A1D47	E	402	2	-	7/8/28/28	0/5/5/5
3	A1D47	K	402	2	-	6/8/28/28	0/5/5/5
3	A1D47	G	402	2	-	3/8/28/28	0/5/5/5
3	A1D47	A	402	-	-	4/8/28/28	0/5/5/5
3	A1D47	J	402	2	-	2/8/28/28	0/5/5/5
3	A1D47	F	402	2	-	2/8/28/28	0/5/5/5
3	A1D47	H	402	2	-	4/8/28/28	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1D47	I	402	2	-	2/8/28/28	0/5/5/5
3	A1D47	D	402	2	-	4/8/28/28	0/5/5/5

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	402	A1D47	C02-N03	9.14	1.46	1.36
3	H	402	A1D47	C02-N03	9.10	1.45	1.36
3	G	402	A1D47	C02-N03	9.03	1.45	1.36
3	E	402	A1D47	C02-N03	8.93	1.45	1.36
3	A	402	A1D47	C02-N03	8.88	1.45	1.36
3	D	402	A1D47	C02-N03	8.76	1.45	1.36
3	F	402	A1D47	C02-N03	8.58	1.45	1.36
3	K	402	A1D47	C02-N03	8.55	1.45	1.36
3	C	402	A1D47	C02-N03	8.40	1.45	1.36
3	J	402	A1D47	C02-N03	8.30	1.45	1.36
3	B	402	A1D47	C02-N03	7.93	1.44	1.36
3	E	402	A1D47	C04-N03	7.60	1.52	1.38
3	H	402	A1D47	C04-N03	7.54	1.52	1.38
3	G	402	A1D47	C04-N03	7.48	1.52	1.38
3	I	402	A1D47	C04-N03	7.43	1.52	1.38
3	F	402	A1D47	C04-N03	7.33	1.52	1.38
3	A	402	A1D47	C04-N03	7.32	1.52	1.38
3	J	402	A1D47	C04-N03	7.29	1.52	1.38
3	B	402	A1D47	C04-N03	7.27	1.52	1.38
3	C	402	A1D47	C04-N03	7.25	1.52	1.38
3	K	402	A1D47	C04-N03	7.05	1.51	1.38
3	D	402	A1D47	C04-N03	7.00	1.51	1.38
3	K	402	A1D47	C19-C18	5.09	1.56	1.46
3	J	402	A1D47	C19-C18	4.41	1.55	1.46
3	I	402	A1D47	C19-C18	4.37	1.55	1.46
3	D	402	A1D47	C05-C17	4.28	1.54	1.45
3	A	402	A1D47	C19-C18	4.19	1.54	1.46
3	G	402	A1D47	C19-C18	4.07	1.54	1.46
3	F	402	A1D47	C19-C18	4.07	1.54	1.46
3	C	402	A1D47	C19-C18	4.04	1.54	1.46
3	H	402	A1D47	C19-C18	3.95	1.54	1.46
3	H	402	A1D47	C05-C17	3.86	1.53	1.45
3	K	402	A1D47	C05-C17	3.86	1.53	1.45
3	E	402	A1D47	C19-C18	3.86	1.54	1.46
3	A	402	A1D47	C05-C17	3.82	1.53	1.45
3	I	402	A1D47	C05-C17	3.78	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	A1D47	C05-C17	3.73	1.53	1.45
3	B	402	A1D47	C19-C18	3.65	1.53	1.46
3	F	402	A1D47	C05-C17	3.56	1.52	1.45
3	C	402	A1D47	C05-C17	3.48	1.52	1.45
3	E	402	A1D47	C05-C17	3.40	1.52	1.45
3	G	402	A1D47	C05-C17	3.36	1.52	1.45
3	J	402	A1D47	C05-C17	3.30	1.52	1.45
3	C	402	A1D47	O07-C06	3.14	1.43	1.37
3	D	402	A1D47	C19-C18	3.12	1.52	1.46
3	F	402	A1D47	O07-C06	2.88	1.42	1.37
3	D	402	A1D47	O01-C02	-2.82	1.18	1.23
3	J	402	A1D47	O07-C06	2.75	1.42	1.37
3	I	402	A1D47	O07-C06	2.70	1.42	1.37
3	K	402	A1D47	O01-C02	-2.69	1.18	1.23
3	H	402	A1D47	O01-C02	-2.65	1.18	1.23
3	J	402	A1D47	O01-C02	-2.60	1.18	1.23
3	B	402	A1D47	O01-C02	-2.59	1.18	1.23
3	E	402	A1D47	O01-C02	-2.57	1.18	1.23
3	G	402	A1D47	O01-C02	-2.56	1.18	1.23
3	B	402	A1D47	O07-C06	2.54	1.41	1.37
3	A	402	A1D47	O01-C02	-2.48	1.18	1.23
3	F	402	A1D47	O01-C02	-2.43	1.19	1.23
3	C	402	A1D47	O01-C02	-2.38	1.19	1.23
3	I	402	A1D47	O01-C02	-2.30	1.19	1.23
3	H	402	A1D47	O07-C06	2.29	1.41	1.37
3	D	402	A1D47	C09-C08	-2.23	1.45	1.51
3	G	402	A1D47	C13-C08	-2.12	1.45	1.51
3	A	402	A1D47	O07-C06	2.10	1.41	1.37
3	K	402	A1D47	O07-C06	2.05	1.41	1.37

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	402	A1D47	C12-C13-C08	6.67	117.68	109.78
3	J	402	A1D47	C04-N03-C02	-6.52	107.28	111.38
3	B	402	A1D47	C12-C13-C08	6.25	117.18	109.78
3	C	402	A1D47	C04-N03-C02	-5.67	107.82	111.38
3	G	402	A1D47	C04-N03-C02	-5.47	107.94	111.38
3	D	402	A1D47	C04-N03-C02	-5.38	108.00	111.38
3	K	402	A1D47	C04-N03-C02	-5.37	108.01	111.38
3	E	402	A1D47	C04-N03-C02	-5.23	108.09	111.38
3	F	402	A1D47	C04-N03-C02	-5.22	108.10	111.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	402	A1D47	C04-N03-C02	-5.21	108.11	111.38
3	A	402	A1D47	C04-N03-C02	-5.18	108.12	111.38
3	E	402	A1D47	C10-C09-C08	5.17	115.90	109.78
3	G	402	A1D47	C12-C13-C08	4.83	115.50	109.78
3	F	402	A1D47	C19-C18-C17	-4.77	120.06	129.63
3	H	402	A1D47	C12-C13-C08	4.76	115.42	109.78
3	B	402	A1D47	C04-N03-C02	-4.69	108.43	111.38
3	C	402	A1D47	C05-C17-C02	4.54	107.89	105.31
3	I	402	A1D47	C10-C09-C08	4.48	115.09	109.78
3	D	402	A1D47	C12-C13-C08	4.39	114.99	109.78
3	K	402	A1D47	C17-C02-N03	4.25	109.27	106.88
3	J	402	A1D47	C17-C02-N03	4.12	109.19	106.88
3	K	402	A1D47	O07-C08-C13	4.01	117.17	108.31
3	E	402	A1D47	O07-C08-C09	3.99	117.12	108.31
3	B	402	A1D47	C19-C18-C17	-3.95	121.71	129.63
3	D	402	A1D47	C17-C02-N03	3.90	109.07	106.88
3	C	402	A1D47	C12-C13-C08	3.87	114.36	109.78
3	J	402	A1D47	C19-C18-C17	-3.82	121.96	129.63
3	E	402	A1D47	C05-C17-C02	3.78	107.45	105.31
3	C	402	A1D47	C10-C09-C08	3.76	114.23	109.78
3	B	402	A1D47	C05-C17-C02	3.74	107.43	105.31
3	H	402	A1D47	C04-N03-C02	-3.72	109.04	111.38
3	B	402	A1D47	O07-C08-C13	3.58	116.23	108.31
3	H	402	A1D47	C05-C17-C02	3.50	107.30	105.31
3	H	402	A1D47	C20-C19-C18	3.46	128.40	118.94
3	E	402	A1D47	C12-C13-C08	3.45	113.86	109.78
3	C	402	A1D47	C19-C18-C17	-3.34	122.93	129.63
3	G	402	A1D47	C10-C09-C08	3.26	113.64	109.78
3	F	402	A1D47	C05-C17-C02	3.24	107.15	105.31
3	J	402	A1D47	C04-C05-C06	3.15	120.79	117.79
3	A	402	A1D47	C19-C18-C17	-3.14	123.33	129.63
3	A	402	A1D47	C17-C02-N03	3.02	108.57	106.88
3	F	402	A1D47	O07-C08-C13	2.93	114.79	108.31
3	C	402	A1D47	C04-C05-C06	2.93	120.58	117.79
3	I	402	A1D47	C19-C18-C17	-2.90	123.81	129.63
3	H	402	A1D47	C27-C19-C18	-2.89	111.38	121.22
3	J	402	A1D47	C09-C08-C13	-2.85	106.23	111.74
3	H	402	A1D47	C18-C17-C02	2.84	131.37	119.96
3	G	402	A1D47	C05-C17-C02	2.83	106.91	105.31
3	F	402	A1D47	C04-C05-C06	2.81	120.46	117.79
3	I	402	A1D47	O07-C06-C05	2.79	123.65	117.70
3	I	402	A1D47	C05-C17-C02	2.77	106.88	105.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	402	A1D47	O07-C06-C14	-2.70	117.54	123.87
3	K	402	A1D47	C18-C17-C02	2.66	130.66	119.96
3	G	402	A1D47	C04-C05-C06	2.63	120.29	117.79
3	K	402	A1D47	O01-C02-N03	-2.59	122.25	126.36
3	I	402	A1D47	C06-O07-C08	-2.59	111.45	120.21
3	E	402	A1D47	C04-C05-C06	2.59	120.25	117.79
3	A	402	A1D47	C12-C13-C08	2.55	112.80	109.78
3	H	402	A1D47	O07-C08-C13	2.54	113.93	108.31
3	I	402	A1D47	O07-C08-C13	2.54	113.93	108.31
3	B	402	A1D47	O11-C12-C13	2.54	117.31	111.72
3	G	402	A1D47	C18-C17-C02	2.48	129.95	119.96
3	A	402	A1D47	C04-C05-C06	2.47	120.14	117.79
3	I	402	A1D47	C18-C17-C02	2.40	129.60	119.96
3	I	402	A1D47	O07-C06-C14	-2.39	118.26	123.87
3	D	402	A1D47	O07-C08-C09	2.39	113.58	108.31
3	J	402	A1D47	O07-C08-C13	2.38	113.56	108.31
3	F	402	A1D47	C17-C02-N03	2.31	108.17	106.88
3	G	402	A1D47	C17-C02-N03	2.29	108.16	106.88
3	J	402	A1D47	C06-C05-C17	-2.26	130.95	136.13
3	K	402	A1D47	C06-C05-C17	-2.22	131.04	136.13
3	G	402	A1D47	C06-C05-C17	-2.21	131.06	136.13
3	H	402	A1D47	O07-C06-C14	-2.18	118.74	123.87
3	I	402	A1D47	C17-C02-N03	2.18	108.10	106.88
3	B	402	A1D47	C04-C05-C06	2.13	119.82	117.79
3	A	402	A1D47	C06-C05-C17	-2.13	131.25	136.13
3	G	402	A1D47	C19-C18-C17	-2.11	125.39	129.63
3	J	402	A1D47	C18-C17-C02	2.10	128.42	119.96
3	H	402	A1D47	O07-C08-C09	2.10	112.95	108.31
3	H	402	A1D47	O07-C06-C05	2.09	122.16	117.70
3	E	402	A1D47	C18-C17-C02	2.07	128.27	119.96
3	E	402	A1D47	C06-C05-C17	-2.06	131.41	136.13
3	D	402	A1D47	C09-C08-C13	2.03	115.65	111.74
3	F	402	A1D47	C06-C05-C17	-2.01	131.52	136.13
3	J	402	A1D47	C05-C17-C02	2.01	106.45	105.31
3	B	402	A1D47	C17-C02-N03	2.01	108.01	106.88

