



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:57 PM UTC

PDB ID : 8GET / pdb_00008get
Title : R. hominis 2 beta-glucuronidase bound to norquetiapine-glucuronide
Authors : Simpson, J.B.; Redinbo, M.R.
Deposited on : 2023-03-07
Resolution : 2.90 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

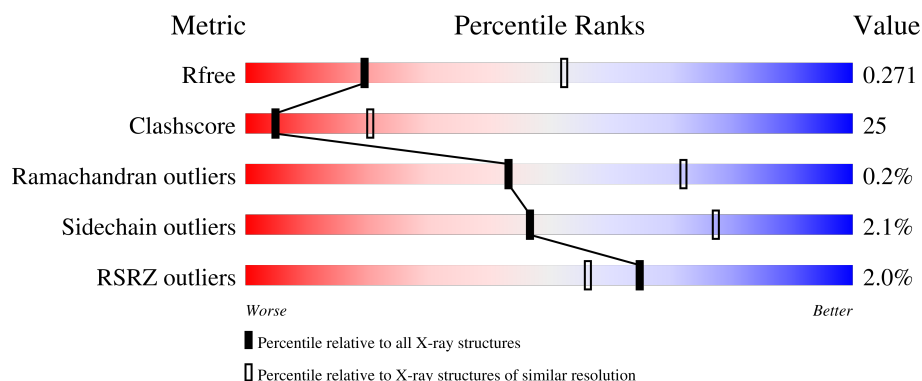
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	757	5% 49% 34% 16%
1	B	757	51% 34% 15%
1	C	757	50% 35% 13%
1	D	757	5% 44% 37% 18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20810 atoms, of which 140 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.

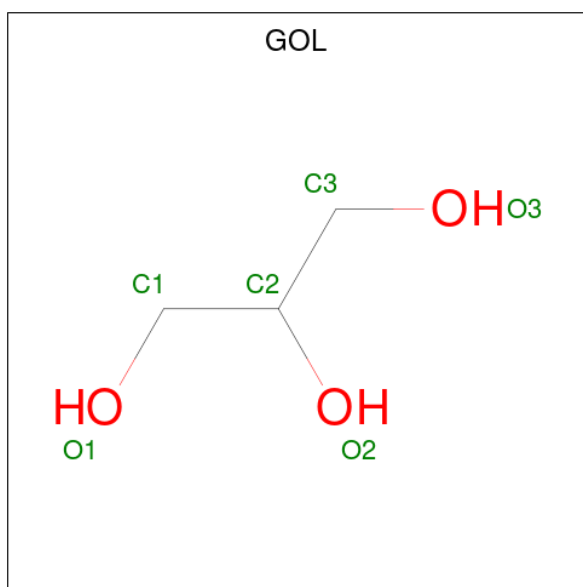
- Molecule 1 is a protein called beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			5127	3262	852	992	21			
1	B	644	Total	C	N	O	S	0	0	0
			5138	3263	853	1002	20			
1	C	659	Total	C	N	O	S	0	0	0
			5256	3339	879	1017	21			
1	D	623	Total	C	N	O	S	0	0	0
			4942	3141	828	955	18			

There are 4 discrepancies between the modelled and reference sequences:

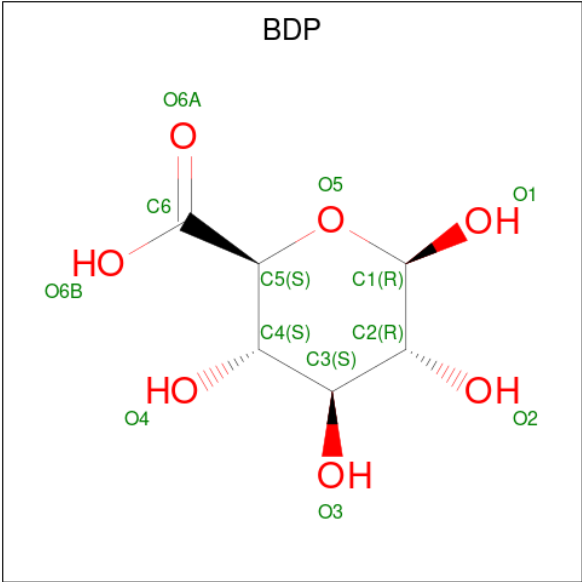
Chain	Residue	Modelled	Actual	Comment	Reference
A	247	ALA	THR	conflict	UNP A0A395V8I7
B	247	ALA	THR	conflict	UNP A0A395V8I7
C	247	ALA	THR	conflict	UNP A0A395V8I7
D	247	ALA	THR	conflict	UNP A0A395V8I7

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



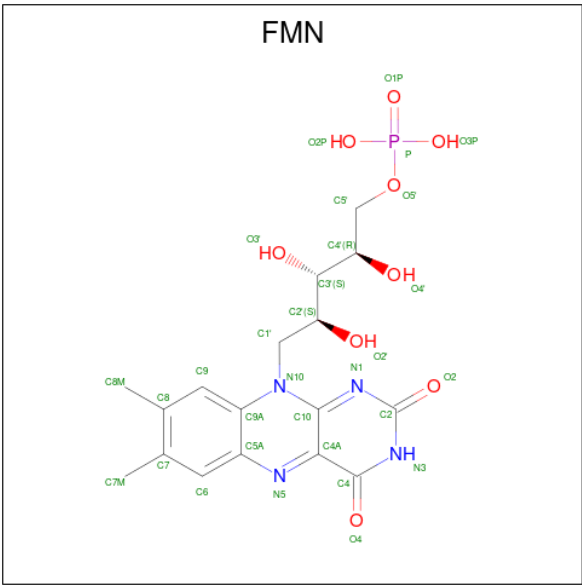
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is beta-D-glucopyranuronic acid (CCD ID: BDP) (formula: C₆H₁₀O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			22	6	9	7		
3	B	1	Total	C	H	O	0	0
			22	6	9	7		
3	D	1	Total	C	H	O	0	0
			22	6	9	7		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



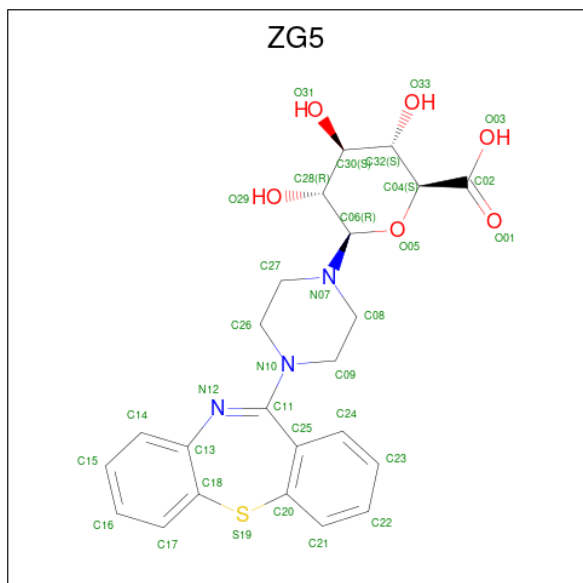
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			50	17	19	4	9		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 11-(4-beta-D-glucopyranuronosylpiperazin-1-yl)dibenzo[b,f][1,4]thiazepine (CCD ID: ZG5) (formula: C₂₃H₂₅N₃O₆S).

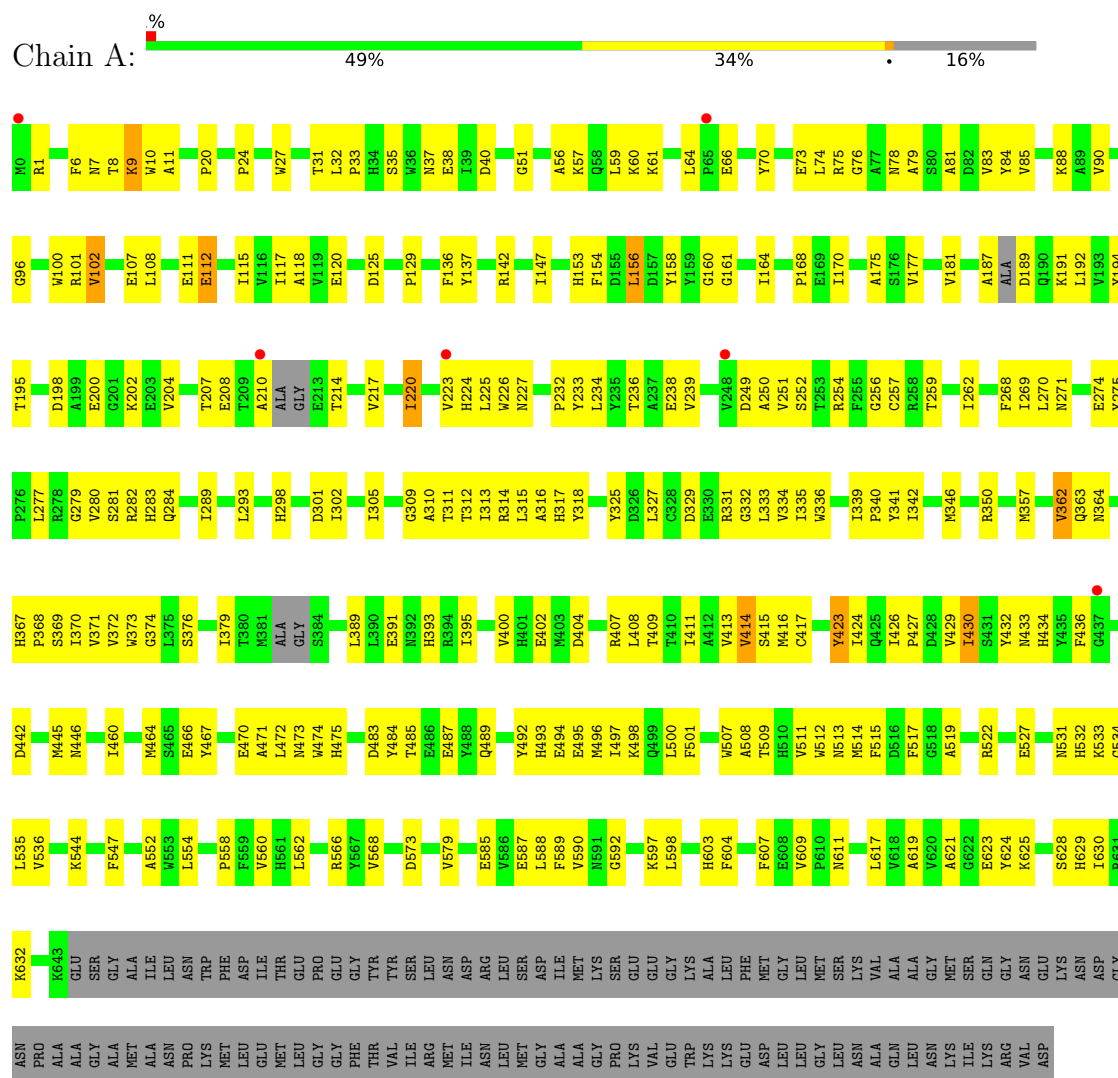


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	S	0	0
			33	23	3	6	1		

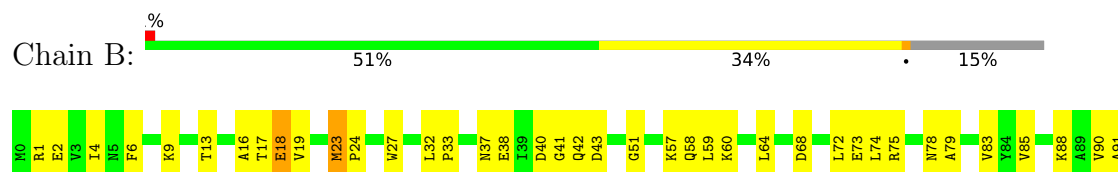
3 Residue-property plots

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: beta-galactosidase



• Molecule 1: beta-galactosidase







4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.47Å 146.29Å 281.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 2.90 48.05 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.0 (48.05-2.90) 89.0 (48.05-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.91Å)	Xtriage
Refinement program	phenix.refine 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.224 , 0.269 0.222 , 0.271	Depositor DCC
R_{free} test set	2000 reflections (2.16%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20810	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, ZG5, BDP, 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	0.16	0/5267	0.33	0/7165
1	B	0.26	0/5281	0.45	1/7194 (0.0%)
1	C	0.17	0/5398	0.34	2/7345 (0.0%)
1	D	0.15	0/5076	0.33	0/6908
All	All	0.19	0/21022	0.37	3/28612 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	GLU	N-CA-C	-7.02	105.14	113.21
1	C	439	TYR	N-CA-C	-5.34	100.72	109.80
1	C	438	TRP	N-CA-C	-5.13	107.68	114.04

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5127	0	4768	237	0
1	B	5138	0	4748	236	0
1	C	5256	0	4894	249	0
1	D	4942	0	4487	281	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	8	8	1	0
2	B	18	24	24	1	0
2	C	12	16	16	5	0
2	D	6	8	8	0	0
3	A	13	9	9	2	0
3	B	13	9	9	3	0
3	D	13	9	8	1	0
4	A	31	19	19	1	0
4	B	31	19	19	4	0
4	C	31	19	19	2	0
5	C	33	0	0	1	0
All	All	20670	140	19036	1002	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 25.

