



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 06:09 PM EST

PDB ID : 8GES
Title : R. hominis 2 beta-glucuronidase bound to UNC10201652-glucuronide
Authors : Simpson, J.B.; Redinbo, M.R.
Deposited on : 2023-03-07
Resolution : 2.70 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
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

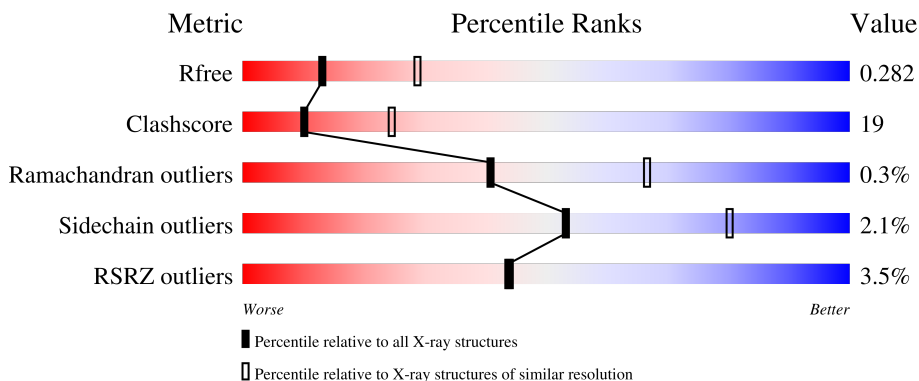
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. 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	756	 60% 25% 15%
1	B	756	 56% 29% 15%
1	C	756	 57% 27% 15%
1	D	756	 45% 36% 17%

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
3	GOL	B	804	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 21102 atoms, of which 241 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 beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	644	5182	3294	865	1003	20	0	0	0
1	D	631	4994	3174	835	966	19	0	0	0
1	C	642	5150	3272	860	997	21	0	0	0
1	B	643	5168	3285	862	1000	21	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	ALA	THR	conflict	UNP A0A395V8I7
A	735	ALA	LYS	conflict	UNP A0A395V8I7
D	248	ALA	THR	conflict	UNP A0A395V8I7
D	735	ALA	LYS	conflict	UNP A0A395V8I7
C	248	ALA	THR	conflict	UNP A0A395V8I7
C	735	ALA	LYS	conflict	UNP A0A395V8I7
B	248	ALA	THR	conflict	UNP A0A395V8I7
B	735	ALA	LYS	conflict	UNP A0A395V8I7

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
2	C	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
2	B	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



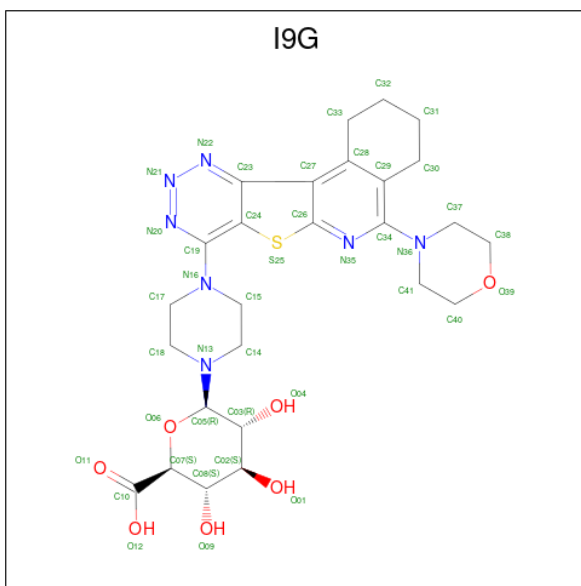
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is 8-(4-beta-D-glucopyranuronosylpiperazin-1-yl)-5-(morpholin-4-yl)-1,2,3,4-tetrahydro[1,2,3]triazino[4',5':4,5]thieno[2,3-c]isoquinoline (three-letter code: I9G) (formula: C₂₆H₃₃N₇O₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	H	N	O	S	0	0
			73	26	32	7	7	1		
4	D	1	Total	C	H	N	O	S	0	0
			73	26	32	7	7	1		
4	C	1	Total	C	H	N	O	S	0	0
			73	26	32	7	7	1		
4	B	1	Total	C	H	N	O	S	0	0
			73	26	32	7	7	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	19	Total O 19 19	0	0
5	D	14	Total O 14 14	0	0
5	C	18	Total O 18 18	0	0
5	B	17	Total O 17 17	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.41Å 145.95Å 281.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 2.70 49.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.96-2.70) 99.3 (49.96-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.231 , 0.282 0.231 , 0.282	Depositor DCC
R_{free} test set	2000 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtrriage
Anisotropy	0.733	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21102	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: I9G, FMN, GOL

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	0.26	0/5325	0.46	0/7243
1	B	0.27	0/5310	0.46	0/7223
1	C	0.26	0/5291	0.46	0/7199
1	D	0.30	0/5129	0.49	0/6986
All	All	0.27	0/21055	0.47	0/28651

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	5182	0	4844	148	0
1	B	5168	0	4828	173	0
1	C	5150	0	4796	158	0
1	D	4994	0	4550	271	0
2	A	31	19	19	2	0
2	B	31	19	19	4	0
2	C	31	19	19	7	0
3	A	18	24	24	3	0
3	B	18	24	24	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	6	8	8	1	0
4	A	41	32	0	0	0
4	B	41	32	0	1	0
4	C	41	32	0	5	0
4	D	41	32	0	1	0
5	A	19	0	0	0	0
5	B	17	0	0	6	0
5	C	18	0	0	0	0
5	D	14	0	0	1	0
All	All	20861	241	19131	753	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 19.