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	A1D47	C02-C17-C18-C19
3	A	402	A1D47	C05-C17-C18-C19

Continued on next page...

Continued from previous page...

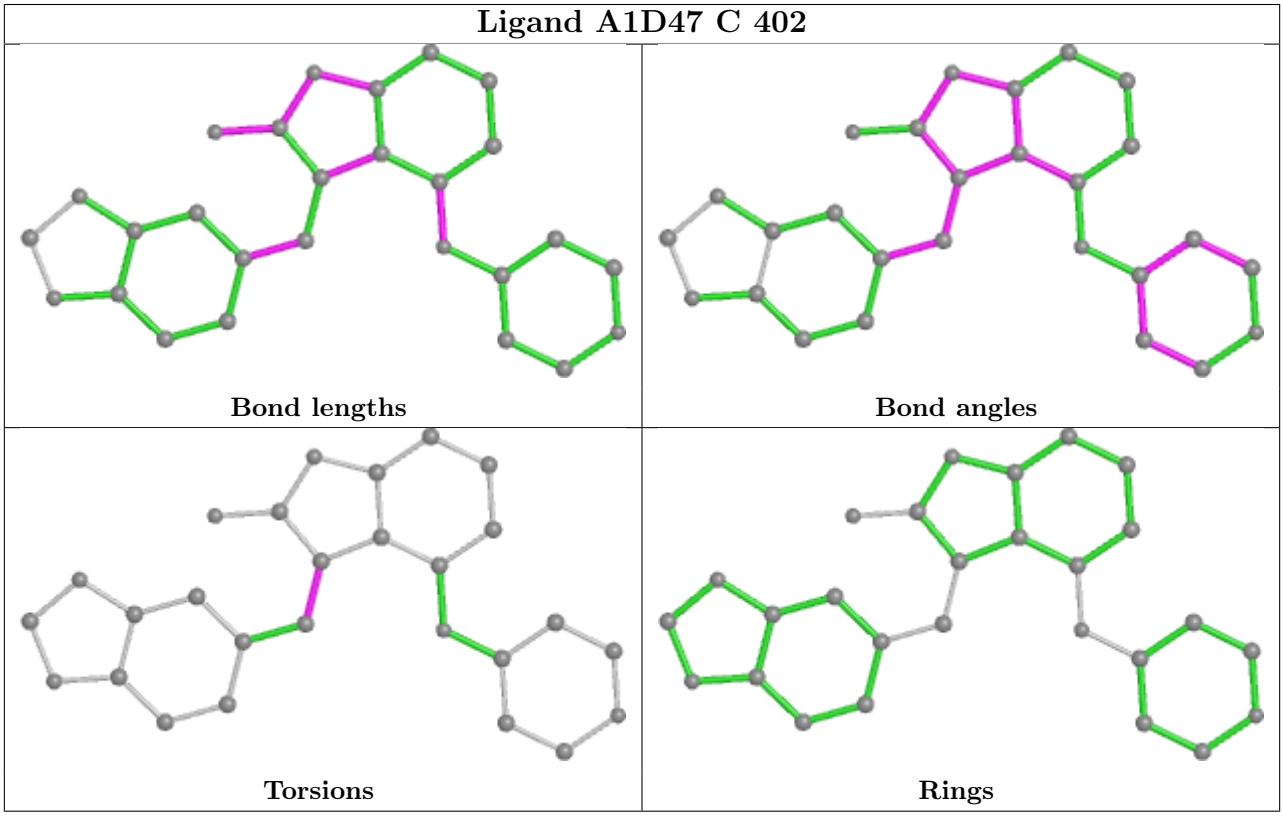
Mol	Chain	Res	Type	Atoms
3	B	402	A1D47	C02-C17-C18-C19
3	B	402	A1D47	C05-C17-C18-C19
3	C	402	A1D47	C02-C17-C18-C19
3	C	402	A1D47	C05-C17-C18-C19
3	D	402	A1D47	C02-C17-C18-C19
3	D	402	A1D47	C05-C17-C18-C19
3	E	402	A1D47	C02-C17-C18-C19
3	E	402	A1D47	C05-C17-C18-C19
3	E	402	A1D47	C09-C08-O07-C06
3	F	402	A1D47	C02-C17-C18-C19
3	F	402	A1D47	C05-C17-C18-C19
3	G	402	A1D47	C02-C17-C18-C19
3	G	402	A1D47	C05-C17-C18-C19
3	H	402	A1D47	C02-C17-C18-C19
3	H	402	A1D47	C05-C17-C18-C19
3	J	402	A1D47	C02-C17-C18-C19
3	J	402	A1D47	C05-C17-C18-C19
3	K	402	A1D47	C02-C17-C18-C19
3	K	402	A1D47	C13-C08-O07-C06
3	E	402	A1D47	C17-C18-C19-C20
3	E	402	A1D47	C17-C18-C19-C27
3	B	402	A1D47	C14-C06-O07-C08
3	I	402	A1D47	C05-C06-O07-C08
3	H	402	A1D47	C14-C06-O07-C08
3	K	402	A1D47	C09-C08-O07-C06
3	K	402	A1D47	C05-C17-C18-C19
3	B	402	A1D47	C05-C06-O07-C08
3	H	402	A1D47	C05-C06-O07-C08
3	I	402	A1D47	C14-C06-O07-C08
3	E	402	A1D47	C05-C06-O07-C08
3	B	402	A1D47	C13-C08-O07-C06
3	D	402	A1D47	C05-C06-O07-C08
3	D	402	A1D47	C14-C06-O07-C08
3	A	402	A1D47	C14-C06-O07-C08
3	E	402	A1D47	C14-C06-O07-C08
3	K	402	A1D47	C14-C06-O07-C08
3	A	402	A1D47	C05-C06-O07-C08
3	K	402	A1D47	C05-C06-O07-C08
3	G	402	A1D47	C13-C08-O07-C06

There are no ring outliers.

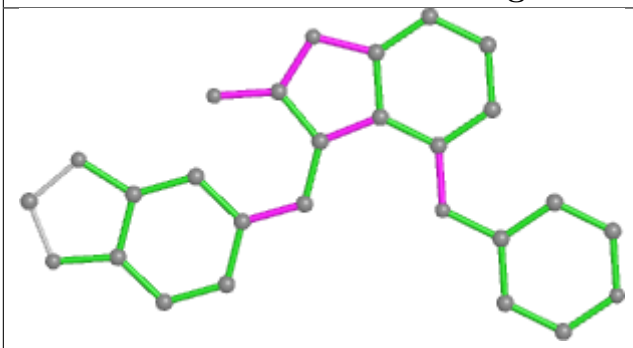
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	402	A1D47	1	0
3	G	402	A1D47	1	0
3	F	402	A1D47	1	0
3	H	402	A1D47	1	0
3	I	402	A1D47	1	0

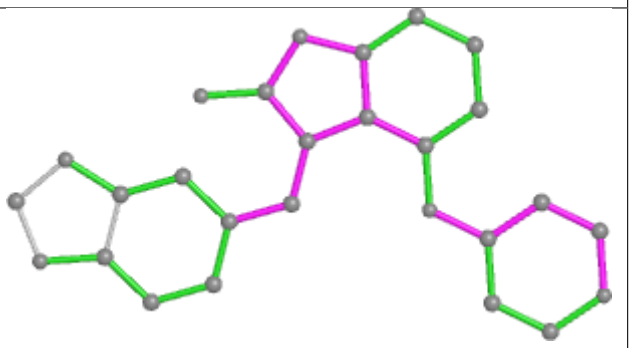
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



