Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 04:37 PM JST

PDB ID	:	5XMS
Title	:	Plasmodium vivax SHMT bound with PLP-glycine and GS498
Authors	:	Chitnumsub, P.; Jaruwat, A.; Leartsakulpanich, U.; Schwertz, G.; Diederich, F.
Deposited on	:	2017-05-16
Resolution	:	2.45 Å(reported)

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

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

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

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

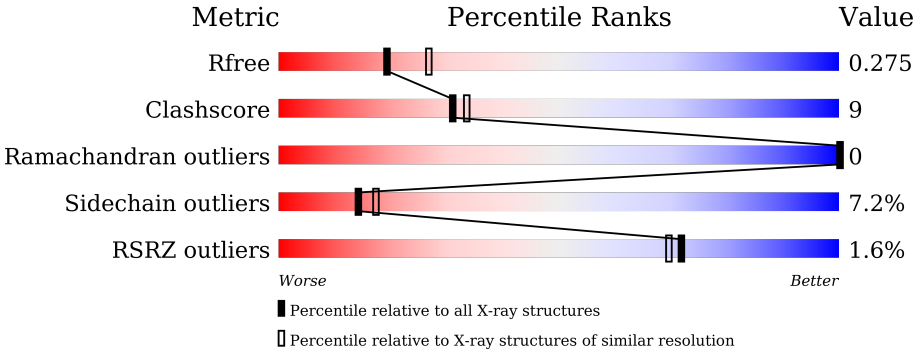
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	442	2% 76% 22% •
1	B	442	2% 78% 20% •
1	C	442	% 77% 20% •

2 Entry composition (i)

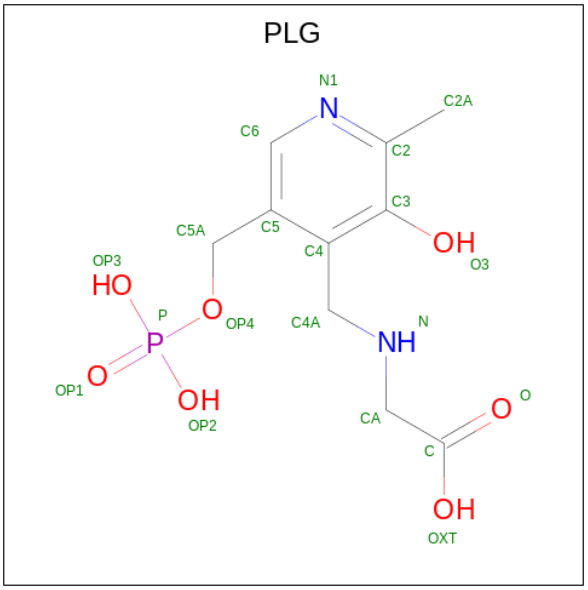
There are 5 unique types of molecules in this entry. The entry contains 10865 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine hydroxymethyltransferase.

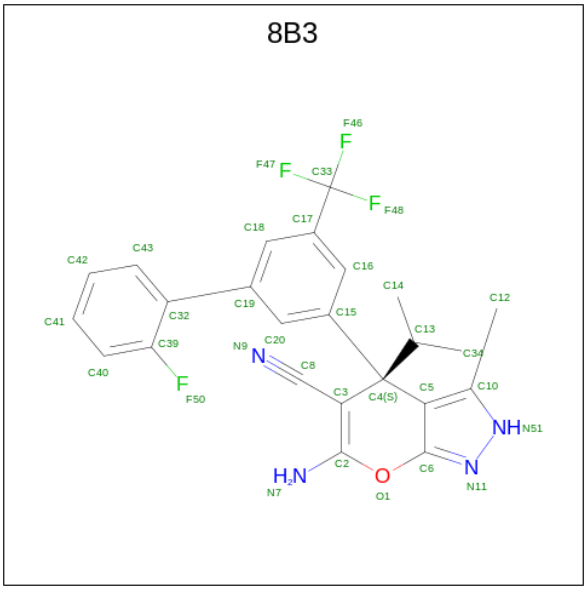
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3458	2186	600	655	17	0	0	0
1	B	442	3458	2186	600	655	17	0	0	0
1	C	442	3458	2186	600	655	17	0	0	0

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: $C_{10}H_{15}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	20	10	2	7	1	0	0
2	B	1	20	10	2	7	1	0	0
2	C	1	20	10	2	7	1	0	0

- Molecule 3 is (4 {S})-6-azanyl-4-[3-(2-fluorophenyl)-5-(trifluoromethyl)phenyl]-3-methyl-4 -propan-2-yl-2 {H}-pyrano[2,3-c]pyrazole-5- carbonitrile (three-letter code: 8B3) (formula: $C_{24}H_{20}F_4N_4O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	33	24	4	4	1	0	0
			Total	C	F	N	O		
3	B	1	33	24	4	4	1	0	0
			Total	C	F	N	O		
3	C	1	33	24	4	4	1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0
			Total	Cl		
4	C	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	110	110	110	0	0
			Total	O		
5	B	110	110	110	0	0
			Total	O		
5	C	110	110	110	0	0

3 Residue-property plots (i)

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

• Molecule 1: Serine hydroxymethyltransferase

Chain A: 2% 76% 22%

M1 P6 L7 I10 D11 E21 E22 R26 E27 N39 G40 A41 V42 V50 Y54 P59 K60 K61 R62 Y63 Y64 F69 I70 D71 E74 Q78 E91 W92 G93 Q97 S100 G101 S102 L109 Y110 V113 M120 C125 S126 G127 G128 H129

L130 T131 K138 K139 T144 M147 F148 D162 A165 V166 R167 E168 M169 S172 F173 K174 P175 K176 V177 I178 I179 C180 G181 Y182 T183 S184 R195 V201 N202 D208 I209 S210 S213 S214 F215 C218 W219 I220 L221 L226 H227 T234 T235 H236 R240 G241

P242 R243 F249 N250 K251 K252 R253 N254 P255 G256 I257 I261 N262 S263 A264 V265 S268 N275 K294 E295 L327 S340 K341 I349 N350 V351 V362 D363 C364 R371 T374 P375 I398 K399 I400 T401 V402 Q405 K410 K411 D414 L419 N422

L425 Q426 Q427 Q430 V433 P442

• Molecule 1: Serine hydroxymethyltransferase

Chain B: 2% 78% 20%

M1 L7 I10 E21 E22 R26 S34 N39 V42 V50 Y54 S55 P59 K60 K61 R62 Y63 Y64 I70 D71 E74 Q78 K79 R80 D89 Q97 S100 G101 S102 L109 V113 M120 H129 L130 T131 K138 K139 T144

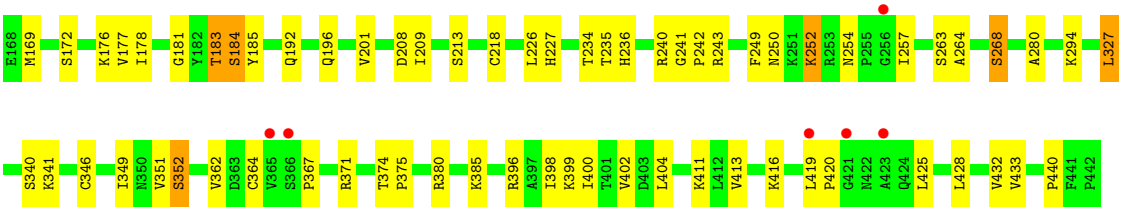
S145 D146 M147 F148 Y153 R167 E168 M169 K174 P175 K176 V177 I178 I179 C180 G181 Y182 T183 S184 Y185 Q192 R195 Q196 I197 C198 V201 N202 A203 D208 I209 S210 S213 C218 N219 H227 V230 T234 T235 H236 R240 G241 F248 F249 N250 R253

N254 S263 A264 V265 H274 N275 N276 K277 K294 K309 Q315 L327 K334 S340 N347 S352 C364 V365 S366 P367 T374 P375 R380 R396 A397 I398 V402 Q405 E406 K410 V413 L419 Q427 L428 P440 F441 P442

• Molecule 1: Serine hydroxymethyltransferase

Chain C: % 77% 20%

M1 P6 L7 I10 E21 E22 R26 E27 T28 I29 N30 E35 K53 Y54 P59 R62 Y63 Y64 D71 E74 Q78 D89 E90 E91 W92 G93 S100 L109 L112 V113 M120 H129 K138 K139 K151 L152 Y153 V161 R167


E168
M169
S172
K176
V177
I178
G181
Y182
T183
S184
Y185
Q192
Q196
V201
D208
I209
S213
C218
L226
H227
T234
T235
H236
R240
G241
P242
R243
F249
N250
K251
K252
R253
N254
P255
G256
I257
S263
A264
S268
A280
K294
L327
S340
K341
C346
I349
N350
V351
S352
V362
D363
C364
V365
S366
P367
R371
T374
P375
R380
K385
R396
A397
I398
K399
I400
T401
V402
D403
L404
K411
L412
V413
K416
L419
P420
G421
M422
A423
Q424
L425
L428
V432
V433
P440
F441
P442

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	101.81Å 58.79Å 235.13Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	30.00 – 2.45 29.16 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.1 (30.00-2.45) 95.1 (29.16-2.45)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	13.22 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.218 , 0.280 0.217 , 0.275	Depositor DCC
R_{free} test set	4837 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 13.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.013 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.013 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.469 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.477 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.014 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10865	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PLG, 8B3

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	0.54	0/3521	0.69	0/4754
1	B	0.55	0/3521	0.69	0/4754
1	C	0.54	0/3521	0.70	0/4754
All	All	0.54	0/10563	0.69	0/14262

There are no bond length outliers.