All (753) 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:166:VAL:HG22	1:C:180:VAL:HG12	1.37	1.06
1:C:588:GLU:HG3	1:C:598:LYS:HG2	1.36	1.06
1:D:175:ALA:H	1:D:221:ILE:HG12	1.14	1.03
1:B:412:ILE:HG12	1:B:428:PRO:HG3	1.39	1.02
1:B:256:PHE:HB2	3:B:804:GOL:H11	1.46	0.94
1:C:168:PRO:HB3	1:C:177:VAL:HG12	1.49	0.94
1:C:3:VAL:HG22	1:C:147:ILE:HG12	1.53	0.90
1:D:340:ILE:HD11	1:D:342:TYR:HB2	1.51	0.90
1:A:563:LEU:HD23	1:A:580:VAL:HG22	1.55	0.88
1:D:619:VAL:HG22	1:D:628:GLU:HG3	1.54	0.88
1:C:279:ARG:HD2	1:C:510:THR:HG22	1.57	0.87
1:B:458:PHE:HB3	1:B:461:ILE:HD12	1.57	0.86
1:D:267:ARG:HA	1:D:505:LYS:HE2	1.58	0.86
1:C:317:ALA:HB1	1:C:318:HIS:ND1	1.91	0.84
1:C:191:GLN:HB3	1:C:243:VAL:O	1.78	0.82
1:A:598:LYS:O	1:A:599:LEU:HD12	1.80	0.82
1:B:229:GLY:HA3	5:B:901:HOH:O	1.79	0.82
1:B:66:GLU:HA	1:B:70:TYR:OH	1.79	0.81
1:D:174:ASP:HB3	1:D:221:ILE:CG2	2.12	0.80
1:D:175:ALA:N	1:D:221:ILE:HG12	1.97	0.79
1:D:514:ASN:O	1:D:535:GLY:HA2	1.83	0.79
1:A:196:THR:HG23	1:A:239:GLU:HB3	1.64	0.79
1:D:430:VAL:HG13	1:D:462:PRO:HB2	1.63	0.79
1:A:6:PHE:CE1	1:A:57:LYS:HE2	2.19	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:GLU:O	1:B:396:ILE:HG13	1.82	0.78
1:D:182:VAL:HG11	1:D:240:VAL:HG21	1.65	0.78
1:C:279:ARG:HD2	1:C:510:THR:CG2	2.13	0.78
1:D:278:LEU:HD13	1:D:313:THR:HG23	1.65	0.77
1:B:368:HIS:HB2	1:B:371:ILE:HD12	1.68	0.76
1:A:514:ASN:O	1:A:535:GLY:HA2	1.86	0.75
1:D:340:ILE:HD11	1:D:342:TYR:CB	2.17	0.75
1:B:636:THR:HG22	5:B:904:HOH:O	1.86	0.75
1:C:281:VAL:HG12	1:C:512:VAL:HB	1.69	0.74
1:C:366:TYR:O	1:C:408:ARG:NH2	2.20	0.74
1:A:392:GLU:O	1:A:396:ILE:HG13	1.87	0.74
1:D:7:ASN:HD21	1:D:143:ASP:HA	1.50	0.74
1:D:340:ILE:CD1	1:D:342:TYR:HB2	2.16	0.74
1:B:66:GLU:HA	1:B:70:TYR:HH	1.51	0.74
1:A:586:GLU:HG2	1:A:600:GLN:HG3	1.69	0.74
1:D:615:GLU:CG	1:D:632:ARG:HG2	2.18	0.73
1:D:351:ARG:HB3	1:D:393:ASN:OD1	1.88	0.73
1:B:563:LEU:HD13	1:B:629:SER:HB2	1.69	0.73
1:A:59:LEU:HD21	1:A:64:LEU:HD11	1.70	0.73
1:B:411:THR:O	1:B:412:ILE:HD13	1.88	0.73
1:D:514:ASN:OD1	1:D:515:MET:N	2.21	0.73
1:D:502:PHE:HE2	1:D:555:LEU:HD21	1.52	0.73
1:B:438:GLY:O	1:B:482:GLN:HG3	1.88	0.73
1:C:306:ILE:HD13	1:C:314:ILE:HD13	1.69	0.73
1:C:168:PRO:CB	1:C:177:VAL:HG12	2.17	0.72
1:D:23:MET:HE3	1:D:24:PRO:HD2	1.72	0.72
1:B:425:ILE:HG23	1:B:431:ILE:HD13	1.69	0.72
1:D:317:ALA:HB1	1:D:318:HIS:ND1	2.05	0.72
1:D:430:VAL:CG1	1:D:462:PRO:HB2	2.20	0.72
1:A:599:LEU:HD13	1:A:608:PHE:CE2	2.25	0.71
1:B:514:ASN:O	1:B:535:GLY:HA2	1.90	0.71
1:D:358:MET:O	1:D:362:VAL:HG23	1.91	0.71
1:D:3:VAL:HG22	1:D:147:ILE:HG12	1.71	0.71
1:D:66:GLU:HA	1:D:66:GLU:OE2	1.91	0.71
1:B:281:VAL:HG12	1:B:512:VAL:HB	1.73	0.71
1:D:501:LEU:HD23	1:D:510:THR:CG2	2.21	0.70
1:C:306:ILE:HG21	1:C:314:ILE:HD11	1.74	0.70
1:D:174:ASP:HB3	1:D:221:ILE:HG23	1.72	0.70
1:D:351:ARG:O	1:D:355:ILE:HD12	1.92	0.70
1:B:412:ILE:CG1	1:B:428:PRO:HG3	2.21	0.70
1:B:91:ALA:HB2	1:B:102:VAL:HG21	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:ILE:HD12	1:C:409:LEU:HD12	1.74	0.69
1:C:306:ILE:HD13	1:C:314:ILE:CD1	2.23	0.69
1:D:409:LEU:HD12	1:D:429:ASP:OD2	1.91	0.69
1:A:88:LYS:HD2	1:A:89:ALA:N	2.07	0.69
1:B:439:TRP:CZ2	1:B:471:GLU:HG3	2.27	0.69
1:D:168:PRO:HA	1:D:177:VAL:HA	1.74	0.69
1:B:574:ASP:O	1:B:612:ASN:N	2.25	0.69
1:D:342:TYR:OH	1:D:346:HIS:ND1	2.22	0.68
1:B:85:VAL:HG22	1:B:115:ILE:CD1	2.23	0.68
1:D:615:GLU:HG3	1:D:632:ARG:HG2	1.73	0.68
1:D:348:PRO:HB3	1:D:389:ASP:OD2	1.94	0.68
1:D:166:VAL:HG11	1:D:256:PHE:CG	2.29	0.68
1:D:168:PRO:CA	1:D:177:VAL:HG13	2.23	0.68
1:B:60:LYS:O	1:B:64:LEU:HD13	1.93	0.68
1:C:591:VAL:HG21	1:C:610:VAL:HG13	1.76	0.68
1:A:343:ILE:HG13	1:A:378:ASN:HD22	1.59	0.68
1:A:205:VAL:HG12	1:A:221:ILE:HG22	1.74	0.67
1:D:426:GLN:HE22	1:D:458:PHE:HE2	1.42	0.67
1:D:155:ASP:OD2	1:D:158:TYR:HB2	1.94	0.67
1:C:184:LEU:HD13	1:C:242:LEU:HD22	1.74	0.67
1:C:392:GLU:O	1:C:396:ILE:HG13	1.94	0.67
1:C:182:VAL:HG11	1:C:240:VAL:HG11	1.75	0.67
1:D:278:LEU:HD13	1:D:313:THR:CG2	2.24	0.67
1:C:431:ILE:HD11	1:C:454:PHE:CZ	2.29	0.67
1:A:439:TRP:CZ2	1:A:471:GLU:HG3	2.30	0.66
1:D:23:MET:CE	1:D:24:PRO:HD2	2.25	0.66
1:A:205:VAL:CG1	1:A:221:ILE:HG22	2.25	0.66
1:C:363:VAL:HA	2:C:801:FMN:HM72	1.78	0.66
1:D:204:GLU:O	1:D:206:ALA:N	2.28	0.66
1:B:60:LYS:HB2	1:B:63:GLU:HG3	1.75	0.66
1:A:279:ARG:HD2	1:A:502:PHE:CD1	2.31	0.66
1:B:572:VAL:O	1:B:633:LYS:HE2	1.95	0.65
1:A:60:LYS:HA	1:A:111:GLU:O	1.96	0.65
1:D:7:ASN:HD22	1:D:32:LEU:HB2	1.62	0.65
1:B:573:GLU:HG3	1:B:575:THR:O	1.96	0.65
1:D:37:ASN:HA	1:D:40:ASP:OD1	1.96	0.65
1:C:610:VAL:HG13	1:C:611:PRO:HD2	1.79	0.65
1:D:78:ASN:HA	1:D:96:GLY:HA3	1.78	0.64
1:C:438:GLY:O	1:C:482:GLN:HG3	1.96	0.64
1:D:1:ARG:NH2	1:D:156:LEU:HD21	2.13	0.64
1:D:361:LEU:HD12	1:D:365:ASN:HD22	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LEU:C	1:C:279:ARG:HD3	2.18	0.64
1:D:463:LEU:HD12	1:D:464:GLY:N	2.13	0.64
1:B:400:MET:HG2	1:B:404:MET:HE3	1.80	0.64
1:D:351:ARG:HA	1:D:354:THR:HG23	1.80	0.64
1:C:314:ILE:HB	1:C:336:ILE:CD1	2.27	0.64
1:A:363:VAL:HA	2:A:801:FMN:HM72	1.79	0.64
1:D:193:LEU:HB3	1:D:210:THR:HG22	1.78	0.64
2:B:802:FMN:N1	2:B:802:FMN:O2'	2.30	0.64
1:B:588:GLU:HB2	1:B:598:LYS:HG2	1.81	0.63
1:A:17:THR:HG21	1:B:355:ILE:HD13	1.80	0.63
1:B:591:VAL:HG12	1:B:618:LEU:HD23	1.80	0.63
1:B:285:GLN:HG2	1:B:319:TYR:CE1	2.33	0.63
1:C:514:ASN:O	1:C:535:GLY:HA2	1.97	0.63
1:B:425:ILE:CG2	1:B:431:ILE:HD13	2.27	0.63
1:A:395:ARG:HG2	1:A:427:ILE:HD13	1.81	0.63
1:D:174:ASP:OD1	1:D:224:VAL:N	2.30	0.63
1:C:183:PHE:C	1:C:184:LEU:HD23	2.18	0.63
1:B:111:GLU:OE1	1:B:112:GLU:HG2	1.97	0.63
1:D:563:LEU:CD2	1:D:627:ASP:HB3	2.29	0.63
1:D:516:PHE:HD1	1:D:537:VAL:HB	1.64	0.63
1:D:165:LYS:O	1:D:180:VAL:HA	1.98	0.62
1:D:174:ASP:HB3	1:D:221:ILE:HG21	1.80	0.62
1:D:203:LYS:O	1:D:205:VAL:HG23	1.99	0.62
1:A:422:ASP:OD1	1:A:424:TYR:HB3	1.99	0.62
1:C:303:ILE:HG21	1:C:328:LEU:HD13	1.82	0.62
2:C:801:FMN:N1	2:C:801:FMN:O2'	2.32	0.62
1:B:343:ILE:HG13	1:B:378:ASN:HD22	1.65	0.62
1:D:129:PRO:HG2	1:D:136:PHE:CE1	2.35	0.62
1:C:411:THR:HB	1:C:430:VAL:HG23	1.79	0.62
1:D:359:LYS:O	1:D:363:VAL:HG23	2.00	0.62
1:D:445:SER:HA	1:D:500:GLN:HE22	1.64	0.62
1:D:182:VAL:CG1	1:D:240:VAL:HG21	2.29	0.62
1:A:500:GLN:O	1:A:504:ARG:HD2	2.00	0.61
1:B:376:LEU:HB2	1:B:412:ILE:HD11	1.82	0.61
1:D:234:TYR:O	1:D:235:LEU:HD12	1.99	0.61
1:C:380:ILE:HG21	1:C:394:HIS:CE1	2.36	0.61
1:A:88:LYS:HD2	1:A:89:ALA:H	1.65	0.61
1:A:400:MET:O	1:A:404:MET:HG3	2.00	0.61
1:C:359:LYS:O	1:C:363:VAL:HG23	2.00	0.61
1:A:496:GLU:O	1:A:500:GLN:HG3	2.00	0.61
1:D:340:ILE:HD12	1:D:342:TYR:H	1.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:GLU:C	1:D:459:PRO:HD3	2.21	0.61
1:C:267:ARG:HH11	1:C:267:ARG:HG2	1.65	0.61
1:D:314:ILE:HD11	1:D:334:LEU:HG	1.82	0.61
1:D:393:ASN:HA	1:D:396:ILE:HD12	1.81	0.61
1:A:476:HIS:HA	1:A:488:GLU:OE1	2.01	0.61
1:A:577:LYS:HE2	1:A:607:HIS:ND1	2.16	0.60
1:D:498:ILE:HG23	1:D:502:PHE:CD1	2.36	0.60
1:C:59:LEU:HD21	1:C:64:LEU:HD11	1.83	0.60
1:B:168:PRO:HD3	3:B:804:GOL:H31	1.82	0.60
1:D:59:LEU:HB2	1:D:115:ILE:CD1	2.31	0.60
1:D:501:LEU:HD23	1:D:510:THR:HG21	1.82	0.60
4:C:803:I9G:C18	4:C:803:I9G:C08	2.80	0.60
1:A:391:LEU:O	1:A:395:ARG:HG3	2.02	0.60
1:D:175:ALA:O	1:D:221:ILE:HB	2.02	0.60
1:D:61:LYS:HE2	1:D:108:LEU:HB3	1.83	0.60
1:D:235:LEU:HD21	1:D:330:ASP:HB3	1.83	0.60
1:D:392:GLU:O	1:D:396:ILE:HG13	2.01	0.60
1:D:175:ALA:H	1:D:221:ILE:CG1	2.03	0.60
1:D:227:TRP:CZ2	1:D:333:GLY:HA2	2.37	0.60
1:D:378:ASN:ND2	1:D:379:GLU:HG3	2.17	0.60
1:C:411:THR:HB	1:C:430:VAL:CG2	2.31	0.60
1:B:356:SER:O	1:B:360:GLU:HG3	2.01	0.60
1:A:498:ILE:HG23	1:A:502:PHE:CD2	2.37	0.59
1:C:285:GLN:HG2	1:C:319:TYR:CE1	2.37	0.59
1:A:494:HIS:O	1:A:498:ILE:HG13	2.02	0.59
1:C:188:ALA:HB3	1:C:191:GLN:OE1	2.02	0.59
1:C:318:HIS:NE2	4:C:803:I9G:O01	2.31	0.59
1:D:1:ARG:HH22	1:D:156:LEU:HD21	1.66	0.59
1:C:3:VAL:HG22	1:C:147:ILE:CG1	2.32	0.59
1:A:16:ALA:HB3	1:A:54:TYR:CD1	2.38	0.59
1:A:191:GLN:HG2	1:A:244:SER:OG	2.03	0.59
1:B:615:GLU:HG2	1:B:632:ARG:HG2	1.84	0.59
1:C:35:SER:O	1:C:38:GLU:HG3	2.02	0.58
1:C:315:ARG:NH1	1:C:467:GLU:HG3	2.18	0.58
1:A:573:GLU:HG3	1:A:575:THR:O	2.02	0.58
1:D:155:ASP:O	1:D:156:LEU:HD23	2.03	0.58
1:D:168:PRO:HA	1:D:177:VAL:HG13	1.84	0.58
1:D:267:ARG:CA	1:D:505:LYS:HE2	2.32	0.58
1:C:128:TYR:CZ	1:C:347:MET:HE2	2.38	0.58
1:B:1:ARG:HB2	1:B:250:ASP:OD1	2.03	0.58
1:A:458:PHE:HB3	1:A:461:ILE:HD12	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:615:GLU:HG2	1:C:632:ARG:HG2	1.85	0.58
1:A:317:ALA:HB1	1:A:318:HIS:ND1	2.19	0.58
1:A:563:LEU:HD13	1:A:629:SER:OG	2.04	0.58
1:D:94:ASP:OD2	1:D:127:VAL:HG21	2.03	0.58
1:D:400:MET:O	1:D:404:MET:HG2	2.04	0.58
1:A:270:ILE:CD1	1:A:275:GLU:HG2	2.34	0.58
1:D:33:PRO:HB3	1:D:141:TYR:O	2.03	0.58
1:D:285:GLN:HG2	1:D:319:TYR:OH	2.03	0.58
1:D:473:LEU:HD22	1:D:526:GLY:O	2.03	0.58
1:B:37:ASN:HA	1:B:40:ASP:OD1	2.04	0.58
1:C:206:ALA:HB1	1:C:219:LEU:HB3	1.86	0.57
1:B:587:VAL:HG22	1:B:622:ALA:HB2	1.86	0.57
1:A:84:TYR:HA	1:A:88:LYS:O	2.05	0.57
1:D:463:LEU:HD12	1:D:464:GLY:H	1.69	0.57
1:B:51:GLY:O	1:B:120:GLU:HA	2.04	0.57
1:B:620:ALA:O	1:B:626:LYS:HA	2.04	0.57
1:D:501:LEU:HD23	1:D:510:THR:HG22	1.86	0.57
1:B:633:LYS:HD3	1:B:634:VAL:N	2.19	0.57
1:D:411:THR:HA	1:D:430:VAL:O	2.03	0.57
1:D:563:LEU:HD22	1:D:627:ASP:HB3	1.86	0.57
1:B:6:PHE:HB3	1:B:144:VAL:HG12	1.86	0.57
1:D:20:PRO:HD2	1:D:116:VAL:HG11	1.86	0.57
1:D:381:THR:HG22	1:D:381:THR:O	2.05	0.57
1:D:188:ALA:HB1	1:D:190:ASP:OD1	2.05	0.57
1:D:197:VAL:O	1:D:205:VAL:HB	2.05	0.57
1:D:495:GLU:HG2	1:D:605:PHE:CD2	2.39	0.57
1:B:243:VAL:HG13	1:B:247:GLU:O	2.04	0.57
1:B:414:VAL:HG13	1:B:424:TYR:OH	2.04	0.57
1:C:168:PRO:HA	1:C:177:VAL:HA	1.87	0.56
1:B:494:HIS:O	1:B:498:ILE:HG13	2.05	0.56
1:A:154:PHE:CD2	1:A:252:VAL:HG13	2.40	0.56
1:C:397:LEU:O	1:C:401:VAL:HG23	2.04	0.56
1:A:174:ASP:OD1	1:A:222:PRO:HA	2.05	0.56
1:C:363:VAL:HG13	2:C:801:FMN:C6	2.36	0.56
1:C:591:VAL:HG22	1:C:618:LEU:HD22	1.88	0.56
1:B:59:LEU:HD21	1:B:64:LEU:HD21	1.86	0.56
1:B:91:ALA:HB2	1:B:102:VAL:CG2	2.36	0.56
1:B:591:VAL:HG12	1:B:618:LEU:CD2	2.36	0.56
1:A:412:ILE:HD12	1:A:414:VAL:HG22	1.87	0.56
1:A:590:PHE:CE2	1:A:595:SER:HB2	2.40	0.56
1:D:424:TYR:O	1:D:427:ILE:HG13	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:O	1:A:509:ALA:HA	2.06	0.56
1:A:359:LYS:HG3	1:A:400:MET:SD	2.45	0.56
1:B:590:PHE:CE1	1:B:595:SER:HB2	2.41	0.56
1:A:285:GLN:HG2	1:A:319:TYR:OH	2.06	0.56
1:D:280:GLY:HA3	1:D:313:THR:O	2.06	0.56
1:C:168:PRO:HB3	1:C:177:VAL:CG1	2.32	0.56
1:D:479:ASP:OD2	1:D:481:LYS:HE3	2.06	0.56
1:C:219:LEU:HD12	1:C:219:LEU:H	1.70	0.56
1:C:343:ILE:HG13	1:C:378:ASN:HD22	1.72	0.56
1:B:303:ILE:HD13	1:B:328:LEU:HB3	1.87	0.56
1:B:431:ILE:HD11	1:B:454:PHE:CZ	2.41	0.55
1:B:400:MET:HG2	1:B:404:MET:CE	2.36	0.55
1:D:164:ILE:HB	1:D:252:VAL:HG11	1.89	0.55
1:D:377:SER:OG	1:D:380:ILE:HB	2.06	0.55
1:C:14:LYS:HG2	1:C:53:CYS:SG	2.47	0.55
1:D:439:TRP:CZ2	1:D:471:GLU:HB2	2.42	0.55
1:C:591:VAL:HG21	1:C:610:VAL:CG1	2.37	0.55
1:D:287:ARG:HG3	1:D:288:TRP:N	2.22	0.55
1:D:594:LYS:HD2	1:D:594:LYS:N	2.21	0.55
1:D:154:PHE:HA	1:D:184:LEU:HD23	1.88	0.55
1:C:561:VAL:HG21	1:C:622:ALA:HB3	1.87	0.55
1:A:577:LYS:CE	1:A:607:HIS:HB3	2.37	0.55
1:B:154:PHE:HA	1:B:184:LEU:HD13	1.89	0.55
1:B:454:PHE:CD1	1:B:463:LEU:HD22	2.42	0.55
1:A:315:ARG:NH1	1:A:467:GLU:HG3	2.22	0.55
1:D:434:ASN:OD1	1:D:466:SER:HB3	2.07	0.55
1:A:1:ARG:HB2	1:A:250:ASP:OD1	2.06	0.54
1:D:340:ILE:HD12	1:D:342:TYR:N	2.23	0.54
1:D:409:LEU:HB3	1:D:429:ASP:HB2	1.89	0.54
1:D:222:PRO:O	1:D:223:ALA:C	2.45	0.54
1:D:263:ILE:HD13	1:D:508:TRP:CE3	2.42	0.54
1:B:16:ALA:HB3	1:B:54:TYR:CD1	2.42	0.54
1:A:577:LYS:HE2	1:A:607:HIS:HB3	1.89	0.54
1:D:50:ARG:HA	1:D:121:ASN:OD1	2.07	0.54
1:D:303:ILE:HG23	1:D:332:ARG:NH1	2.23	0.54
4:C:803:I9G:C18	4:C:803:I9G:C07	2.86	0.54
1:A:352:GLU:HG3	1:B:17:THR:O	2.07	0.54
1:D:72:LEU:HD12	1:D:146:ILE:CD1	2.37	0.54
1:D:593:GLY:C	1:D:594:LYS:HD2	2.27	0.54
1:B:182:VAL:O	1:B:215:THR:HB	2.08	0.54
1:B:177:VAL:HG22	1:B:219:LEU:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:GLU:OE2	1:A:598:LYS:HD2	2.08	0.53
1:D:493:TYR:O	1:D:497:MET:HG2	2.07	0.53
1:D:254:THR:HG21	1:D:367:ASN:OD1	2.08	0.53
1:D:194:VAL:HG22	1:D:209:GLU:HG3	1.90	0.53
1:B:365:ASN:HB3	1:B:368:HIS:HD2	1.73	0.53
1:A:323:GLN:OE1	1:A:365:ASN:ND2	2.40	0.53
1:D:69:CYS:HB2	1:D:149:VAL:HG23	1.91	0.53
1:D:388:GLU:O	1:D:392:GLU:HB2	2.09	0.53
1:D:602:GLU:HB2	5:D:906:HOH:O	2.07	0.53
1:A:60:LYS:HE2	1:A:112:GLU:OE2	2.09	0.53
1:C:0:MET:HB2	1:C:249:VAL:O	2.09	0.53
1:C:379:GLU:HB3	1:C:415:VAL:HB	1.90	0.53
1:A:85:VAL:HG22	1:A:115:ILE:HD12	1.91	0.52
1:B:63:GLU:O	1:B:64:LEU:HD12	2.09	0.52
1:A:190:ASP:OD1	1:A:190:ASP:N	2.42	0.52
1:A:198:LYS:HE2	1:A:202:GLY:O	2.10	0.52
1:D:387:ASP:O	1:D:391:LEU:HG	2.09	0.52
1:C:278:LEU:O	1:C:279:ARG:HD3	2.10	0.52
1:B:160:GLY:O	1:B:364:GLN:HG2	2.09	0.52
1:D:166:VAL:HG11	1:D:256:PHE:CD2	2.44	0.52
1:C:341:PRO:O	1:C:343:ILE:HG22	2.09	0.52
1:A:142:ARG:HD3	1:A:322:ASP:OD2	2.10	0.52
1:A:496:GLU:OE2	1:A:499:LYS:NZ	2.32	0.52
3:A:804:GOL:H2	1:B:92:HIS:CE1	2.44	0.52
1:D:51:GLY:O	1:D:120:GLU:HA	2.09	0.52
1:B:254:THR:HG21	1:B:367:ASN:ND2	2.24	0.52
1:D:61:LYS:NZ	1:D:108:LEU:HB2	2.24	0.52
1:B:197:VAL:HG23	1:B:219:LEU:HD22	1.91	0.52
1:A:59:LEU:HD11	1:A:146:ILE:HD13	1.91	0.52
1:D:74:LEU:HD22	1:D:100:TRP:CZ2	2.45	0.52
1:D:394:HIS:O	1:D:398:ASN:HB2	2.09	0.52
1:C:373:VAL:HA	1:C:409:LEU:O	2.09	0.52
1:B:373:VAL:HG12	1:B:409:LEU:HB2	1.92	0.52
1:B:498:ILE:O	1:B:502:PHE:HB2	2.09	0.52
1:C:150:ASN:OD1	1:C:151:LYS:N	2.43	0.52
1:A:270:ILE:HD13	1:A:275:GLU:HG2	1.91	0.51
1:C:152:SER:HB3	1:C:186:ASN:O	2.11	0.51
1:B:60:LYS:HE2	1:B:112:GLU:OE1	2.10	0.51
1:B:177:VAL:HG23	1:B:177:VAL:O	2.08	0.51
1:B:585:PRO:O	1:B:600:GLN:HG2	2.09	0.51
1:C:50:ARG:HA	1:C:121:ASN:OD1	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:TYR:HD2	1:D:292:ASN:HB3	1.75	0.51
1:B:174:ASP:OD1	1:B:222:PRO:HA	2.10	0.51
1:A:203:LYS:HD2	1:A:203:LYS:N	2.25	0.51
1:D:373:VAL:CG1	1:D:411:THR:HG22	2.40	0.51
1:B:197:VAL:HG11	1:B:221:ILE:HD11	1.93	0.51
1:B:621:VAL:HG22	1:B:626:LYS:CD	2.41	0.51
1:A:59:LEU:HD22	1:A:108:LEU:HD22	1.92	0.51
1:D:236:TYR:O	1:D:256:PHE:N	2.35	0.51
1:D:438:GLY:O	1:D:482:GLN:NE2	2.43	0.51
1:C:390:LEU:HD23	1:C:390:LEU:O	2.10	0.51
1:A:267:ARG:HD2	1:A:275:GLU:OE2	2.11	0.51
1:A:599:LEU:HB2	1:A:608:PHE:CZ	2.46	0.51
1:B:243:VAL:CG1	1:B:246:GLU:HA	2.41	0.51
1:B:343:ILE:HG12	1:B:344:SER:N	2.25	0.51
1:B:417:MET:SD	1:B:417:MET:N	2.84	0.51
1:D:10:TRP:CE2	1:D:57:LYS:HD3	2.46	0.51
1:D:368:HIS:HB2	1:D:371:ILE:HG13	1.92	0.51
1:B:32:LEU:HA	1:B:33:PRO:C	2.32	0.51
1:C:371:ILE:HB	1:C:408:ARG:NH1	2.26	0.51
1:B:67:ALA:HB1	1:B:149:VAL:O	2.11	0.51
1:C:439:TRP:CZ2	1:C:471:GLU:HG3	2.46	0.50
1:C:400:MET:HA	1:C:403:GLU:OE1	2.12	0.50
1:B:33:PRO:HB2	1:B:293:ALA:HB1	1.94	0.50
1:D:285:GLN:HG2	1:D:319:TYR:CZ	2.47	0.50
1:B:315:ARG:NH1	1:B:467:GLU:HG3	2.26	0.50
1:D:236:TYR:HB3	1:D:256:PHE:CZ	2.46	0.50
1:D:498:ILE:HG23	1:D:502:PHE:CG	2.46	0.50
1:B:68:ASP:HB2	1:B:151:LYS:N	2.26	0.50
1:D:220:SER:O	1:D:221:ILE:HB	2.12	0.50
1:D:368:HIS:CB	1:D:371:ILE:HG13	2.42	0.50
1:D:372:VAL:C	1:D:408:ARG:HG2	2.32	0.50
1:D:575:THR:HG23	1:D:610:VAL:C	2.32	0.50
1:B:230:LYS:N	5:B:901:HOH:O	2.45	0.50
1:B:328:LEU:O	1:B:332:ARG:HG2	2.11	0.50
1:C:239:GLU:HG2	1:C:253:SER:HB2	1.94	0.50
1:A:193:LEU:N	1:A:210:THR:O	2.38	0.50
1:C:175:ALA:O	1:C:220:SER:OG	2.21	0.50
1:B:261:PHE:CE2	1:B:372:VAL:HB	2.47	0.50
1:D:72:LEU:HD12	1:D:146:ILE:HD11	1.94	0.50
1:D:306:ILE:HA	1:D:515:MET:HE1	1.93	0.50
1:C:51:GLY:O	1:C:120:GLU:HA	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:PRO:HB2	1:D:293:ALA:HB1	1.94	0.50
1:D:315:ARG:HB2	1:D:511:HIS:CG	2.47	0.50
1:D:430:VAL:HG13	1:D:462:PRO:CB	2.38	0.50
1:D:88:LYS:O	1:D:90:VAL:HG13	2.12	0.49
1:D:500:GLN:O	1:D:504:ARG:HD2	2.12	0.49
1:A:188:ALA:HB1	1:A:190:ASP:OD1	2.11	0.49
1:D:433:TYR:HB3	1:D:435:HIS:CD2	2.47	0.49
1:B:263:ILE:HD12	1:B:409:LEU:HD12	1.93	0.49
1:B:439:TRP:CH2	1:B:471:GLU:HB2	2.47	0.49
1:C:561:VAL:CG2	1:C:622:ALA:HB3	2.41	0.49
1:D:590:PHE:CE1	1:D:595:SER:HB2	2.47	0.49
1:D:598:LYS:HG2	1:C:597:GLY:HA2	1.92	0.49
1:D:615:GLU:HG2	1:D:632:ARG:HG2	1.94	0.49
1:B:256:PHE:HB2	3:B:804:GOL:C1	2.32	0.49
1:B:363:VAL:HA	2:B:802:FMN:HM72	1.94	0.49
1:D:414:VAL:HG11	1:D:433:TYR:CZ	2.47	0.49
1:C:420:ILE:HG13	1:C:458:PHE:HE2	1.77	0.49
1:B:5:ASN:HD21	1:B:7:ASN:HB2	1.77	0.49
1:A:51:GLY:O	1:A:120:GLU:HA	2.12	0.49
1:D:78:ASN:HA	1:D:96:GLY:CA	2.43	0.49
1:C:128:TYR:CE1	1:C:347:MET:HE2	2.47	0.49
1:D:190:ASP:OD1	1:D:190:ASP:N	2.45	0.49
1:B:536:LEU:O	1:B:545:LYS:HG3	2.13	0.49
1:D:165:LYS:HG3	1:D:366:TYR:CE2	2.48	0.49
1:D:303:ILE:HD12	1:D:328:LEU:HB3	1.95	0.49
1:A:473:LEU:HB2	1:A:475:TRP:CD1	2.48	0.48
1:A:51:GLY:O	1:A:120:GLU:HG2	2.13	0.48