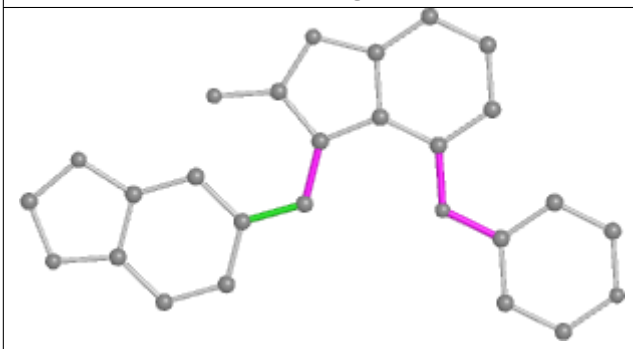
Ligand A1D47 B 402



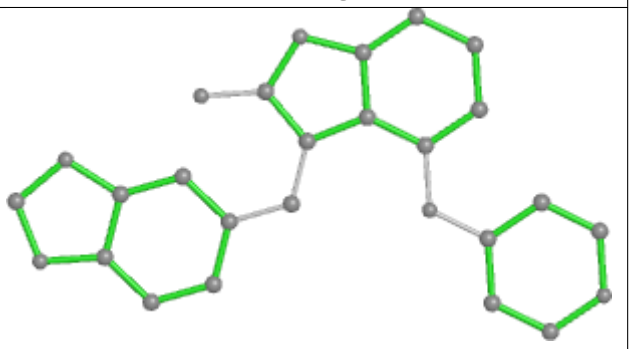
Bond lengths



Bond angles

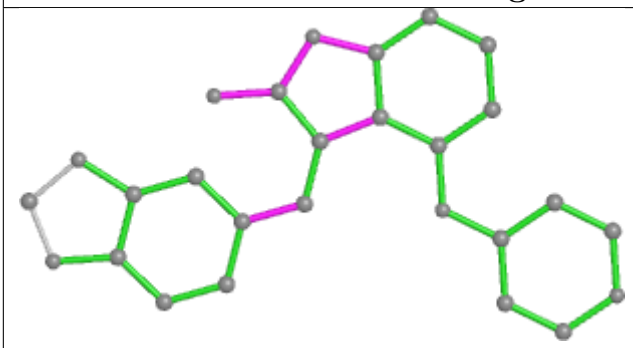


Torsions

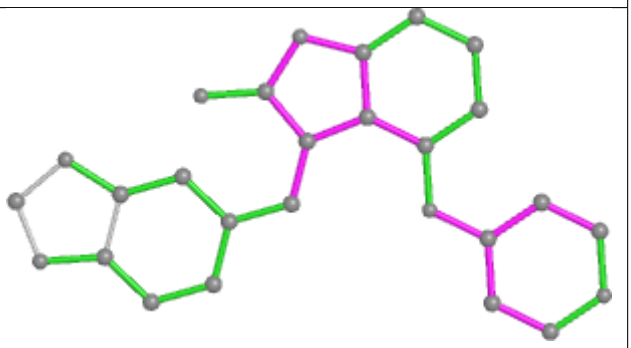


Rings

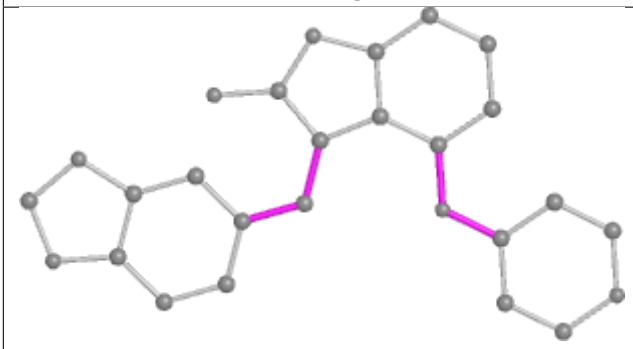
Ligand A1D47 E 402



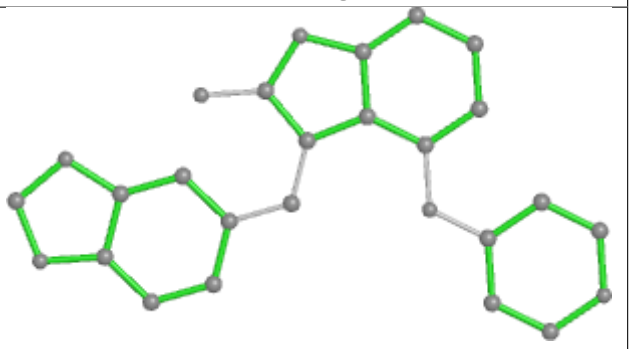
Bond lengths



Bond angles

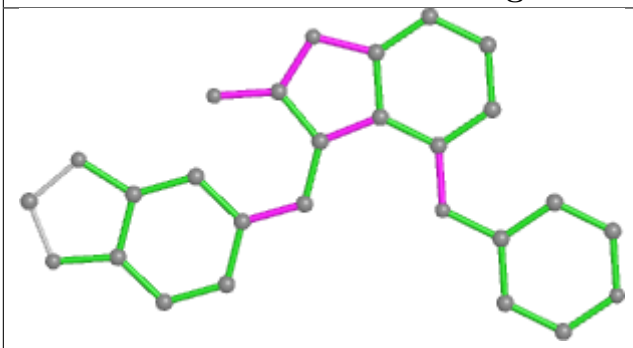


Torsions

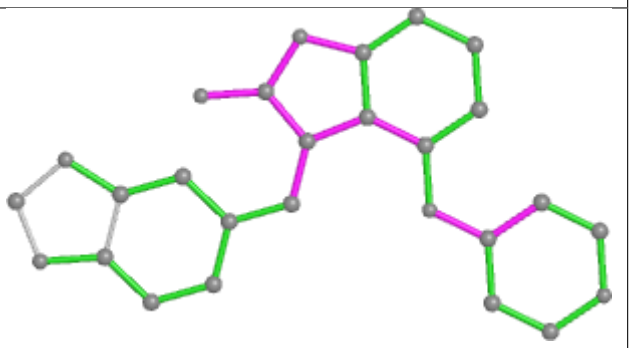


Rings

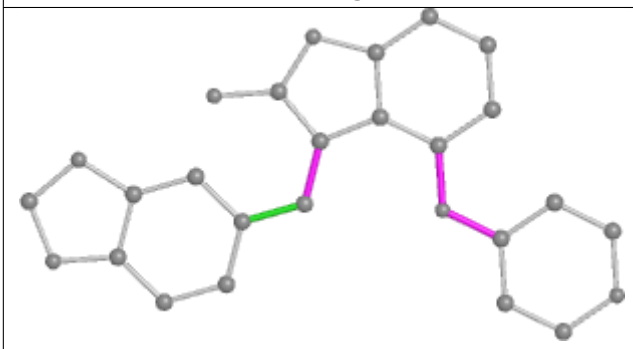
Ligand A1D47 K 402



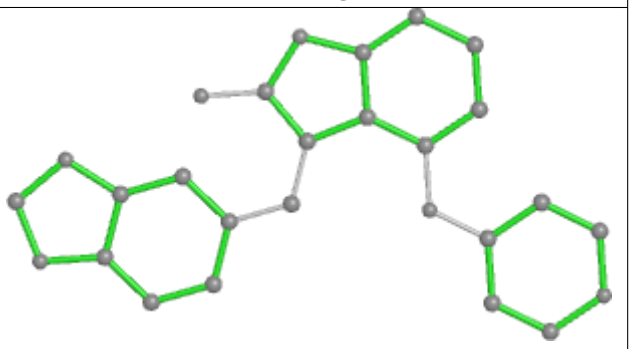
Bond lengths



Bond angles

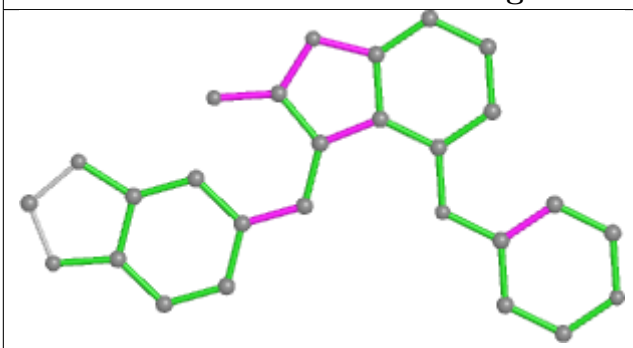


Torsions

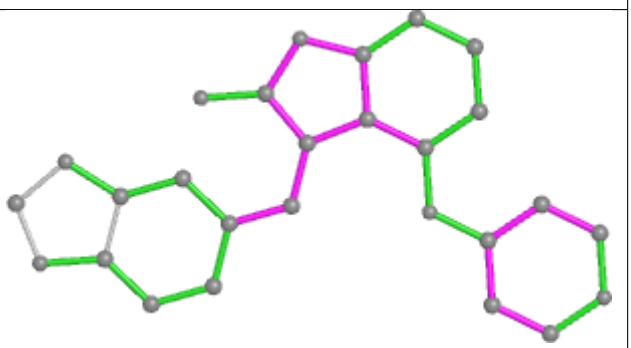


Rings

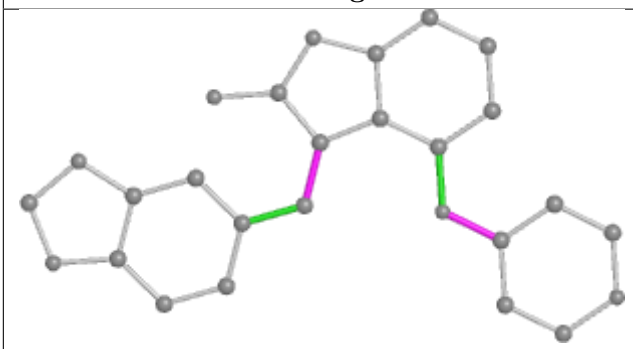
Ligand A1D47 G 402



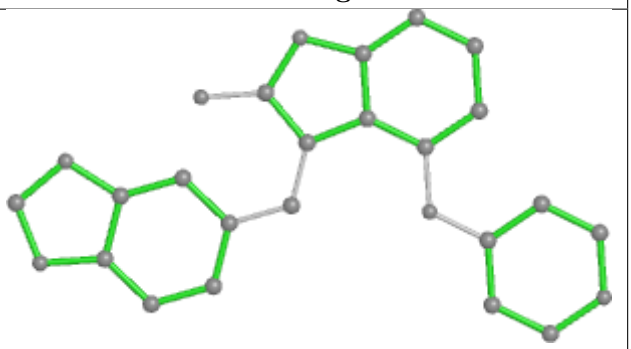
Bond lengths



Bond angles

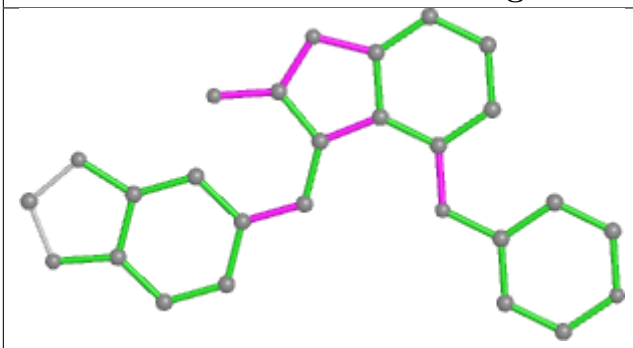


Torsions

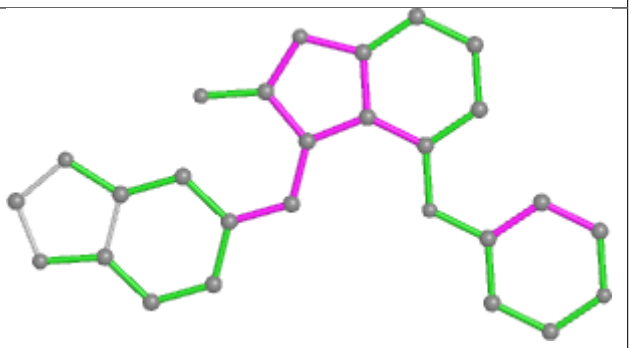


Rings

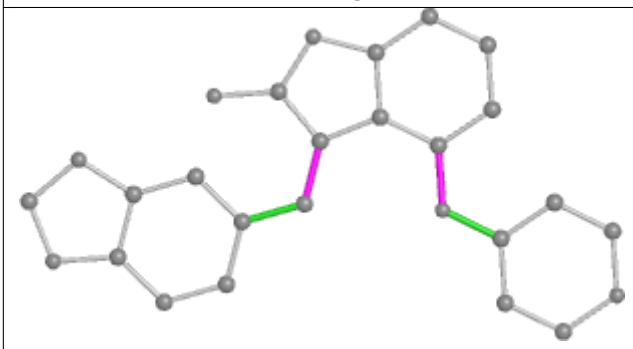
Ligand A1D47 A 402



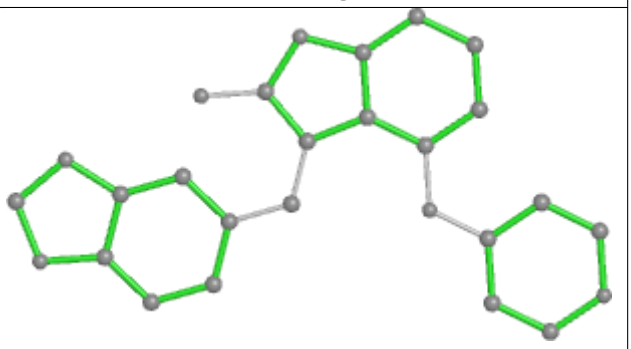
Bond lengths



Bond angles

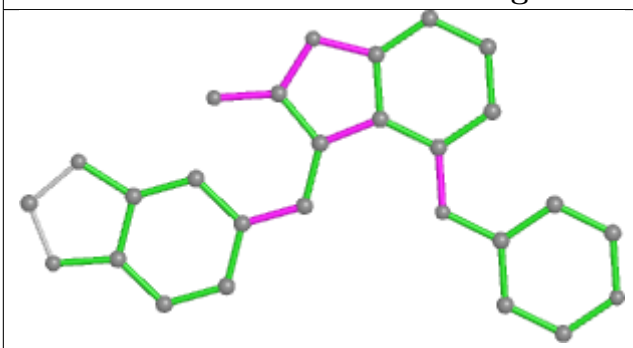


Torsions

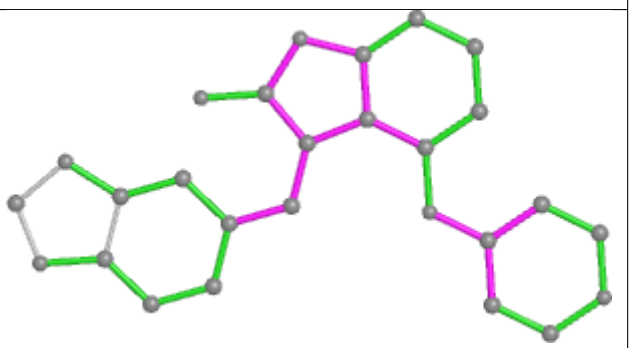


Rings

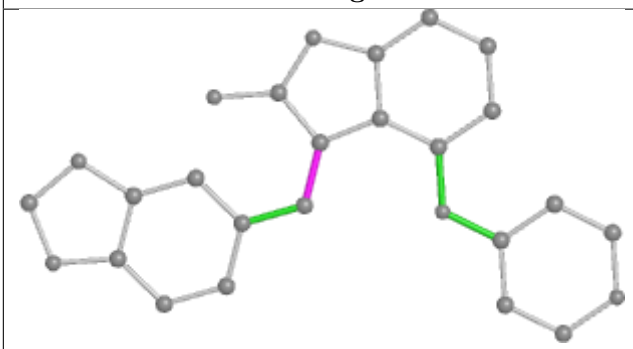
Ligand A1D47 J 402



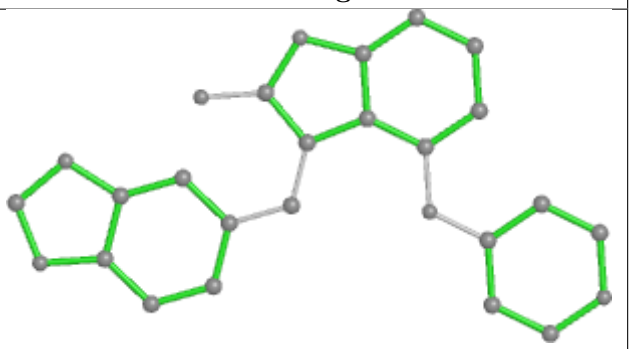
Bond lengths



Bond angles

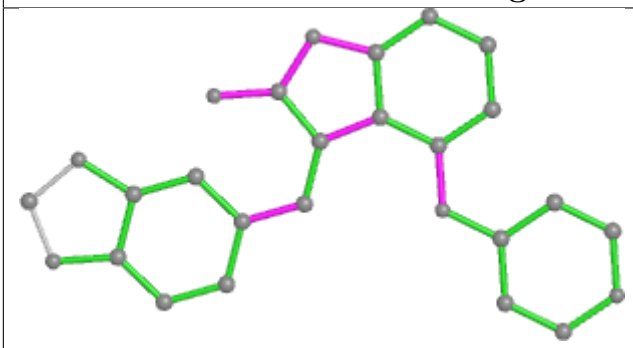


Torsions

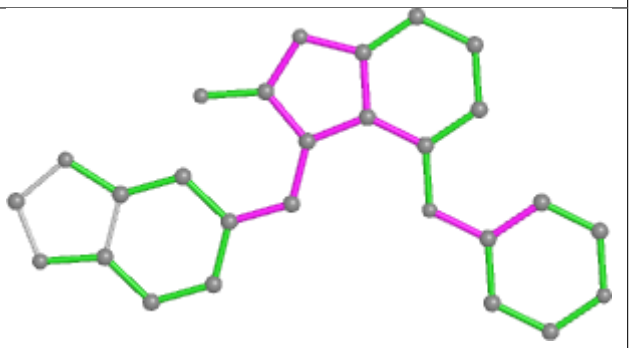


Rings

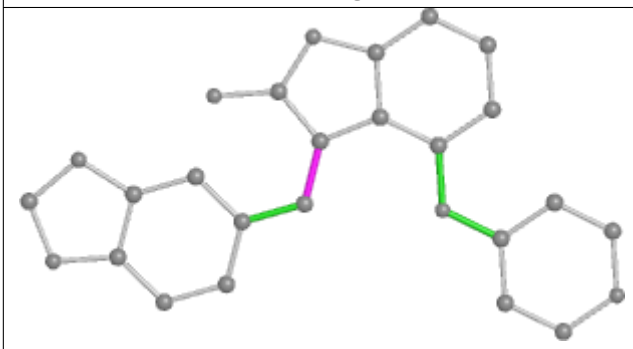
Ligand A1D47 F 402



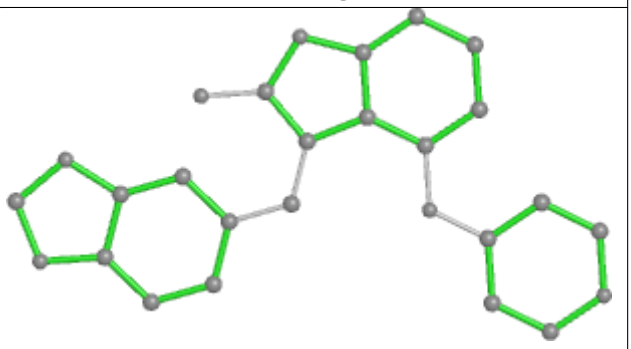
Bond lengths