All (1002) 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:B:168:PRO:HB3	1:B:177:VAL:HG12	1.35	1.07
1:C:339:ILE:HD13	1:C:357:MET:HE2	1.38	1.03
1:B:371:VAL:HG23	1:B:372:VAL:HG13	1.39	1.02
1:C:166:VAL:HG22	1:C:179:VAL:HG12	1.41	1.02
1:C:367:HIS:HB2	1:C:370:ILE:HD12	1.43	0.98
1:B:175:ALA:HB3	1:B:223:VAL:HG11	1.48	0.95
1:A:367:HIS:HB2	1:A:370:ILE:HD12	1.50	0.94
1:B:72:LEU:HD23	1:B:74:LEU:HD11	1.46	0.93
1:C:562:LEU:HD13	1:C:628:SER:HB3	1.52	0.92
1:C:493:HIS:O	1:C:497:ILE:HG13	1.72	0.90
1:C:68:ASP:HB3	1:C:151:LYS:HG3	1.53	0.89
1:C:261:GLU:HG2	1:C:269:ILE:HB	1.55	0.89
1:C:434:HIS:HB2	1:C:464:MET:HE1	1.54	0.89
1:B:183:LEU:HD21	1:B:241:LEU:HD11	1.55	0.88
1:D:183:LEU:HD21	1:D:241:LEU:HD21	1.54	0.88
1:D:395:ILE:HD12	1:D:395:ILE:H	1.37	0.88
1:D:471:ALA:HB3	1:D:544:LYS:HE3	1.56	0.88
1:C:281:SER:HB3	1:C:314:ARG:HB3	1.54	0.88
1:B:590:VAL:HG11	1:B:609:VAL:HG11	1.56	0.87
1:A:493:HIS:O	1:A:497:ILE:HG13	1.75	0.86
1:A:8:THR:HA	1:A:31:THR:HG23	1.57	0.86
1:B:91:ALA:HB2	1:B:102:VAL:HG21	1.58	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ASP:OD1	1:C:199:ALA:N	2.09	0.85
1:A:562:LEU:HD23	1:A:579:VAL:HG22	1.57	0.84
1:B:181:VAL:HG21	1:B:239:VAL:HG11	1.60	0.84
1:D:168:PRO:HA	1:D:177:VAL:HA	1.58	0.84
1:B:358:LYS:O	1:B:362:VAL:HG23	1.78	0.83
1:C:411:ILE:HD13	1:C:427:PRO:HG3	1.59	0.83
1:A:277:LEU:HD22	1:A:334:VAL:HG21	1.60	0.83
1:B:168:PRO:CB	1:B:177:VAL:HG12	2.09	0.82
1:B:501:PHE:CE2	1:B:554:LEU:HD21	2.14	0.82
1:D:280:VAL:HG12	1:D:511:VAL:CG1	2.09	0.82
1:C:101:ARG:HE	1:C:156:LEU:HB3	1.44	0.82
1:B:204:VAL:HG11	1:B:220:ILE:HG23	1.62	0.81
1:D:305:ILE:HG12	1:D:514:MET:HE2	1.62	0.81
1:C:305:ILE:HG13	1:C:514:MET:HE2	1.60	0.81
1:A:164:ILE:HD12	1:A:181:VAL:HG12	1.62	0.81
1:C:196:VAL:HG11	1:C:220:ILE:HD11	1.63	0.81
1:D:78:ASN:HA	1:D:96:GLY:HA3	1.64	0.80
1:D:154:PHE:CE1	1:D:249:ASP:HB2	2.17	0.80
1:D:371:VAL:HG23	1:D:372:VAL:HG13	1.64	0.80
1:C:333:LEU:O	1:C:369:SER:HB2	1.82	0.80
1:C:464:MET:HG3	1:C:500:LEU:HD21	1.64	0.80
1:D:341:TYR:HB3	1:D:375:LEU:O	1.81	0.80
1:B:636:PHE:CZ	1:B:640:TYR:HB2	2.18	0.79
1:D:154:PHE:CZ	1:D:241:LEU:HD23	2.16	0.79
1:B:280:VAL:HG12	1:B:511:VAL:CG1	2.12	0.79
1:C:101:ARG:HH21	1:C:156:LEU:HA	1.46	0.79
1:C:305:ILE:CG1	1:C:514:MET:HE2	2.13	0.79
1:C:59:LEU:HD11	1:C:64:LEU:HD22	1.64	0.78
1:A:281:SER:HB3	1:A:314:ARG:HB3	1.65	0.77
1:B:615:SER:HB2	1:B:630:ILE:HG12	1.65	0.77
1:B:636:PHE:HE2	1:B:641:SER:HB2	1.48	0.77
1:C:305:ILE:HG21	1:C:313:ILE:HD11	1.65	0.77
1:D:302:ILE:HD11	1:D:331:ARG:HG3	1.65	0.77
1:D:399:MET:O	1:D:403:MET:HG3	1.82	0.77
1:B:574:THR:HA	1:B:610:PRO:HA	1.65	0.77
1:A:513:ASN:O	1:A:534:GLY:HA2	1.84	0.77
1:A:592:GLY:HA2	2:A:801:GOL:H11	1.67	0.77
1:A:60:LYS:HD3	1:A:111:GLU:OE2	1.85	0.77
1:A:262:ILE:HD12	1:A:408:LEU:HD22	1.67	0.76
1:A:340:PRO:O	1:A:342:ILE:HG22	1.84	0.76
1:B:501:PHE:HE2	1:B:554:LEU:HD21	1.50	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:GLY:HA2	1:D:506:ILE:HG23	1.67	0.76
1:C:530:GLN:NE2	1:C:538:PHE:HB2	2.00	0.76
1:C:350:ARG:O	1:C:354:ILE:HD12	1.86	0.75
1:D:357:MET:O	1:D:361:VAL:HG23	1.86	0.75
1:A:170:ILE:HD11	1:A:225:LEU:HD21	1.67	0.75
1:D:470:GLU:HG2	1:D:533:LYS:HG3	1.67	0.74
1:D:623:GLU:O	1:D:623:GLU:HG3	1.86	0.74
1:B:590:VAL:HG11	1:B:609:VAL:CG1	2.17	0.74
1:A:379:ILE:HG23	1:A:389:LEU:HD11	1.66	0.74
1:B:362:VAL:HG13	4:B:805:FMN:C6	2.18	0.74
1:B:284:GLN:HG2	1:B:318:TYR:CE1	2.22	0.74
1:C:513:ASN:O	1:C:534:GLY:HA2	1.88	0.73
1:A:302:ILE:HD11	1:A:331:ARG:HG3	1.70	0.73
1:C:68:ASP:CB	1:C:151:LYS:HG3	2.17	0.73
1:D:230:LYS:HE3	1:D:230:LYS:HA	1.71	0.73
1:B:636:PHE:CE2	1:B:641:SER:HB2	2.23	0.73
1:D:432:TYR:HB3	1:D:434:HIS:CD2	2.23	0.73
1:D:451:ASP:O	1:D:455:LYS:HG2	1.88	0.73
1:D:73:GLU:HB2	1:D:147:ILE:HD11	1.71	0.72
1:D:192:LEU:HD23	1:D:241:LEU:HD22	1.70	0.72
1:B:495:GLU:O	1:B:499:GLN:HG3	1.90	0.72
1:D:513:ASN:O	1:D:534:GLY:HA2	1.90	0.72
1:A:168:PRO:HB3	1:A:177:VAL:HG12	1.72	0.72
1:B:1:ARG:HG3	1:B:149:VAL:HG12	1.69	0.72
1:D:266:ARG:HA	1:D:504:LYS:HZ3	1.54	0.72
1:D:59:LEU:HD11	1:D:64:LEU:HD21	1.70	0.72
1:D:419:ILE:HD11	1:D:453:PHE:CD2	2.24	0.72
1:D:423:TYR:HA	1:D:426:ILE:CD1	2.20	0.72
1:A:415:SER:HB2	1:A:434:HIS:ND1	2.05	0.71
1:C:378:GLU:HB3	1:C:414:VAL:HB	1.73	0.71
1:B:391:GLU:O	1:B:395:ILE:HD12	1.90	0.71
1:B:404:ASP:OD2	1:B:407:ARG:HD2	1.90	0.71
1:B:207:THR:HG22	1:B:218:LEU:HD21	1.73	0.71
1:D:339:ILE:HD11	1:D:341:TYR:HB2	1.71	0.71
1:A:277:LEU:CD2	1:A:334:VAL:HG21	2.21	0.71
1:B:104:ILE:HD12	1:B:108:LEU:HD21	1.72	0.71
1:D:230:LYS:HD2	1:D:230:LYS:N	2.06	0.71
1:B:166:VAL:HG12	1:B:168:PRO:HD3	1.73	0.70
1:D:225:LEU:HD12	1:D:271:ASN:CG	2.17	0.70
1:A:573:ASP:OD1	1:A:632:LYS:HE2	1.92	0.70
1:A:562:LEU:CD2	1:A:579:VAL:HG22	2.20	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ARG:NH2	1:C:284:GLN:HA	2.07	0.70
1:A:101:ARG:NH2	1:A:161:GLY:O	2.21	0.70
1:A:305:ILE:CG1	1:A:514:MET:HE2	2.22	0.70
1:C:411:ILE:CD1	1:C:427:PRO:HG3	2.20	0.70
1:C:467:TYR:CD2	1:C:496:MET:HG2	2.26	0.70
1:D:225:LEU:H	1:D:225:LEU:HD23	1.56	0.70
1:D:273:GLU:OE1	1:D:273:GLU:N	2.24	0.70
1:A:269:ILE:HD13	1:A:274:GLU:HA	1.74	0.70
1:C:443:VAL:HG23	1:C:496:MET:CE	2.22	0.69
1:B:78:ASN:HA	1:B:96:GLY:HA3	1.74	0.69
1:B:438:TRP:CZ2	1:B:470:GLU:HG3	2.28	0.69
1:D:339:ILE:CD1	1:D:341:TYR:HB2	2.23	0.69
1:C:88:LYS:HD3	1:C:107:GLU:OE1	1.91	0.69
1:B:33:PRO:HB2	1:B:292:ALA:HB1	1.74	0.69
1:D:341:TYR:CE1	1:D:379:ILE:HD11	2.27	0.69
1:D:350:ARG:HG2	1:D:354:ILE:CD1	2.22	0.69
1:D:493:HIS:HA	1:D:496:MET:HB2	1.75	0.69
1:B:262:ILE:HD12	1:B:408:LEU:HD12	1.74	0.69
1:D:360:LEU:HD12	1:D:364:ASN:HD22	1.58	0.69
1:B:168:PRO:HA	1:B:177:VAL:HA	1.75	0.69
1:B:150:ASN:OD1	1:B:151:LYS:N	2.25	0.68
1:B:280:VAL:HG12	1:B:511:VAL:HG12	1.74	0.68
1:C:302:ILE:HD13	1:C:327:LEU:HB3	1.74	0.68
1:C:302:ILE:HG23	1:C:331:ARG:HH12	1.57	0.68
1:A:379:ILE:HG21	1:A:393:HIS:HE1	1.59	0.68
1:B:32:LEU:HA	1:B:33:PRO:C	2.19	0.68
1:B:220:ILE:HB	1:B:223:VAL:HG12	1.74	0.68
1:B:168:PRO:HB3	1:B:177:VAL:CG1	2.20	0.68
1:B:305:ILE:HD13	1:B:514:MET:HE2	1.74	0.68
1:B:483:ASP:CG	1:B:485:THR:HG23	2.19	0.67
1:C:396:LEU:O	1:C:400:VAL:HG23	1.95	0.67
1:D:233:TYR:O	1:D:234:LEU:HD23	1.93	0.67
1:C:78:ASN:HA	1:C:96:GLY:HA3	1.75	0.67
1:B:170:ILE:HD11	1:B:257:CYS:HB3	1.75	0.67
1:D:164:ILE:HD11	1:D:239:VAL:HG13	1.77	0.67
1:D:313:ILE:HD11	1:D:333:LEU:HD13	1.77	0.67
1:A:471:ALA:HB2	1:A:489:GLN:HB2	1.77	0.67
1:C:6:PHE:CE1	1:C:57:LYS:HE2	2.30	0.67
1:D:72:LEU:HA	1:D:146:ILE:HD13	1.75	0.67
1:A:1:ARG:HB2	1:A:249:ASP:OD1	1.94	0.67
1:B:68:ASP:HB3	1:B:151:LYS:HD3	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ILE:HB	1:B:223:VAL:CG1	2.25	0.67
1:C:576:LYS:CE	1:C:606:HIS:HB3	2.26	0.67
1:D:589:PHE:CE1	1:D:594:SER:HB2	2.29	0.67
1:B:513:ASN:O	1:B:534:GLY:HA2	1.95	0.66
1:A:316:ALA:HB1	1:A:317:HIS:ND1	2.10	0.66
1:B:333:LEU:O	1:B:369:SER:HB2	1.96	0.66
1:C:3:VAL:HG22	1:C:147:ILE:HG13	1.77	0.66
1:A:339:ILE:HD13	1:A:357:MET:HE2	1.77	0.66
1:D:142:ARG:HD3	1:D:321:ASP:OD1	1.96	0.66
1:D:198:ASP:CB	1:D:236:THR:H	2.08	0.66
1:A:585:GLU:OE2	1:A:597:LYS:HD2	1.95	0.66
1:D:443:VAL:HG23	1:D:496:MET:HE2	1.77	0.66
1:A:305:ILE:HG13	1:A:514:MET:HE2	1.78	0.66
1:A:195:THR:HG23	1:A:238:GLU:HB2	1.78	0.66
1:D:360:LEU:HD12	1:D:364:ASN:ND2	2.11	0.66
1:A:125:ASP:C	1:A:346:MET:HE3	2.20	0.66
1:A:497:ILE:HD12	1:A:604:PHE:HZ	1.60	0.66
1:C:242:VAL:HG12	1:C:244:GLY:O	1.96	0.66
1:D:33:PRO:HB2	1:D:292:ALA:HB1	1.78	0.66
1:C:166:VAL:HG11	1:C:255:PHE:CD2	2.31	0.65
1:A:66:GLU:HA	1:A:70:TYR:OH	1.96	0.65
1:C:23:MET:HE2	1:C:58:GLN:HG3	1.79	0.65
1:C:167:THR:HG22	1:C:365:TYR:HE2	1.62	0.65
1:A:413:VAL:HG12	1:A:414:VAL:O	1.96	0.65
1:C:391:GLU:O	1:C:395:ILE:HG13	1.97	0.65
1:C:530:GLN:HE21	1:C:538:PHE:HB2	1.60	0.65
1:D:37:ASN:HA	1:D:40:ASP:OD1	1.96	0.65
1:D:147:ILE:HG22	1:D:149:VAL:HG13	1.78	0.65
1:C:583:LEU:HD13	1:C:584:PRO:HD2	1.79	0.65
1:A:153:HIS:ND1	1:A:156:LEU:HD12	2.12	0.65
1:B:2:GLU:OE1	1:B:4:ILE:CG1	2.45	0.65
1:D:36:TRP:HZ2	1:D:121:ASN:HD22	1.45	0.64
1:B:316:ALA:HB1	1:B:317:HIS:ND1	2.12	0.64
1:A:302:ILE:HG21	1:A:327:LEU:HD13	1.79	0.64
1:B:58:GLN:HG2	1:B:114:LEU:HD12	1.78	0.64
1:D:632:LYS:HD2	1:D:633:VAL:O	1.97	0.64
1:B:37:ASN:HA	1:B:40:ASP:OD1	1.97	0.64
1:D:259:THR:O	1:D:271:ASN:N	2.24	0.64
1:D:446:ASN:ND2	1:D:496:MET:HE1	2.11	0.64
1:D:500:LEU:HD23	1:D:509:THR:HG22	1.78	0.64
1:A:367:HIS:HB2	1:A:370:ILE:CD1	2.25	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:HD23	1:B:186:ALA:CB	2.28	0.64
1:D:589:PHE:HE1	1:D:594:SER:HB2	1.63	0.64
1:C:97:TYR:O	1:C:319:GLN:HB3	1.97	0.64
1:A:391:GLU:O	1:A:395:ILE:HG13	1.98	0.64
1:D:284:GLN:HG2	1:D:318:TYR:CE1	2.33	0.63
1:D:266:ARG:HA	1:D:504:LYS:NZ	2.12	0.63
1:D:586:VAL:HG22	1:D:621:ALA:HB2	1.80	0.63
1:A:302:ILE:CD1	1:A:331:ARG:HG3	2.28	0.63
1:D:73:GLU:HB2	1:D:147:ILE:CD1	2.28	0.63
1:A:154:PHE:HD2	1:A:251:VAL:HG13	1.63	0.63
1:A:475:HIS:HA	1:A:487:GLU:OE1	1.98	0.63
1:A:284:GLN:HG2	1:A:318:TYR:CE1	2.34	0.63
1:A:236:THR:HG22	1:A:254:ARG:HG2	1.80	0.62