1:D:458:PHE:N	1:D:459:PRO:HD3	2.29	0.48
1:A:32:LEU:HA	1:A:33:PRO:C	2.34	0.48
1:C:227:TRP:CZ2	1:C:333:GLY:HA2	2.49	0.48
1:D:474:ASN:OD1	1:D:476:HIS:HE1	1.97	0.48
1:C:498:ILE:HD11	1:C:551:TYR:CD1	2.48	0.48
1:B:317:ALA:HB1	1:B:318:HIS:ND1	2.28	0.48
1:A:184:LEU:HD22	1:A:242:LEU:HD13	1.94	0.48
1:B:343:ILE:CG1	1:B:378:ASN:HD22	2.27	0.48
1:B:369:PRO:HD3	3:B:804:GOL:O1	2.14	0.48
1:A:210:THR:OG1	1:A:214:GLU:HB3	2.14	0.48
1:A:434:ASN:CG	1:A:467:GLU:HB2	2.34	0.48
1:C:207:LYS:N	1:C:219:LEU:HD23	2.28	0.48
1:C:473:LEU:HD21	1:C:533:HIS:CD2	2.49	0.48
1:A:175:ALA:HB3	1:A:221:ILE:HG13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ILE:N	1:A:370:SER:O	2.36	0.48
1:C:267:ARG:HG2	1:C:267:ARG:NH1	2.28	0.48
1:B:85:VAL:HG22	1:B:115:ILE:HD13	1.96	0.48
1:B:191:GLN:NE2	1:B:242:LEU:HD21	2.28	0.48
1:D:340:ILE:CD1	1:D:342:TYR:CB	2.86	0.48
1:B:35:SER:O	1:B:38:GLU:HG3	2.13	0.48
1:A:464:GLY:HA2	1:A:507:ILE:HG23	1.95	0.48
1:D:432:SER:HB2	1:D:466:SER:OG	2.13	0.48
1:C:194:VAL:O	1:C:240:VAL:HA	2.13	0.47
1:B:419:ASP:OD1	1:B:421:HIS:N	2.33	0.47
1:D:620:ALA:O	1:D:626:LYS:HA	2.14	0.47
1:B:318:HIS:HA	1:B:339:GLU:OE2	2.14	0.47
1:B:343:ILE:CD1	1:B:378:ASN:HD22	2.27	0.47
1:B:516:PHE:HD1	1:B:537:VAL:HB	1.78	0.47
1:A:78:ASN:HA	1:A:79:ALA:HA	1.58	0.47
1:D:438:GLY:O	1:D:439:TRP:C	2.51	0.47
1:D:441:GLY:HA3	4:D:801:I9G:C38	2.44	0.47
1:C:493:TYR:CE1	1:C:497:MET:HG3	2.48	0.47
1:B:281:VAL:O	1:B:314:ILE:HA	2.14	0.47
1:B:427:ILE:HB	1:B:428:PRO:HD3	1.96	0.47
1:A:192:LYS:HB2	1:A:243:VAL:HG22	1.96	0.47
1:A:494:HIS:HE1	1:A:512:VAL:HG13	1.80	0.47
1:D:32:LEU:HA	1:D:33:PRO:C	2.34	0.47
1:D:263:ILE:HD12	1:D:430:VAL:HG21	1.96	0.47
1:D:376:LEU:HB2	1:D:412:ILE:HG22	1.95	0.47
1:C:263:ILE:HD12	1:C:409:LEU:CD1	2.43	0.47
1:D:502:PHE:CE2	1:D:555:LEU:HD21	2.41	0.47
1:C:36:TRP:CZ3	1:C:139:GLY:HA2	2.50	0.47
1:C:476:HIS:HA	1:C:488:GLU:OE1	2.14	0.47
1:B:337:TRP:HH2	1:B:432:SER:HB2	1.79	0.47
1:D:254:THR:HG21	1:D:367:ASN:CB	2.44	0.47
1:C:65:PRO:O	1:C:70:TYR:OH	2.24	0.47
1:B:88:LYS:O	1:B:90:VAL:HG13	2.14	0.47
1:B:162:PRO:O	1:B:252:VAL:HG21	2.15	0.47
1:A:279:ARG:HD3	1:A:510:THR:OG1	2.15	0.47
1:D:1:ARG:HB2	1:D:250:ASP:OD1	2.15	0.47
1:D:72:LEU:CD2	1:D:74:LEU:HD11	2.44	0.47
1:D:137:TYR:CD2	1:D:292:ASN:HB3	2.49	0.47
1:D:265:PRO:O	1:D:455:HIS:NE2	2.45	0.47
1:D:367:ASN:N	1:D:367:ASN:HD22	2.12	0.47
1:C:40:ASP:HA	1:C:43:ASP:OD2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ASP:HB3	4:C:803:I9G:C08	2.45	0.47
1:C:610:VAL:HG13	1:C:611:PRO:CD	2.43	0.47
1:B:13:THR:HG21	1:B:27:TRP:CE2	2.50	0.47
1:B:561:VAL:HG23	1:B:625:TYR:HB3	1.97	0.47
1:D:531:GLN:OE1	1:D:539:PHE:HB2	2.14	0.47
1:C:81:ALA:HA	1:C:118:ALA:O	2.15	0.47
1:B:416:SER:HB2	1:B:434:ASN:O	2.15	0.47
1:C:318:HIS:HA	1:C:339:GLU:OE2	2.15	0.47
1:A:278:LEU:O	1:A:279:ARG:NH1	2.46	0.47
1:D:4:ILE:CG1	1:D:146:ILE:HB	2.45	0.47
1:D:59:LEU:HB2	1:D:115:ILE:HD11	1.97	0.47
1:D:224:VAL:O	1:D:226:LEU:HD12	2.14	0.47
1:D:337:TRP:CD1	1:D:337:TRP:C	2.89	0.47
1:D:513:TRP:HA	1:D:514:ASN:HA	1.64	0.47
1:D:379:GLU:HG2	1:D:434:ASN:HD22	1.80	0.46
1:D:336:ILE:HG12	1:D:370:SER:HB2	1.96	0.46
1:D:368:HIS:HB2	1:D:371:ILE:CD1	2.44	0.46
1:C:294:LEU:HD12	1:C:299:HIS:HE1	1.79	0.46
1:C:513:TRP:HA	1:C:514:ASN:HA	1.69	0.46
1:B:230:LYS:HG2	1:B:332:ARG:O	2.16	0.46
1:B:334:LEU:O	1:B:370:SER:HB2	2.14	0.46
1:A:374:TRP:NE1	1:A:408:ARG:HD2	2.30	0.46
1:D:301:GLU:O	1:D:305:LEU:HD23	2.16	0.46
1:D:303:ILE:CD1	1:D:328:LEU:HB3	2.45	0.46
1:C:168:PRO:CA	1:C:177:VAL:HG12	2.45	0.46
1:C:372:VAL:HG23	1:C:373:VAL:HG13	1.97	0.46
1:C:433:TYR:HB3	1:C:435:HIS:CD2	2.50	0.46
1:A:287:ARG:NH2	1:A:541:ARG:HG2	2.31	0.46
1:C:181:GLU:HG3	1:C:216:LYS:HG2	1.97	0.46
1:D:327:ASP:O	1:D:331:GLU:HG3	2.15	0.46
1:C:472:ALA:HB2	1:C:490:GLN:CB	2.45	0.46
1:B:59:LEU:HD21	1:B:64:LEU:CD2	2.45	0.46
1:A:341:PRO:O	1:A:343:ILE:HG22	2.15	0.46
1:A:616:SER:HB2	1:A:631:ILE:HG13	1.98	0.46
1:C:327:ASP:O	1:C:331:GLU:HG3	2.15	0.46
1:C:83:VAL:O	1:C:90:VAL:HG22	2.15	0.46
1:C:184:LEU:CD1	1:C:242:LEU:HD22	2.44	0.46
1:C:308:GLU:HG2	1:C:552:LYS:HE3	1.98	0.46
1:C:568:TYR:CZ	1:C:571:ARG:HG2	2.51	0.46
1:B:588:GLU:CB	1:B:598:LYS:HG2	2.45	0.46
1:A:343:ILE:HG12	1:A:344:SER:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:LYS:HA	1:D:203:LYS:O	2.15	0.46
1:B:373:VAL:HA	1:B:409:LEU:O	2.14	0.46
1:B:434:ASN:CG	1:B:467:GLU:HB2	2.36	0.46
1:B:495:GLU:HG2	1:B:605:PHE:CD2	2.50	0.46
1:D:285:GLN:HG2	1:D:319:TYR:CE1	2.51	0.46
1:D:398:ASN:OD1	1:D:427:ILE:HG22	2.16	0.46
1:B:78:ASN:HA	1:B:79:ALA:HA	1.60	0.46
1:A:35:SER:O	1:A:38:GLU:HG3	2.15	0.46
1:D:316:LEU:HB3	1:D:321:HIS:CD2	2.52	0.45
1:C:60:LYS:HA	1:C:111:GLU:O	2.16	0.45
1:B:149:VAL:HA	5:B:905:HOH:O	2.16	0.45
1:A:411:THR:HB	1:A:430:VAL:CG2	2.47	0.45
1:D:473:LEU:HD11	1:D:533:HIS:ND1	2.32	0.45
1:D:563:LEU:HD23	1:D:627:ASP:HB3	1.98	0.45
1:C:195:TYR:O	1:C:207:LYS:HA	2.16	0.45
1:B:391:LEU:O	1:B:395:ARG:HG3	2.17	0.45
1:A:92:HIS:CG	3:A:804:GOL:H11	2.51	0.45
1:A:243:VAL:HA	1:A:247:GLU:O	2.16	0.45
1:D:61:LYS:HE3	1:D:108:LEU:O	2.16	0.45
1:A:271:LEU:HD23	1:A:276:TYR:CD2	2.51	0.45
1:A:427:ILE:HB	1:A:428:PRO:HD3	1.98	0.45
1:D:476:HIS:HA	1:D:488:GLU:OE1	2.15	0.45
1:B:230:LYS:HE3	1:B:307:CYS:SG	2.56	0.45
1:D:390:LEU:HD23	1:D:394:HIS:CE1	2.52	0.45
1:D:411:THR:OG1	1:D:412:ILE:N	2.50	0.45
1:A:61:LYS:HB3	1:A:111:GLU:OE2	2.16	0.45
1:A:536:LEU:O	1:A:545:LYS:HG3	2.16	0.45
1:D:600:GLN:O	1:C:599:LEU:HD13	2.17	0.45
1:A:88:LYS:HE3	1:A:89:ALA:O	2.16	0.45
1:A:303:ILE:HD11	1:A:334:LEU:HD12	1.97	0.45
1:D:340:ILE:HG22	1:D:361:LEU:HD22	1.98	0.45
1:C:381:THR:HG21	1:C:424:TYR:CE1	2.52	0.45
1:B:376:LEU:HB2	1:B:412:ILE:CD1	2.45	0.45
1:A:17:THR:HG21	1:B:355:ILE:CD1	2.45	0.45
1:A:75:ARG:HB2	1:A:142:ARG:HB3	1.98	0.45
1:D:435:HIS:ND1	1:D:437:PHE:CE2	2.85	0.45
1:D:619:VAL:CG2	1:D:628:GLU:HG3	2.38	0.45
1:A:199:ASP:OD1	1:A:200:ALA:N	2.49	0.45
1:A:334:LEU:O	1:A:370:SER:HB2	2.17	0.45
1:A:416:SER:HB2	1:A:434:ASN:O	2.17	0.45
1:C:374:TRP:CE2	1:C:408:ARG:HD2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LYS:HE2	1:B:110:GLU:O	2.16	0.45
1:B:80:SER:HB3	1:B:94:ASP:OD1	2.17	0.45
1:B:285:GLN:HG2	1:B:319:TYR:CZ	2.52	0.45
1:B:591:VAL:HG23	1:B:591:VAL:O	2.16	0.45
1:A:412:ILE:HG12	1:A:428:PRO:HG3	1.99	0.45
1:A:481:LYS:HD2	1:A:481:LYS:HA	1.57	0.45
1:D:13:THR:HG21	1:D:27:TRP:CZ2	2.52	0.45
1:A:1:ARG:HB2	1:A:149:VAL:HG12	1.99	0.44
1:A:414:VAL:HG12	1:A:415:VAL:O	2.17	0.44
1:D:142:ARG:HD3	1:D:322:ASP:OD1	2.16	0.44
1:D:221:ILE:HD11	1:D:224:VAL:CB	2.46	0.44
1:D:464:GLY:HA2	1:D:507:ILE:HG23	1.98	0.44
1:C:374:TRP:NE1	1:C:408:ARG:HD2	2.32	0.44
2:C:801:FMN:O2'	2:C:801:FMN:C10	2.65	0.44
1:B:33:PRO:HB3	1:B:141:TYR:O	2.17	0.44
1:D:159:TYR:O	1:D:364:GLN:NE2	2.51	0.44
1:D:318:HIS:O	1:D:341:PRO:HA	2.17	0.44
1:C:24:PRO:HG2	1:C:27:TRP:CE3	2.52	0.44
1:C:59:LEU:CD2	1:C:64:LEU:HD11	2.48	0.44
1:A:182:VAL:O	1:A:215:THR:HB	2.17	0.44
1:A:373:VAL:HA	1:A:409:LEU:O	2.17	0.44
1:D:420:ILE:CG2	1:D:454:PHE:HD1	2.29	0.44
1:A:584:LEU:HB3	1:A:585:PRO:HD2	1.99	0.44
1:D:451:MET:HE2	1:D:507:ILE:HD13	1.98	0.44
1:D:92:HIS:NE2	1:D:94:ASP:OD1	2.51	0.44
1:B:633:LYS:HD3	1:B:634:VAL:H	1.82	0.44
1:D:351:ARG:HA	1:D:354:THR:CG2	2.47	0.44
1:B:194:VAL:HG22	1:B:209:GLU:HG3	1.99	0.44
1:B:418:CYS:SG	1:B:424:TYR:HE2	2.41	0.44
1:B:513:TRP:HA	1:B:514:ASN:HA	1.62	0.44
1:A:577:LYS:HE2	1:A:607:HIS:CG	2.52	0.44
1:D:283:ARG:HD3	1:D:284:HIS:O	2.18	0.44
1:C:37:ASN:HA	1:C:40:ASP:OD1	2.18	0.44
1:C:263:ILE:CD1	1:C:409:LEU:HD12	2.44	0.44
1:C:315:ARG:HH11	1:C:467:GLU:HG3	1.83	0.44
1:B:10:TRP:CE3	1:B:55:TYR:HB3	2.52	0.44
1:B:376:LEU:HD12	1:B:412:ILE:HD11	1.99	0.44
2:B:802:FMN:H1'1	2:B:802:FMN:H9	1.75	0.44
1:D:184:LEU:HD13	1:D:187:ALA:CB	2.48	0.44
1:D:439:TRP:HZ2	1:D:485:TYR:CE2	2.36	0.44
1:D:563:LEU:HD23	1:D:627:ASP:C	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ALA:HA	1:A:118:ALA:O	2.18	0.44
1:D:469:GLY:HA3	1:D:513:TRP:O	2.17	0.44
1:C:281:VAL:O	1:C:314:ILE:HA	2.17	0.44
1:D:78:ASN:HA	1:D:79:ALA:HA	1.54	0.43
1:C:159:TYR:CZ	1:C:359:LYS:HD2	2.53	0.43
1:A:192:LYS:HE2	1:A:243:VAL:HG21	2.00	0.43
1:A:468:TYR:CZ	1:A:512:VAL:HG22	2.53	0.43
1:A:634:VAL:HG22	1:A:635:ASP:N	2.33	0.43
1:D:236:TYR:CE2	1:D:258:CYS:SG	3.11	0.43
1:D:414:VAL:HG12	1:D:415:VAL:O	2.18	0.43
1:C:256:PHE:HB2	3:C:802:GOL:H12	1.99	0.43
1:C:390:LEU:HD23	1:C:390:LEU:C	2.39	0.43
1:C:557:ASP:O	1:C:559:PRO:HD3	2.18	0.43
1:B:621:VAL:HG22	1:B:626:LYS:HD3	1.99	0.43
1:D:286:ASP:O	1:D:541:ARG:NH2	2.51	0.43
1:D:317:ALA:HB1	1:D:318:HIS:CG	2.52	0.43
1:D:451:MET:CE	1:D:507:ILE:HD13	2.47	0.43
1:D:463:LEU:O	1:D:507:ILE:HA	2.17	0.43
1:B:278:LEU:O	1:B:509:ALA:HA	2.19	0.43
1:D:236:TYR:O	1:D:255:ARG:HA	2.18	0.43
1:C:404:MET:HB3	2:C:801:FMN:HM82	2.00	0.43
1:B:243:VAL:HG11	1:B:246:GLU:HA	1.99	0.43
1:B:257:GLY:N	3:B:804:GOL:O1	2.48	0.43
1:A:412:ILE:HD12	1:A:414:VAL:CG2	2.48	0.43
1:C:386:SER:HB3	1:C:391:LEU:CD2	2.49	0.43
1:C:531:GLN:HB2	1:C:533:HIS:NE2	2.33	0.43
1:C:620:ALA:O	1:C:626:LYS:HA	2.18	0.43
1:B:502:PHE:CZ	1:B:555:LEU:HD11	2.53	0.43
1:D:374:TRP:HE1	1:D:408:ARG:HD2	1.83	0.43
1:C:368:HIS:HB2	1:C:371:ILE:HG13	2.00	0.43
1:C:386:SER:HA	1:C:390:LEU:HD13	2.01	0.43
1:B:518:PHE:HZ	4:B:803:I9G:O09	2.00	0.43
1:A:192:LYS:HB2	1:A:243:VAL:CG2	2.47	0.43
1:A:205:VAL:HG11	1:A:221:ILE:HG22	1.99	0.43
1:B:444:VAL:HG23	1:B:493:TYR:CE1	2.53	0.43
1:A:395:ARG:CG	1:A:427:ILE:HD13	2.49	0.43
1:D:478:SER:C	1:D:480:PRO:HD3	2.39	0.43
1:B:3:VAL:C	1:B:4:ILE:HD13	2.39	0.43
1:A:78:ASN:HB3	1:A:137:TYR:O	2.19	0.43
1:D:200:ALA:C	1:D:202:GLY:N	2.72	0.43
1:C:305:LEU:CD2	1:C:544:LYS:HE3	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LEU:HD21	1:B:117:ILE:HD13	1.99	0.43
1:B:279:ARG:HD3	1:B:510:THR:OG1	2.19	0.43
1:A:168:PRO:HD3	3:A:802:GOL:H2	2.00	0.43
1:A:188:ALA:N	1:A:191:GLN:OE1	2.52	0.43
1:A:379:GLU:HB3	1:A:415:VAL:HB	2.01	0.43
1:D:8:THR:O	1:D:57:LYS:HE2	2.19	0.43
1:D:110:GLU:CD	1:D:111:GLU:H	2.22	0.43
1:D:268:GLY:O	1:D:270:ILE:HD12	2.19	0.43
1:D:274:GLU:OE2	1:D:274:GLU:HA	2.19	0.43
1:C:361:LEU:HD12	1:C:365:ASN:ND2	2.34	0.43
1:B:317:ALA:HB1	1:B:318:HIS:HA	2.01	0.43
2:B:802:FMN:N1	2:B:802:FMN:C2'	2.82	0.43
2:A:801:FMN:H1'1	2:A:801:FMN:H9	1.74	0.42
1:D:424:TYR:HA	1:D:427:ILE:HG13	2.00	0.42
1:C:142:ARG:HD3	1:C:322:ASP:OD2	2.19	0.42
1:C:261:PHE:HA	1:C:270:ILE:O	2.18	0.42
1:B:41:GLY:HA2	1:B:48:TYR:HB3	2.02	0.42
1:A:337:TRP:CD1	1:A:337:TRP:C	2.92	0.42
1:A:468:TYR:OH	1:A:512:VAL:HG22	2.20	0.42
1:D:287:ARG:HG3	1:D:288:TRP:H	1.84	0.42
1:D:327:ASP:OD1	1:D:368:HIS:HE1	2.02	0.42
1:C:133:ASP:OD1	1:C:523:ARG:NE	2.50	0.42
1:D:434:ASN:OD1	1:D:467:GLU:HB2	2.19	0.42
1:B:303:ILE:HG21	1:B:328:LEU:HD13	2.01	0.42
1:B:392:GLU:OE1	1:B:392:GLU:HA	2.20	0.42
1:B:458:PHE:CB	1:B:461:ILE:HD12	2.37	0.42
1:A:78:ASN:HA	1:A:96:GLY:HA3	2.00	0.42
1:D:13:THR:HB	1:D:27:TRP:CD2	2.55	0.42
1:D:81:ALA:HA	1:D:118:ALA:O	2.19	0.42
1:D:168:PRO:HB3	1:D:177:VAL:HG22	2.01	0.42
1:D:237:THR:O	1:D:237:THR:HG23	2.20	0.42
1:A:390:LEU:O	1:A:390:LEU:HD23	2.19	0.42
1:A:482:GLN:HB2	1:A:489:TYR:OH	2.20	0.42
1:A:563:LEU:HD23	1:A:580:VAL:CG2	2.38	0.42
1:D:168:PRO:N	1:D:177:VAL:HG13	2.34	0.42
1:C:261:PHE:CE2	1:C:372:VAL:HB	2.54	0.42
1:B:42:GLN:HE21	1:B:291:GLY:HA2	1.85	0.42
1:B:90:VAL:HG11	1:B:107:GLU:HG3	2.01	0.42
1:B:316:LEU:HB3	1:B:321:HIS:CD2	2.54	0.42
1:D:164:ILE:HB	1:D:252:VAL:CG1	2.48	0.42
1:C:168:PRO:HA	1:C:177:VAL:HG12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:LEU:HD12	1:D:146:ILE:HD13	2.02	0.42
1:D:237:THR:HA	1:D:255:ARG:HA	2.01	0.42
1:D:478:SER:O	1:D:480:PRO:HD3	2.19	0.42
1:D:516:PHE:CD1	1:D:537:VAL:HB	2.50	0.42
1:B:474:ASN:HB3	3:B:805:GOL:H32	2.00	0.42
1:A:570:ASP:OD1	1:A:632:ARG:NH1	2.53	0.42
1:D:83:VAL:HG22	1:D:117:ILE:HG12	2.02	0.42
1:D:495:GLU:HG2	1:D:605:PHE:CE2	2.55	0.42
1:C:78:ASN:ND2	1:C:137:TYR:O	2.43	0.42
1:C:188:ALA:H	1:C:191:GLN:HE22	1.67	0.42
1:C:424:TYR:HA	1:C:427:ILE:HG13	2.01	0.42
1:A:11:ALA:HB1	1:A:27:TRP:HB2	2.02	0.42
1:D:35:SER:O	1:D:38:GLU:HG3	2.19	0.42
1:D:14:LYS:HZ3	1:D:36:TRP:HD1	1.66	0.41
1:D:200:ALA:C	1:D:202:GLY:H	2.23	0.41
1:D:340:ILE:HB	1:D:341:PRO:HD2	2.02	0.41
1:D:373:VAL:CG1	1:D:411:THR:CG2	2.98	0.41
1:C:101:ARG:CZ	1:C:156:LEU:HD23	2.50	0.41
1:C:178:GLU:HB2	1:C:218:VAL:HG22	2.01	0.41
1:C:411:THR:OG1	1:C:412:ILE:N	2.53	0.41
1:B:2:GLU:HG2	1:B:4:ILE:CD1	2.49	0.41
1:B:495:GLU:HG2	1:B:605:PHE:CE2	2.55	0.41
1:A:13:THR:HG21	1:A:27:TRP:CZ2	2.55	0.41
1:A:577:LYS:HE2	1:A:607:HIS:CB	2.49	0.41
1:D:3:VAL:HG22	1:D:147:ILE:HG23	2.02	0.41
1:D:73:GLU:C	1:D:74:LEU:HD12	2.40	0.41
1:D:227:TRP:CD1	1:D:235:LEU:CD1	3.02	0.41
1:D:281:VAL:O	1:D:314:ILE:HA	2.19	0.41
1:C:352:GLU:OE1	1:C:352:GLU:N	2.34	0.41
1:C:590:PHE:O	1:C:618:LEU:HA	2.20	0.41
1:B:166:VAL:HG22	1:B:180:VAL:HG22	2.01	0.41
1:B:563:LEU:HD13	1:B:629:SER:CB	2.44	0.41
1:A:473:LEU:HD11	1:A:533:HIS:CE1	2.55	0.41
1:B:556:SER:OG	1:B:558:GLU:HB2	2.19	0.41
1:A:225:HIS:HB2	1:A:234:TYR:CD2	2.55	0.41
1:A:540:ASP:OD1	1:A:542:LYS:HB2	2.20	0.41
1:D:69:CYS:HB2	1:D:149:VAL:CG2	2.49	0.41
1:D:184:LEU:HD13	1:D:187:ALA:HB1	2.02	0.41
1:C:78:ASN:HA	1:C:96:GLY:HA3	2.01	0.41
1:C:411:THR:CB	1:C:430:VAL:HG23	2.47	0.41
1:B:1:ARG:HG3	1:B:149:VAL:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:VAL:CG1	1:B:240:VAL:HG21	2.50	0.41
1:B:434:ASN:OD1	1:B:467:GLU:HB2	2.20	0.41
1:B:531:GLN:NE2	1:B:539:PHE:HB2	2.35	0.41
1:D:4:ILE:HG12	1:D:146:ILE:HB	2.02	0.41
1:D:236:TYR:HD2	1:D:258:CYS:HG	1.61	0.41
1:C:41:GLY:HA2	1:C:48:TYR:HB3	2.01	0.41
1:C:42:GLN:HE21	1:C:291:GLY:HA2	1.85	0.41
1:A:33:PRO:HB3	1:A:141:TYR:O	2.21	0.41
1:A:411:THR:OG1	1:A:412:ILE:N	2.54	0.41
1:D:137:TYR:HE2	1:D:286:ASP:HB3	1.86	0.41
1:D:275:GLU:OE2	1:D:505:LYS:NZ	2.54	0.41
1:C:183:PHE:O	1:C:184:LEU:HD23	2.20	0.41
1:B:73:GLU:HB2	1:B:147:ILE:HD11	2.02	0.41
1:B:315:ARG:HB2	1:B:511:HIS:CD2	2.56	0.41
1:A:227:TRP:CZ2	1:A:333:GLY:HA2	2.55	0.41
1:D:439:TRP:O	1:D:482:GLN:NE2	2.53	0.41
1:D:495:GLU:O	1:D:499:LYS:HG3	2.20	0.41
1:C:72:LEU:O	1:C:101:ARG:HA	2.21	0.41
2:C:801:FMN:H9	2:C:801:FMN:H1'1	1.77	0.41
1:A:390:LEU:HD23	1:A:390:LEU:C	2.41	0.41
1:A:620:ALA:O	1:A:626:LYS:HA	2.21	0.41
1:D:41:GLY:HA2	1:D:48:TYR:HB3	2.02	0.41
1:D:309:LEU:C	1:D:309:LEU:HD23	2.41	0.41
1:C:59:LEU:HD11	1:C:146:ILE:HD12	2.03	0.41
1:C:210:THR:OG1	1:C:214:GLU:HB3	2.21	0.41
1:C:363:VAL:HG13	2:C:801:FMN:H6	2.00	0.41
1:B:276:TYR:CE2	5:B:901:HOH:O	2.70	0.41
1:B:285:GLN:HG2	1:B:319:TYR:OH	2.20	0.41
1:A:44:GLY:HA2	1:A:521:ASP:O	2.21	0.41
1:A:380:ILE:HG21	1:A:394:HIS:CE1	2.55	0.41
1:D:7:ASN:ND2	1:D:143:ASP:HA	2.26	0.41
1:D:24:PRO:HG2	1:D:27:TRP:CE3	2.56	0.41
1:D:69:CYS:HA	1:D:105:THR:CG2	2.50	0.41
1:D:374:TRP:NE1	1:D:408:ARG:HD2	2.36	0.41
1:C:32:LEU:HA	1:C:33:PRO:C	2.40	0.41
1:C:361:LEU:HD12	1:C:361:LEU:O	2.21	0.41
1:C:412:ILE:HG12	1:C:431:ILE:HG22	2.02	0.41
1:B:149:VAL:CA	5:B:905:HOH:O	2.69	0.41
1:B:153:HIS:ND1	1:B:154:PHE:O	2.49	0.41
1:B:476:HIS:HA	1:B:488:GLU:OE1	2.21	0.41
1:D:184:LEU:HB3	1:D:187:ALA:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:643:LEU:O	1:D:643:LEU:HD23	2.21	0.41
1:C:371:ILE:O	1:C:408:ARG:NH1	2.53	0.41
1:B:102:VAL:O	1:B:102:VAL:HG13	2.20	0.41
1:A:17:THR:O	1:A:17:THR:CG2	2.69	0.40
1:A:41:GLY:HA2	1:A:48:TYR:HB3	2.03	0.40
1:C:125:ASP:HA	1:C:347:MET:SD	2.61	0.40
1:C:544:LYS:HD3	1:C:548:PHE:CE1	2.56	0.40
1:B:85:VAL:HG22	1:B:115:ILE:HD12	2.00	0.40
1:B:309:LEU:HD21	1:B:551:TYR:HB3	2.02	0.40
1:A:200:ALA:HB2	1:A:234:TYR:CZ	2.57	0.40
1:D:164:ILE:CG2	1:D:254:THR:OG1	2.69	0.40
1:D:210:THR:HG23	1:D:211:ALA:N	2.36	0.40
1:D:317:ALA:HB1	1:D:318:HIS:HA	2.02	0.40
1:A:1:ARG:HG3	1:A:149:VAL:CG1	2.52	0.40
1:A:60:LYS:CE	1:A:112:GLU:OE2	2.70	0.40
1:A:599:LEU:HB2	1:A:608:PHE:CE2	2.56	0.40
1:D:432:SER:HA	1:D:464:GLY:O	2.22	0.40
1:C:133:ASP:HB3	4:C:803:I9G:O09	2.21	0.40
1:C:330:ASP:OD1	1:C:370:SER:OG	2.28	0.40
1:D:23:MET:HB2	1:D:58:GLN:OE1	2.21	0.40
1:D:154:PHE:HE1	1:D:250:ASP:C	2.25	0.40
1:C:74:LEU:HD21	1:C:117:ILE:HD13	2.02	0.40
1:C:337:TRP:CH2	1:C:466:SER:HB3	2.57	0.40
1:B:184:LEU:HD13	1:B:184:LEU:HA	1.91	0.40
1:A:411:THR:HB	1:A:430:VAL:HG22	2.02	0.40
1:A:458:PHE:N	1:A:459:PRO:HD3	2.36	0.40
1:D:430:VAL:HG12	1:D:431:ILE:H	1.87	0.40
1:D:452:ASP:O	1:D:456:LYS:N	2.50	0.40
1:D:598:LYS:HG2	1:C:597:GLY:CA	2.51	0.40
1:C:2:GLU:HG2	1:C:4:ILE:HD11	2.03	0.40
1:B:600:GLN:HA	1:B:606:PHE:HE2	1.87	0.40
1:B:642:SER:OG	1:B:644:LYS:HG3	2.22	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	642/756 (85%)	613 (96%)	28 (4%)	1 (0%)	47	73
1	B	639/756 (84%)	609 (95%)	30 (5%)	0	100	100
1	C	636/756 (84%)	608 (96%)	28 (4%)	0	100	100
1	D	615/756 (81%)	563 (92%)	46 (8%)	6 (1%)	15	37
All	All	2532/3024 (84%)	2393 (94%)	132 (5%)	7 (0%)	41	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	205	VAL
1	D	224	VAL
1	A	9	LYS
1	D	222	PRO
1	D	344	SER
1	D	439	TRP
1	D	221	ILE