There are no bond angle outliers.

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	3458	0	3477	66	0
1	B	3458	0	3477	64	0
1	C	3458	0	3477	64	1
2	A	20	0	11	1	0
2	B	20	0	11	2	0
2	C	20	0	11	1	0
3	A	33	0	0	0	0
3	B	33	0	0	0	0
3	C	33	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
5	A	110	0	0	1	0
5	B	110	0	0	1	0
5	C	110	0	0	6	1
All	All	10865	0	10464	190	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (190) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LYS:NZ	5:C:601:HOH:O	1.90	0.99
1:C:167:ARG:NH1	5:C:602:HOH:O	2.04	0.89
1:C:22:GLU:OE1	1:C:26:ARG:NH2	2.06	0.88
1:B:315:GLN:O	1:B:334:LYS:NZ	2.13	0.79
1:B:174:LYS:HD3	1:B:201:VAL:HG13	1.63	0.79
1:B:120:MET:SD	1:B:169:MET:HE3	2.27	0.75
1:A:174:LYS:HD3	1:A:201:VAL:HG13	1.69	0.74
1:A:113:VAL:HG11	1:A:177:VAL:HG23	1.71	0.71
1:B:22:GLU:OE1	1:B:26:ARG:NH2	2.26	0.67
1:B:153:TYR:HB3	1:B:169:MET:CE	2.25	0.67
1:B:7:LEU:HA	1:B:10:ILE:HG22	1.77	0.66
1:C:184:SER:HB3	1:C:371:ARG:HD3	1.79	0.64
1:C:7:LEU:HA	1:C:10:ILE:CG2	2.29	0.63
1:B:405:GLN:CD	1:B:410:LYS:HD3	2.18	0.63
1:C:59:PRO:HA	1:C:71:ASP:OD1	1.99	0.62
1:C:6:PRO:O	1:C:10:ILE:HG22	1.98	0.62
1:A:7:LEU:HA	1:A:10:ILE:CG2	2.30	0.62
1:B:210:SER:HB3	1:B:234:THR:OG1	1.99	0.62
1:B:50:VAL:HG22	1:B:275:ASN:HB3	1.82	0.61
1:B:120:MET:HE2	1:B:178:ILE:HG12	1.81	0.61
1:C:120:MET:SD	1:C:169:MET:HE3	2.40	0.61
1:A:7:LEU:HA	1:A:10:ILE:HG22	1.83	0.59
1:A:398:ILE:O	1:A:402:VAL:HG23	2.03	0.59
1:B:74:GLU:O	1:B:78:GLN:HG3	2.03	0.59
1:B:183:THR:HB	2:B:501:PLG:O3	2.03	0.59
1:C:209:ILE:HD12	1:C:213:SER:HA	1.84	0.59
1:B:113:VAL:CG1	1:B:177:VAL:HG23	2.32	0.59
1:A:209:ILE:HD12	1:A:213:SER:HA	1.84	0.58
1:C:113:VAL:CG1	1:C:177:VAL:HG23	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:NZ	5:A:602:HOH:O	2.37	0.57
1:C:341:LYS:NZ	5:C:603:HOH:O	2.37	0.57
1:A:6:PRO:O	1:A:10:ILE:HG22	2.03	0.57
1:A:400:ILE:HG21	1:A:425:LEU:HD21	1.87	0.57
1:C:7:LEU:HA	1:C:10:ILE:HG22	1.87	0.57
1:A:22:GLU:OE1	1:A:26:ARG:NH2	2.39	0.56
1:C:109:LEU:O	1:C:113:VAL:HG22	2.05	0.56
1:C:235:THR:O	1:C:241:GLY:N	2.38	0.56
1:A:91:GLU:HG3	1:A:252:LYS:HB2	1.88	0.56
1:A:113:VAL:CG1	1:A:177:VAL:CG2	2.84	0.56
1:A:422:ASN:O	1:A:426:GLN:HG3	2.06	0.55
1:B:7:LEU:HA	1:B:10:ILE:CG2	2.37	0.55
1:B:153:TYR:HB3	1:B:169:MET:HE2	1.88	0.55
1:B:209:ILE:HD12	1:B:213:SER:HA	1.88	0.55
1:B:174:LYS:HD3	1:B:201:VAL:CG1	2.35	0.55
1:B:234:THR:HB	1:B:236:HIS:CE1	2.42	0.55
1:B:235:THR:O	1:B:241:GLY:N	2.36	0.55
1:C:120:MET:HE2	1:C:178:ILE:HG12	1.89	0.55
1:B:34:SER:OG	2:B:501:PLG:O	2.18	0.54
1:A:120:MET:SD	1:A:169:MET:HE3	2.48	0.54
1:C:234:THR:HB	1:C:236:HIS:CE1	2.42	0.54
1:A:127:GLY:O	1:A:182:TYR:HB3	2.08	0.54
1:A:210:SER:HB3	1:A:234:THR:OG1	2.08	0.54
1:C:396:ARG:CZ	1:C:428:LEU:HD13	2.37	0.54
1:C:153:TYR:HB3	1:C:169:MET:CE	2.38	0.53
1:A:234:THR:HB	1:A:236:HIS:CE1	2.44	0.53
1:C:113:VAL:HG12	1:C:176:LYS:HB2	1.90	0.53
1:A:109:LEU:HD21	1:A:179:ILE:HD11	1.90	0.53
1:A:50:VAL:HG22	1:A:275:ASN:HB3	1.90	0.53
1:C:226:LEU:HB2	1:C:227:HIS:CD2	2.43	0.53
1:B:167:ARG:HB2	1:B:197:ILE:CD1	2.39	0.53
1:A:113:VAL:CG1	1:A:177:VAL:HG23	2.38	0.52
1:C:91:GLU:HG3	1:C:252:LYS:HB2	1.90	0.52
1:A:226:LEU:HB2	1:A:227:HIS:CD2	2.45	0.52
1:C:113:VAL:HG11	1:C:177:VAL:HG23	1.92	0.52
1:B:102:SER:HA	1:B:131:THR:HG21	1.93	0.51
1:B:64:TYR:CD1	1:B:64:TYR:N	2.78	0.51
1:C:236:HIS:ND1	1:C:243:ARG:HA	2.26	0.51
1:A:7:LEU:CA	1:A:10:ILE:HG22	2.41	0.50
1:C:192:GLN:HG2	5:C:605:HOH:O	2.10	0.50
1:C:64:TYR:CD1	1:C:64:TYR:N	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:TYR:HB3	1:C:169:MET:HE2	1.93	0.50
1:A:64:TYR:CD1	1:A:64:TYR:N	2.79	0.49
1:B:398:ILE:O	1:B:402:VAL:HG23	2.11	0.49
1:C:400:ILE:HG21	1:C:425:LEU:HD21	1.95	0.49
1:C:398:ILE:O	1:C:402:VAL:HG23	2.12	0.49
1:A:110:TYR:OH	1:B:146:ASP:OD2	2.26	0.49
1:A:427:GLN:HE21	1:A:427:GLN:HA	1.78	0.49
1:A:113:VAL:HA	1:A:176:LYS:HE3	1.94	0.48
1:A:147:MET:HE2	1:A:148:PHE:CZ	2.49	0.48
1:B:195:ARG:HB2	1:B:227:HIS:HB3	1.96	0.48
1:B:153:TYR:HB3	1:B:169:MET:HE1	1.95	0.48
1:C:113:VAL:HA	1:C:176:LYS:HE2	1.95	0.47
1:B:39:ASN:OD1	1:B:42:VAL:HG23	2.14	0.47
1:C:129:HIS:HA	1:C:183:THR:HG21	1.95	0.47
1:C:380:ARG:O	1:C:440:PRO:HD2	2.14	0.47
1:B:181:GLY:HA3	1:B:208:ASP:O	2.15	0.47
1:C:192:GLN:HA	1:C:227:HIS:ND1	2.29	0.47
1:C:29:ILE:HD12	1:C:432:VAL:HG13	1.96	0.47
1:A:405:GLN:CD	1:A:410:LYS:HD3	2.35	0.47
1:B:113:VAL:HG11	1:B:177:VAL:HG23	1.95	0.47
1:C:349:ILE:HG13	1:C:351:VAL:HG23	1.97	0.47
1:B:109:LEU:HD21	1:B:179:ILE:HD11	1.96	0.47
1:B:192:GLN:HA	1:B:227:HIS:ND1	2.30	0.47
1:A:69:PHE:HB2	1:B:21:GLU:HG2	1.96	0.46
1:A:97:GLN:HB2	1:A:265:VAL:HG11	1.96	0.46
1:B:364:CYS:O	1:B:367:PRO:HD3	2.15	0.46
1:A:60:LYS:N	1:A:71:ASP:OD2	2.48	0.46
1:A:27:GLU:HG2	1:A:433:VAL:HG13	1.95	0.46
1:A:102:SER:HA	1:A:131:THR:HG21	1.96	0.46
1:A:131:THR:O	1:A:144:THR:HG21	2.16	0.46
1:A:129:HIS:HB2	1:A:183:THR:HG22	1.98	0.46
1:A:349:ILE:HG13	1:A:351:VAL:HG23	1.98	0.46
1:A:183:THR:HB	2:A:501:PLG:O3	2.16	0.45
1:A:327:LEU:HD12	1:A:327:LEU:C	2.37	0.45
1:B:218:CYS:HB3	1:B:294:LYS:HD2	1.98	0.45
1:C:183:THR:HB	2:C:501:PLG:O3	2.16	0.45
1:A:235:THR:O	1:A:241:GLY:N	2.43	0.45
1:C:113:VAL:HG12	1:C:176:LYS:CB	2.45	0.45
1:A:129:HIS:HA	1:A:183:THR:HG21	1.97	0.45
1:A:184:SER:HB3	1:A:371:ARG:HD3	1.98	0.45
1:C:89:ASP:C	1:C:89:ASP:OD1	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:MET:CE	1:A:148:PHE:CZ	3.00	0.45
1:C:364:CYS:O	1:C:367:PRO:HD3	2.17	0.45
1:B:64:TYR:N	1:B:64:TYR:HD1	2.14	0.45
1:A:427:GLN:O	1:A:427:GLN:NE2	2.50	0.45
1:B:427:GLN:HE21	1:B:427:GLN:HA	1.81	0.45
1:B:7:LEU:CA	1:B:10:ILE:HG22	2.46	0.44
1:B:174:LYS:CD	1:B:201:VAL:HG13	2.40	0.44
1:A:41:ALA:CB	1:B:10:ILE:HG21	2.47	0.44
1:C:7:LEU:O	1:C:7:LEU:HD12	2.16	0.44
1:B:97:GLN:HB2	1:B:265:VAL:HG11	2.00	0.44
1:B:327:LEU:C	1:B:327:LEU:HD12	2.38	0.44
1:B:374:THR:N	1:B:375:PRO:CD	2.80	0.44
1:C:404:LEU:CD1	1:C:419:LEU:HD23	2.47	0.44
1:A:374:THR:N	1:A:375:PRO:HD3	2.33	0.44
1:C:181:GLY:HA3	1:C:208:ASP:O	2.17	0.44
1:A:362:VAL:HG12	1:A:362:VAL:O	2.18	0.44
1:A:236:HIS:ND1	1:A:243:ARG:HA	2.33	0.44
1:C:64:TYR:N	1:C:64:TYR:HD1	2.16	0.44
1:A:39:ASN:OD1	1:A:42:VAL:HG23	2.18	0.43
1:B:50:VAL:HG22	1:B:275:ASN:CB	2.48	0.43
1:C:161:VAL:HG23	1:C:185:TYR:CZ	2.54	0.43
1:C:264:ALA:HA	1:C:268:SER:HB2	2.01	0.43
1:A:374:THR:N	1:A:375:PRO:CD	2.82	0.43
1:A:181:GLY:HA3	1:A:208:ASP:O	2.19	0.43
1:B:89:ASP:OD1	1:B:89:ASP:C	2.57	0.43
1:C:10:ILE:HD12	1:C:10:ILE:O	2.18	0.43
1:C:74:GLU:O	1:C:78:GLN:HG3	2.19	0.43
1:B:201:VAL:HG12	1:B:201:VAL:O	2.19	0.43
1:C:416:LYS:O	1:C:420:PRO:HD3	2.18	0.43
1:C:196:GLN:NE2	5:C:605:HOH:O	2.44	0.43
1:A:201:VAL:HG12	1:A:201:VAL:O	2.19	0.43
1:B:144:THR:O	1:B:148:PHE:HB2	2.19	0.43
1:C:7:LEU:CA	1:C:10:ILE:HG22	2.48	0.43
1:A:93:GLY:HA3	1:A:249:PHE:CE2	2.53	0.42
1:A:125:CYS:SG	1:A:364:CYS:SG	3.17	0.42
1:A:162:ASP:OD2	1:A:165:ALA:HB2	2.19	0.42
1:A:257:ILE:HD13	1:A:261:ILE:HG13	2.01	0.42
1:B:113:VAL:HG12	1:B:176:LYS:HB3	2.00	0.42
1:C:218:CYS:HB3	1:C:294:LYS:HD2	2.01	0.42
1:B:109:LEU:O	1:B:113:VAL:HG22	2.19	0.42
1:C:201:VAL:O	1:C:201:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:THR:O	1:B:144:THR:HG21	2.20	0.42
1:B:198:CYS:HB3	1:B:203:ALA:O	2.19	0.42
1:B:374:THR:N	1:B:375:PRO:HD3	2.34	0.42
1:C:27:GLU:HG2	1:C:433:VAL:HG13	2.01	0.42
1:A:215:PHE:CB	1:A:221:LEU:HD12	2.50	0.42
1:B:50:VAL:HG23	1:B:70:ILE:CD1	2.50	0.42
1:C:93:GLY:HA3	1:C:249:PHE:CE2	2.55	0.42
1:A:113:VAL:HG13	1:A:177:VAL:CG2	2.49	0.42
1:A:109:LEU:O	1:A:113:VAL:HG22	2.20	0.42
1:B:230:VAL:HG13	1:B:248:PHE:O	2.19	0.42
1:B:274:HIS:O	1:B:277:LYS:HB2	2.20	0.42
1:B:380:ARG:O	1:B:440:PRO:HD2	2.20	0.42
1:B:396:ARG:CZ	1:B:428:LEU:HD13	2.49	0.42
1:A:218:CYS:HB3	1:A:294:LYS:HD2	2.02	0.42
1:B:60:LYS:N	1:B:71:ASP:OD2	2.48	0.41
1:C:242:PRO:HG3	1:C:280:ALA:HB3	2.01	0.41
1:B:129:HIS:HA	1:B:183:THR:HG21	2.01	0.41
1:B:240:ARG:HD3	5:B:695:HOH:O	2.20	0.41
1:C:112:LEU:HD21	1:C:257:ILE:HD11	2.02	0.41
1:C:184:SER:HB3	1:C:371:ARG:CD	2.46	0.41
1:C:374:THR:N	1:C:375:PRO:CD	2.83	0.41
1:C:30:ASN:HA	1:C:352:SER:HB2	2.02	0.41
1:C:327:LEU:C	1:C:327:LEU:HD12	2.41	0.41
1:C:404:LEU:HD13	1:C:419:LEU:HD23	2.03	0.41
1:A:74:GLU:O	1:A:78:GLN:HG3	2.20	0.41
1:C:346:CYS:HA	1:C:349:ILE:HG12	2.03	0.41
1:A:11:ASP:OD2	1:B:80:ARG:NH1	2.50	0.41
1:A:195:ARG:HB2	1:A:227:HIS:HB3	2.03	0.41
1:B:182:TYR:HB2	1:B:185:TYR:HB2	2.03	0.40
1:A:218:CYS:HB2	1:A:220:ILE:CD1	2.51	0.40
1:A:227:HIS:CD2	1:A:227:HIS:N	2.90	0.40
1:B:59:PRO:O	1:B:60:LYS:HB2	2.21	0.40
1:C:64:TYR:HD2	5:C:601:HOH:O	2.05	0.40
1:C:129:HIS:HB2	1:C:183:THR:HG22	2.02	0.40
1:C:226:LEU:HB2	1:C:227:HIS:HD2	1.82	0.40
1:A:59:PRO:O	1:A:60:LYS:HB2	2.22	0.40
1:A:120:MET:HG2	1:A:169:MET:HE3	2.04	0.40
1:B:59:PRO:HA	1:B:71:ASP:OD2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:GLU:OE2	5:C:601:HOH:O[2_656]	2.19	0.01