1:C:35:SER:O	1:C:38:GLU:HG3	1.99	0.62
1:A:275:TYR:HE1	1:A:311:THR:HG21	1.64	0.62
1:D:302:ILE:CD1	1:D:331:ARG:HG3	2.29	0.62
1:D:419:ILE:HD11	1:D:453:PHE:HD2	1.63	0.62
1:A:83:VAL:HG22	1:A:117:ILE:HG12	1.81	0.62
1:C:626:ASP:OD1	1:C:627:GLU:N	2.33	0.62
1:B:183:LEU:HD23	1:B:186:ALA:HB2	1.80	0.62
1:B:349:GLY:O	1:B:353:THR:HG23	2.00	0.62
1:C:358:LYS:O	1:C:362:VAL:HG23	1.99	0.62
1:D:166:VAL:HG11	1:D:255:PHE:CG	2.34	0.62
1:D:333:LEU:O	1:D:369:SER:HB2	1.98	0.62
1:B:284:GLN:HG2	1:B:318:TYR:HE1	1.61	0.62
1:A:73:GLU:HB2	1:A:147:ILE:HD11	1.82	0.62
1:C:223:VAL:HG13	1:C:225:LEU:HD21	1.81	0.62
1:A:101:ARG:HH11	1:A:156:LEU:HD23	1.64	0.62
1:A:181:VAL:O	1:A:214:THR:HB	1.99	0.62
1:B:72:LEU:CD2	1:B:74:LEU:HD11	2.27	0.62
1:A:24:PRO:HG2	1:A:27:TRP:CE3	2.34	0.62
1:C:154:PHE:CD2	1:C:251:VAL:HG22	2.35	0.62
1:A:256:GLY:N	1:A:368:PRO:HG3	2.15	0.61
1:A:279:GLY:O	1:A:511:VAL:HG23	1.99	0.61
1:C:183:LEU:CD1	1:C:241:LEU:HD22	2.29	0.61
1:D:350:ARG:HG2	1:D:354:ILE:HD11	1.81	0.61
1:A:168:PRO:CB	1:A:177:VAL:HG12	2.30	0.61
1:B:280:VAL:HG21	1:B:305:ILE:HD11	1.82	0.61
1:C:167:THR:HG22	1:C:365:TYR:CE2	2.35	0.61
1:C:583:LEU:CD1	1:C:584:PRO:HD2	2.30	0.61
1:C:166:VAL:CG2	1:C:179:VAL:HG12	2.25	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:ILE:HD12	1:D:413:VAL:HG23	1.82	0.61
1:B:275:TYR:HE1	1:B:311:THR:HB	1.65	0.61
1:D:277:LEU:HD11	1:D:334:VAL:HG11	1.82	0.61
1:B:23:MET:HB2	1:B:114:LEU:HD11	1.83	0.61
1:B:354:ILE:HG23	1:B:399:MET:HE2	1.83	0.61
1:C:313:ILE:HD12	1:C:333:LEU:HD13	1.81	0.61
1:D:192:LEU:CD1	1:D:212:GLY:HA2	2.31	0.61
1:D:300:GLU:O	1:D:304:LEU:HD12	2.01	0.61
1:B:430:ILE:HD11	1:B:453:PHE:CZ	2.35	0.61
1:D:429:VAL:HG12	1:D:461:PRO:HB2	1.82	0.61
1:D:456:GLU:C	1:D:457:PHE:HD1	2.08	0.61
1:A:202:LYS:HD2	1:A:202:LYS:N	2.14	0.61
1:A:587:GLU:HG2	1:A:589:PHE:CE2	2.36	0.61
1:D:350:ARG:O	1:D:354:ILE:HD12	2.00	0.61
1:A:101:ARG:NH1	1:A:156:LEU:HA	2.16	0.61
1:D:154:PHE:CD1	1:D:249:ASP:HB2	2.36	0.61
1:A:423:TYR:HA	1:A:426:ILE:HD12	1.81	0.60
1:A:35:SER:O	1:A:38:GLU:HG3	2.01	0.60
1:A:224:HIS:HB2	1:A:233:TYR:CD2	2.37	0.60
1:B:68:ASP:CB	1:B:151:LYS:HG2	2.31	0.60
1:C:501:PHE:CE2	1:C:554:LEU:HD21	2.36	0.60
1:B:91:ALA:HB2	1:B:102:VAL:CG2	2.30	0.60
1:C:576:LYS:HE2	1:C:606:HIS:HB3	1.82	0.60
1:D:32:LEU:HA	1:D:33:PRO:C	2.25	0.60
1:C:226:TRP:CZ2	1:C:332:GLY:HA2	2.37	0.60
1:B:453:PHE:CD1	1:B:462:LEU:HD22	2.36	0.60
1:A:423:TYR:HA	1:A:426:ILE:CD1	2.32	0.60
1:B:590:VAL:CG1	1:B:609:VAL:HG11	2.28	0.60
1:C:181:VAL:O	1:C:214:THR:HB	2.02	0.60
1:C:306:CYS:SG	1:C:331:ARG:HD2	2.42	0.60
1:D:268:PHE:HE2	1:D:270:LEU:HB2	1.67	0.60
1:D:155:ASP:OD2	1:D:158:TYR:HB2	2.01	0.60
1:A:331:ARG:HB2	1:A:333:LEU:HD12	1.82	0.59
1:B:2:GLU:OE1	1:B:4:ILE:HG13	2.02	0.59
1:B:357:MET:CE	1:B:375:LEU:HD23	2.32	0.59
1:A:280:VAL:O	1:A:313:ILE:HA	2.03	0.59
1:B:2:GLU:CD	1:B:4:ILE:HG12	2.27	0.59
1:C:207:THR:HG22	1:C:208:GLU:H	1.67	0.59
1:C:241:LEU:O	1:C:248:VAL:HG22	2.01	0.59
1:B:473:ASN:OD1	1:B:473:ASN:O	2.20	0.59
1:C:722:ILE:HD12	1:C:722:ILE:H	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:LEU:O	1:D:400:VAL:HG13	2.01	0.59
1:B:68:ASP:HB3	1:B:151:LYS:CD	2.33	0.59
1:D:298:HIS:O	1:D:302:ILE:HG22	2.02	0.59
1:B:23:MET:HE3	1:B:114:LEU:HD11	1.84	0.59
1:C:280:VAL:O	1:C:313:ILE:HA	2.02	0.59
1:D:153:HIS:HA	1:D:249:ASP:OD2	2.03	0.59
1:D:314:ARG:HD2	1:D:336:TRP:CZ3	2.38	0.59
1:A:170:ILE:HD11	1:A:225:LEU:CD2	2.32	0.59
1:B:446:ASN:CG	1:B:496:MET:HE1	2.28	0.59
1:A:187:ALA:HB1	1:A:189:ASP:OD1	2.02	0.58
1:B:543:LYS:HD2	1:B:547:PHE:CE1	2.39	0.58
1:C:517:PHE:CE1	1:C:531:ASN:HB3	2.39	0.58
1:D:314:ARG:HD2	1:D:336:TRP:CE3	2.38	0.58
1:D:354:ILE:HD12	1:D:354:ILE:H	1.68	0.58
1:A:225:LEU:HD13	1:A:271:ASN:OD1	2.04	0.58
1:B:294:LEU:HD12	1:B:297:HIS:HE1	1.68	0.58
1:C:493:HIS:HE1	1:C:511:VAL:HG13	1.67	0.58
1:D:472:LEU:HD13	1:D:525:GLY:O	2.04	0.58
1:A:302:ILE:CD1	1:A:327:LEU:HB3	2.33	0.58
1:A:362:VAL:HA	4:A:803:FMN:HM72	1.86	0.58
1:D:286:ARG:CZ	1:D:540:ARG:HD3	2.33	0.58
1:C:2:GLU:HG2	1:C:4:ILE:HD11	1.85	0.58
1:D:164:ILE:CD1	1:D:239:VAL:HG13	2.33	0.58
1:D:175:ALA:O	1:D:220:ILE:HA	2.04	0.58
1:D:35:SER:O	1:D:38:GLU:HG3	2.04	0.57
1:D:443:VAL:HG21	1:D:495:GLU:HB2	1.86	0.57
1:A:270:LEU:HD13	1:A:275:TYR:CD2	2.38	0.57
1:B:611:ASN:OD1	1:B:630:ILE:HD12	2.03	0.57
1:C:183:LEU:HD11	1:C:241:LEU:HD22	1.85	0.57
1:C:598:LEU:HB2	1:C:607:PHE:CE2	2.38	0.57
1:A:495:GLU:HA	1:A:498:LYS:HE3	1.87	0.57
1:D:51:GLY:O	1:D:120:GLU:HA	2.04	0.57
1:D:128:TYR:CZ	1:D:346:MET:HE2	2.38	0.57
1:B:6:PHE:CE2	1:B:57:LYS:HD3	2.39	0.57
1:C:436:PHE:HB2	1:C:446:ASN:ND2	2.20	0.57
1:C:496:MET:HG3	1:C:500:LEU:HD13	1.86	0.57
1:A:611:ASN:OD1	1:A:630:ILE:HD12	2.03	0.57
1:B:400:VAL:HG21	1:B:409:THR:HG22	1.85	0.57
1:B:2:GLU:OE1	1:B:4:ILE:HG12	2.04	0.57
1:D:501:PHE:HE2	1:D:554:LEU:HD11	1.70	0.57
1:A:154:PHE:CD2	1:A:251:VAL:HG13	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ILE:HG21	1:A:393:HIS:CE1	2.38	0.57
1:B:13:THR:HG21	1:B:16:ALA:HB2	1.87	0.57
1:B:73:GLU:OE1	1:B:101:ARG:NH1	2.38	0.57
1:D:13:THR:HG21	1:D:27:TRP:CE2	2.40	0.57
1:D:167:THR:HG1	1:D:365:TYR:HH	1.49	0.57
1:D:424:ILE:CG2	1:D:430:ILE:HD13	2.35	0.57
1:A:154:PHE:HE2	1:A:250:ALA:HA	1.70	0.56
1:D:574:THR:HA	1:D:610:PRO:HA	1.86	0.56
1:A:101:ARG:NH1	1:A:156:LEU:HD23	2.18	0.56
1:B:204:VAL:CG1	1:B:220:ILE:HG23	2.34	0.56
1:B:419:ILE:O	1:B:424:ILE:HD11	2.05	0.56
1:C:262:ILE:HD12	1:C:408:LEU:HD12	1.87	0.56
1:C:305:ILE:HD13	1:C:313:ILE:HD11	1.86	0.56
1:D:193:VAL:HG23	1:D:193:VAL:O	2.04	0.56
1:A:312:THR:HB	1:A:334:VAL:HG23	1.87	0.56
1:B:23:MET:HE2	1:B:24:PRO:HD2	1.87	0.56
1:B:285:ASP:HB2	1:B:290:GLY:O	2.04	0.56
1:C:467:TYR:CE2	1:C:496:MET:HG2	2.40	0.56
1:D:164:ILE:HD12	1:D:251:VAL:HG13	1.86	0.56
1:D:285:ASP:HB2	1:D:290:GLY:O	2.06	0.56
1:D:549:ALA:HB2	1:D:580:TYR:CE2	2.39	0.56
1:B:399:MET:O	1:B:403:MET:HG3	2.05	0.56
1:C:101:ARG:NE	1:C:156:LEU:HB3	2.19	0.56
1:B:85:VAL:HG22	1:B:115:ILE:HD13	1.86	0.56
1:A:32:LEU:HA	1:A:33:PRO:C	2.31	0.56
1:A:78:ASN:HA	1:A:96:GLY:HA3	1.87	0.56
1:C:197:LYS:HE3	1:C:238:GLU:OE1	2.06	0.56
1:D:253:THR:HG21	1:D:366:ASN:ND2	2.20	0.56
1:B:551:LYS:HG2	1:B:559:PHE:CE2	2.41	0.56
1:A:623:GLU:OE1	1:A:623:GLU:N	2.37	0.56
1:B:379:ILE:HG23	1:B:389:LEU:HD11	1.85	0.56
1:C:495:GLU:O	1:C:499:GLN:HG3	2.06	0.56
1:C:198:ASP:OD1	1:C:233:TYR:OH	2.21	0.56
1:B:92:HIS:NE2	1:B:94:ASP:OD2	2.34	0.56
1:D:36:TRP:HZ2	1:D:121:ASN:ND2	2.04	0.56
1:D:469:CYS:HB3	1:D:489:GLN:CG	2.36	0.56
1:D:503:ARG:HB2	1:D:506:ILE:HD12	1.88	0.56
1:A:434:HIS:HB2	1:A:464:MET:HE1	1.87	0.55
1:A:225:LEU:HD22	1:A:257:CYS:O	2.05	0.55
1:C:59:LEU:HD11	1:C:64:LEU:CD2	2.33	0.55
1:C:223:VAL:HG22	1:C:225:LEU:HD23	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:TYR:CD2	1:D:291:ASN:HB3	2.41	0.55
1:D:226:TRP:CZ2	1:D:332:GLY:HA2	2.41	0.55
1:B:469:CYS:C	1:B:533:LYS:HG2	2.31	0.55
1:B:481:GLN:HA	1:B:488:TYR:CE2	2.42	0.55
1:C:9:LYS:O	1:C:57:LYS:HD2	2.05	0.55
1:D:301:ASP:O	1:D:305:ILE:HG13	2.06	0.55
1:D:471:ALA:HB3	1:D:544:LYS:CE	2.34	0.55
1:A:483:ASP:HB2	1:A:485:THR:HG23	1.87	0.55
1:C:168:PRO:HA	1:C:177:VAL:HA	1.87	0.55
1:B:51:GLY:O	1:B:120:GLU:HA	2.07	0.55
1:A:472:LEU:CD1	1:A:484:TYR:HB3	2.37	0.55
1:A:302:ILE:HD12	1:A:327:LEU:HB3	1.89	0.55
1:D:169:GLU:O	1:D:175:ALA:HA	2.05	0.55
1:C:88:LYS:O	1:C:90:VAL:HG23	2.06	0.54
1:D:230:LYS:N	1:D:230:LYS:CD	2.70	0.54
1:D:280:VAL:HG12	1:D:511:VAL:HG13	1.89	0.54
1:B:536:VAL:HG12	1:B:537:THR:H	1.71	0.54
1:C:316:ALA:HB1	1:C:317:HIS:HA	1.88	0.54
1:D:192:LEU:CD2	1:D:241:LEU:HD22	2.36	0.54
1:D:443:VAL:HG23	1:D:496:MET:CE	2.37	0.54
1:B:38:GLU:HG2	1:B:289:ILE:C	2.32	0.54
1:B:75:ARG:O	1:B:142:ARG:HD2	2.07	0.54
1:C:302:ILE:HG23	1:C:331:ARG:NH1	2.22	0.54
1:B:536:VAL:HG12	1:B:537:THR:N	2.22	0.54
1:C:362:VAL:HG13	4:C:1604:FMN:C6	2.38	0.54
1:C:476:THR:HG22	1:C:485:THR:HG21	1.89	0.54
1:D:60:LYS:HA	1:D:111:GLU:O	2.08	0.54
1:D:283:HIS:HD2	1:D:517:PHE:CD2	2.26	0.54
1:B:362:VAL:HA	4:B:805:FMN:HM72	1.89	0.54
1:B:367:HIS:HB2	1:B:370:ILE:HD12	1.89	0.54
1:D:277:LEU:O	1:D:508:ALA:HA	2.05	0.54
1:A:517:PHE:CZ	1:A:531:ASN:HB3	2.43	0.54
1:C:282:ARG:HH21	1:C:284:GLN:HA	1.71	0.54
1:C:200:GLU:OE1	1:C:200:GLU:HA	2.07	0.54
1:C:471:ALA:HB2	1:C:489:GLN:HB2	1.90	0.54
1:C:542:TYR:OH	1:C:566:ARG:HD2	2.08	0.54
1:A:560:VAL:HG21	1:A:621:ALA:HB3	1.89	0.53
1:D:339:ILE:HD12	1:D:341:TYR:H	1.73	0.53
1:D:583:LEU:HB3	1:D:584:PRO:HD2	1.88	0.53
1:A:192:LEU:O	1:A:208:GLU:HA	2.09	0.53
1:B:168:PRO:CA	1:B:177:VAL:HG12	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ILE:HB	1:C:335:ILE:CD1	2.39	0.53
1:C:316:ALA:HB1	1:C:317:HIS:ND1	2.23	0.53
1:D:354:ILE:HG23	1:D:399:MET:SD	2.49	0.53
1:A:473:ASN:CG	1:A:566:ARG:HH21	2.16	0.53
1:B:354:ILE:HG23	1:B:399:MET:CE	2.37	0.53
1:B:615:SER:HB2	1:B:630:ILE:CG1	2.38	0.53
1:C:235:TYR:HB2	1:C:255:PHE:CE1	2.43	0.53
1:D:119:VAL:HG21	1:D:140:LEU:CD1	2.38	0.53
1:D:340:PRO:O	1:D:342:ILE:HG22	2.08	0.53
1:D:386:ASP:O	1:D:390:LEU:HG	2.09	0.53