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	545/640 (85%)	538 (99%)	7 (1%)	69	87
1	B	544/640 (85%)	538 (99%)	6 (1%)	73	90
1	C	541/640 (84%)	524 (97%)	17 (3%)	40	69
1	D	511/640 (80%)	495 (97%)	16 (3%)	40	69
All	All	2141/2560 (84%)	2095 (98%)	46 (2%)	53	80

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	176	SER
1	A	337	TRP
1	A	345	SER
1	A	595	SER
1	A	626	LYS
1	A	642	SER
1	D	14	LYS
1	D	100	TRP
1	D	210	THR
1	D	218	VAL
1	D	313	THR
1	D	314	ILE
1	D	315	ARG
1	D	337	TRP
1	D	386	SER
1	D	393	ASN
1	D	398	ASN
1	D	429	ASP
1	D	433	TYR
1	D	466	SER
1	D	586	GLU
1	D	594	LYS
1	C	100	TRP
1	C	120	GLU
1	C	176	SER
1	C	199	ASP
1	C	253	SER
1	C	259	ARG
1	C	337	TRP
1	C	356	SER
1	C	387	ASP
1	C	393	ASN
1	C	424	TYR
1	C	466	SER
1	C	470	CYS
1	C	539	PHE
1	C	557	ASP
1	C	632	ARG
1	C	642	SER
1	B	63	GLU
1	B	100	TRP
1	B	337	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	393	ASN
1	B	424	TYR
1	B	632	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	447	ASN
1	D	476	HIS
1	C	447	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](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	I9G	D	801	-	41,47,47	2.20	9 (21%)	45,70,70	1.49	6 (13%)
2	FMN	B	802	-	33,33,33	1.13	2 (6%)	48,50,50	1.35	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	802	-	5,5,5	0.77	0	5,5,5	0.90	0
3	GOL	A	803	-	5,5,5	0.97	0	5,5,5	1.15	1 (20%)
3	GOL	C	802	-	5,5,5	0.80	0	5,5,5	0.98	0
4	I9G	A	805	-	41,47,47	2.22	11 (26%)	45,70,70	1.72	6 (13%)
3	GOL	B	801	-	5,5,5	0.81	0	5,5,5	1.10	1 (20%)
4	I9G	B	803	-	41,47,47	2.26	11 (26%)	45,70,70	1.79	10 (22%)
3	GOL	B	805	-	5,5,5	0.83	0	5,5,5	0.83	0
2	FMN	C	801	-	33,33,33	1.09	2 (6%)	48,50,50	1.47	9 (18%)
3	GOL	B	804	-	5,5,5	0.86	0	5,5,5	1.25	1 (20%)
3	GOL	A	804	-	5,5,5	0.78	0	5,5,5	1.03	0
4	I9G	C	803	-	41,47,47	2.87	11 (26%)	45,70,70	2.93	21 (46%)
2	FMN	A	801	-	33,33,33	1.10	2 (6%)	48,50,50	1.34	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	I9G	D	801	-	-	2/16/61/61	0/7/7/7
2	FMN	B	802	-	-	12/18/18/18	0/3/3/3
3	GOL	A	802	-	-	2/4/4/4	-
3	GOL	A	803	-	-	2/4/4/4	-
3	GOL	C	802	-	-	2/4/4/4	-
4	I9G	A	805	-	-	4/16/61/61	0/7/7/7
3	GOL	B	801	-	-	2/4/4/4	-
4	I9G	B	803	-	-	2/16/61/61	0/7/7/7
3	GOL	B	805	-	-	3/4/4/4	-
2	FMN	C	801	-	-	7/18/18/18	0/3/3/3
3	GOL	B	804	-	-	2/4/4/4	-
3	GOL	A	804	-	-	2/4/4/4	-
4	I9G	C	803	-	-	4/16/61/61	0/7/7/7
2	FMN	A	801	-	-	9/18/18/18	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	I9G	O06-C05	12.33	1.62	1.42
4	B	803	I9G	O06-C05	7.10	1.53	1.42
4	D	801	I9G	O06-C05	6.83	1.53	1.42
4	A	805	I9G	O06-C05	6.83	1.53	1.42
4	C	803	I9G	C14-N13	-6.10	1.35	1.47
4	C	803	I9G	O06-C07	5.43	1.52	1.43
4	D	801	I9G	C19-N16	5.18	1.52	1.37
4	B	803	I9G	C14-N13	-5.14	1.37	1.47
4	C	803	I9G	C19-N16	5.10	1.52	1.37
4	B	803	I9G	C19-N16	5.01	1.52	1.37
4	D	801	I9G	C18-N13	-4.99	1.37	1.47
4	A	805	I9G	C18-N13	-4.88	1.37	1.47
4	A	805	I9G	C19-N16	4.83	1.51	1.37
4	D	801	I9G	C14-N13	-4.82	1.37	1.47
4	A	805	I9G	C14-N13	-4.77	1.37	1.47
4	B	803	I9G	C18-N13	-4.65	1.38	1.47
4	B	803	I9G	C34-N36	4.22	1.48	1.37
4	C	803	I9G	C34-N36	4.21	1.48	1.37
4	D	801	I9G	C34-N36	4.07	1.47	1.37
4	C	803	I9G	C18-N13	-4.06	1.39	1.47
4	A	805	I9G	C34-N36	4.05	1.47	1.37
2	B	802	FMN	C4A-N5	4.02	1.38	1.30
2	A	801	FMN	C4A-N5	3.81	1.38	1.30
2	C	801	FMN	C4A-N5	3.67	1.37	1.30
4	A	805	I9G	C03-C05	3.30	1.56	1.52
4	A	805	I9G	C30-C29	2.93	1.56	1.51
4	D	801	I9G	C03-C05	2.81	1.56	1.52
4	B	803	I9G	C30-C29	2.80	1.56	1.51
4	B	803	I9G	C34-N35	2.79	1.34	1.31
2	B	802	FMN	C10-N1	2.71	1.38	1.33
4	B	803	I9G	O06-C07	2.61	1.47	1.43
4	A	805	I9G	C28-C27	2.59	1.47	1.42
2	A	801	FMN	C10-N1	2.59	1.38	1.33
4	C	803	I9G	C03-C05	2.58	1.56	1.52
4	D	801	I9G	N20-N21	2.56	1.35	1.32
4	C	803	I9G	C34-N35	2.55	1.34	1.31
4	B	803	I9G	C03-C05	2.53	1.56	1.52
4	A	805	I9G	C34-N35	2.42	1.34	1.31
4	B	803	I9G	C28-C27	2.39	1.46	1.42
4	C	803	I9G	N20-N21	2.39	1.35	1.32
4	D	801	I9G	C30-C29	2.36	1.55	1.51
4	C	803	I9G	C30-C29	2.35	1.55	1.51
2	C	801	FMN	C10-N1	2.31	1.37	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	I9G	C28-C27	2.28	1.46	1.42
4	A	805	I9G	N20-N21	2.15	1.35	1.32
4	A	805	I9G	C03-C02	-2.05	1.47	1.52
4	D	801	I9G	C34-N35	2.03	1.33	1.31
4	B	803	I9G	C03-C02	-2.00	1.47	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	803	I9G	O04-C03-C05	6.44	121.73	109.23
4	B	803	I9G	C02-C03-C05	6.30	118.23	108.98
4	C	803	I9G	C18-N13-C14	6.05	120.14	109.08
4	A	805	I9G	C02-C03-C05	5.78	117.47	108.98
4	D	801	I9G	O06-C05-C03	5.13	118.07	110.15
4	C	803	I9G	O09-C08-C07	-5.08	98.36	109.74
4	C	803	I9G	O06-C07-C08	-4.98	100.65	109.57
4	C	803	I9G	O01-C02-C03	4.73	121.27	110.35
4	C	803	I9G	O04-C03-C02	-4.72	99.43	110.35
4	C	803	I9G	C18-N13-C05	4.65	125.94	115.09
4	C	803	I9G	O06-C07-C10	-4.58	93.56	105.88
4	C	803	I9G	C17-C18-N13	4.40	119.00	110.59
4	B	803	I9G	O06-C07-C08	4.24	117.16	109.57
4	C	803	I9G	C14-C15-N16	4.19	118.84	110.70
4	C	803	I9G	O11-C10-C07	4.16	136.07	120.81
4	A	805	I9G	O06-C05-C03	4.05	116.40	110.15
4	A	805	I9G	C14-C15-N16	3.94	118.36	110.70
4	C	803	I9G	C02-C03-C05	-3.90	103.25	108.98
4	D	801	I9G	C02-C03-C05	3.73	114.46	108.98
4	C	803	I9G	C08-C02-C03	3.54	117.00	110.82
4	C	803	I9G	O12-C10-O11	-3.50	116.13	124.09
4	D	801	I9G	O06-C07-C08	3.49	115.81	109.57
2	C	801	FMN	C4-N3-C2	-3.43	119.30	125.64
2	C	801	FMN	C10-N1-C2	3.34	123.59	116.90
2	A	801	FMN	C4-N3-C2	-3.29	119.56	125.64
2	C	801	FMN	C4A-C10-N1	-3.27	117.14	124.73
4	A	805	I9G	O06-C07-C08	3.19	115.28	109.57
2	C	801	FMN	C4A-C10-N10	3.16	121.10	116.48
2	B	802	FMN	C4-N3-C2	-3.09	119.93	125.64
2	C	801	FMN	C4A-C4-N3	3.07	120.99	113.19
2	B	802	FMN	C5A-C9A-N10	2.97	121.03	117.95
2	A	801	FMN	C4A-C10-N1	-2.96	117.86	124.73
4	C	803	I9G	N35-C34-N36	2.86	119.66	117.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FMN	C4A-C4-N3	2.84	120.41	113.19
4	C	803	I9G	C02-C08-C07	2.84	114.10	109.25
2	B	802	FMN	C4A-C4-N3	2.83	120.38	113.19
2	B	802	FMN	C9A-C5A-N5	-2.83	119.36	122.43
4	C	803	I9G	C34-N35-C26	2.75	121.70	116.74
4	B	803	I9G	C34-N35-C26	2.74	121.68	116.74
4	C	803	I9G	C32-C33-C28	2.66	116.54	112.49
2	C	801	FMN	O4-C4-C4A	-2.66	119.56	126.60
4	B	803	I9G	C18-C17-N16	2.65	115.85	110.70
2	B	802	FMN	O4-C4-C4A	-2.62	119.64	126.60
4	B	803	I9G	N35-C34-N36	2.61	119.48	117.62
4	B	803	I9G	C41-N36-C37	-2.60	105.78	111.52
4	D	801	I9G	C34-N35-C26	2.56	121.36	116.74
4	C	803	I9G	O01-C02-C08	-2.50	104.58	110.35
2	A	801	FMN	C5A-C9A-N10	2.48	120.52	117.95
2	A	801	FMN	O4-C4-C4A	-2.48	120.02	126.60
2	B	802	FMN	C4A-C10-N1	-2.48	118.98	124.73
4	A	805	I9G	C34-N35-C26	2.48	121.21	116.74
2	A	801	FMN	C10-N1-C2	2.45	121.81	116.90
4	C	803	I9G	C15-C14-N13	2.44	115.26	110.59
2	A	801	FMN	C4A-C10-N10	2.37	119.94	116.48
2	C	801	FMN	C10-C4A-N5	-2.36	119.85	124.86
4	D	801	I9G	C18-C17-N16	2.35	115.26	110.70
4	D	801	I9G	C33-C28-C27	-2.34	118.27	122.37
2	B	802	FMN	C1'-N10-C9A	-2.34	116.62	120.51
4	B	803	I9G	C40-C41-N36	2.28	114.23	110.02
4	A	805	I9G	O04-C03-C05	-2.26	104.84	109.23
2	A	801	FMN	C4-C4A-C10	2.21	120.51	116.79
3	B	804	GOL	C3-C2-C1	-2.19	103.19	111.70
4	B	803	I9G	O04-C03-C05	-2.19	104.98	109.23
4	B	803	I9G	O39-C40-C41	2.18	116.60	111.80
4	B	803	I9G	C40-O39-C38	2.18	117.16	109.89
2	A	801	FMN	C9A-C5A-N5	-2.17	120.07	122.43
4	C	803	I9G	C17-N16-C15	-2.16	106.75	111.52
2	C	801	FMN	C5A-C9A-N10	2.14	120.17	117.95
2	A	801	FMN	C10-C4A-N5	-2.13	120.34	124.86
3	A	803	GOL	C3-C2-C1	-2.03	103.80	111.70
2	C	801	FMN	C4-C4A-C10	2.03	120.19	116.79
3	B	801	GOL	C3-C2-C1	-2.02	103.84	111.70
2	B	802	FMN	C10-N1-C2	2.00	120.91	116.90