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	440/442 (100%)	430 (98%)	10 (2%)	0	100	100
1	B	440/442 (100%)	429 (98%)	11 (2%)	0	100	100
1	C	440/442 (100%)	430 (98%)	10 (2%)	0	100	100
All	All	1320/1326 (100%)	1289 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	381/381 (100%)	354 (93%)	27 (7%)	14	17
1	B	381/381 (100%)	356 (93%)	25 (7%)	16	20
1	C	381/381 (100%)	351 (92%)	30 (8%)	12	14
All	All	1143/1143 (100%)	1061 (93%)	82 (7%)	14	17

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	10	ILE
1	A	21	GLU
1	A	22	GLU
1	A	54	TYR
1	A	62	ARG
1	A	100	SER
1	A	138	LYS
1	A	139	LYS
1	A	167	ARG
1	A	172	SER
1	A	183	THR
1	A	184	SER
1	A	240	ARG
1	A	250	ASN
1	A	252	LYS
1	A	253	ARG
1	A	254	ASN
1	A	257	ILE
1	A	263	SER
1	A	268	SER
1	A	295	GLU
1	A	327	LEU
1	A	340	SER
1	A	411	LYS
1	A	427	GLN
1	A	430	GLN
1	B	21	GLU
1	B	22	GLU
1	B	26	ARG
1	B	54	TYR
1	B	55	SER
1	B	62	ARG
1	B	71	ASP
1	B	100	SER
1	B	139	LYS
1	B	169	MET
1	B	183	THR
1	B	184	SER
1	B	240	ARG
1	B	250	ASN
1	B	253	ARG
1	B	254	ASN