1:B:174:ASP:OD1	1:B:221:PRO:HA	2.07	0.53
1:C:314:ARG:NH2	1:C:338:GLU:OE1	2.36	0.53
1:D:83:VAL:HG22	1:D:117:ILE:HG12	1.90	0.53
1:C:51:GLY:O	1:C:120:GLU:HA	2.09	0.53
1:C:155:ASP:HA	1:C:184:THR:OG1	2.08	0.53
1:C:278:ARG:HD2	1:C:501:PHE:CD1	2.43	0.53
1:C:55:TYR:CE2	1:C:140:LEU:HG	2.43	0.53
1:C:436:PHE:HB2	1:C:446:ASN:HD21	1.73	0.53
1:C:727:LEU:HD12	1:C:727:LEU:O	2.09	0.53
1:A:11:ALA:HB3	1:A:56:ALA:HB3	1.89	0.53
1:A:154:PHE:CD2	1:A:251:VAL:HG22	2.44	0.53
1:B:474:TRP:CE2	1:B:642:LEU:HD13	2.44	0.53
1:D:24:PRO:HG2	1:D:27:TRP:CE3	2.44	0.53
1:A:598:LEU:HB2	1:A:607:PHE:CE2	2.44	0.53
1:C:37:ASN:HA	1:C:40:ASP:OD1	2.08	0.53
1:D:101:ARG:CD	1:D:156:LEU:HD22	2.39	0.53
1:D:429:VAL:HG12	1:D:461:PRO:CG	2.39	0.53
1:D:472:LEU:HD21	1:D:532:HIS:ND1	2.23	0.53
1:D:497:ILE:HA	1:D:501:PHE:CD1	2.44	0.53
1:D:503:ARG:HB3	1:D:505:TYR:CE2	2.43	0.53
1:A:6:PHE:CE1	1:A:57:LYS:HE2	2.44	0.53
1:D:165:LYS:HB3	1:D:180:GLU:HB2	1.91	0.53
1:A:24:PRO:HG2	1:A:27:TRP:CZ3	2.44	0.52
1:A:217:VAL:HG13	1:A:217:VAL:O	2.09	0.52
1:A:335:ILE:HG12	1:A:369:SER:OG	2.09	0.52
1:A:78:ASN:ND2	1:A:137:TYR:O	2.28	0.52
1:A:432:TYR:HB3	1:A:434:HIS:CD2	2.44	0.52
1:B:158:TYR:CZ	4:B:805:FMN:O2'	2.60	0.52
1:B:583:LEU:HB3	1:B:584:PRO:HD2	1.91	0.52
1:C:618:VAL:HG11	2:C:1602:GOL:H12	1.91	0.52
1:B:453:PHE:HD1	1:B:462:LEU:HD22	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ILE:HG23	1:C:430:ILE:HD13	1.91	0.52
1:B:444:SER:HA	1:B:499:GLN:HE22	1.74	0.52
1:C:209:THR:HB	1:C:213:GLU:HG2	1.92	0.52
1:C:411:ILE:HD12	1:C:423:TYR:CE2	2.44	0.52
1:A:168:PRO:HA	1:A:177:VAL:HA	1.91	0.52
1:B:474:TRP:CZ2	1:B:642:LEU:HD13	2.45	0.52
1:B:575:THR:HG22	1:B:609:VAL:O	2.10	0.52
1:D:154:PHE:HE2	1:D:239:VAL:HG22	1.73	0.52
1:D:279:GLY:HA3	1:D:312:THR:O	2.10	0.52
1:B:280:VAL:HG21	1:B:305:ILE:CD1	2.39	0.52
1:A:279:GLY:HA3	1:A:312:THR:O	2.10	0.52
1:A:404:ASP:OD2	1:A:407:ARG:HB2	2.10	0.52
1:A:423:TYR:O	1:A:426:ILE:HD12	2.10	0.52
1:A:282:ARG:HD2	1:A:301:ASP:OD2	2.10	0.52
1:D:162:PRO:O	1:D:251:VAL:HG21	2.09	0.52
1:B:110:GLU:C	1:B:112:GLU:H	2.18	0.52
1:B:446:ASN:OD1	1:B:496:MET:HE1	2.10	0.52
1:D:126:ARG:HA	1:D:349:GLY:CA	2.40	0.52
1:A:500:LEU:HD23	1:A:509:THR:CG2	2.40	0.51
1:B:59:LEU:HD11	1:B:64:LEU:HD13	1.92	0.51
1:D:294:LEU:HB2	1:D:297:HIS:ND1	2.24	0.51
1:B:305:ILE:HD13	1:B:514:MET:CE	2.40	0.51
1:D:164:ILE:HD12	1:D:251:VAL:CG1	2.40	0.51
1:D:165:LYS:HE3	1:D:365:TYR:CE2	2.46	0.51
1:A:175:ALA:HB2	1:A:223:VAL:CG2	2.41	0.51
1:A:282:ARG:HG2	1:A:283:HIS:O	2.10	0.51
1:A:309:GLY:O	1:A:554:LEU:HB3	2.10	0.51
1:B:83:VAL:O	1:B:90:VAL:HG22	2.09	0.51
1:C:325:TYR:HB3	1:C:367:HIS:CD2	2.44	0.51
1:A:7:ASN:HB3	1:A:32:LEU:HB2	1.91	0.51
1:A:59:LEU:HD23	1:A:59:LEU:C	2.35	0.51
1:B:317:HIS:HA	1:B:338:GLU:OE2	2.10	0.51
1:C:433:ASN:CG	1:C:466:GLU:HB2	2.36	0.51
1:D:340:PRO:HG3	1:D:356:GLN:OE1	2.10	0.51
1:A:158:TYR:HE2	1:A:362:VAL:HG21	1.75	0.51
1:A:372:VAL:HA	1:A:408:LEU:O	2.10	0.51
1:C:23:MET:HE1	1:C:57:LYS:HA	1.92	0.51
1:D:284:GLN:HG2	1:D:318:TYR:OH	2.11	0.51
1:D:426:ILE:HD12	1:D:426:ILE:H	1.76	0.51
1:A:562:LEU:HD13	1:A:628:SER:HB2	1.93	0.51
1:B:418:ASP:OD2	1:B:420:HIS:HB2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:SER:HB2	1:B:433:ASN:O	2.11	0.51
1:D:154:PHE:HE1	1:D:249:ASP:HB2	1.69	0.51
1:D:423:TYR:HA	1:D:426:ILE:HD11	1.91	0.51
1:B:618:VAL:HG22	1:B:627:GLU:HG3	1.93	0.51
1:D:129:PRO:HG3	1:D:340:PRO:HB3	1.93	0.51
1:D:358:LYS:O	1:D:362:VAL:HG23	2.11	0.51
1:D:539:ASP:CG	1:D:541:LYS:HB2	2.35	0.51
1:A:170:ILE:CD1	1:A:225:LEU:HD21	2.37	0.51
1:A:277:LEU:HD22	1:A:334:VAL:CG2	2.36	0.51
1:B:362:VAL:HG13	4:B:805:FMN:H6	1.93	0.51
1:C:419:ILE:CG2	1:C:453:PHE:HD2	2.24	0.51
1:D:72:LEU:CD2	1:D:74:LEU:HD11	2.40	0.51
1:D:438:TRP:CE3	1:D:438:TRP:HA	2.46	0.51
1:A:311:THR:O	1:A:334:VAL:HG22	2.11	0.50
1:A:473:ASN:HA	1:A:566:ARG:HH22	1.76	0.50
1:D:137:TYR:HD2	1:D:291:ASN:HB3	1.76	0.50
1:B:316:ALA:HB1	1:B:317:HIS:HA	1.94	0.50
1:D:129:PRO:HD3	1:D:340:PRO:CB	2.41	0.50
1:D:560:VAL:HG21	1:D:621:ALA:HB3	1.92	0.50
1:A:350:ARG:HD2	1:B:17:THR:HG21	1.93	0.50
1:A:568:VAL:HG13	1:A:629:HIS:O	2.11	0.50
1:C:90:VAL:HG12	1:C:102:VAL:HG21	1.92	0.50
1:D:268:PHE:CE2	1:D:270:LEU:HB2	2.46	0.50
1:D:467:TYR:CD2	1:D:496:MET:HG3	2.47	0.50
1:B:59:LEU:HD11	1:B:64:LEU:CD1	2.42	0.50
1:C:75:ARG:O	1:C:142:ARG:HD2	2.12	0.50
1:C:474:TRP:CZ2	1:C:642:LEU:HD13	2.45	0.50
1:D:373:TRP:O	1:D:409:THR:HA	2.12	0.50
1:A:310:ALA:HA	1:A:554:LEU:HD13	1.93	0.50
1:A:436:PHE:HB2	1:A:446:ASN:OD1	2.11	0.50
1:C:277:LEU:HD22	1:C:312:THR:HB	1.93	0.50
1:C:286:ARG:NH1	1:C:300:GLU:OE1	2.30	0.50
1:C:315:LEU:HD21	1:C:324:PHE:CE2	2.46	0.50
1:D:5:ASN:OD1	1:D:6:PHE:N	2.44	0.50
1:D:32:LEU:CD1	1:D:34:HIS:HB3	2.41	0.50
1:D:230:LYS:HE3	1:D:230:LYS:CA	2.40	0.50
1:B:73:GLU:OE1	1:B:147:ILE:HD11	2.12	0.50
1:A:341:TYR:CE1	1:A:379:ILE:HD11	2.47	0.50
1:A:527:GLU:HB3	1:A:532:HIS:CE1	2.46	0.50
1:D:336:TRP:CD1	1:D:336:TRP:C	2.89	0.50
1:D:469:CYS:HB3	1:D:489:GLN:HG2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:VAL:HG12	1:D:511:VAL:HG12	1.90	0.50
1:B:305:ILE:HG21	1:B:313:ILE:HD11	1.94	0.49
1:B:590:VAL:HG12	1:B:617:LEU:CD2	2.42	0.49
1:D:150:ASN:HB2	1:D:248:VAL:HG13	1.93	0.49
1:D:407:ARG:C	1:D:408:LEU:HD23	2.36	0.49
1:A:10:TRP:CE2	1:A:57:LYS:HD3	2.47	0.49
1:A:107:GLU:HA	1:A:107:GLU:OE1	2.13	0.49
1:B:13:THR:HG21	1:B:27:TRP:CZ2	2.47	0.49
1:B:380:THR:CG2	1:B:380:THR:O	2.61	0.49
1:A:9:LYS:O	1:A:57:LYS:HD2	2.11	0.49
1:A:535:LEU:O	1:A:544:LYS:HG3	2.11	0.49
1:B:395:ILE:O	1:B:399:MET:HB2	2.12	0.49
1:B:443:VAL:O	1:B:499:GLN:NE2	2.43	0.49
1:C:314:ARG:HA	1:C:336:TRP:HB3	1.94	0.49
1:D:474:TRP:CE2	1:D:642:LEU:HB2	2.47	0.49
1:D:500:LEU:HD23	1:D:509:THR:CG2	2.40	0.49
1:A:402:GLU:O	1:A:402:GLU:HG2	2.12	0.49
1:B:313:ILE:HB	1:B:335:ILE:CD1	2.43	0.49
1:D:20:PRO:HG3	1:D:27:TRP:CH2	2.47	0.49
1:B:360:LEU:O	1:B:364:ASN:ND2	2.32	0.49
1:B:617:LEU:HD11	1:B:630:ILE:HG21	1.95	0.49
1:C:438:TRP:CZ2	1:C:470:GLU:HG3	2.48	0.49
1:D:36:TRP:CZ2	1:D:121:ASN:ND2	2.80	0.49
1:D:284:GLN:HG2	1:D:318:TYR:CZ	2.47	0.49
1:A:51:GLY:O	1:A:120:GLU:HA	2.11	0.49
1:A:160:GLY:O	1:A:363:GLN:HG2	2.13	0.49
1:B:413:VAL:CG1	1:B:417:CYS:HB3	2.42	0.49
1:A:284:GLN:HG2	1:A:318:TYR:HE1	1.74	0.49
1:C:262:ILE:CD1	1:C:408:LEU:HD12	2.43	0.49
1:C:450:MET:SD	1:C:462:LEU:HD21	2.52	0.49
1:D:413:VAL:HG12	1:D:414:VAL:O	2.12	0.49
1:A:61:LYS:HE2	1:A:108:LEU:O	2.13	0.49
1:C:196:VAL:HG12	1:C:204:VAL:HG23	1.94	0.49
1:C:389:LEU:O	1:C:389:LEU:HD23	2.12	0.49
1:D:392:ASN:HA	1:D:395:ILE:HD13	1.93	0.49
1:A:233:TYR:O	1:A:234:LEU:HD23	2.13	0.49
1:A:313:ILE:HD11	1:A:333:LEU:HD22	1.94	0.49
1:B:300:GLU:O	1:B:304:LEU:HD12	2.13	0.49
1:C:443:VAL:HG23	1:C:496:MET:HE1	1.95	0.49
1:C:596:GLY:HA2	1:D:597:LYS:O	2.13	0.49
1:C:613:GLY:O	1:C:631:ARG:HA	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:SER:HB3	1:A:433:ASN:O	2.13	0.49
1:B:493:HIS:O	1:B:497:ILE:HG13	2.13	0.49
1:C:166:VAL:HG11	1:C:255:PHE:CG	2.47	0.49
1:B:282:ARG:HG2	1:B:283:HIS:N	2.27	0.48
1:B:431:SER:HB2	1:B:465:SER:OG	2.13	0.48
1:C:280:VAL:HG12	1:C:511:VAL:HB	1.94	0.48
1:C:305:ILE:HA	1:C:514:MET:HE2	1.94	0.48
1:C:556:ASP:O	1:C:558:PRO:HD3	2.13	0.48
1:D:493:HIS:O	1:D:497:ILE:HG13	2.13	0.48
1:B:531:ASN:HD21	3:B:804:BDP:C6	2.26	0.48
1:C:32:LEU:HA	1:C:33:PRO:C	2.37	0.48
1:C:440:GLY:N	1:C:719:PHE:HE1	2.11	0.48
1:D:589:PHE:HD1	1:D:594:SER:HA	1.76	0.48
1:A:168:PRO:HB3	1:A:177:VAL:CG1	2.42	0.48
1:A:473:ASN:OD1	1:A:566:ARG:NH2	2.46	0.48
1:C:496:MET:HE2	1:C:496:MET:HA	1.95	0.48
1:D:497:ILE:HG23	1:D:501:PHE:CD1	2.49	0.48
1:A:37:ASN:HA	1:A:40:ASP:OD1	2.12	0.48
1:A:175:ALA:HB2	1:A:223:VAL:HG21	1.95	0.48
1:C:372:VAL:HA	1:C:408:LEU:O	2.13	0.48
1:C:399:MET:O	1:C:403:MET:HG3	2.13	0.48
1:D:429:VAL:HG12	1:D:461:PRO:CB	2.43	0.48
1:C:223:VAL:HG13	1:C:225:LEU:CD2	2.43	0.48
1:D:13:THR:HG21	1:D:27:TRP:CZ2	2.48	0.48
1:A:293:LEU:HD23	1:A:298:HIS:CE1	2.49	0.48
1:B:18:GLU:O	1:B:18:GLU:HG3	2.12	0.48
1:B:88:LYS:O	1:B:90:VAL:HG13	2.13	0.48
1:D:181:VAL:HG11	1:D:239:VAL:HG21	1.96	0.48
1:A:558:PRO:HB2	1:A:624:TYR:CZ	2.48	0.48
1:B:127:VAL:O	1:B:130:GLN:HG2	2.14	0.48
1:D:280:VAL:O	1:D:313:ILE:HA	2.13	0.48
1:B:336:TRP:CD1	1:B:336:TRP:C	2.92	0.48
1:C:154:PHE:HE2	1:C:250:ALA:HA	1.77	0.48
1:C:305:ILE:HD13	1:C:313:ILE:CD1	2.42	0.48
1:A:175:ALA:HB3	1:A:220:ILE:HG23	1.95	0.48
1:A:204:VAL:HG12	1:A:204:VAL:O	2.12	0.48
1:B:590:VAL:CG1	1:B:609:VAL:HG21	2.44	0.48
1:C:720:THR:HG22	1:C:723:ARG:HB3	1.96	0.48
1:A:112:GLU:OE1	1:A:112:GLU:N	2.46	0.48
1:D:573:ASP:O	1:D:611:ASN:N	2.33	0.48
1:B:411:ILE:HG23	1:B:427:PRO:HG3	1.94	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:VAL:HG11	1:C:239:VAL:HG11	1.95	0.47
1:D:411:ILE:CD1	1:D:413:VAL:HG23	2.44	0.47
1:D:483:ASP:HB2	1:D:485:THR:HG23	1.95	0.47
1:B:494:GLU:OE2	1:B:580:TYR:OH	2.26	0.47
1:C:278:ARG:HD3	1:C:509:THR:HG23	1.94	0.47
1:D:150:ASN:OD1	1:D:151:LYS:N	2.48	0.47
1:D:230:LYS:HD2	1:D:230:LYS:H	1.75	0.47
1:D:438:TRP:HE1	1:D:470:GLU:HG3	1.79	0.47