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FMN	C2'-C1'-N10-C10
2	A	801	FMN	N10-C1'-C2'-O2'
2	A	801	FMN	C2'-C3'-C4'-O4'
2	A	801	FMN	C2'-C3'-C4'-C5'
2	A	801	FMN	O3'-C3'-C4'-O4'
2	A	801	FMN	O3'-C3'-C4'-C5'
2	A	801	FMN	C3'-C4'-C5'-O5'
2	A	801	FMN	O4'-C4'-C5'-O5'
2	C	801	FMN	C2'-C1'-N10-C10
2	C	801	FMN	N10-C1'-C2'-O2'
2	C	801	FMN	N10-C1'-C2'-C3'
2	C	801	FMN	C5'-O5'-P-O1P
2	B	802	FMN	C2'-C1'-N10-C10
2	B	802	FMN	N10-C1'-C2'-O2'
2	B	802	FMN	N10-C1'-C2'-C3'
2	B	802	FMN	C2'-C3'-C4'-O4'
2	B	802	FMN	O3'-C3'-C4'-O4'
3	A	802	GOL	C1-C2-C3-O3
3	A	803	GOL	C1-C2-C3-O3
3	A	804	GOL	C1-C2-C3-O3
3	C	802	GOL	C1-C2-C3-O3
3	B	804	GOL	C1-C2-C3-O3
4	D	801	I9G	C29-C34-N36-C37
4	D	801	I9G	N35-C34-N36-C37
4	C	803	I9G	C03-C05-N13-C14
4	C	803	I9G	O06-C05-N13-C14
4	C	803	I9G	C29-C34-N36-C37
4	C	803	I9G	N35-C34-N36-C37
2	B	802	FMN	O3'-C3'-C4'-C5'
2	B	802	FMN	C2'-C3'-C4'-C5'
3	A	802	GOL	O2-C2-C3-O3
3	B	805	GOL	O2-C2-C3-O3
4	A	805	I9G	N35-C34-N36-C41
3	B	801	GOL	C1-C2-C3-O3
3	B	805	GOL	C1-C2-C3-O3
3	A	803	GOL	O2-C2-C3-O3
3	C	802	GOL	O2-C2-C3-O3
4	A	805	I9G	C29-C34-N36-C41
3	A	804	GOL	O2-C2-C3-O3
3	B	804	GOL	O2-C2-C3-O3
4	A	805	I9G	N35-C34-N36-C37
2	C	801	FMN	C5'-O5'-P-O3P