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Mol	Chain	Res	Type
1	B	263	SER
1	B	309	LYS
1	B	327	LEU
1	B	340	SER
1	B	347	ASN
1	B	352	SER
1	B	406	GLU
1	B	413	VAL
1	B	427	GLN
1	C	7	LEU
1	C	21	GLU
1	C	22	GLU
1	C	54	TYR
1	C	62	ARG
1	C	64	TYR
1	C	89	ASP
1	C	90	GLU
1	C	100	SER
1	C	138	LYS
1	C	139	LYS
1	C	151	LYS
1	C	167	ARG
1	C	172	SER
1	C	183	THR
1	C	184	SER
1	C	240	ARG
1	C	250	ASN
1	C	252	LYS
1	C	254	ASN
1	C	263	SER
1	C	268	SER
1	C	327	LEU
1	C	340	SER
1	C	352	SER
1	C	362	VAL
1	C	385	LYS
1	C	399	LYS
1	C	411	LYS
1	C	413	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	227	HIS
1	A	289	HIS
1	A	347	ASN
1	A	426	GLN
1	A	427	GLN
1	B	196	GLN
1	B	227	HIS
1	B	299	GLN
1	B	321	ASN
1	B	424	GLN
1	B	427	GLN
1	C	78	GLN
1	C	196	GLN
1	C	227	HIS
1	C	347	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLG	C	501	-	20,20,20	2.68	4 (20%)	25,28,28	2.58	10 (40%)
3	8B3	B	502	-	31,36,36	2.57	2 (6%)	43,56,56	1.98	10 (23%)
3	8B3	C	502	-	31,36,36	2.56	2 (6%)	43,56,56	1.69	8 (18%)
2	PLG	B	501	-	20,20,20	2.78	3 (15%)	25,28,28	2.49	8 (32%)
2	PLG	A	501	-	20,20,20	2.60	4 (20%)	25,28,28	2.33	8 (32%)
3	8B3	A	502	-	31,36,36	2.66	2 (6%)	43,56,56	1.99	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLG	C	501	-	-	5/12/12/12	0/1/1/1
3	8B3	B	502	-	-	2/22/44/44	0/4/4/4
3	8B3	C	502	-	-	1/22/44/44	0/4/4/4
2	PLG	B	501	-	-	3/12/12/12	0/1/1/1
2	PLG	A	501	-	-	5/12/12/12	0/1/1/1
3	8B3	A	502	-	-	0/22/44/44	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	8B3	C8-C3	-12.36	1.25	1.42
3	C	502	8B3	C8-C3	-11.96	1.26	1.42
3	B	502	8B3	C8-C3	-11.58	1.26	1.42
2	B	501	PLG	C3-C2	8.61	1.49	1.40
2	C	501	PLG	C3-C2	8.09	1.49	1.40
3	B	502	8B3	O1-C2	7.66	1.45	1.36
2	A	501	PLG	C3-C2	7.45	1.48	1.40
3	A	502	8B3	O1-C2	7.26	1.44	1.36
3	C	502	8B3	O1-C2	6.90	1.44	1.36
2	C	501	PLG	C5-C4	6.46	1.49	1.40
2	B	501	PLG	C5-C4	6.26	1.49	1.40
2	A	501	PLG	C5-C4	5.87	1.48	1.40
2	A	501	PLG	C3-C4	5.73	1.48	1.40
2	B	501	PLG	C3-C4	4.93	1.47	1.40
2	C	501	PLG	C3-C4	4.57	1.47	1.40
2	A	501	PLG	OXT-C	-2.36	1.22	1.30
2	C	501	PLG	OXT-C	-2.12	1.23	1.30

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	PLG	C4A-N-CA	9.05	122.03	112.58
3	B	502	8B3	O1-C2-N7	7.70	115.75	110.22
2	A	501	PLG	C4A-N-CA	7.66	120.57	112.58
3	A	502	8B3	O1-C2-N7	7.39	115.53	110.22
2	B	501	PLG	C4A-N-CA	6.06	118.91	112.58
3	C	502	8B3	O1-C2-N7	5.68	114.30	110.22
2	B	501	PLG	OP4-C5A-C5	5.30	119.45	109.35
3	B	502	8B3	C3-C2-N7	-4.89	122.57	127.47
3	A	502	8B3	C3-C2-N7	-4.84	122.62	127.47
2	B	501	PLG	C4A-C4-C5	4.46	124.67	119.71
2	B	501	PLG	C6-C5-C4	4.16	121.06	118.12
2	B	501	PLG	C3-C4-C5	-4.08	114.81	118.72
3	C	502	8B3	C3-C2-N7	-3.81	123.65	127.47
2	A	501	PLG	C6-N1-C2	3.63	125.89	119.17
3	B	502	8B3	C8-C3-C2	3.36	122.09	117.64
3	A	502	8B3	C8-C3-C2	3.29	122.00	117.64
2	C	501	PLG	C6-N1-C2	3.18	125.05	119.17
3	C	502	8B3	C10-C5-C6	-3.15	100.68	104.01
2	C	501	PLG	C4A-C4-C5	3.14	123.21	119.71
3	A	502	8B3	C5-C4-C3	3.14	110.72	104.34
3	C	502	8B3	C14-C13-C4	2.98	115.60	112.40
2	C	501	PLG	OP4-C5A-C5	2.98	115.02	109.35
3	A	502	8B3	C13-C4-C3	-2.95	105.59	110.32
3	B	502	8B3	C5-C4-C3	2.89	110.22	104.34
3	B	502	8B3	C10-C5-C6	-2.87	100.98	104.01
3	C	502	8B3	C5-C4-C3	2.84	110.12	104.34
3	A	502	8B3	C10-C5-C6	-2.83	101.03	104.01
2	A	501	PLG	OP4-C5A-C5	2.79	114.66	109.35
3	A	502	8B3	C43-C32-C39	2.78	120.11	116.10
2	C	501	PLG	C3-C4-C5	-2.77	116.06	118.72
2	A	501	PLG	C3-C2-N1	-2.75	117.22	120.77
2	C	501	PLG	OP3-P-OP2	2.66	117.80	107.64
2	B	501	PLG	OP3-P-OP4	-2.60	99.83	106.73
3	C	502	8B3	C8-C3-C2	2.54	121.01	117.64
3	B	502	8B3	C13-C4-C3	-2.53	106.26	110.32
2	C	501	PLG	OXT-C-CA	2.46	121.29	112.74
3	A	502	8B3	C40-C39-C32	-2.43	120.33	123.30
2	A	501	PLG	OXT-C-CA	2.40	121.06	112.74
3	C	502	8B3	C13-C4-C3	-2.38	106.50	110.32
3	C	502	8B3	C40-C39-C32	-2.35	120.43	123.30
2	B	501	PLG	C6-N1-C2	2.33	123.49	119.17
2	A	501	PLG	OP3-P-OP4	-2.32	100.57	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	PLG	C6-C5-C4	2.30	119.74	118.12
2	A	501	PLG	C3-C4-C5	-2.29	116.52	118.72
3	B	502	8B3	F46-C33-F48	2.26	114.01	105.72
3	B	502	8B3	C14-C13-C4	2.21	114.77	112.40
3	A	502	8B3	C6-O1-C2	2.16	120.72	118.38
2	A	501	PLG	OP3-P-OP2	2.16	115.89	107.64
3	B	502	8B3	C43-C32-C39	2.09	119.11	116.10
3	B	502	8B3	C40-C39-C32	-2.08	120.76	123.30
2	B	501	PLG	C4-C4A-N	2.08	115.46	111.58
2	C	501	PLG	OXT-C-O	-2.05	118.18	123.30
2	C	501	PLG	OP3-P-OP4	-2.05	101.28	106.73
3	A	502	8B3	F46-C33-F47	2.03	113.17	105.72

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLG	C5-C4-C4A-N
2	A	501	PLG	C5A-OP4-P-OP1
2	C	501	PLG	C5A-OP4-P-OP1
2	C	501	PLG	C5A-OP4-P-OP3
2	B	501	PLG	C5-C4-C4A-N
2	C	501	PLG	C5-C4-C4A-N
2	A	501	PLG	C3-C4-C4A-N
2	B	501	PLG	C3-C4-C4A-N
2	C	501	PLG	C3-C4-C4A-N
2	B	501	PLG	C6-C5-C5A-OP4
2	C	501	PLG	C5A-OP4-P-OP2
3	B	502	8B3	C16-C15-C4-C5
3	B	502	8B3	C20-C15-C4-C5
3	C	502	8B3	C20-C15-C4-C5
2	A	501	PLG	C5A-OP4-P-OP2
2	A	501	PLG	C5A-OP4-P-OP3

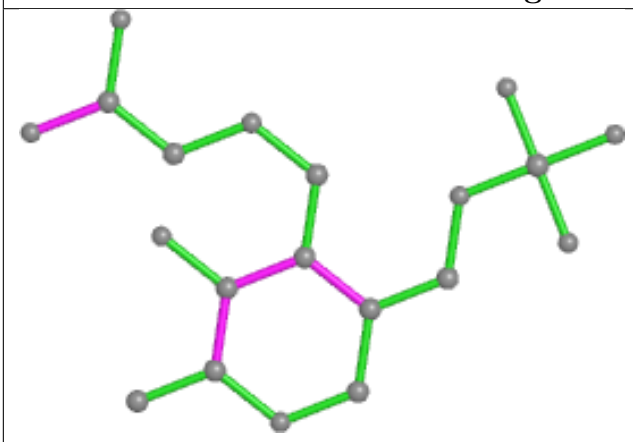
There are no ring outliers.

3 monomers are involved in 4 short contacts:

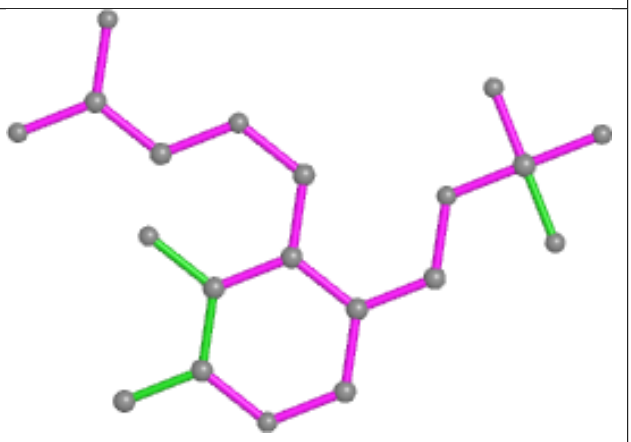
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	PLG	1	0
2	B	501	PLG	2	0
2	A	501	PLG	1	0

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.