1:C:83:VAL:HG22	1:C:117:ILE:HG12	1.96	0.47
1:C:591:ASN:OD1	1:C:615:SER:HA	2.15	0.47
1:C:611:ASN:O	1:C:632:LYS:HD3	2.15	0.47
1:A:411:ILE:HD12	1:A:413:VAL:HG23	1.96	0.47
1:A:470:GLU:HG2	1:A:533:LYS:CG	2.44	0.47
1:C:101:ARG:HH21	1:C:156:LEU:CA	2.22	0.47
1:C:522:ARG:NH1	1:C:524:GLU:OE2	2.41	0.47
1:D:614:GLU:HG2	1:D:631:ARG:CB	2.44	0.47
1:A:84:TYR:HA	1:A:88:LYS:O	2.15	0.47
1:B:162:PRO:O	1:B:251:VAL:HG21	2.14	0.47
1:D:478:ASP:OD2	1:D:480:LYS:HE3	2.14	0.47
1:D:587:GLU:HB3	1:D:620:VAL:CG2	2.44	0.47
1:A:194:TYR:HB2	1:A:207:THR:HG22	1.95	0.47
1:A:232:PRO:HB3	1:A:332:GLY:CA	2.45	0.47
1:A:277:LEU:O	1:A:508:ALA:HA	2.14	0.47
1:B:68:ASP:O	1:B:105:THR:HG21	2.15	0.47
1:B:584:PRO:O	1:B:599:GLN:HG2	2.14	0.47
1:C:180:GLU:HA	1:C:214:THR:O	2.14	0.47
1:D:259:THR:OG1	1:D:271:ASN:HA	2.14	0.47
1:D:270:LEU:HD23	1:D:275:TYR:CD2	2.50	0.47
1:B:380:THR:O	1:B:380:THR:HG22	2.14	0.47
1:B:466:GLU:OE1	3:B:804:BDP:H1	2.15	0.47
1:B:549:ALA:HB2	1:B:580:TYR:CE2	2.50	0.47
1:C:590:VAL:HG13	1:C:590:VAL:O	2.15	0.47
1:D:372:VAL:HG23	1:D:372:VAL:O	2.15	0.47
1:A:90:VAL:HG12	1:A:102:VAL:HG21	1.97	0.47
1:A:189:ASP:OD1	1:A:189:ASP:N	2.47	0.47
1:A:198:ASP:OD1	1:A:200:GLU:HG2	2.14	0.47
1:A:376:SER:HB3	1:A:393:HIS:NE2	2.30	0.47
1:B:315:LEU:HD12	1:B:325:TYR:CE1	2.49	0.47
1:C:16:ALA:HB3	1:C:54:TYR:CD1	2.50	0.47
1:C:133:ASP:CG	1:C:522:ARG:HH21	2.22	0.47
1:C:367:HIS:HB2	1:C:370:ILE:CD1	2.31	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:PHE:HE2	1:C:554:LEU:HD21	1.78	0.47
1:D:364:ASN:HB2	1:D:373:TRP:HH2	1.80	0.47
1:B:346:MET:HE2	1:B:346:MET:HB2	1.68	0.47
1:B:512:TRP:HA	1:B:513:ASN:HA	1.76	0.47
1:C:73:GLU:HB2	1:C:147:ILE:CD1	2.44	0.47
1:C:81:ALA:HA	1:C:118:ALA:O	2.14	0.47
1:D:248:VAL:HG12	1:D:249:ASP:N	2.29	0.47
1:A:81:ALA:HA	1:A:118:ALA:O	2.14	0.46
1:A:446:ASN:HD22	1:A:464:MET:HE1	1.81	0.46
1:A:470:GLU:HG2	1:A:533:LYS:HG2	1.97	0.46
1:B:74:LEU:HD21	1:B:117:ILE:HD13	1.97	0.46
1:B:111:GLU:CG	1:B:111:GLU:O	2.62	0.46
1:D:623:GLU:O	1:D:623:GLU:CG	2.61	0.46
1:A:312:THR:CB	1:A:334:VAL:HG23	2.45	0.46
1:A:519:ALA:HB3	1:A:522:ARG:HG3	1.97	0.46
1:D:192:LEU:HD12	1:D:211:ALA:O	2.14	0.46
1:D:464:MET:HG2	1:D:500:LEU:HD21	1.96	0.46
1:A:588:LEU:HD21	1:A:609:VAL:HG21	1.97	0.46
1:B:58:GLN:HG2	1:B:114:LEU:CD1	2.45	0.46
1:D:165:LYS:HE3	1:D:365:TYR:CZ	2.50	0.46
1:A:336:TRP:C	1:A:336:TRP:CD1	2.93	0.46
1:B:40:ASP:HA	1:B:43:ASP:OD2	2.15	0.46
1:C:7:ASN:CG	1:C:32:LEU:HB2	2.39	0.46
1:C:305:ILE:HA	1:C:514:MET:CE	2.45	0.46
1:C:336:TRP:CD1	1:C:336:TRP:C	2.93	0.46
1:D:286:ARG:HB3	1:D:289:ILE:HD11	1.97	0.46
1:A:494:GLU:HG2	1:A:604:PHE:CE2	2.51	0.46
1:A:562:LEU:HD23	1:A:562:LEU:HA	1.76	0.46
1:B:68:ASP:OD2	1:B:151:LYS:HG2	2.15	0.46
1:B:617:LEU:HD12	1:B:628:SER:OG	2.15	0.46
1:C:24:PRO:HG2	1:C:27:TRP:CE3	2.50	0.46
1:D:236:THR:HG22	1:D:254:ARG:HG2	1.97	0.46
1:A:497:ILE:HD12	1:A:604:PHE:CZ	2.46	0.46
1:B:474:TRP:O	1:B:485:THR:HB	2.14	0.46
1:C:23:MET:SD	1:C:24:PRO:HD2	2.56	0.46
1:C:171:LYS:HE2	1:C:176:SER:OG	2.15	0.46
1:C:262:ILE:HD12	1:C:408:LEU:CD1	2.46	0.46
1:B:437:GLY:O	1:B:488:TYR:OH	2.29	0.46
1:C:125:ASP:HA	1:C:346:MET:SD	2.55	0.46
1:D:395:ILE:HD12	1:D:395:ILE:N	2.19	0.46
1:D:611:ASN:OD1	1:D:630:ILE:HD12	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ILE:CD1	1:B:514:MET:HE2	2.44	0.46
1:B:421:ASP:OD1	1:B:422:PRO:HD2	2.16	0.46
1:B:588:LEU:HD11	1:B:617:LEU:HB3	1.97	0.46
4:C:1604:FMN:O2'	4:C:1604:FMN:H9	2.15	0.46
1:D:10:TRP:CE2	1:D:57:LYS:HD2	2.51	0.46
1:D:225:LEU:H	1:D:225:LEU:CD2	2.26	0.46
1:D:477:SER:O	1:D:479:PRO:HD3	2.16	0.46
1:A:442:ASP:H	1:A:445:MET:HE3	1.80	0.46
1:A:619:ALA:O	1:A:625:LYS:HA	2.16	0.46
1:B:372:VAL:HA	1:B:408:LEU:O	2.15	0.46
1:B:475:HIS:HA	1:B:487:GLU:OE1	2.16	0.46
1:B:562:LEU:HD21	1:B:619:ALA:CB	2.46	0.46
1:C:496:MET:HE2	1:C:496:MET:CA	2.46	0.46
1:D:164:ILE:HD11	1:D:239:VAL:CG1	2.45	0.46
1:D:289:ILE:HD12	1:D:293:LEU:HD12	1.97	0.46
1:A:75:ARG:O	1:A:142:ARG:HD2	2.16	0.46
1:A:329:ASP:OD1	1:A:369:SER:HB3	2.16	0.46
1:A:411:ILE:CD1	1:A:413:VAL:HG23	2.46	0.46
1:B:436:PHE:HB2	1:B:446:ASN:OD1	2.16	0.46
1:C:209:THR:CB	1:C:213:GLU:HG2	2.46	0.46
1:D:24:PRO:HG2	1:D:27:TRP:CZ3	2.51	0.46
1:D:101:ARG:HD2	1:D:156:LEU:HD22	1.98	0.46
1:D:265:GLU:C	1:D:267:GLY:H	2.24	0.46
1:B:360:LEU:HD12	1:B:364:ASN:ND2	2.30	0.45
1:B:481:GLN:HB2	1:B:488:TYR:OH	2.15	0.45
1:D:269:ILE:HG23	1:D:273:GLU:O	2.16	0.45
1:A:226:TRP:CZ2	1:A:332:GLY:HA2	2.50	0.45
1:D:424:ILE:HG23	1:D:430:ILE:HD13	1.98	0.45
1:D:453:PHE:CD1	1:D:462:LEU:HD13	2.51	0.45
1:A:411:ILE:HG12	1:A:427:PRO:HG3	1.97	0.45
1:B:270:LEU:HD23	1:B:275:TYR:CD2	2.51	0.45
1:C:389:LEU:HD23	1:C:389:LEU:C	2.41	0.45
1:C:493:HIS:CE1	1:C:511:VAL:HG13	2.50	0.45
1:D:193:VAL:HG22	1:D:240:ALA:HB3	1.98	0.45
1:D:503:ARG:HG3	1:D:503:ARG:HH11	1.82	0.45
1:A:191:LYS:HD2	1:A:208:GLU:OE2	2.17	0.45
1:C:196:VAL:HG12	1:C:204:VAL:CG2	2.47	0.45
1:C:282:ARG:O	1:C:282:ARG:HG3	2.17	0.45
1:D:373:TRP:HE1	1:D:407:ARG:HD2	1.81	0.45
1:A:515:PHE:HD1	1:A:536:VAL:HB	1.82	0.45
1:A:560:VAL:HG21	1:A:621:ALA:CB	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLN:HE21	1:C:112:GLU:HB3	1.81	0.45
1:D:336:TRP:HB2	1:D:372:VAL:CG2	2.47	0.45
1:A:426:ILE:HB	1:A:427:PRO:HD3	1.98	0.45
1:B:209:THR:HB	1:B:213:GLU:CD	2.42	0.45
1:C:385:SER:OG	1:C:421:ASP:OD1	2.33	0.45
1:C:249:ASP:OD1	1:C:250:ALA:N	2.46	0.45
1:D:395:ILE:H	1:D:395:ILE:CD1	2.15	0.45
1:B:220:ILE:CG2	1:B:223:VAL:HG12	2.48	0.45
1:C:196:VAL:CG1	1:C:220:ILE:HD11	2.39	0.45
1:D:277:LEU:CD1	1:D:334:VAL:HG11	2.46	0.45
1:A:270:LEU:HD23	1:A:271:ASN:N	2.32	0.44
1:C:315:LEU:HD12	1:C:325:TYR:CE1	2.52	0.44
1:D:126:ARG:HA	1:D:349:GLY:HA3	1.98	0.44
1:D:411:ILE:HG12	1:D:427:PRO:HG3	1.99	0.44
1:A:238:GLU:HG2	1:A:252:SER:HB2	1.99	0.44
1:B:329:ASP:CG	1:B:368:PRO:HD2	2.43	0.44
1:B:438:TRP:CE2	1:B:470:GLU:HG3	2.51	0.44
1:B:457:PHE:HB3	1:B:460:ILE:HG13	1.99	0.44
1:B:576:LYS:HB3	1:B:576:LYS:HE2	1.77	0.44
1:C:450:MET:HE1	1:C:462:LEU:HG	1.99	0.44
1:A:223:VAL:CG1	1:A:225:LEU:HD23	2.47	0.44
1:A:312:THR:HB	1:A:334:VAL:CG2	2.47	0.44
1:B:391:GLU:OE2	1:B:394:ARG:NH2	2.48	0.44
1:B:493:HIS:HA	1:B:496:MET:HB2	1.99	0.44
1:B:617:LEU:HD11	1:B:630:ILE:CG2	2.47	0.44
1:C:1:ARG:HD3	1:C:249:ASP:OD1	2.17	0.44
1:D:457:PHE:N	1:D:457:PHE:CD1	2.84	0.44
1:A:191:LYS:HA	1:A:210:ALA:HA	2.00	0.44
1:A:371:VAL:HA	1:A:407:ARG:HG2	1.98	0.44
1:A:414:VAL:HG22	1:A:416:MET:H	1.81	0.44
1:B:19:VAL:HG13	1:B:116:VAL:HG21	2.00	0.44
1:B:282:ARG:HG2	1:B:283:HIS:O	2.17	0.44
1:C:719:PHE:HB3	1:C:723:ARG:HG2	1.99	0.44
1:D:226:TRP:O	1:D:271:ASN:ND2	2.51	0.44
1:A:254:ARG:HE	1:A:254:ARG:HB2	1.59	0.44
1:A:483:ASP:CB	1:A:485:THR:HG23	2.48	0.44
1:B:137:TYR:CD2	1:B:291:ASN:HB3	2.52	0.44
1:B:220:ILE:O	1:B:223:VAL:HG13	2.17	0.44
1:C:198:ASP:HB3	1:C:202:LYS:HB2	1.99	0.44
1:D:141:TYR:HD1	1:D:141:TYR:H	1.65	0.44
1:D:338:GLU:O	1:D:360:LEU:HD22	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:TYR:O	1:A:496:MET:HG2	2.18	0.44
1:C:260:PHE:HA	1:C:269:ILE:O	2.18	0.44
1:C:312:THR:HA	1:C:334:VAL:O	2.18	0.44
1:C:424:ILE:HG22	1:C:424:ILE:O	2.18	0.44
1:C:530:GLN:HE21	1:C:538:PHE:CB	2.29	0.44
1:A:73:GLU:HB2	1:A:147:ILE:CD1	2.45	0.44
1:A:76:GLY:HA3	1:A:142:ARG:HG3	1.99	0.44
1:A:544:LYS:O	1:A:547:PHE:HB3	2.18	0.44
1:B:175:ALA:CB	1:B:223:VAL:HG11	2.32	0.44
1:B:407:ARG:C	1:B:408:LEU:HD23	2.42	0.44
1:B:557:GLU:OE1	1:B:557:GLU:HA	2.17	0.44
1:D:11:ALA:HB3	1:D:56:ALA:HB3	2.00	0.44
1:D:32:LEU:HD22	1:D:32:LEU:H	1.83	0.44
1:B:175:ALA:HB3	1:B:223:VAL:CG1	2.35	0.44
1:C:530:GLN:HB3	1:C:532:HIS:NE2	2.31	0.44
1:D:270:LEU:HD23	1:D:275:TYR:HD2	1.83	0.44
1:D:366:ASN:O	1:D:368:PRO:HD3	2.18	0.44
1:D:614:GLU:HG2	1:D:631:ARG:HB3	1.99	0.44
1:A:195:THR:CG2	1:A:238:GLU:HB2	2.46	0.44
1:A:429:VAL:HG21	1:A:507:TRP:CZ2	2.52	0.44
1:A:531:ASN:OD1	1:A:533:LYS:HB2	2.18	0.44
1:A:598:LEU:HB2	1:A:607:PHE:CZ	2.53	0.44
1:C:418:ASP:OD1	1:C:419:ILE:N	2.51	0.44
1:C:438:TRP:O	1:C:723:ARG:NH2	2.51	0.44
1:D:339:ILE:HD12	1:D:341:TYR:HB2	2.00	0.44
1:D:429:VAL:HG12	1:D:461:PRO:HG2	1.99	0.44
1:D:522:ARG:HD2	1:D:524:GLU:OE2	2.16	0.44
1:A:339:ILE:HB	1:A:340:PRO:HD2	2.00	0.43
1:A:460:ILE:HD13	1:A:460:ILE:HA	1.82	0.43
1:B:68:ASP:HB3	1:B:151:LYS:HG2	1.98	0.43
1:C:450:MET:CE	1:C:462:LEU:HG	2.48	0.43
1:C:519:ALA:HB1	2:C:1603:GOL:O1	2.17	0.43
1:D:572:GLU:O	1:D:572:GLU:HG2	2.18	0.43
1:A:20:PRO:HG3	1:A:27:TRP:CH2	2.53	0.43
1:B:443:VAL:HG23	1:B:496:MET:HE2	2.00	0.43
1:C:404:ASP:OD2	1:C:407:ARG:HG3	2.18	0.43
1:D:93:HIS:NE2	1:D:95:GLY:O	2.48	0.43
1:D:192:LEU:HD12	1:D:212:GLY:HA2	2.01	0.43
1:A:170:ILE:HD12	1:A:259:THR:HG23	1.99	0.43
1:B:37:ASN:HD22	1:B:40:ASP:CG	2.26	0.43
1:B:111:GLU:O	1:B:111:GLU:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:HD11	1:B:329:ASP:O	2.17	0.43
1:B:278:ARG:HD2	1:B:501:PHE:CE1	2.53	0.43
1:B:568:VAL:HG23	1:B:569:ASP:N	2.33	0.43
1:C:202:LYS:HD3	1:C:202:LYS:HA	1.75	0.43
1:A:552:ALA:HB1	1:A:603:HIS:HB3	1.99	0.43
1:B:78:ASN:HA	1:B:79:ALA:HA	1.63	0.43