Continued on next page...

Continued from previous page...

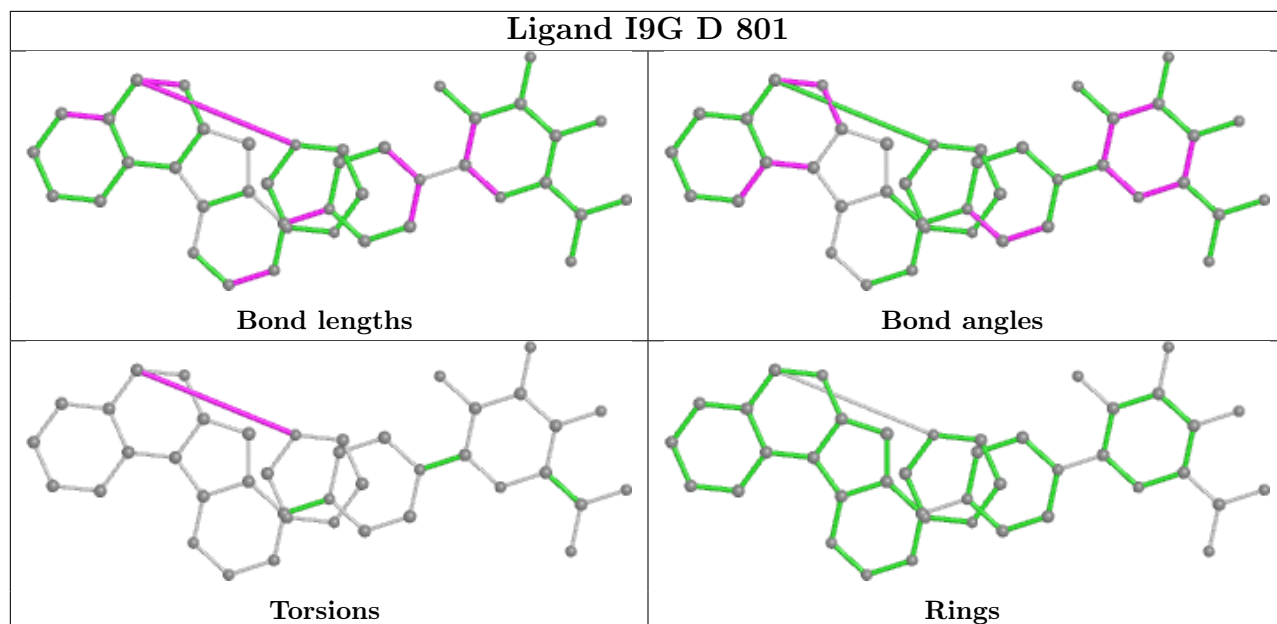
Mol	Chain	Res	Type	Atoms
2	A	801	FMN	N10-C1'-C2'-C3'
2	B	802	FMN	O4'-C4'-C5'-O5'
2	B	802	FMN	O2'-C2'-C3'-O3'
3	B	805	GOL	O1-C1-C2-C3
3	B	801	GOL	O2-C2-C3-O3
4	A	805	I9G	C29-C34-N36-C37
2	B	802	FMN	C2'-C1'-N10-C9A
2	C	801	FMN	C5'-O5'-P-O2P
2	B	802	FMN	O2'-C2'-C3'-C4'
4	B	803	I9G	O06-C07-C10-O11
4	B	803	I9G	O06-C07-C10-O12
2	C	801	FMN	C1'-C2'-C3'-O3'
2	B	802	FMN	C1'-C2'-C3'-O3'

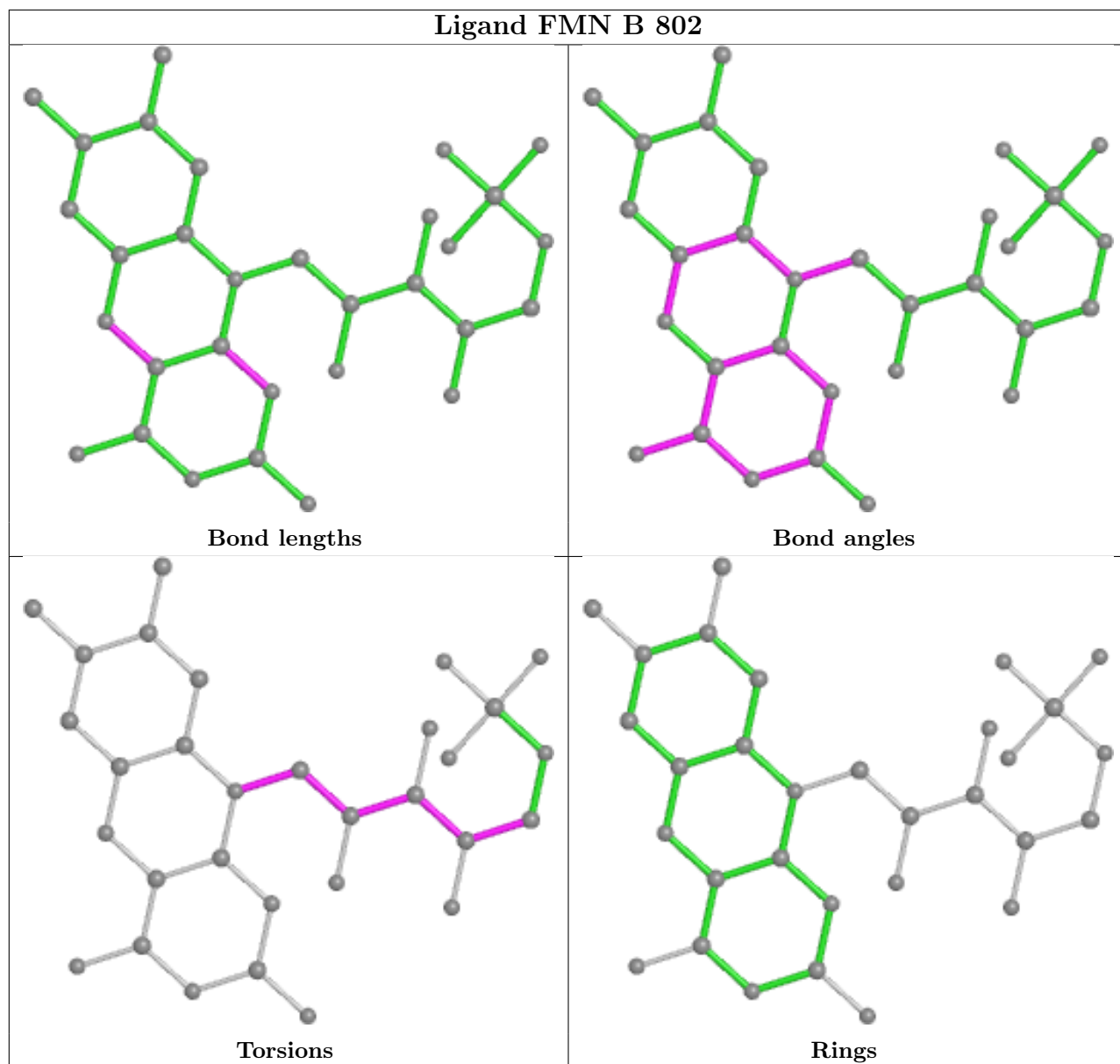
There are no ring outliers.

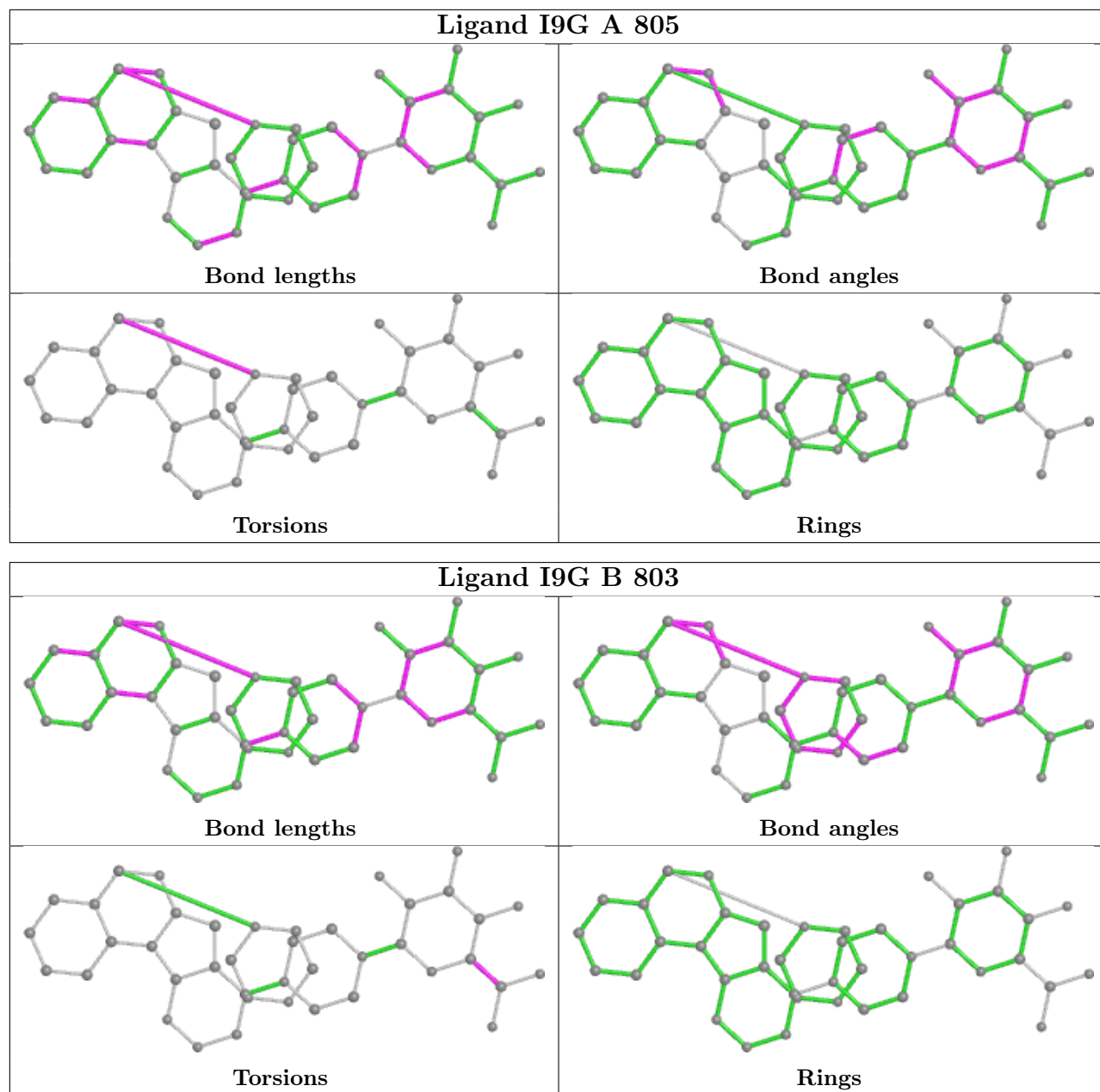
11 monomers are involved in 30 short contacts:

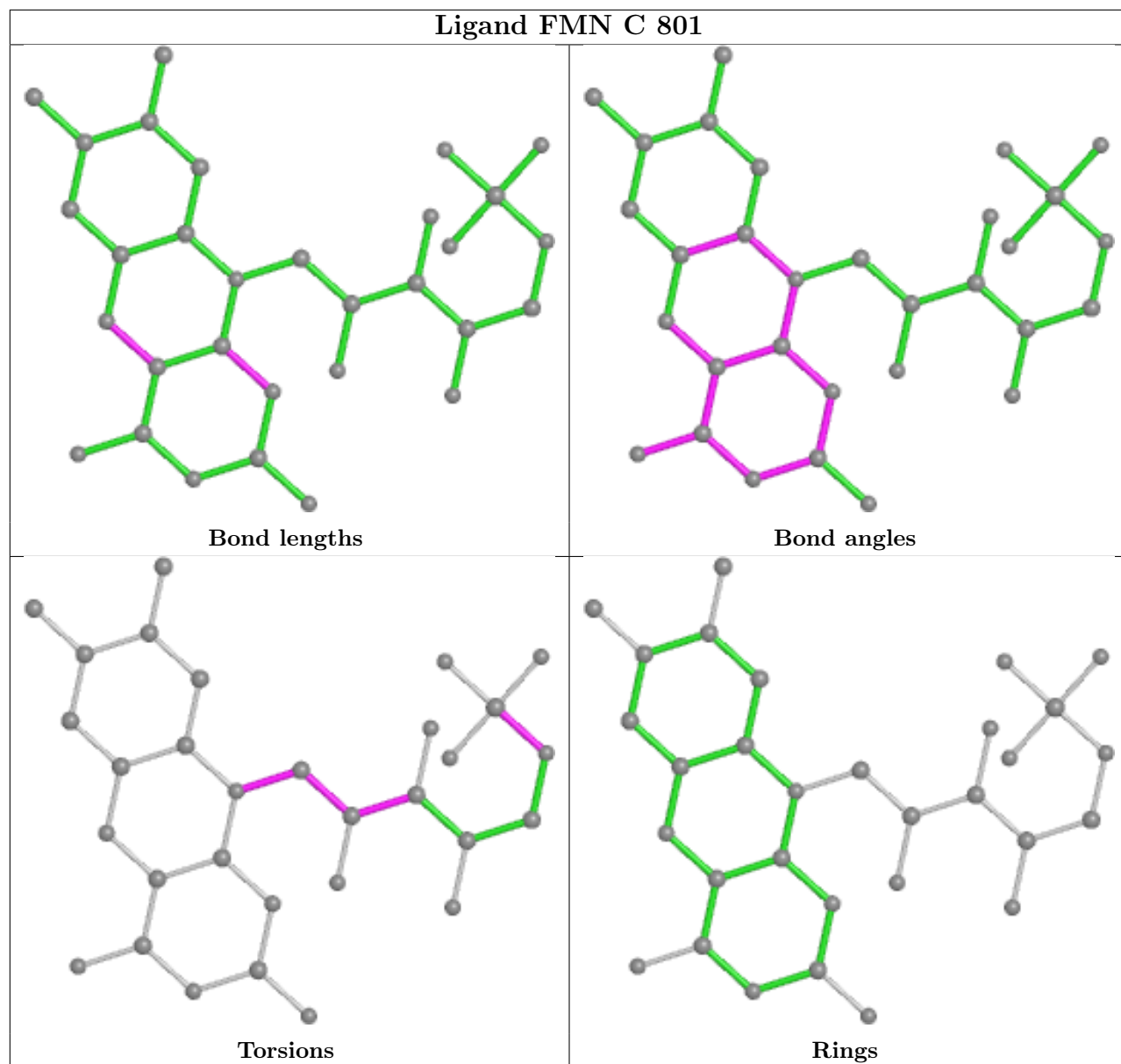
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	801	I9G	1	0
2	B	802	FMN	4	0
3	A	802	GOL	1	0
3	C	802	GOL	1	0
4	B	803	I9G	1	0
3	B	805	GOL	1	0
2	C	801	FMN	7	0
3	B	804	GOL	5	0
3	A	804	GOL	2	0
4	C	803	I9G	5	0
2	A	801	FMN	2	0

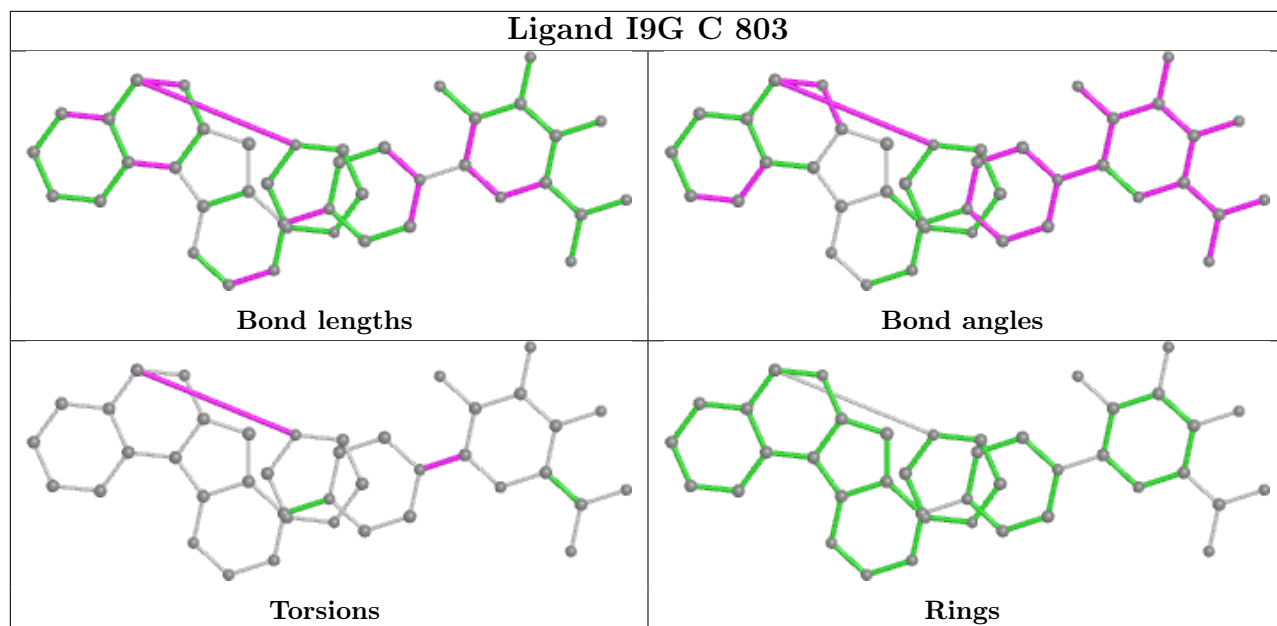
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

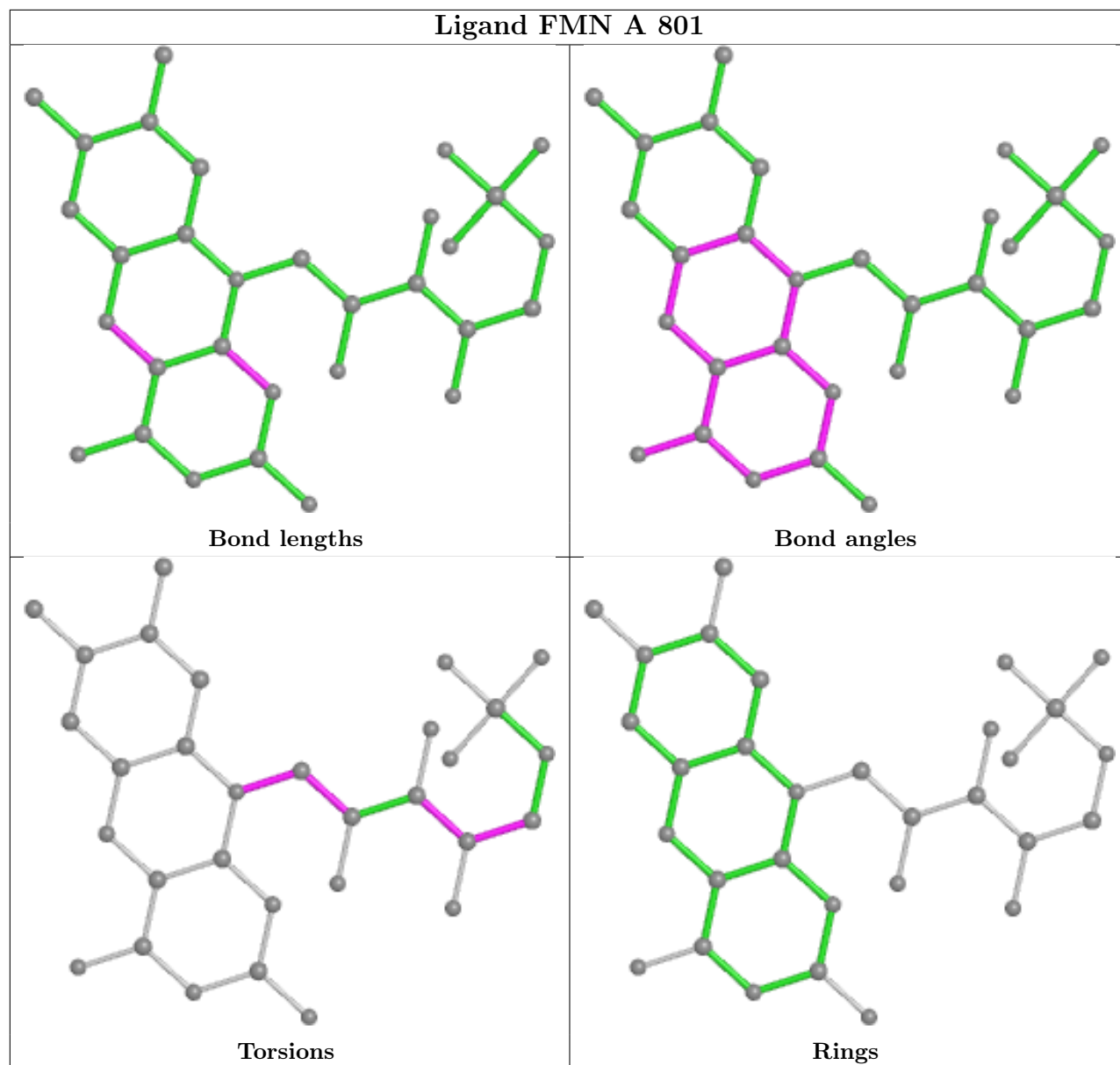












5.7 Other polymers [i](#)

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, 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	644/756 (85%)	0.20	10 (1%) 72 74	41, 57, 83, 114	0
1	B	643/756 (85%)	0.35	17 (2%) 56 57	42, 59, 83, 106	0
1	C	642/756 (84%)	0.24	15 (2%) 60 62	43, 60, 90, 123	0
1	D	631/756 (83%)	0.50	47 (7%) 14 12	52, 74, 101, 116	0
All	All	2560/3024 (84%)	0.32	89 (3%) 44 44	41, 62, 93, 123	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	222	PRO	4.5
1	C	613	VAL	4.2
1	D	236	TYR	4.0
1	D	420	ILE	3.9
1	D	14	LYS	3.6
1	D	211	ALA	3.6
1	D	149	VAL	3.6
1	D	637	PHE	3.5
1	D	194	VAL	3.5
1	D	180	VAL	3.5
1	D	461	ILE	3.4
1	C	242	LEU	3.3
1	D	65	PRO	3.3
1	B	242	LEU	3.3
1	D	197	VAL	3.2
1	D	220	SER	3.2
1	D	193	LEU	3.2
1	B	637	PHE	3.2
1	D	406	HIS	3.1
1	D	240	VAL	3.1
1	B	193	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	384	GLY	3.1
1	C	243	VAL	3.0
1	D	421	HIS	2.9
1	D	219	LEU	2.9
1	D	195	TYR	2.9
1	D	146	ILE	2.9
1	D	204	GLU	2.9
1	D	218	VAL	2.9
1	C	246	GLU	2.7
1	B	249	VAL	2.7
1	B	209	GLU	2.7
1	D	224	VAL	2.7
1	C	221	ILE	2.7
1	D	128	TYR	2.6
1	D	263	ILE	2.6
1	B	631	ILE	2.6
1	D	376	LEU	2.6
1	D	148	ALA	2.6
1	D	164	ILE	2.6
1	C	192	LYS	2.6
1	B	611	PRO	2.6
1	C	175	ALA	2.5
1	D	397	LEU	2.5
1	B	473	LEU	2.5
1	C	247	GLU	2.5
1	B	246	GLU	2.5
1	A	173	ALA	2.5
1	D	205	VAL	2.4
1	D	342	TYR	2.4
1	D	173	ALA	2.4
1	C	219	LEU	2.4
1	A	245	GLY	2.4
1	A	188	ALA	2.4
1	B	273	GLY	2.4
1	D	644	LYS	2.4
1	A	218	VAL	2.3
1	D	385	SER	2.3
1	B	219	LEU	2.3
1	B	610	VAL	2.3
1	A	244	SER	2.3
1	D	96	GLY	2.3
1	D	61	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	196	THR	2.2
1	B	591	VAL	2.2
1	D	168	PRO	2.2
1	D	454	PHE	2.2
1	D	62	SER	2.2
1	D	437	PHE	2.2
1	A	112	GLU	2.2
1	A	212	ALA	2.2
1	A	601	ALA	2.2
1	D	223	ALA	2.2
1	D	108	LEU	2.1
1	B	208	THR	2.1
1	A	624	GLU	2.1
1	B	111	GLU	2.1
1	C	151	LYS	2.1
1	D	176	SER	2.1
1	C	224	VAL	2.1
1	C	206	ALA	2.1
1	D	458	PHE	2.1
1	C	173	ALA	2.0
1	C	618	LEU	2.0
1	C	149	VAL	2.0
1	B	424	TYR	2.0
1	B	618	LEU	2.0
1	D	166	VAL	2.0
1	D	401	VAL	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 [\(i\)](#)

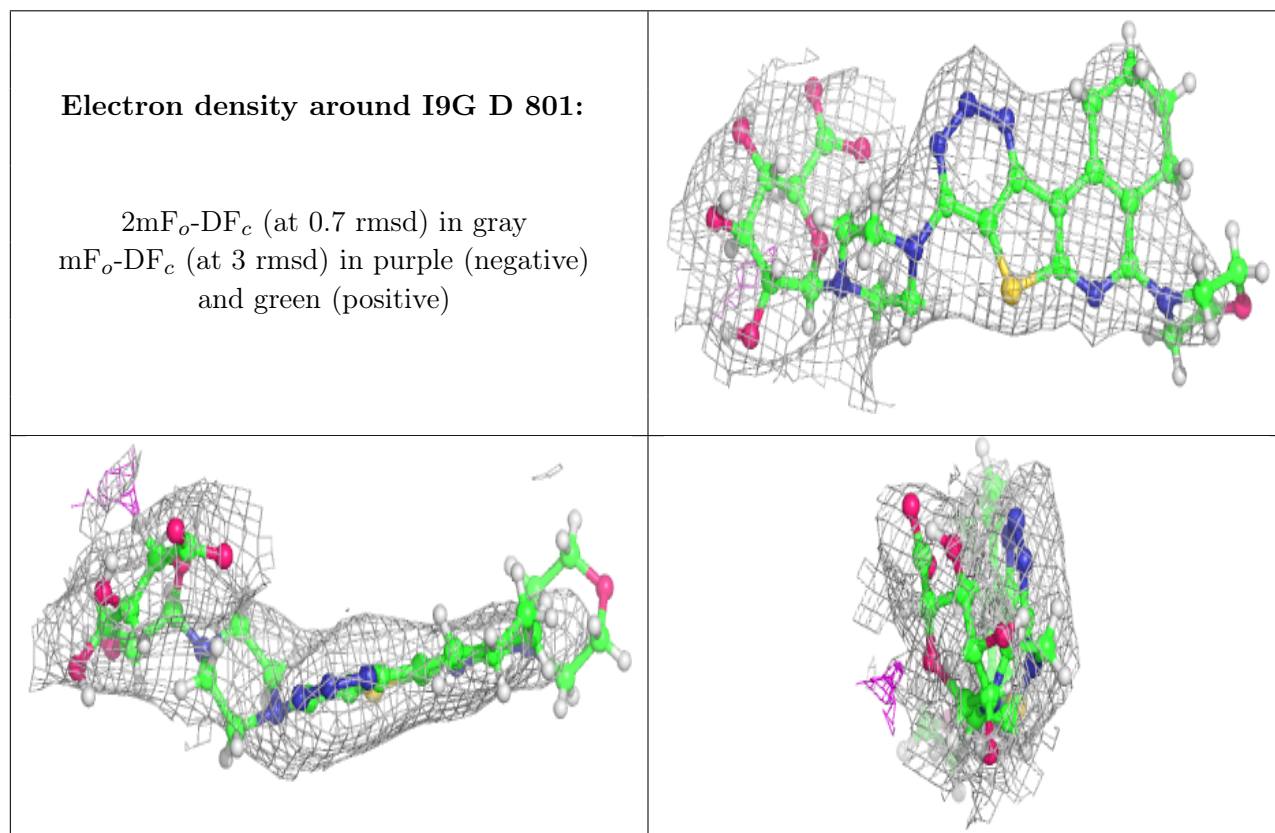
There are no monosaccharides in this entry.