Bond angles

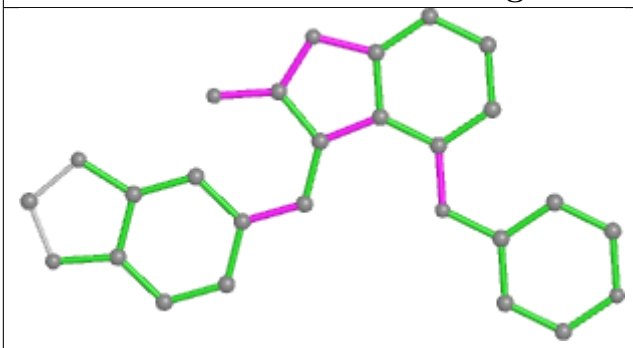


Torsions

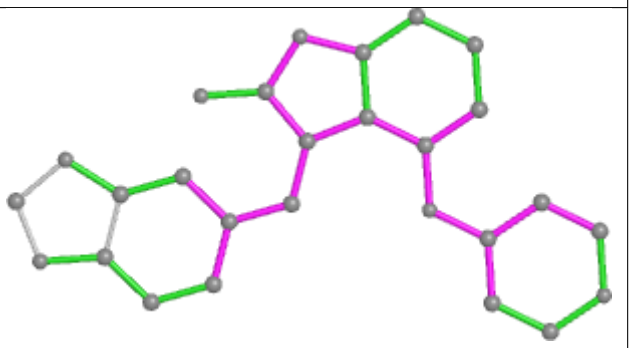


Rings

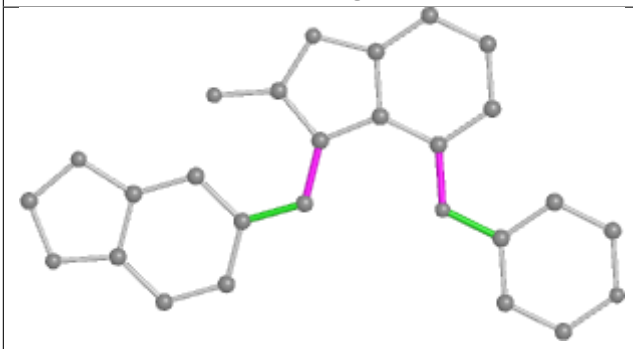
Ligand A1D47 H 402



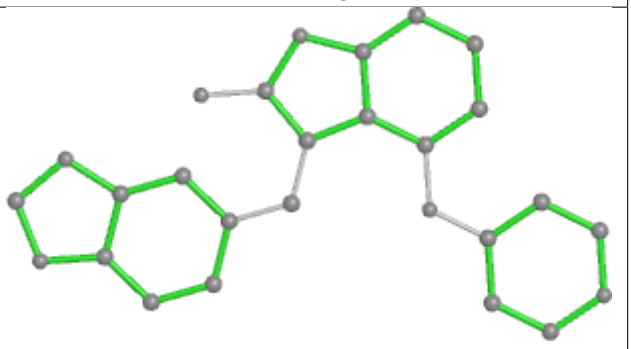
Bond lengths



Bond angles

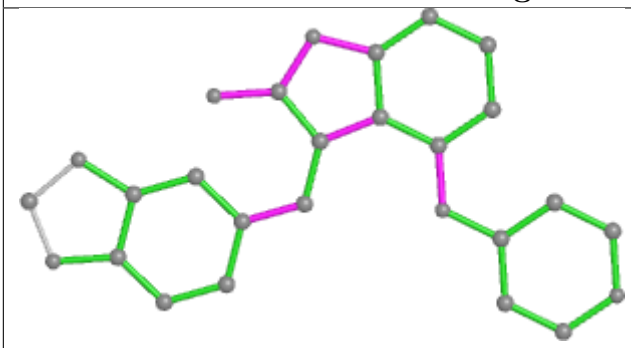


Torsions

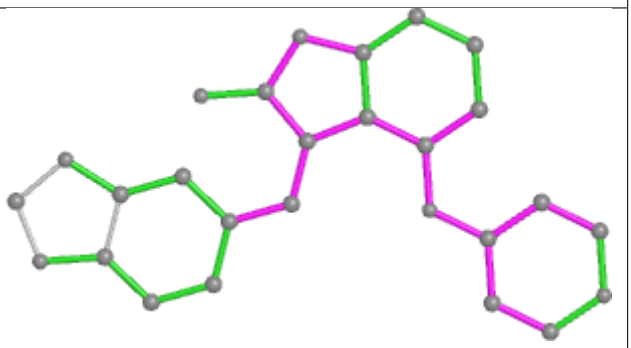


Rings

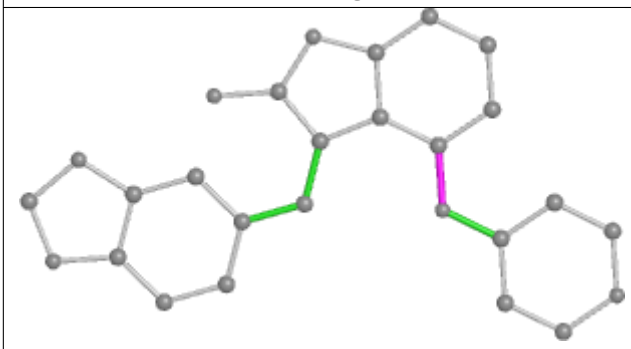
Ligand A1D47 I 402



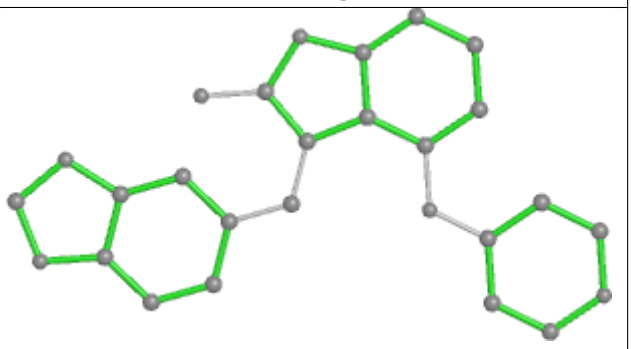
Bond lengths



Bond angles

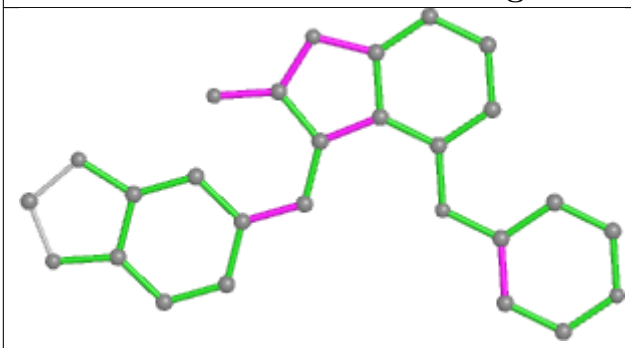


Torsions

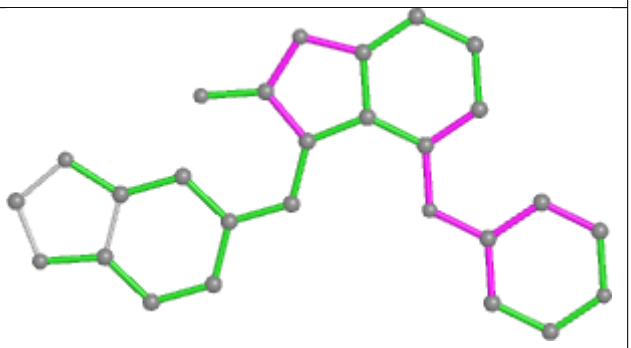


Rings

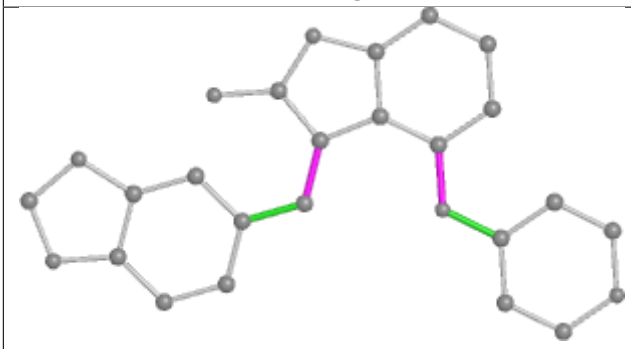
Ligand A1D47 D 402



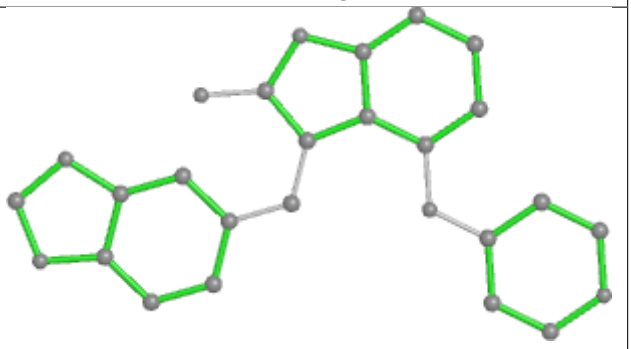
Bond lengths



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	312/313 (99%)	-0.45	2 (0%)	89	81	12, 33, 68, 125	0
1	B	312/313 (99%)	-0.46	4 (1%)	77	65	21, 41, 73, 128	0
1	C	312/313 (99%)	-0.41	5 (1%)	72	59	20, 42, 73, 138	0
1	D	312/313 (99%)	-0.40	4 (1%)	77	65	19, 44, 78, 147	0
1	E	312/313 (99%)	-0.17	5 (1%)	72	59	44, 78, 122, 162	0
1	F	312/313 (99%)	-0.18	5 (1%)	72	59	27, 55, 92, 143	0
1	G	312/313 (99%)	-0.15	4 (1%)	77	65	40, 76, 106, 165	0
1	H	312/313 (99%)	0.55	20 (6%)	19	14	86, 121, 145, 191	0
1	I	312/313 (99%)	-0.23	1 (0%)	94	89	32, 62, 95, 141	0
1	J	312/313 (99%)	0.22	13 (4%)	36	26	57, 91, 126, 179	0
1	K	312/313 (99%)	0.69	33 (10%)	6	6	85, 128, 153, 196	0
All	All	3432/3443 (99%)	-0.09	96 (2%)	53	39	12, 66, 135, 196	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	71	PRO	8.9
1	D	70	VAL	7.6
1	G	70	VAL	7.0
1	K	72	LEU	6.3