1:B:277:LEU:HD11	1:B:334:VAL:HG11	2.01	0.43
1:B:322:GLN:NE2	1:B:322:GLN:HA	2.34	0.43
1:B:335:ILE:HD13	1:B:335:ILE:HA	1.81	0.43
1:C:315:LEU:HD21	1:C:324:PHE:HE2	1.83	0.43
1:C:569:ASP:OD1	1:C:631:ARG:NH1	2.51	0.43
1:C:625:LYS:NZ	2:C:1602:GOL:H2	2.34	0.43
1:D:260:PHE:HA	1:D:269:ILE:O	2.19	0.43
1:D:436:PHE:HB2	1:D:446:ASN:ND2	2.33	0.43
1:D:472:LEU:HD21	1:D:532:HIS:CG	2.54	0.43
1:D:587:GLU:HA	1:D:596:GLY:O	2.18	0.43
1:A:494:GLU:HG2	1:A:604:PHE:CD2	2.53	0.43
1:A:500:LEU:HD23	1:A:509:THR:HG21	2.01	0.43
1:D:129:PRO:HD3	1:D:340:PRO:HB3	1.99	0.43
1:D:560:VAL:CG2	1:D:621:ALA:HB3	2.48	0.43
1:A:164:ILE:HD11	1:A:239:VAL:CG2	2.48	0.43
1:B:220:ILE:CB	1:B:223:VAL:HG12	2.43	0.43
1:B:527:GLU:HB3	1:B:532:HIS:CE1	2.53	0.43
1:D:438:TRP:HZ3	1:D:482:GLY:H	1.67	0.43
1:D:443:VAL:CG2	1:D:495:GLU:HB2	2.47	0.43
1:D:470:GLU:HA	1:D:532:HIS:O	2.19	0.43
1:A:471:ALA:HB2	1:A:489:GLN:CB	2.45	0.43
1:A:512:TRP:HA	1:A:513:ASN:HA	1.70	0.43
1:C:196:VAL:HG23	1:C:218:LEU:HD13	2.01	0.43
1:D:81:ALA:HA	1:D:118:ALA:O	2.19	0.43
1:D:235:TYR:HB3	1:D:255:PHE:CZ	2.53	0.43
1:B:42:GLN:NE2	1:B:290:GLY:HA2	2.32	0.43
1:B:168:PRO:HA	1:B:177:VAL:HG12	1.99	0.43
1:B:481:GLN:HB2	1:B:488:TYR:CZ	2.53	0.43
1:D:387:GLU:OE1	1:D:387:GLU:HA	2.18	0.43
1:D:426:ILE:HB	1:D:427:PRO:HD3	2.01	0.43
1:D:497:ILE:O	1:D:501:PHE:HB2	2.18	0.43
1:A:85:VAL:HG22	1:A:115:ILE:HD12	2.00	0.43
1:A:335:ILE:HD13	1:A:335:ILE:HA	1.83	0.43
1:B:516:ASP:CG	1:B:532:HIS:HA	2.43	0.43
1:C:720:THR:CG2	1:C:723:ARG:H	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PRO:HG2	1:A:136:PHE:CE1	2.54	0.43
1:A:280:VAL:HG21	1:A:514:MET:HB2	2.01	0.43
1:A:413:VAL:HG11	1:A:432:TYR:CZ	2.54	0.43
1:B:389:LEU:HD23	1:B:389:LEU:C	2.44	0.43
1:C:12:PHE:CZ	1:C:36:TRP:HB3	2.54	0.43
1:C:41:GLY:HA2	1:C:48:TYR:HB3	2.01	0.43
1:C:560:VAL:HG21	1:C:621:ALA:HB3	2.00	0.43
1:C:581:SER:OG	1:C:583:LEU:HB2	2.18	0.43
1:A:78:ASN:HA	1:A:79:ALA:HA	1.64	0.42
1:A:497:ILE:HG23	1:A:501:PHE:CD1	2.53	0.42
1:B:590:VAL:HG11	1:B:609:VAL:HG21	2.01	0.42
1:C:426:ILE:N	1:C:427:PRO:HD2	2.34	0.42
1:D:183:LEU:CD2	1:D:241:LEU:HD11	2.48	0.42
1:D:390:LEU:C	1:D:392:ASN:H	2.27	0.42
1:A:90:VAL:HG12	1:A:102:VAL:CG2	2.49	0.42
1:A:154:PHE:CE2	1:A:251:VAL:HG22	2.54	0.42
1:A:373:TRP:NE1	1:A:407:ARG:HD2	2.34	0.42
1:B:59:LEU:HD12	1:B:60:LYS:N	2.34	0.42
1:C:78:ASN:HA	1:C:79:ALA:HA	1.64	0.42
1:C:521:ALA:HB2	2:C:1603:GOL:O2	2.19	0.42
1:A:413:VAL:CG1	1:A:417:CYS:HB3	2.49	0.42
1:D:443:VAL:CG2	1:D:496:MET:HE2	2.48	0.42
1:D:467:TYR:HD2	1:D:496:MET:HG3	1.84	0.42
1:A:277:LEU:HD13	1:A:334:VAL:HG21	2.01	0.42
1:C:719:PHE:CD1	1:C:719:PHE:N	2.85	0.42
1:D:408:LEU:HD23	1:D:408:LEU:N	2.34	0.42
1:D:428:ASP:OD1	1:D:428:ASP:N	2.50	0.42
1:A:400:VAL:HG11	1:A:409:THR:HG22	2.01	0.42
1:A:424:ILE:HG23	1:A:430:ILE:HD13	2.01	0.42
1:C:133:ASP:O	1:C:517:PHE:HE2	2.02	0.42
1:D:91:ALA:HB2	1:D:102:VAL:HG11	2.01	0.42
1:D:587:GLU:O	1:D:620:VAL:HG22	2.18	0.42
1:C:432:TYR:HB3	1:C:434:HIS:CD2	2.54	0.42
1:C:527:GLU:HB3	1:C:532:HIS:CE1	2.54	0.42
1:A:170:ILE:HD12	1:A:259:THR:CG2	2.50	0.42
1:A:515:PHE:CD1	1:A:536:VAL:HB	2.55	0.42
1:C:1:ARG:HD2	1:C:149:VAL:HG12	2.01	0.42
1:C:78:ASN:CA	1:C:96:GLY:HA3	2.48	0.42
1:C:361:VAL:O	1:C:365:TYR:HB2	2.20	0.42
1:D:150:ASN:CB	1:D:248:VAL:HG13	2.50	0.42
1:D:225:LEU:HD23	1:D:225:LEU:N	2.29	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:PHE:HD1	1:D:457:PHE:N	2.17	0.42
1:B:181:VAL:O	1:B:214:THR:HB	2.20	0.42
1:B:413:VAL:HG12	1:B:414:VAL:O	2.18	0.42
1:D:74:LEU:HG	1:D:144:VAL:HG22	2.00	0.42
1:A:74:LEU:HD22	1:A:100:TRP:CZ2	2.54	0.42
1:A:466:GLU:OE1	3:A:802:BDP:H1	2.19	0.42
1:B:469:CYS:HB3	1:B:489:GLN:HG3	2.00	0.42
1:B:551:LYS:HD3	1:B:559:PHE:CD2	2.54	0.42
1:C:170:ILE:N	1:C:170:ILE:HD13	2.35	0.42
1:C:269:ILE:HD13	1:C:274:GLU:HA	2.02	0.42
1:C:604:PHE:CD1	1:C:604:PHE:N	2.88	0.42
1:D:264:PRO:HD3	1:D:461:PRO:HG3	2.02	0.42
1:A:357:MET:HE1	1:A:374:GLY:O	2.20	0.42
1:A:424:ILE:O	1:A:424:ILE:HG22	2.19	0.42
1:B:74:LEU:HD12	1:B:74:LEU:N	2.35	0.42
1:C:277:LEU:O	1:C:508:ALA:HA	2.20	0.42
1:C:619:ALA:O	1:C:625:LYS:HA	2.20	0.42
1:D:94:ASP:HB3	1:D:127:VAL:HG13	2.01	0.42
1:B:177:VAL:HG23	1:B:177:VAL:O	2.19	0.41
1:C:534:GLY:O	1:C:544:LYS:HD2	2.19	0.41
1:D:12:PHE:CZ	1:D:36:TRP:HB3	2.54	0.41
1:B:474:TRP:CH2	2:B:803:GOL:H32	2.56	0.41
1:C:1:ARG:HD2	1:C:149:VAL:CG1	2.50	0.41
1:A:512:TRP:NE1	3:A:802:BDP:H5	2.36	0.41
1:B:493:HIS:HE1	1:B:511:VAL:HG23	1.86	0.41
1:B:504:LYS:O	1:B:504:LYS:HG2	2.20	0.41
1:C:326:ASP:O	1:C:330:GLU:HG3	2.20	0.41
1:C:611:ASN:ND2	1:C:632:LYS:HD2	2.34	0.41
1:C:617:LEU:HD11	1:C:630:ILE:CG2	2.51	0.41
1:D:190:GLN:OE1	1:D:192:LEU:HD11	2.20	0.41
1:D:192:LEU:HA	1:D:240:ALA:O	2.20	0.41
1:D:265:GLU:OE1	1:D:265:GLU:HA	2.19	0.41
1:D:345:HIS:CE1	1:D:389:LEU:HA	2.55	0.41
1:A:227:ASN:OD1	1:A:270:LEU:HD22	2.20	0.41
1:A:305:ILE:HG12	1:A:514:MET:HE2	1.97	0.41
1:A:467:TYR:OH	1:A:511:VAL:HG22	2.20	0.41
1:C:73:GLU:HB3	1:C:145:ASN:HB2	2.02	0.41
1:C:399:MET:HE2	1:C:399:MET:HB3	1.84	0.41
1:C:494:GLU:OE2	1:C:580:TYR:OH	2.29	0.41
1:C:562:LEU:HD23	1:C:579:VAL:HG22	2.03	0.41
1:D:32:LEU:HD12	1:D:34:HIS:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:PRO:CB	1:D:292:ALA:HB1	2.49	0.41
1:D:312:THR:HA	1:D:334:VAL:O	2.19	0.41
1:A:225:LEU:HD13	1:A:271:ASN:CG	2.45	0.41
1:B:419:ILE:CG2	1:B:453:PHE:HD2	2.33	0.41
1:C:147:ILE:HG22	1:C:149:VAL:HG13	2.02	0.41
1:C:343:SER:O	1:C:379:ILE:HD12	2.21	0.41
1:C:414:VAL:HG13	1:C:417:CYS:HB2	2.03	0.41
1:D:308:LEU:C	1:D:308:LEU:HD23	2.46	0.41
1:D:469:CYS:HB3	1:D:489:GLN:HG3	2.01	0.41
1:D:533:LYS:HE3	3:D:801:BDP:O6B	2.20	0.41
1:A:314:ARG:NH1	1:A:466:GLU:HG3	2.36	0.41
1:A:472:LEU:HB2	1:A:474:TRP:CD1	2.55	0.41
1:B:533:LYS:HZ2	3:B:804:BDP:C6	2.32	0.41
1:C:521:ALA:CB	2:C:1603:GOL:H2	2.51	0.41
1:A:341:TYR:CD1	1:A:379:ILE:HD11	2.56	0.41
1:C:305:ILE:HG12	1:C:514:MET:HE2	1.99	0.41
1:C:339:ILE:HB	1:C:340:PRO:HD2	2.03	0.41
1:C:410:THR:OG1	1:C:411:ILE:N	2.54	0.41
1:C:426:ILE:N	1:C:427:PRO:CD	2.84	0.41
1:A:302:ILE:HD13	1:A:327:LEU:HB3	2.02	0.41
1:B:277:LEU:O	1:B:508:ALA:HA	2.20	0.41
1:C:64:LEU:HD12	1:C:64:LEU:HA	1.83	0.41
1:C:335:ILE:HD13	1:C:335:ILE:HA	1.88	0.41
1:A:268:PHE:CG	1:A:277:LEU:HG	2.56	0.41
1:A:497:ILE:HG13	1:A:497:ILE:H	1.63	0.41
1:B:426:ILE:HB	1:B:427:PRO:HD3	2.01	0.41
1:C:10:TRP:CE3	1:C:55:TYR:HB3	2.55	0.41
1:C:58:GLN:NE2	1:C:112:GLU:HB3	2.35	0.41
1:C:170:ILE:HD11	1:C:257:CYS:HB3	2.02	0.41
1:C:198:ASP:HB3	1:C:202:LYS:H	1.86	0.41
1:C:512:TRP:HA	1:C:513:ASN:HA	1.78	0.41
1:C:530:GLN:NE2	1:C:538:PHE:CB	2.76	0.41
1:C:730:ALA:HB3	5:C:1601:ZG5:C22	2.51	0.41
1:D:213:GLU:H	1:D:213:GLU:HG2	1.61	0.41
1:D:562:LEU:HD12	1:D:626:ASP:C	2.46	0.41
1:A:562:LEU:CD1	1:A:628:SER:HB2	2.50	0.41
1:B:315:LEU:HB3	1:B:320:HIS:CD2	2.56	0.41
1:B:496:MET:O	1:B:500:LEU:HG	2.21	0.41
1:C:64:LEU:HD12	1:C:65:PRO:HD2	2.03	0.41
1:C:340:PRO:O	1:C:342:ILE:HG22	2.20	0.41
1:D:83:VAL:O	1:D:90:VAL:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:VAL:O	1:D:239:VAL:HA	2.21	0.41
1:D:305:ILE:HD12	1:D:313:ILE:HD13	2.03	0.41
1:A:64:LEU:HD12	1:A:64:LEU:HA	1.89	0.40
1:B:411:ILE:CG2	1:B:427:PRO:HG3	2.51	0.40
1:B:619:ALA:O	1:B:625:LYS:HA	2.21	0.40
1:C:354:ILE:HG23	1:C:399:MET:SD	2.61	0.40
1:A:315:LEU:HD12	1:A:325:TYR:CE1	2.56	0.40
1:A:364:ASN:HA	1:A:367:HIS:HD2	1.85	0.40
1:A:611:ASN:HD21	1:A:632:LYS:HA	1.87	0.40
1:B:365:TYR:CE2	1:B:404:ASP:OD1	2.75	0.40
1:B:494:GLU:HG2	1:B:604:PHE:CE2	2.55	0.40
1:C:284:GLN:HG2	1:C:318:TYR:OH	2.22	0.40
1:C:291:ASN:OD1	1:C:291:ASN:N	2.54	0.40
1:B:41:GLY:HA3	1:B:135:THR:HG21	2.04	0.40
1:B:280:VAL:O	1:B:313:ILE:HA	2.21	0.40
1:B:494:GLU:HG2	1:B:604:PHE:CD2	2.56	0.40
1:C:603:HIS:C	1:C:604:PHE:HD1	2.29	0.40
1:D:6:PHE:HB3	1:D:144:VAL:O	2.22	0.40
1:D:226:TRP:N	1:D:257:CYS:O	2.41	0.40
1:D:446:ASN:CG	1:D:496:MET:HE1	2.46	0.40
1:A:275:TYR:CD1	1:A:275:TYR:C	2.99	0.40
1:A:590:VAL:HG22	1:A:617:LEU:HD22	2.03	0.40
1:B:110:GLU:O	1:B:113:ASN:ND2	2.54	0.40
1:C:167:THR:O	1:C:167:THR:OG1	2.34	0.40
1:C:403:MET:HE3	1:C:403:MET:HB3	1.96	0.40
1:C:463:GLY:HA2	1:C:506:ILE:HG23	2.02	0.40
1:D:590:VAL:HG13	1:D:590:VAL:O	2.21	0.40
1:B:33:PRO:HB3	1:B:141:TYR:O	2.21	0.40
1:B:560:VAL:O	1:B:626:ASP:HB2	2.22	0.40
1:B:590:VAL:HG11	1:B:609:VAL:CG2	2.51	0.40
1:B:591:ASN:HD21	1:B:615:SER:HA	1.86	0.40
1:C:213:GLU:HG3	1:C:215:LYS:O	2.21	0.40
1:C:549:ALA:HB2	1:C:580:TYR:CE2	2.56	0.40
1:C:586:VAL:HG22	1:C:621:ALA:HB2	2.04	0.40
1:D:99:THR:O	1:D:160:GLY:HA3	2.22	0.40
1:D:378:GLU:HB3	1:D:414:VAL:HB	2.03	0.40
1:D:571:VAL:HG22	1:D:633:VAL:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	631/757 (83%)	581 (92%)	49 (8%)	1 (0%)	43	72
1	B	642/757 (85%)	596 (93%)	43 (7%)	3 (0%)	24	54
1	C	653/757 (86%)	609 (93%)	44 (7%)	0	100	100
1	D	605/757 (80%)	545 (90%)	59 (10%)	1 (0%)	43	72
All	All	2531/3028 (84%)	2331 (92%)	195 (8%)	5 (0%)	43	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	9	LYS
1	D	221	PRO
1	A	9	LYS
1	B	506	ILE
1	B	584	PRO