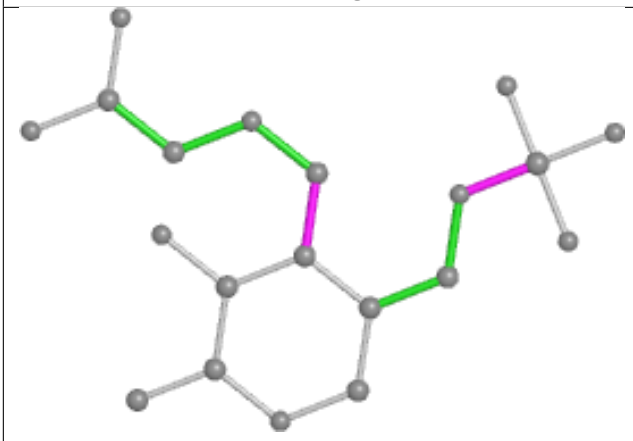
Ligand PLG C 501



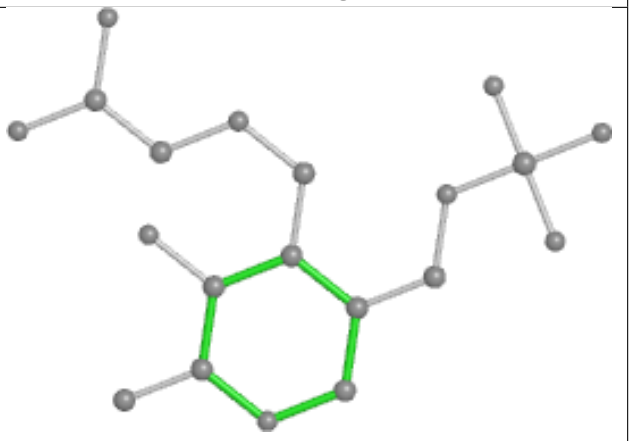
Bond lengths



Bond angles

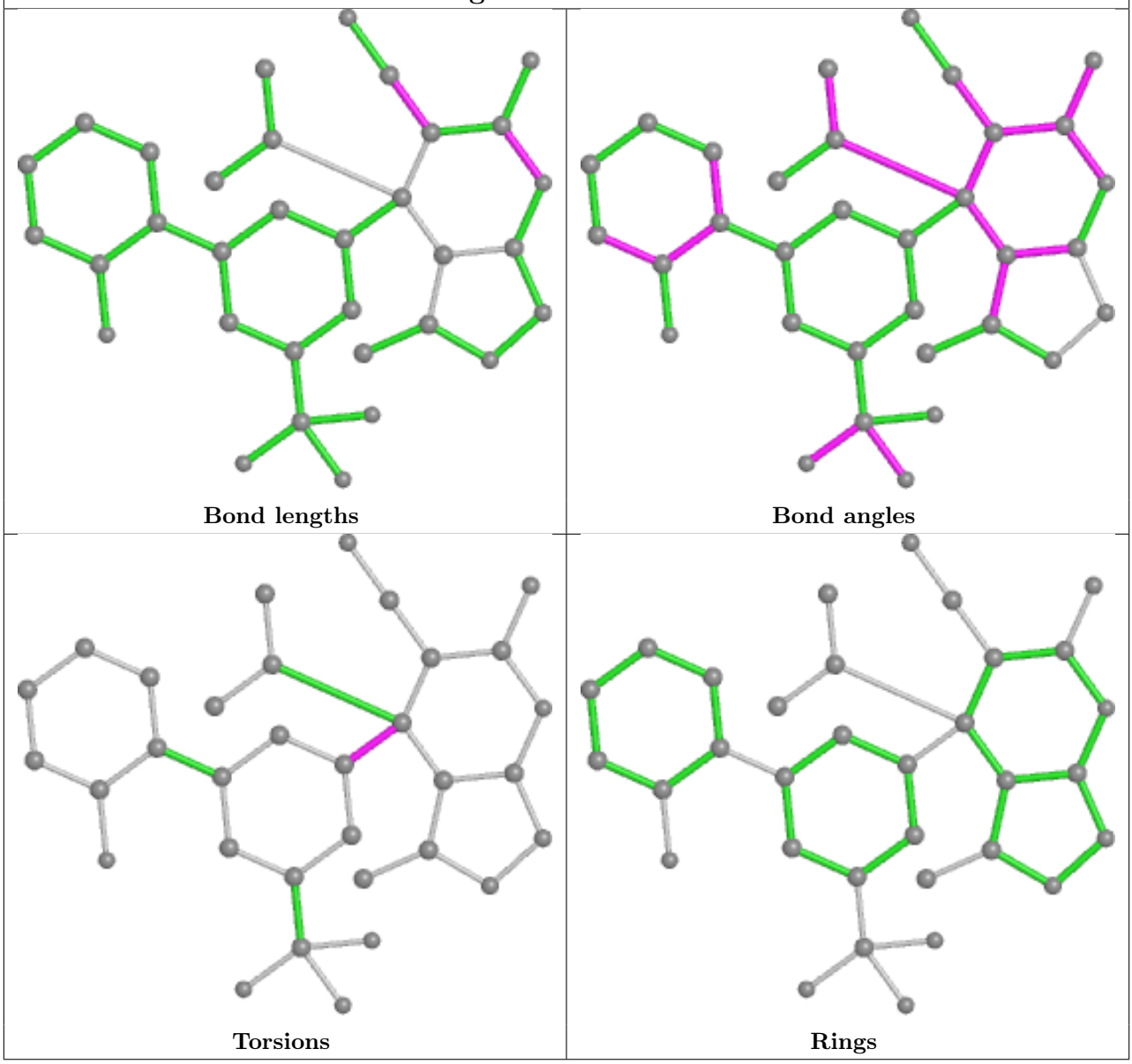


Torsions

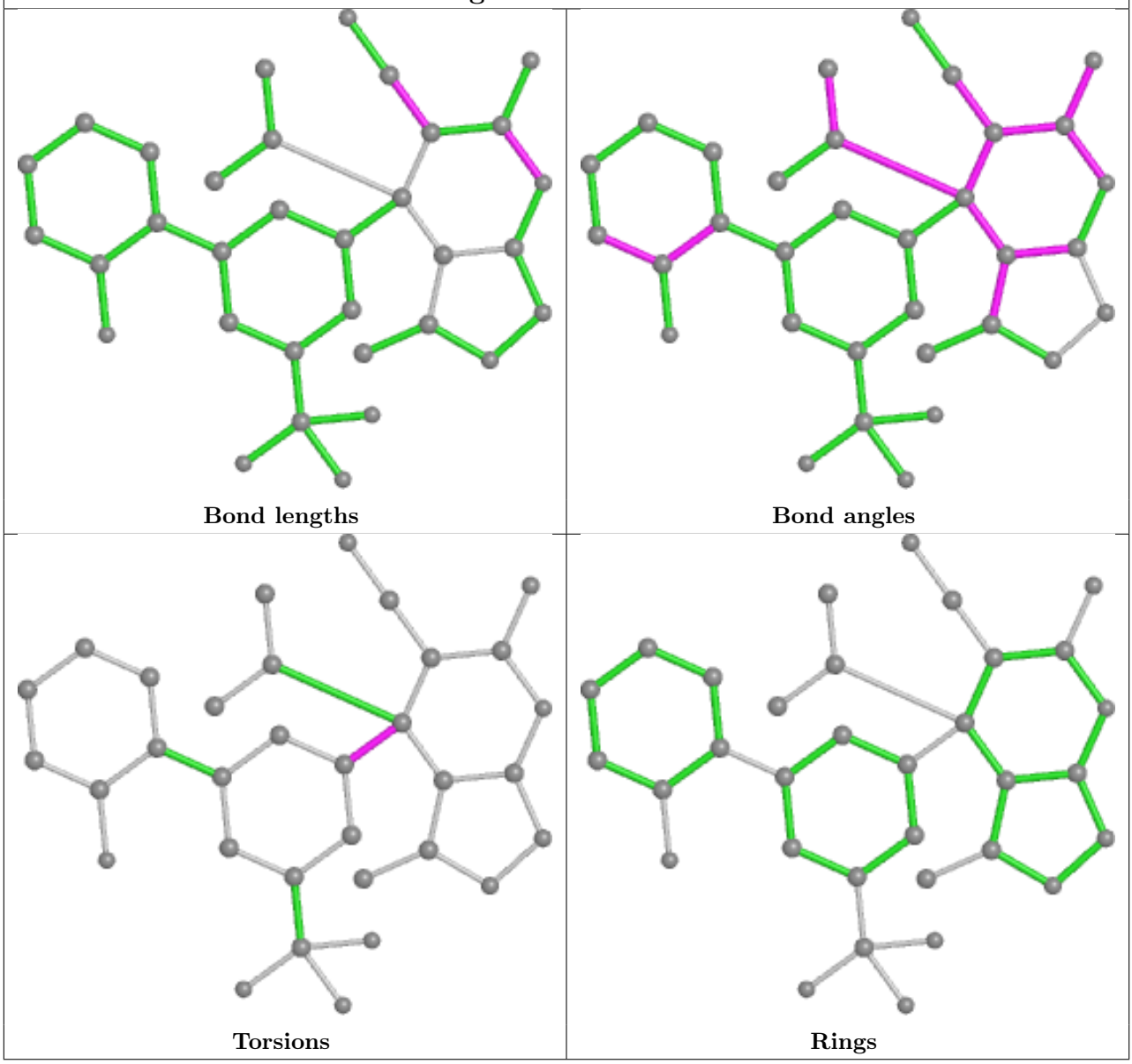


Rings

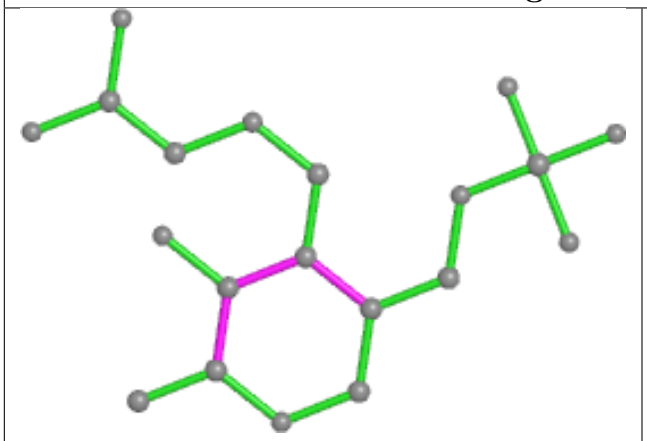
Ligand 8B3 B 502



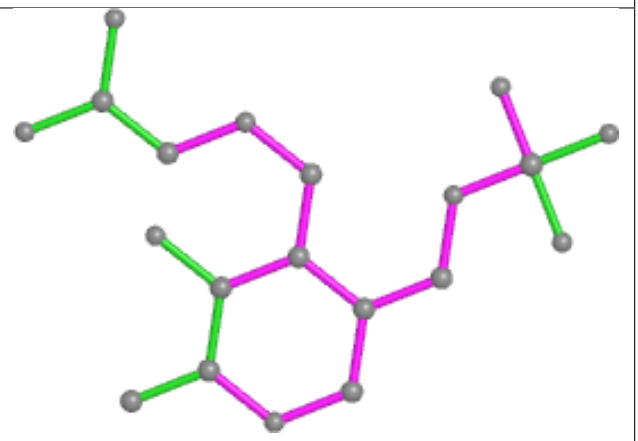
Ligand 8B3 C 502



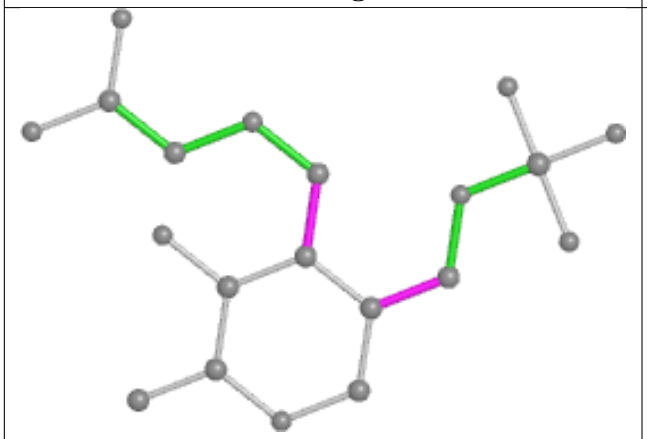
Ligand PLG B 501



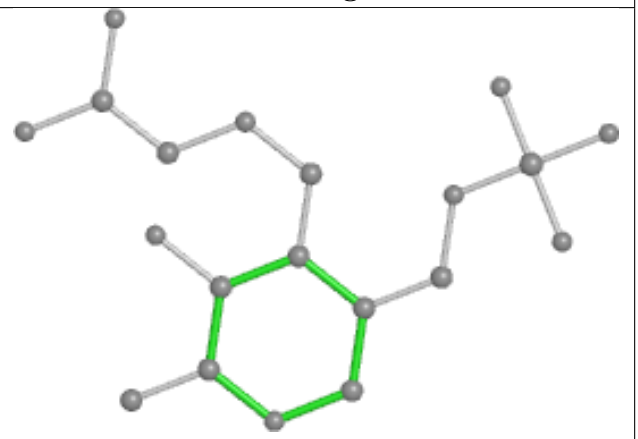
Bond lengths



Bond angles

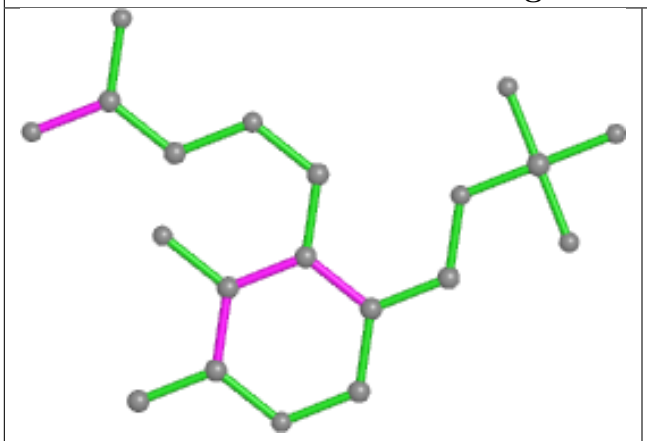


Torsions

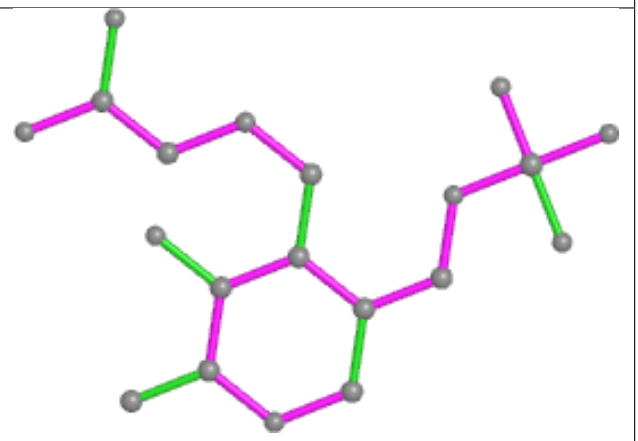


Rings

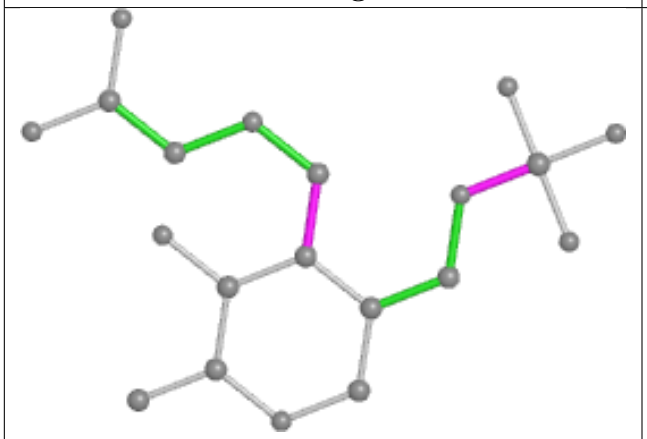
Ligand PLG A 501



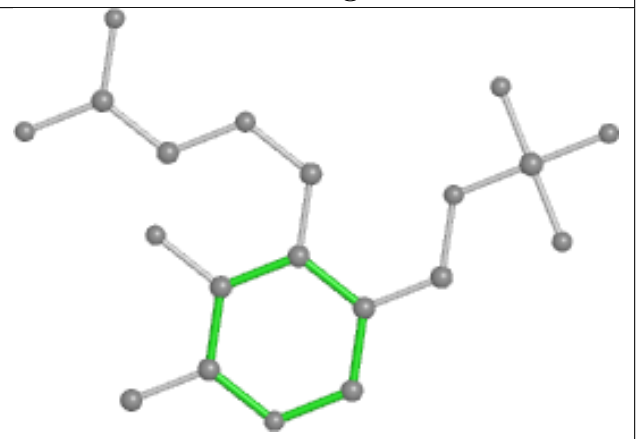
Bond lengths



Bond angles

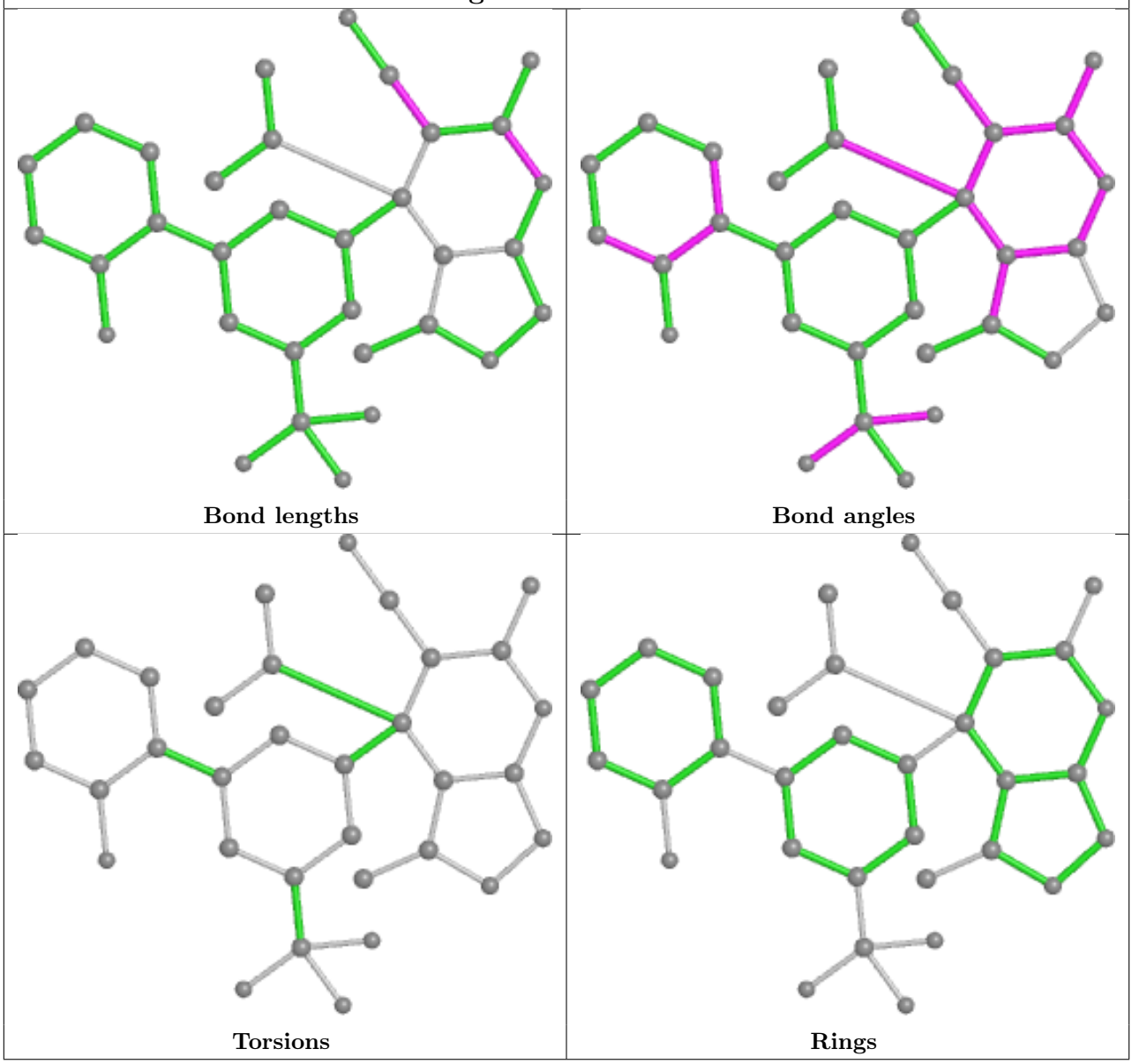