1	A	70	VAL	6.2
1	J	71	PRO	6.2
1	K	70	VAL	6.0
1	K	71	PRO	5.9
1	H	70	VAL	5.7
1	J	70	VAL	5.4
1	F	322	GLY	5.4
1	D	71	PRO	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	71	PRO	5.2
1	J	72	LEU	5.1
1	E	70	VAL	5.1
1	B	71	PRO	5.0
1	H	71	PRO	4.8
1	C	70	VAL	4.7
1	K	382	LEU	4.5
1	J	322	GLY	4.5
1	C	71	PRO	4.4
1	K	179	THR	4.1
1	F	71	PRO	4.0
1	J	78	GLU	4.0
1	J	169	TYR	3.8
1	A	71	PRO	3.8
1	F	320	PRO	3.7
1	H	322	GLY	3.7
1	H	382	LEU	3.7
1	C	322	GLY	3.5
1	K	153	ALA	3.5
1	K	192	ALA	3.3
1	K	351	HIS	3.3
1	K	98	LEU	3.3
1	K	130	TRP	3.2
1	J	321	PHE	3.2
1	K	146	VAL	3.2
1	B	70	VAL	3.2
1	K	307	SER	3.0
1	H	319	GLU	2.9
1	K	152	VAL	2.9
1	D	73	ILE	2.9
1	F	70	VAL	2.9
1	F	321	PHE	2.9
1	K	102	LEU	2.8
1	J	228	LEU	2.8
1	H	140	SER	2.7
1	B	72	LEU	2.7
1	J	73	ILE	2.7
1	H	247	MET	2.6
1	K	165	LEU	2.6
1	E	307	SER	2.6
1	K	223	ASP	2.6
1	H	152	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	216	THR	2.6
1	K	155	LEU	2.6
1	H	238	TYR	2.5
1	K	172	LYS	2.5
1	J	327	ASP	2.4
1	D	72	LEU	2.4
1	H	72	LEU	2.4
1	K	88	LEU	2.4
1	G	73	ILE	2.4
1	K	255	GLY	2.4
1	K	193	LEU	2.4
1	H	226	GLU	2.4
1	C	178	SER	2.4
1	I	322	GLY	2.4
1	H	132	VAL	2.3
1	J	151	VAL	2.3
1	K	219	LEU	2.3
1	H	133	GLU	2.3
1	K	115	VAL	2.3
1	K	171	SER	2.3
1	K	119	LEU	2.3
1	K	181	PHE	2.3
1	K	353	PRO	2.3
1	C	321	PHE	2.2
1	H	258	ARG	2.2
1	E	312	VAL	2.2
1	B	73	ILE	2.2
1	H	243	LEU	2.2
1	H	153	ALA	2.2
1	J	231	TRP	2.2
1	H	230	GLU	2.2
1	K	180	PRO	2.2
1	E	308	HIS	2.1
1	H	131	HIS	2.1
1	H	231	TRP	2.1
1	K	114	GLN	2.1
1	K	225	GLU	2.0
1	G	72	LEU	2.0
1	H	259	ILE	2.0
1	K	148	PHE	2.0
1	K	381	GLY	2.0