5.3.2 Protein sidechains

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	539/642 (84%)	530 (98%)	9 (2%)	53	82
1	B	537/642 (84%)	530 (99%)	7 (1%)	61	86
1	C	549/642 (86%)	536 (98%)	13 (2%)	43	75
1	D	504/642 (78%)	489 (97%)	15 (3%)	36	70
All	All	2129/2568 (83%)	2085 (98%)	44 (2%)	47	77

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	VAL
1	A	112	GLU
1	A	156	LEU
1	A	220	ILE
1	A	289	ILE
1	A	362	VAL
1	A	414	VAL
1	A	423	TYR
1	A	430	ILE
1	B	18	GLU
1	B	23	MET
1	B	152	SER
1	B	243	SER
1	B	364	ASN
1	B	384	SER
1	B	522	ARG
1	C	146	ILE
1	C	214	THR
1	C	281	SER
1	C	385	SER
1	C	403	MET
1	C	414	VAL
1	C	426	ILE
1	C	430	ILE
1	C	465	SER
1	C	535	LEU
1	C	615	SER
1	C	720	THR
1	C	723	ARG
1	D	98	SER
1	D	184	THR
1	D	213	GLU
1	D	236	THR
1	D	239	VAL
1	D	251	VAL
1	D	335	ILE
1	D	339	ILE
1	D	425	GLN
1	D	428	ASP
1	D	430	ILE
1	D	573	ASP
1	D	609	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	634	ASP
1	D	635	THR

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	145	ASN
1	A	298	HIS
1	A	322	GLN
1	A	392	ASN
1	A	446	ASN
1	B	603	HIS
1	B	629	HIS
1	C	58	GLN
1	C	131	ASN
1	C	481	GLN
1	C	530	GLN
1	C	629	HIS
1	D	392	ASN
1	D	420	HIS
1	D	473	ASN
1	D	475	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	FMN	C	1604	-	33,33,33	1.06	2 (6%)	48,50,50	1.29	8 (16%)
2	GOL	C	1603	-	5,5,5	0.78	0	5,5,5	1.01	0
2	GOL	B	803	-	5,5,5	0.66	0	5,5,5	0.89	0
2	GOL	C	1602	-	5,5,5	0.94	0	5,5,5	1.08	0
4	FMN	A	803	-	33,33,33	1.03	2 (6%)	48,50,50	1.22	6 (12%)
2	GOL	A	801	-	5,5,5	0.89	0	5,5,5	1.00	0
3	BDP	D	801	-	13,13,13	1.40	1 (7%)	18,19,19	1.09	1 (5%)
4	FMN	B	805	-	33,33,33	1.11	2 (6%)	48,50,50	1.36	11 (22%)
3	BDP	A	802	-	13,13,13	1.44	2 (15%)	18,19,19	2.12	4 (22%)
2	GOL	B	801	-	5,5,5	0.52	0	5,5,5	0.93	0
3	BDP	B	804	-	13,13,13	1.37	2 (15%)	18,19,19	1.55	3 (16%)
2	GOL	B	802	-	5,5,5	0.82	0	5,5,5	1.04	0
2	GOL	D	802	-	5,5,5	0.90	0	5,5,5	1.08	0
5	ZG5	C	1601	-	36,37,37	1.74	5 (13%)	47,54,54	3.08	16 (34%)