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.

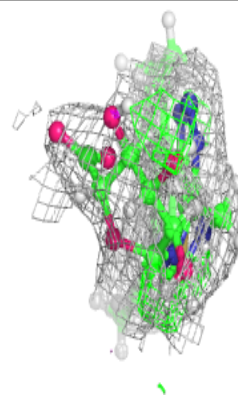
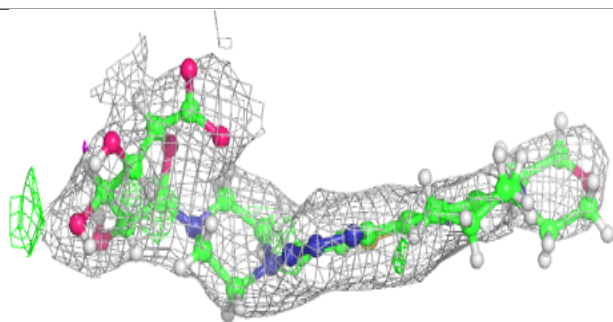
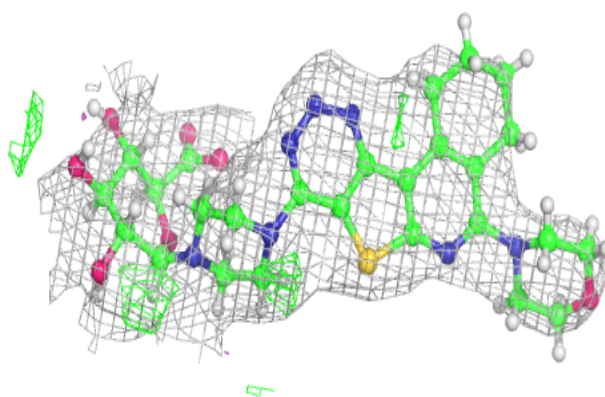
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	803	6/6	0.75	0.30	55,66,77,82	0
3	GOL	B	801	6/6	0.75	0.31	62,80,92,98	0
4	I9G	D	801	41/41	0.77	0.26	67,87,121,126	73
3	GOL	A	804	6/6	0.79	0.31	48,60,72,77	14
4	I9G	B	803	41/41	0.79	0.27	53,73,100,106	73
4	I9G	C	803	41/41	0.80	0.31	47,71,99,100	73
3	GOL	B	805	6/6	0.81	0.30	64,78,94,94	0
4	I9G	A	805	41/41	0.82	0.30	48,65,85,90	73
2	FMN	C	801	31/31	0.84	0.26	79,95,120,126	0
2	FMN	A	801	31/31	0.86	0.24	63,76,102,110	0
3	GOL	A	802	6/6	0.91	0.32	59,73,82,89	0
3	GOL	B	804	6/6	0.92	0.21	50,65,75,78	0
3	GOL	C	802	6/6	0.92	0.30	76,92,95,100	0
2	FMN	B	802	31/31	0.92	0.20	54,71,92,111	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.

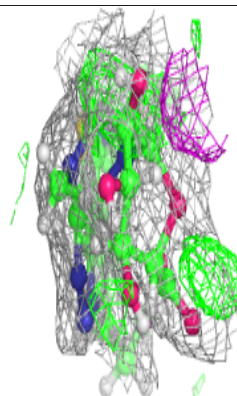
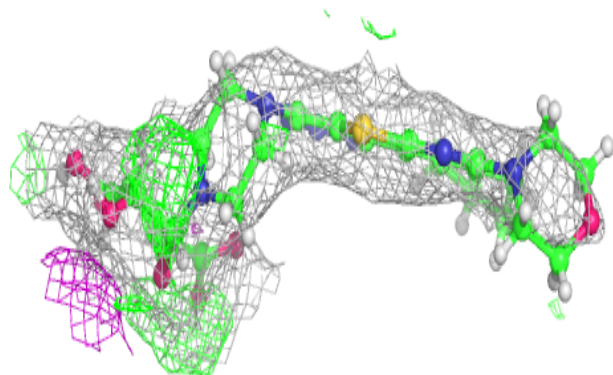
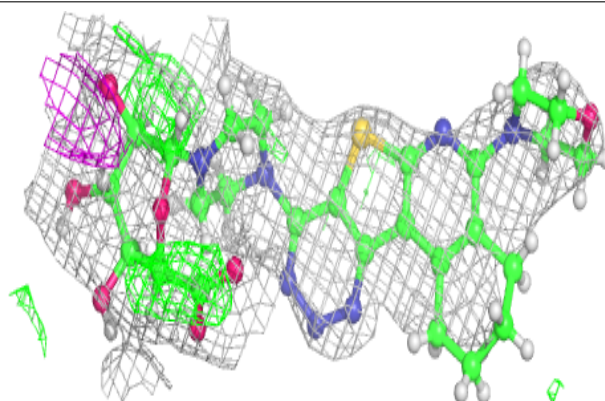


Electron density around I9G B 803:

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

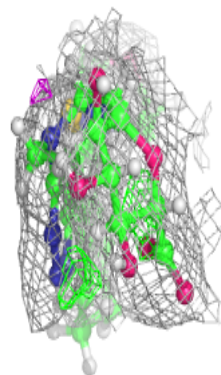
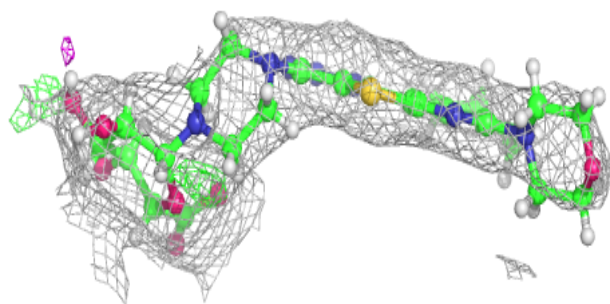
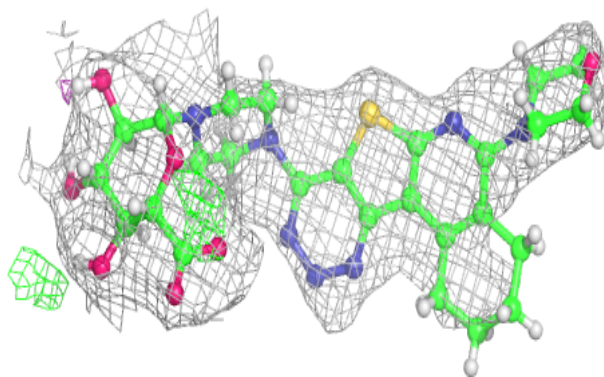
**Electron density around I9G C 803:**

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



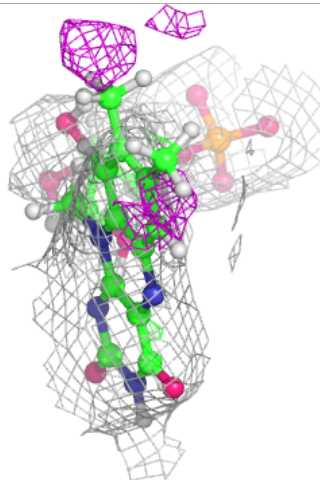
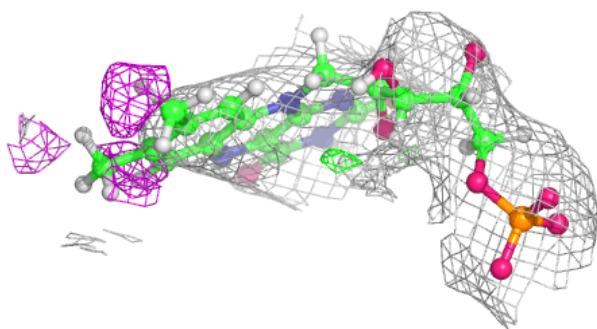
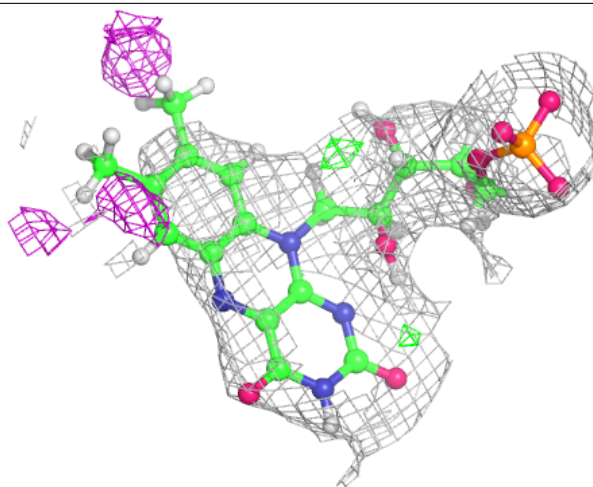
Electron density around I9G A 805:

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



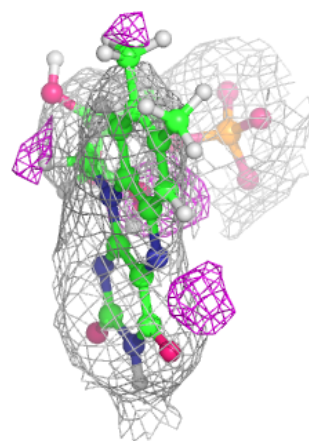
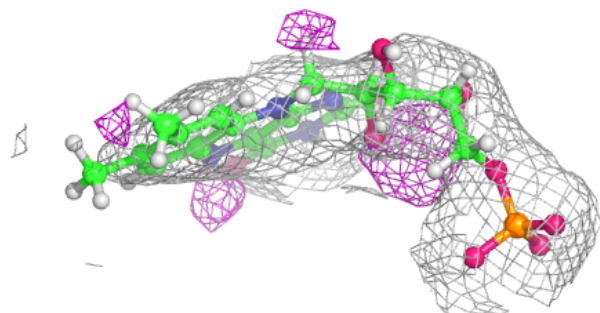
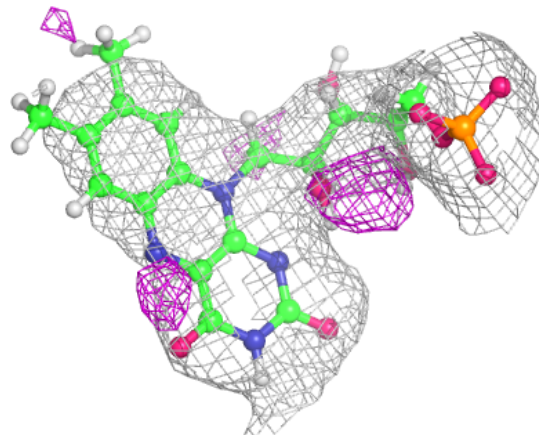
Electron density around FMN C 801:

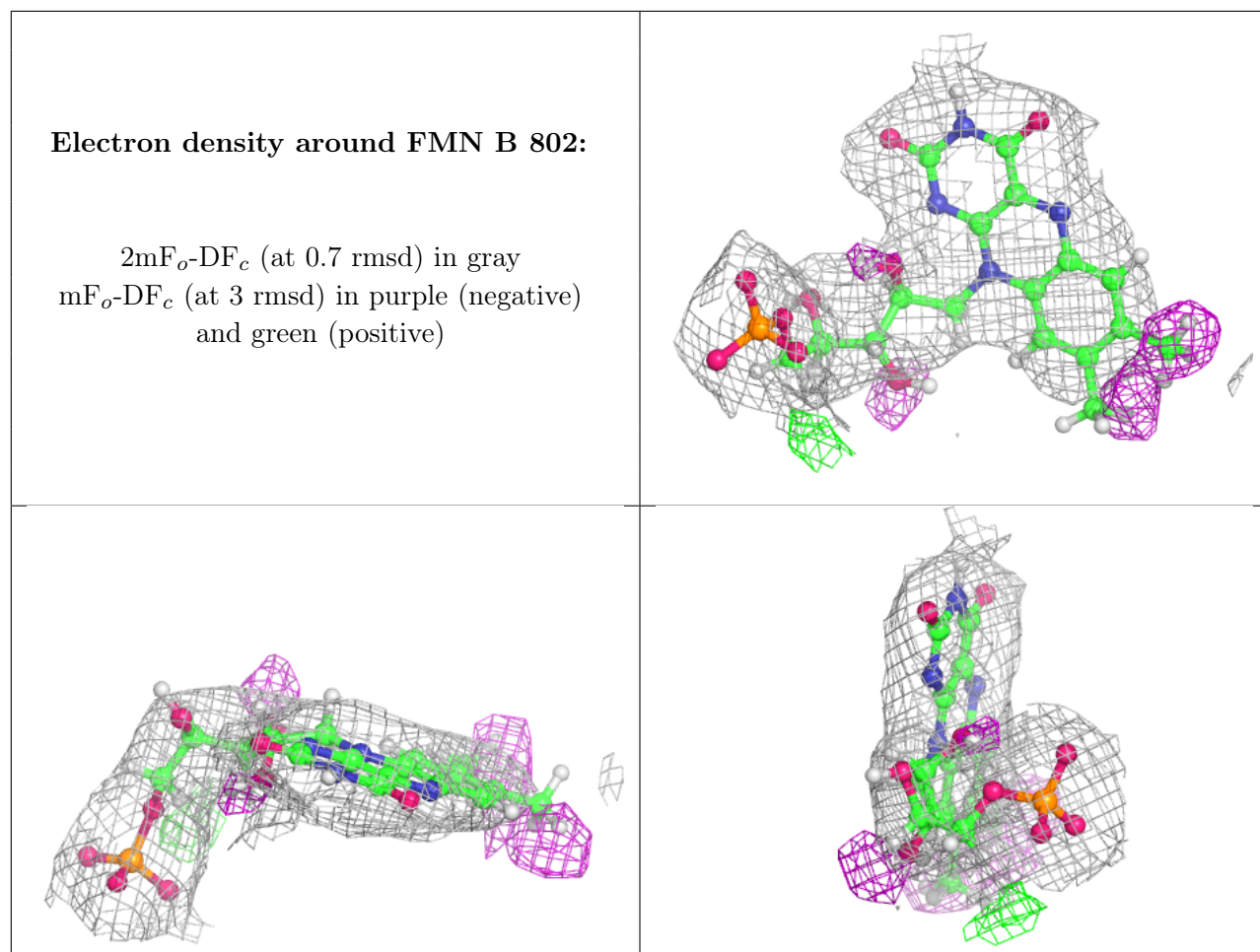
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN A 801:

$2mF_o-DF_c$ (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.