1	J	258	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

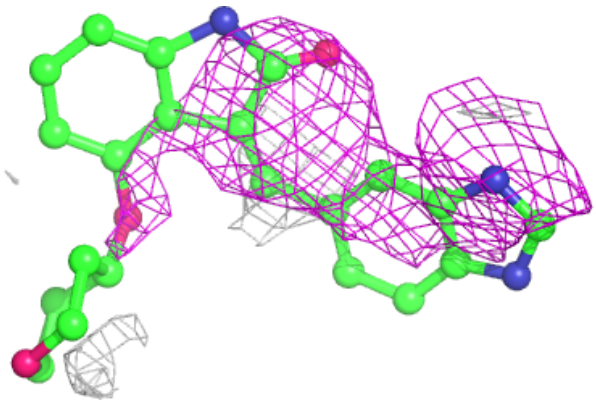
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

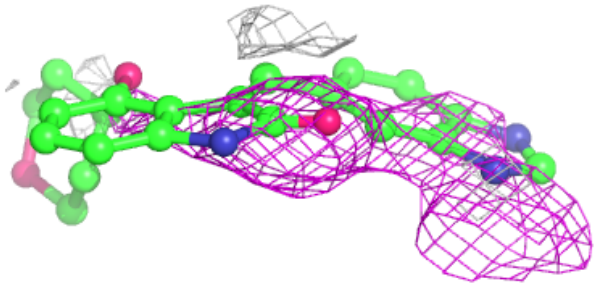
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	A1D47	K	402	27/27	0.29	1.18	111,129,140,144	0
2	ZN	K	401	1/1	0.36	0.56	182,182,182,182	0
3	A1D47	J	402	27/27	0.60	0.96	93,113,129,132	0
3	A1D47	H	402	27/27	0.62	0.69	95,114,143,158	0
2	ZN	H	401	1/1	0.70	0.53	193,193,193,193	0
3	A1D47	D	402	27/27	0.75	0.58	54,86,96,98	0
3	A1D47	I	402	27/27	0.75	0.53	56,88,109,115	0
3	A1D47	A	402	27/27	0.76	0.55	44,86,107,111	0
2	ZN	J	401	1/1	0.76	0.31	144,144,144,144	0
3	A1D47	E	402	27/27	0.77	0.67	68,96,106,110	0
3	A1D47	F	402	27/27	0.78	0.63	59,87,100,102	0
3	A1D47	G	402	27/27	0.78	0.45	65,91,101,104	0
3	A1D47	C	402	27/27	0.79	0.46	51,86,97,97	0
3	A1D47	B	402	27/27	0.80	0.67	55,81,107,117	0
2	ZN	E	401	1/1	0.80	0.39	147,147,147,147	0
2	ZN	D	401	1/1	0.85	0.20	115,115,115,115	0
2	ZN	C	401	1/1	0.90	0.31	132,132,132,132	0
2	ZN	F	401	1/1	0.91	0.46	137,137,137,137	0
2	ZN	I	401	1/1	0.92	0.25	108,108,108,108	0
2	ZN	A	401	1/1	0.95	0.28	108,108,108,108	0
2	ZN	B	401	1/1	0.95	0.30	109,109,109,109	0
2	ZN	G	401	1/1	0.95	0.44	151,151,151,151	0

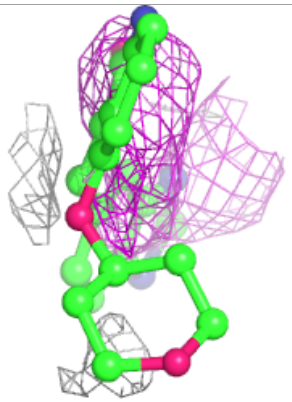
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1D47 K 402:

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

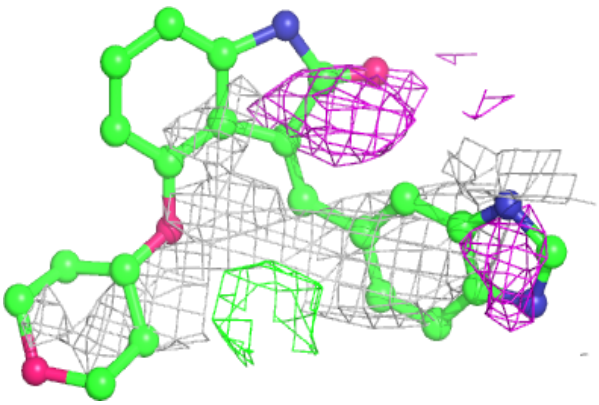


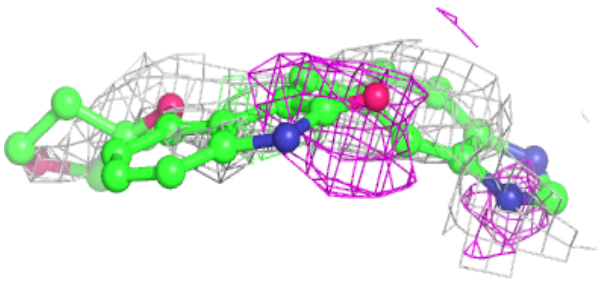


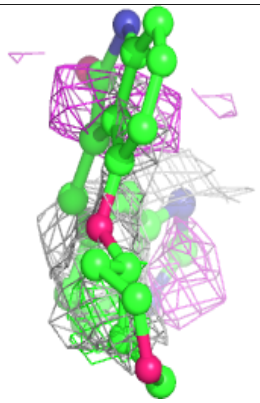


Electron density around A1D47 J 402:

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

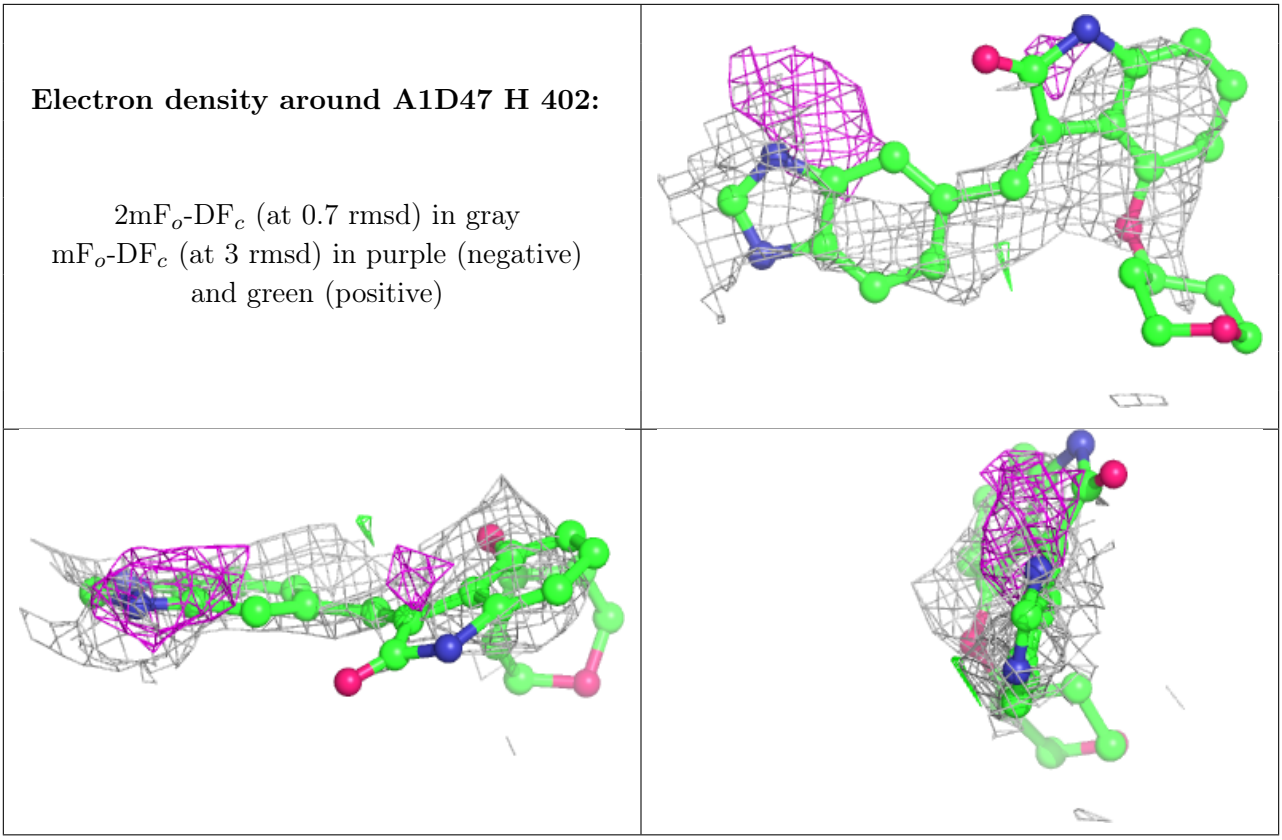






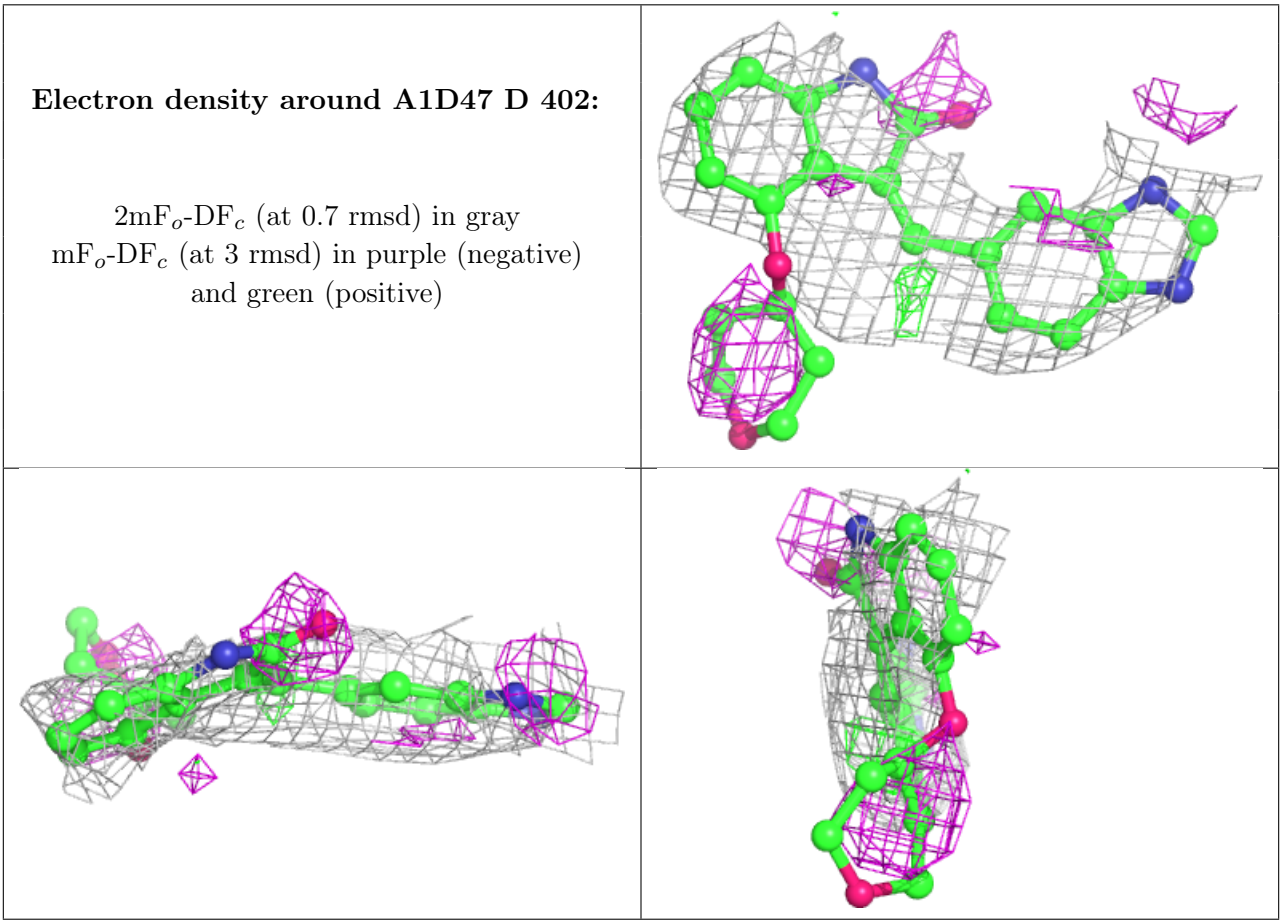
Electron density around A1D47 H 402:

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



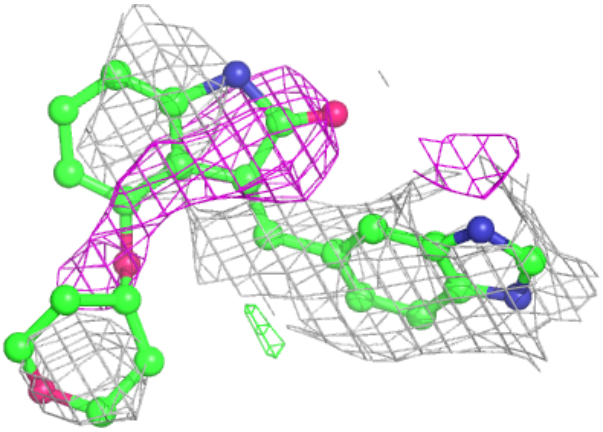
Electron density around A1D47 D 402:

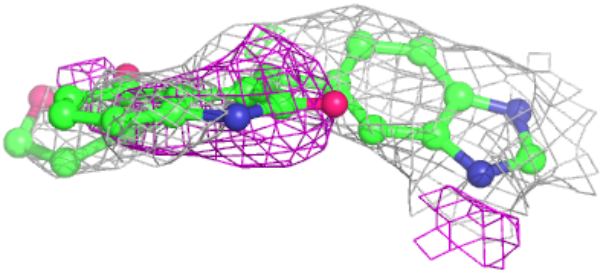
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

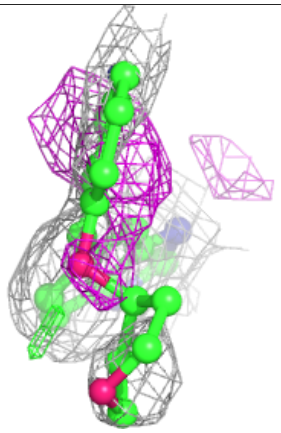


Electron density around A1D47 I 402:

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

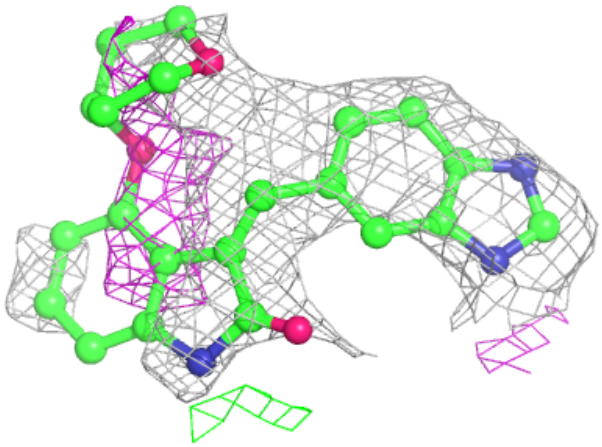


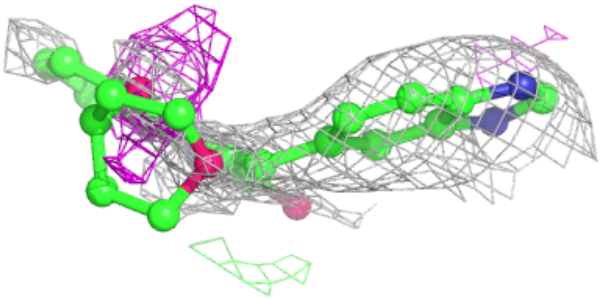




Electron density around A1D47 A 402:

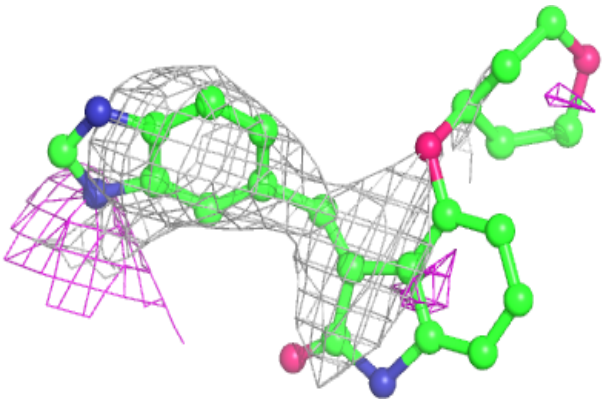
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

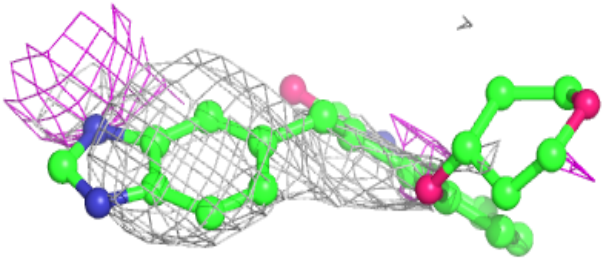


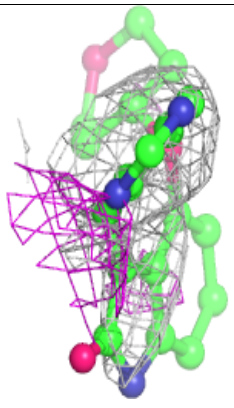


Electron density around A1D47 E 402:

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

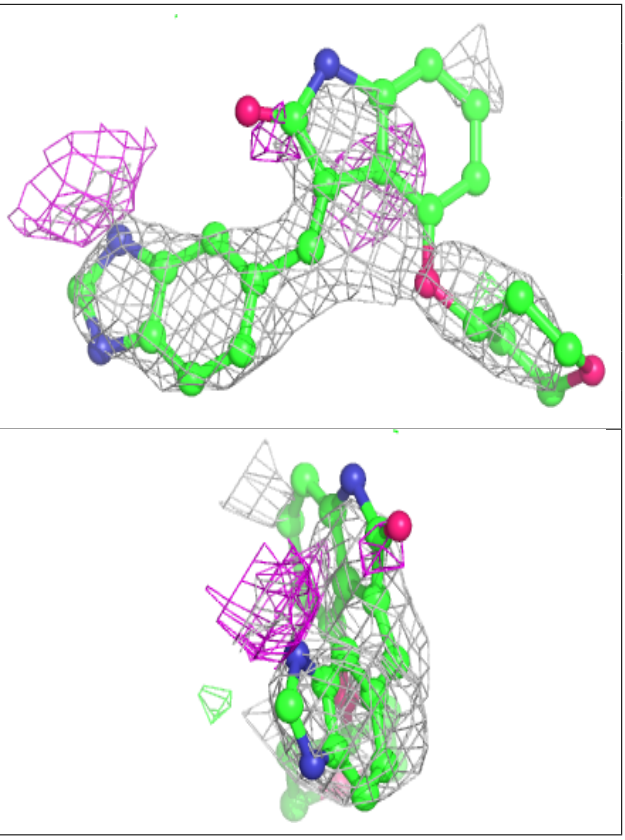


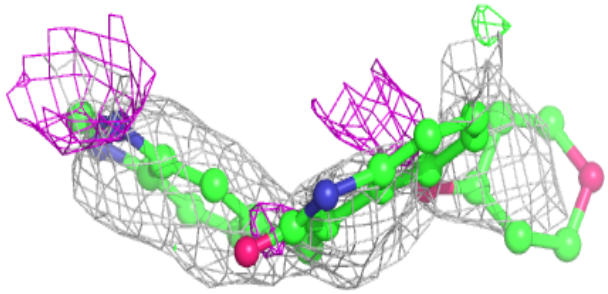




Electron density around A1D47 F 402:

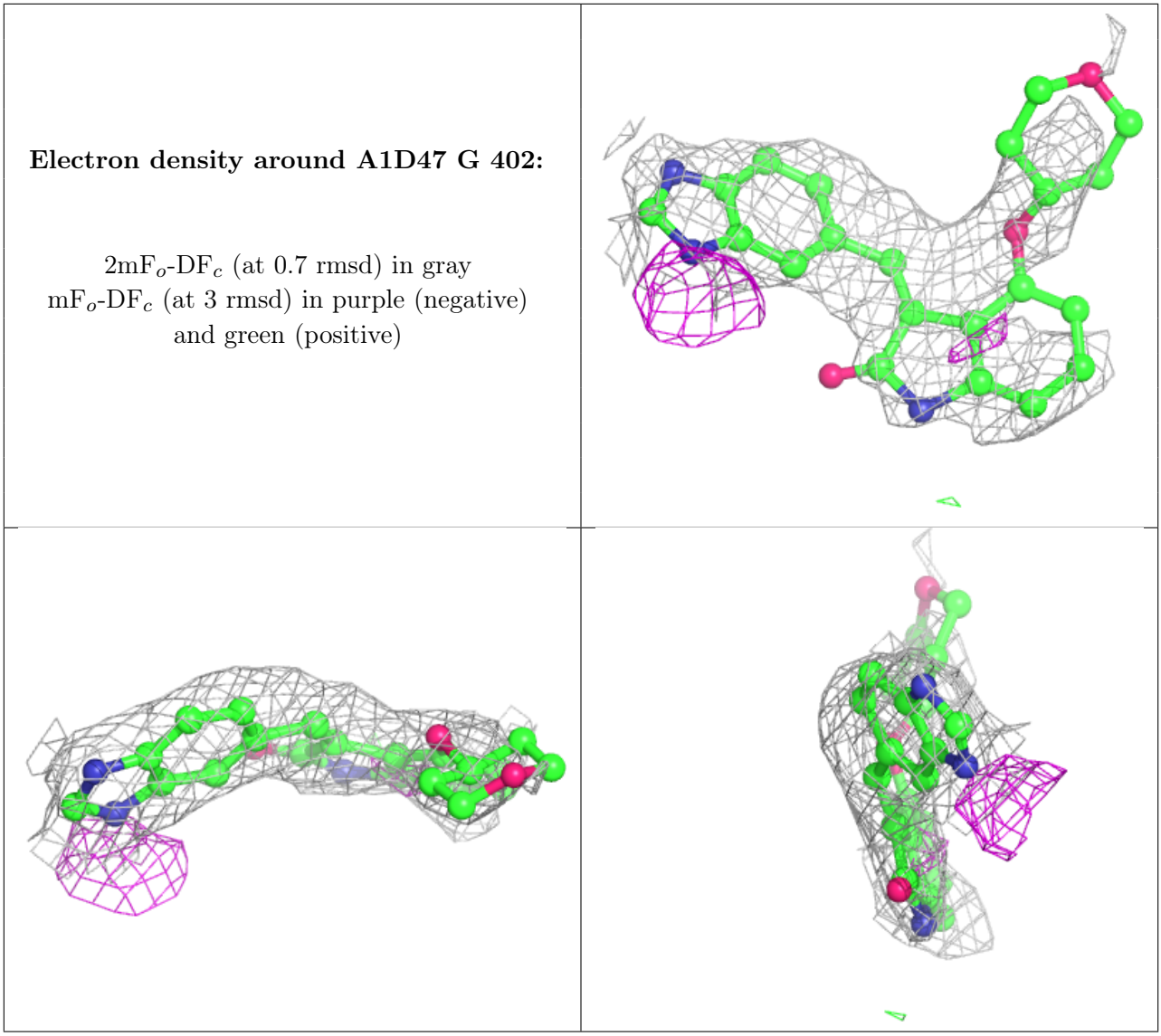
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





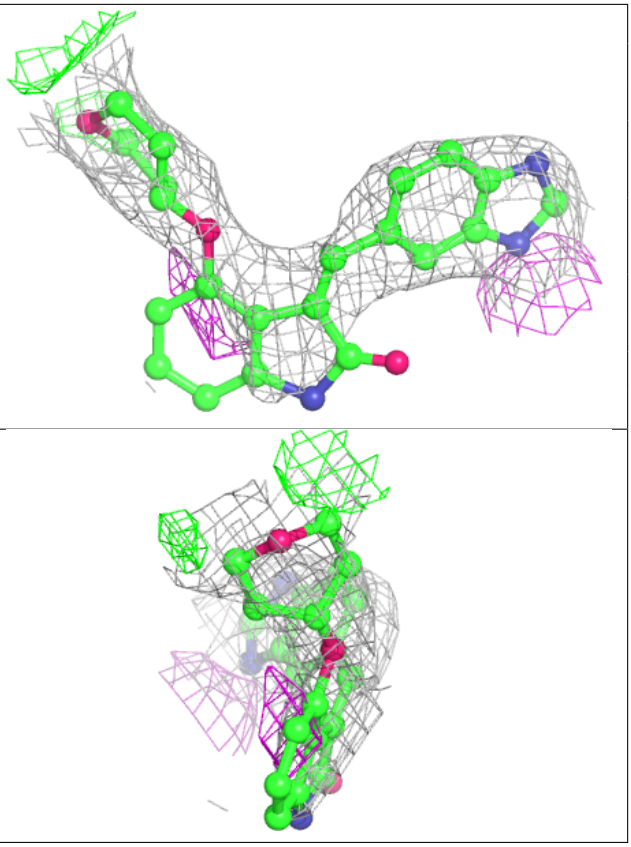
Electron density around A1D47 G 402:

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



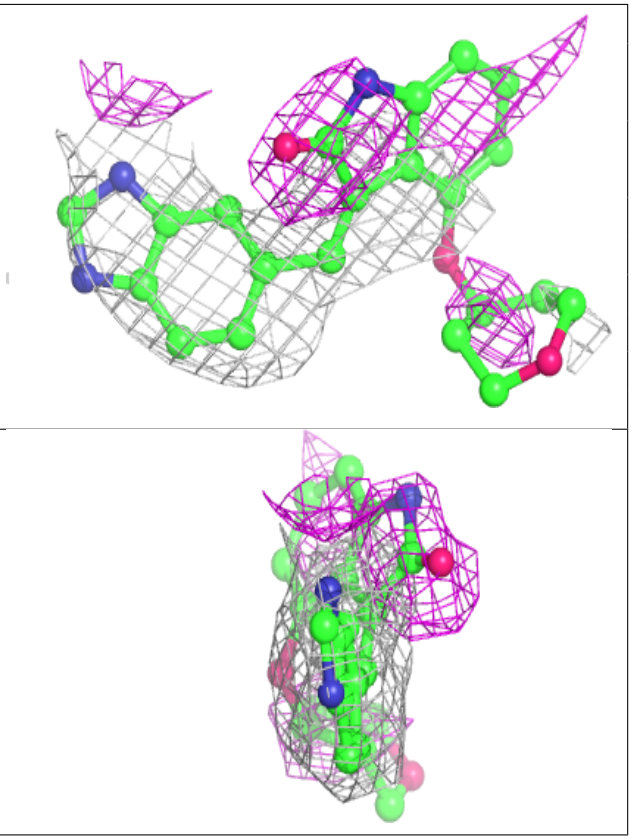
Electron density around A1D47 C 402:

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



Electron density around A1D47 B 402:

$2mF_o$-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.