Torsions



Rings

Ligand 8B3 A 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	442/442 (100%)	0.13	8 (1%)	68	65	20, 32, 53, 76	0
1	B	442/442 (100%)	0.04	7 (1%)	72	69	19, 32, 50, 74	0
1	C	442/442 (100%)	0.05	6 (1%)	75	74	19, 32, 52, 79	0
All	All	1326/1326 (100%)	0.07	21 (1%)	72	69	19, 32, 52, 79	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	419	LEU	4.7
1	A	419	LEU	3.6
1	C	423	ALA	3.5
1	A	256	GLY	3.1
1	A	414	ASP	3.1
1	C	421	GLY	3.0
1	B	202	ASN	2.7
1	A	363	ASP	2.7
1	C	366	SER	2.7
1	B	419	LEU	2.6
1	A	202	ASN	2.6
1	A	138	LYS	2.5
1	B	365	VAL	2.5
1	C	365	VAL	2.4
1	B	366	SER	2.3
1	C	256	GLY	2.2
1	A	426	GLN	2.2
1	A	257	ILE	2.1
1	B	364	CYS	2.0
1	B	138	LYS	2.0
1	B	219	ASN	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)

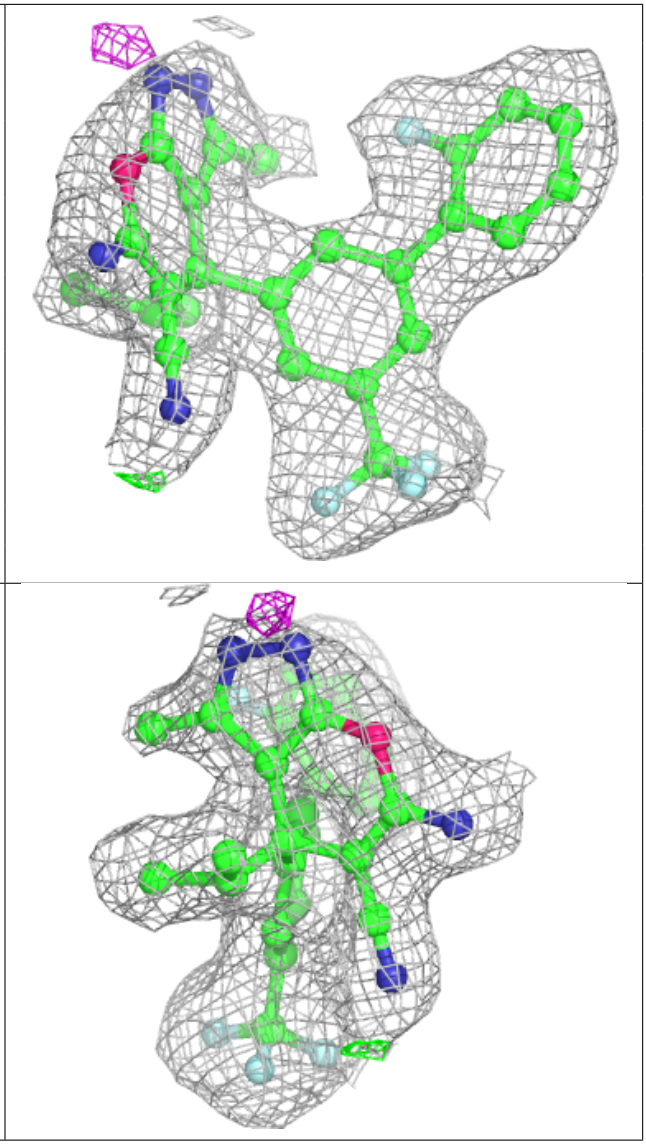
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	A	503	1/1	0.86	0.09	33,33,33,33	0
4	CL	C	503	1/1	0.88	0.15	31,31,31,31	1
3	8B3	C	502	33/33	0.92	0.14	24,25,29,34	0
3	8B3	B	502	33/33	0.94	0.15	25,27,30,32	0
3	8B3	A	502	33/33	0.94	0.14	23,25,29,33	0
2	PLG	C	501	20/20	0.95	0.15	19,25,29,30	0
2	PLG	A	501	20/20	0.95	0.16	19,24,27,29	0
2	PLG	B	501	20/20	0.95	0.13	21,26,28,29	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.

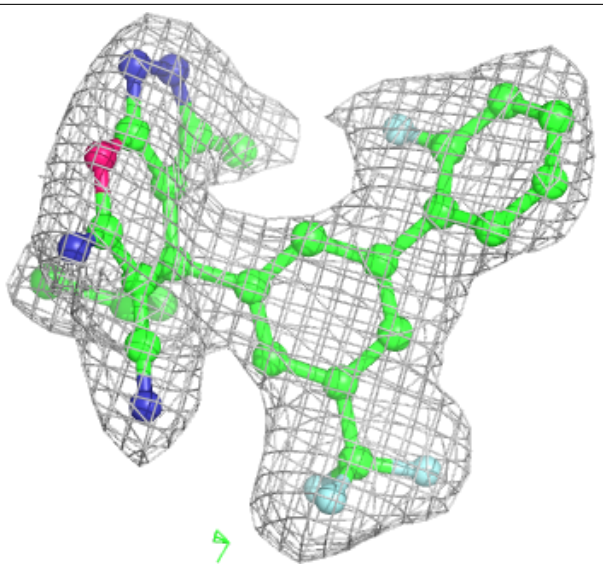
Electron density around 8B3 C 502:

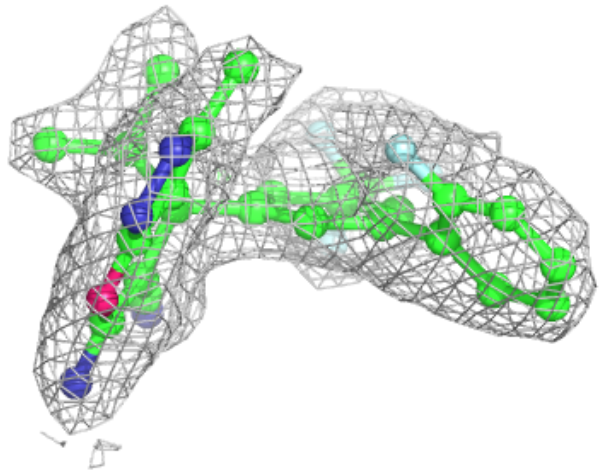
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

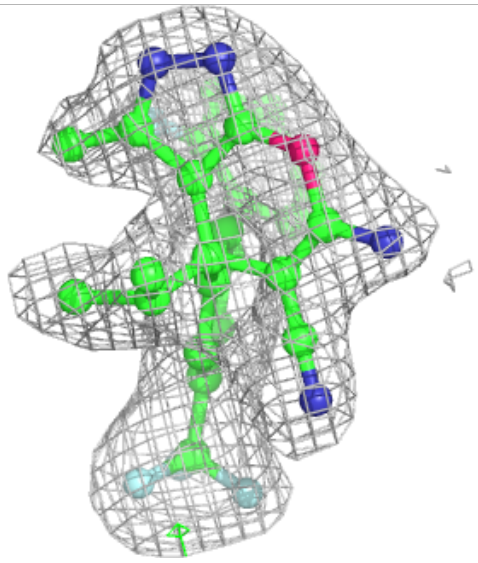


Electron density around 8B3 B 502:

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

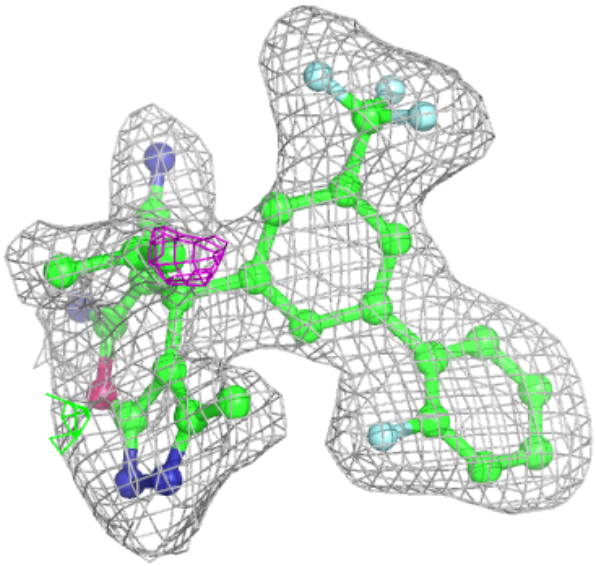


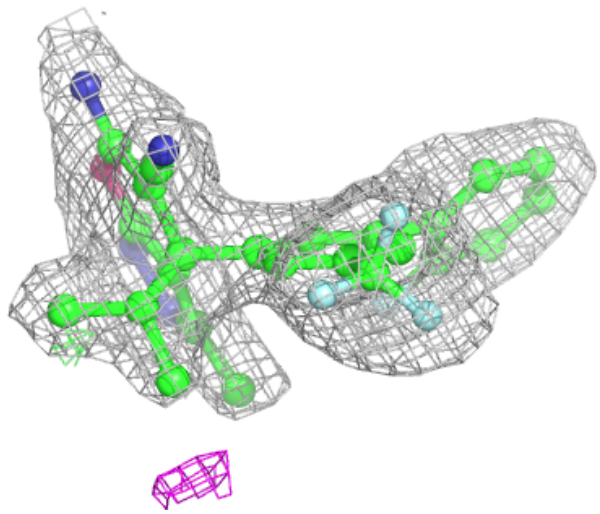


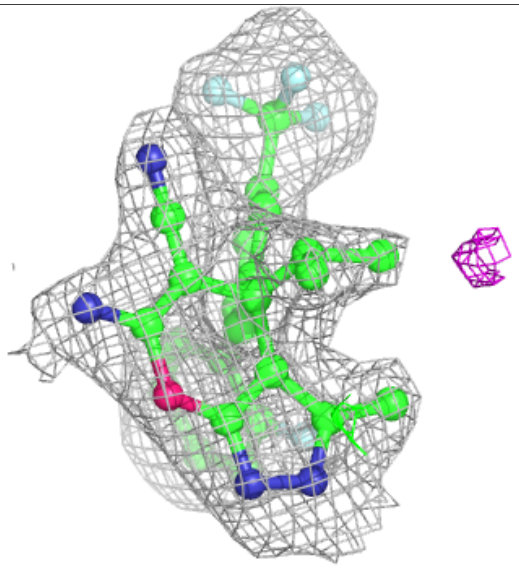


Electron density around 8B3 A 502:

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

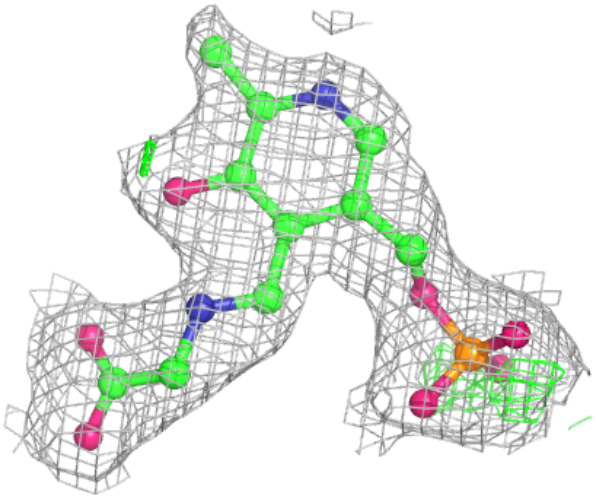


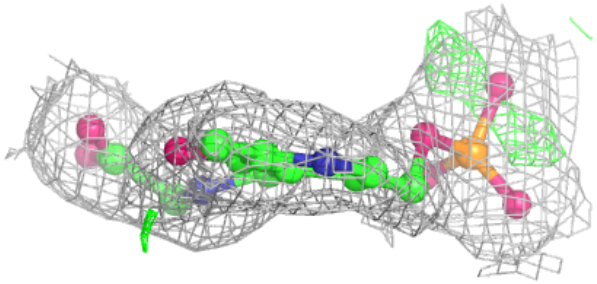


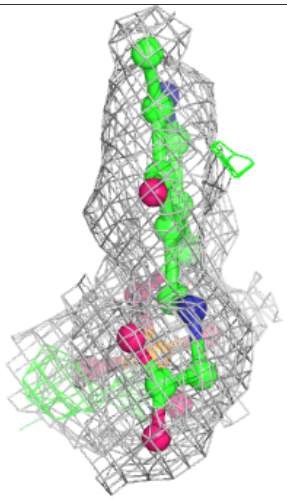


Electron density around PLG C 501:

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

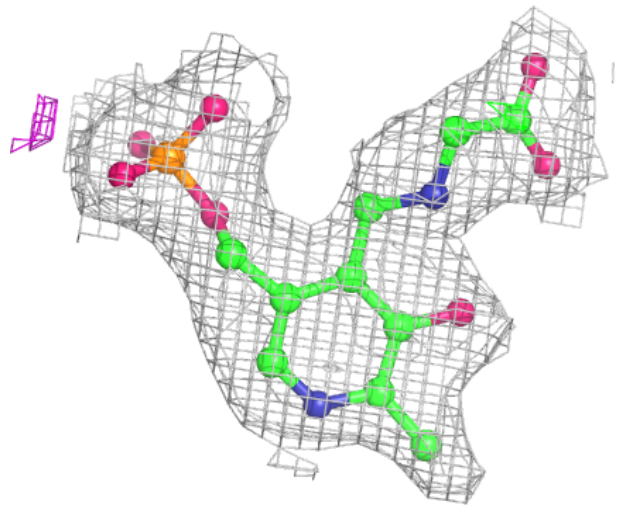


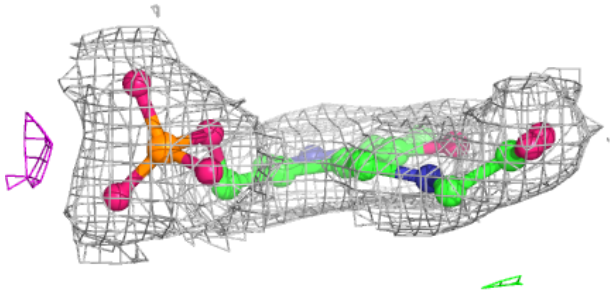


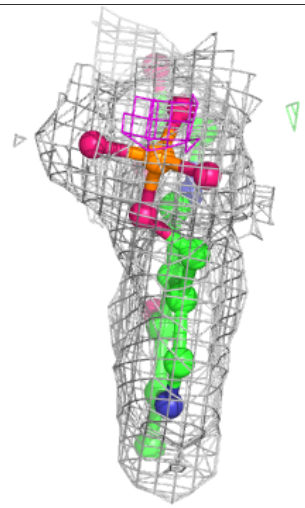


Electron density around PLG A 501:

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

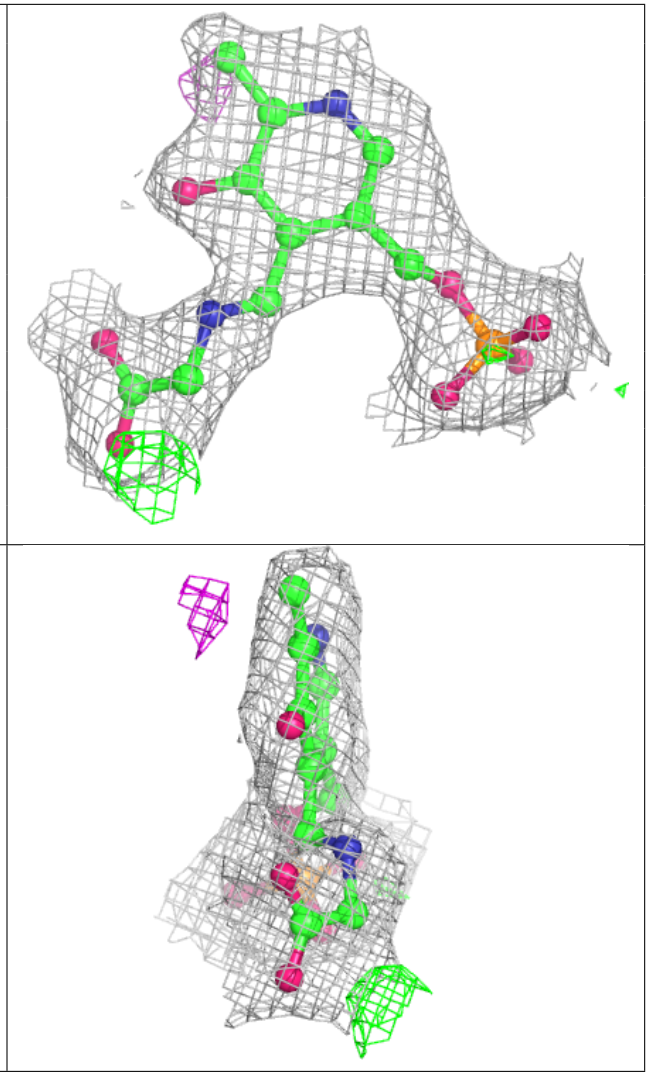






Electron density around PLG B 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.