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	FMN	C	1604	-	-	9/18/18/18	0/3/3/3
2	GOL	C	1603	-	-	2/4/4/4	-
2	GOL	B	803	-	-	2/4/4/4	-
2	GOL	C	1602	-	-	0/4/4/4	-
4	FMN	A	803	-	-	7/18/18/18	0/3/3/3
2	GOL	A	801	-	-	2/4/4/4	-
3	BDP	D	801	-	-	1/4/24/24	0/1/1/1
4	FMN	B	805	-	-	8/18/18/18	0/3/3/3
3	BDP	A	802	-	-	1/4/24/24	0/1/1/1
2	GOL	B	801	-	-	2/4/4/4	-
3	BDP	B	804	-	-	0/4/24/24	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	802	-	-	0/4/4/4	-
2	GOL	D	802	-	-	2/4/4/4	-
5	ZG5	C	1601	-	-	7/12/54/54	0/4/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1601	ZG5	C11-N10	6.66	1.51	1.37
5	C	1601	ZG5	C11-N12	3.93	1.32	1.29
4	B	805	FMN	C4A-N5	3.37	1.38	1.30
4	C	1604	FMN	C4A-N5	3.36	1.38	1.30
4	A	803	FMN	C4A-N5	3.33	1.37	1.30
3	A	802	BDP	O5-C1	3.21	1.50	1.42
3	D	801	BDP	O5-C1	3.01	1.50	1.42
3	B	804	BDP	O5-C1	2.93	1.50	1.42
5	C	1601	ZG5	C18-S19	2.91	1.80	1.78
4	B	805	FMN	C10-N1	2.81	1.38	1.33
5	C	1601	ZG5	C20-S19	2.80	1.80	1.78
5	C	1601	ZG5	C25-C20	-2.74	1.36	1.40
4	C	1604	FMN	C10-N1	2.70	1.38	1.33
4	A	803	FMN	C10-N1	2.64	1.38	1.33
3	A	802	BDP	O5-C5	2.29	1.47	1.43
3	B	804	BDP	O5-C5	2.09	1.47	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1601	ZG5	N10-C11-N12	-12.79	108.31	118.22
5	C	1601	ZG5	C13-N12-C11	10.25	137.04	122.98
3	A	802	BDP	C1-O5-C5	4.83	119.32	112.22
5	C	1601	ZG5	C20-C25-C11	4.57	129.94	121.90
5	C	1601	ZG5	C26-C27-N07	4.34	118.24	110.61
5	C	1601	ZG5	C18-C13-N12	3.87	128.25	123.47
3	A	802	BDP	O5-C1-C2	3.82	117.02	110.30
5	C	1601	ZG5	C22-C23-C24	-3.78	115.57	120.24
3	A	802	BDP	O5-C5-C4	3.69	116.78	109.48
5	C	1601	ZG5	C23-C24-C25	3.47	126.06	119.80
5	C	1601	ZG5	C25-C11-N12	-3.42	122.91	125.98
3	B	804	BDP	O5-C1-C2	3.38	116.25	110.30
3	A	802	BDP	O2-C2-C3	-3.35	102.49	110.38
4	A	803	FMN	C4-N3-C2	-3.18	120.00	125.64
4	C	1604	FMN	C4-N3-C2	-3.15	120.05	125.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1601	ZG5	C26-N10-C09	-3.13	106.31	112.68
4	B	805	FMN	C4-N3-C2	-3.12	120.10	125.64
5	C	1601	ZG5	C20-S19-C18	2.95	110.61	99.96
4	B	805	FMN	C5A-C9A-N10	2.92	120.61	117.97
4	A	803	FMN	C4A-C10-N10	2.77	120.45	116.48
4	C	1604	FMN	C5'-C4'-C3'	-2.74	107.05	112.22
3	B	804	BDP	O2-C2-C3	-2.73	103.94	110.38
3	D	801	BDP	O2-C2-C3	-2.72	103.97	110.38
4	C	1604	FMN	C4A-C10-N10	2.65	120.27	116.48
5	C	1601	ZG5	O33-C32-C30	-2.61	104.23	110.38
4	A	803	FMN	C4A-C4-N3	2.60	119.86	113.25
3	B	804	BDP	C1-C2-C3	2.58	115.62	110.36
4	C	1604	FMN	C4A-C4-N3	2.58	119.82	113.25
4	B	805	FMN	C4A-C10-N1	-2.44	118.60	124.59
4	C	1604	FMN	O4-C4-C4A	-2.44	120.09	126.53
4	A	803	FMN	O4-C4-C4A	-2.43	120.13	126.53
4	B	805	FMN	C4A-C4-N3	2.42	119.41	113.25
4	B	805	FMN	O4-C4-C4A	-2.41	120.16	126.53
4	B	805	FMN	C4-C4A-C10	2.41	121.07	116.93
4	B	805	FMN	C1'-C2'-C3'	2.41	116.20	109.66
5	C	1601	ZG5	O05-C04-C02	2.38	113.59	106.14
4	B	805	FMN	C4A-C10-N10	2.38	119.89	116.48
4	A	803	FMN	C10-C4A-N5	-2.33	120.04	124.81
5	C	1601	ZG5	C15-C14-C13	2.33	123.25	118.97
4	C	1604	FMN	C10-C4A-N5	-2.32	120.08	124.81
5	C	1601	ZG5	O31-C30-C32	-2.31	104.94	110.38
4	C	1604	FMN	C4A-C10-N1	-2.30	118.94	124.59
4	C	1604	FMN	C5A-C9A-N10	2.28	120.03	117.97
5	C	1601	ZG5	C24-C25-C11	-2.23	113.54	119.00
5	C	1601	ZG5	C14-C13-C18	-2.22	115.77	118.95
4	A	803	FMN	C4A-C10-N1	-2.19	119.21	124.59
4	B	805	FMN	C10-C4A-N5	-2.18	120.35	124.81
4	B	805	FMN	C9A-C5A-N5	-2.16	120.17	122.45
4	B	805	FMN	O4'-C4'-C3'	2.03	114.01	109.25

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	C1-C2-C3-O3
2	B	803	GOL	C1-C2-C3-O3
2	B	803	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

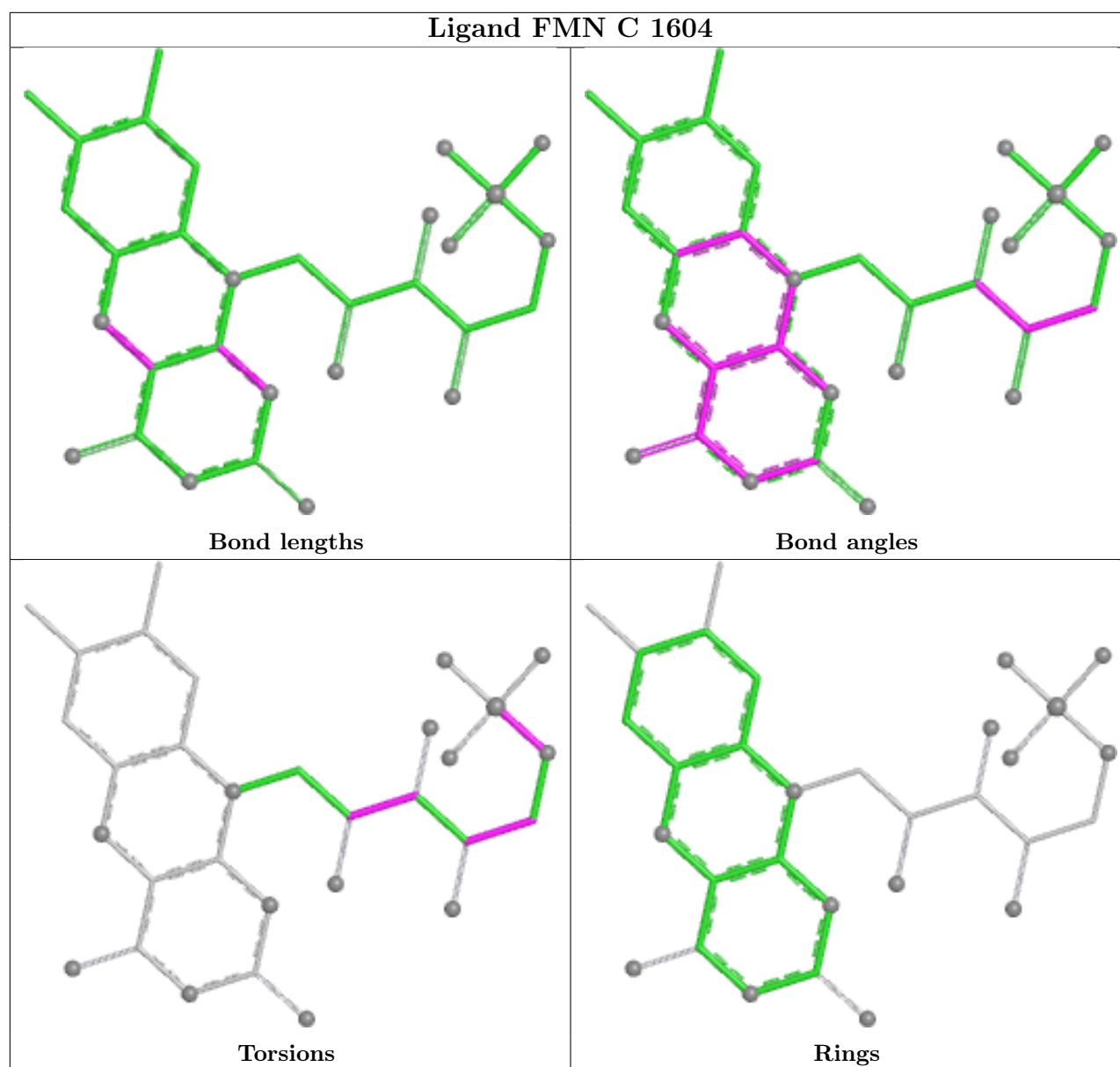
Mol	Chain	Res	Type	Atoms
2	D	802	GOL	C1-C2-C3-O3
4	A	803	FMN	C1'-C2'-C3'-O3'
4	A	803	FMN	C1'-C2'-C3'-C4'
4	A	803	FMN	O2'-C2'-C3'-O3'
4	A	803	FMN	O2'-C2'-C3'-C4'
4	A	803	FMN	C5'-O5'-P-O1P
4	A	803	FMN	C5'-O5'-P-O2P
4	B	805	FMN	C1'-C2'-C3'-O3'
4	B	805	FMN	C1'-C2'-C3'-C4'
4	B	805	FMN	O2'-C2'-C3'-O3'
4	B	805	FMN	O2'-C2'-C3'-C4'
4	B	805	FMN	C2'-C3'-C4'-O4'
4	B	805	FMN	C2'-C3'-C4'-C5'
4	B	805	FMN	O3'-C3'-C4'-O4'
4	B	805	FMN	O3'-C3'-C4'-C5'
4	C	1604	FMN	C1'-C2'-C3'-O3'
4	C	1604	FMN	C1'-C2'-C3'-C4'
4	C	1604	FMN	O2'-C2'-C3'-O3'
4	C	1604	FMN	O2'-C2'-C3'-C4'
4	C	1604	FMN	C3'-C4'-C5'-O5'
4	C	1604	FMN	O4'-C4'-C5'-O5'
4	C	1604	FMN	C5'-O5'-P-O1P
4	C	1604	FMN	C5'-O5'-P-O2P
4	C	1604	FMN	C5'-O5'-P-O3P
5	C	1601	ZG5	C28-C06-N07-C08
5	C	1601	ZG5	C28-C06-N07-C27
5	C	1601	ZG5	O05-C06-N07-C27
5	C	1601	ZG5	N12-C11-N10-C09
2	C	1603	GOL	C1-C2-C3-O3
5	C	1601	ZG5	N12-C11-N10-C26
2	A	801	GOL	O2-C2-C3-O3
2	D	802	GOL	O2-C2-C3-O3
2	B	801	GOL	C1-C2-C3-O3
3	A	802	BDP	O5-C5-C6-O6A
5	C	1601	ZG5	O01-C02-C04-O05
5	C	1601	ZG5	O05-C06-N07-C08
2	C	1603	GOL	O2-C2-C3-O3
4	A	803	FMN	C5'-O5'-P-O3P
3	D	801	BDP	O5-C5-C6-O6B
2	B	801	GOL	O2-C2-C3-O3

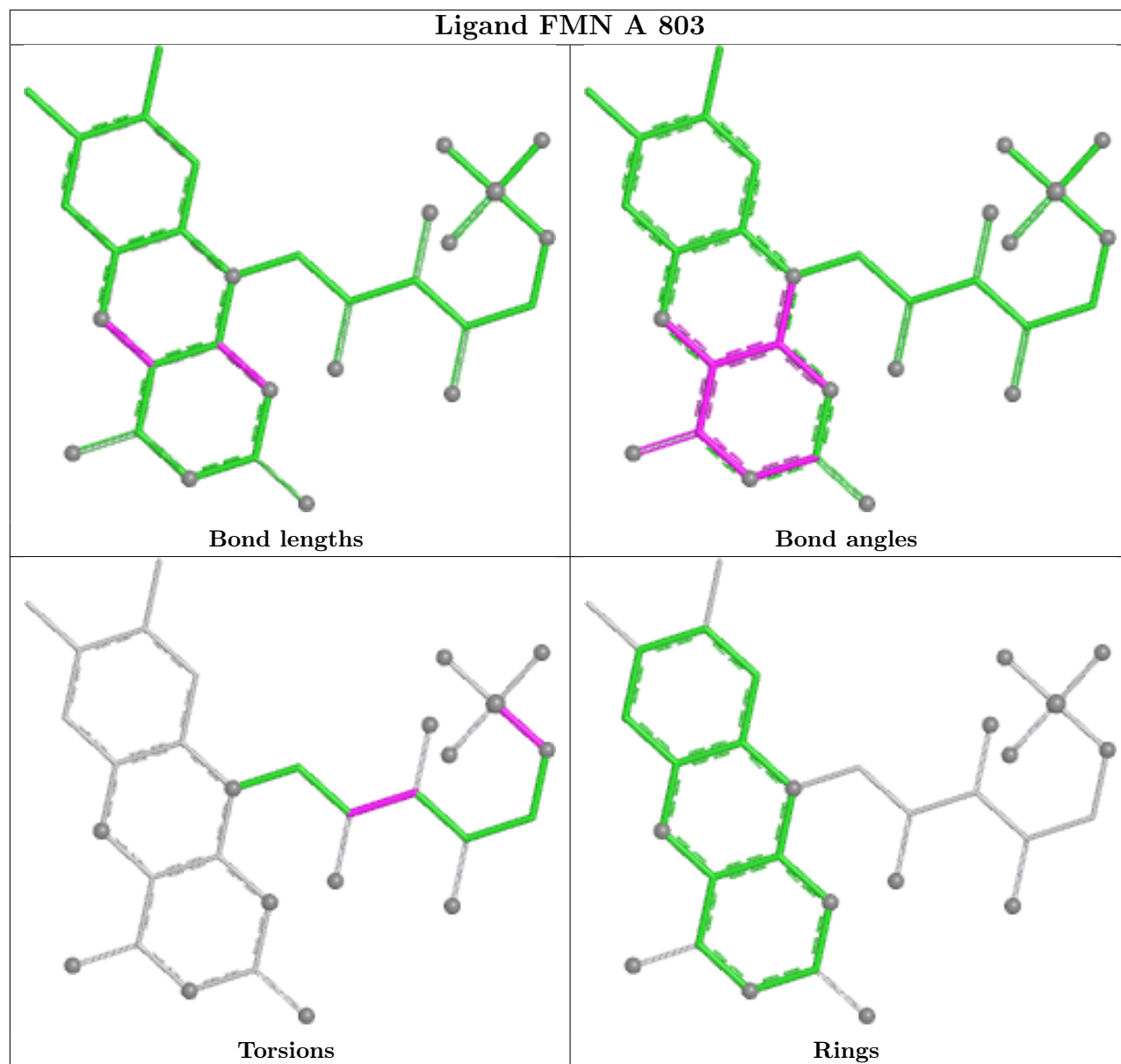
There are no ring outliers.

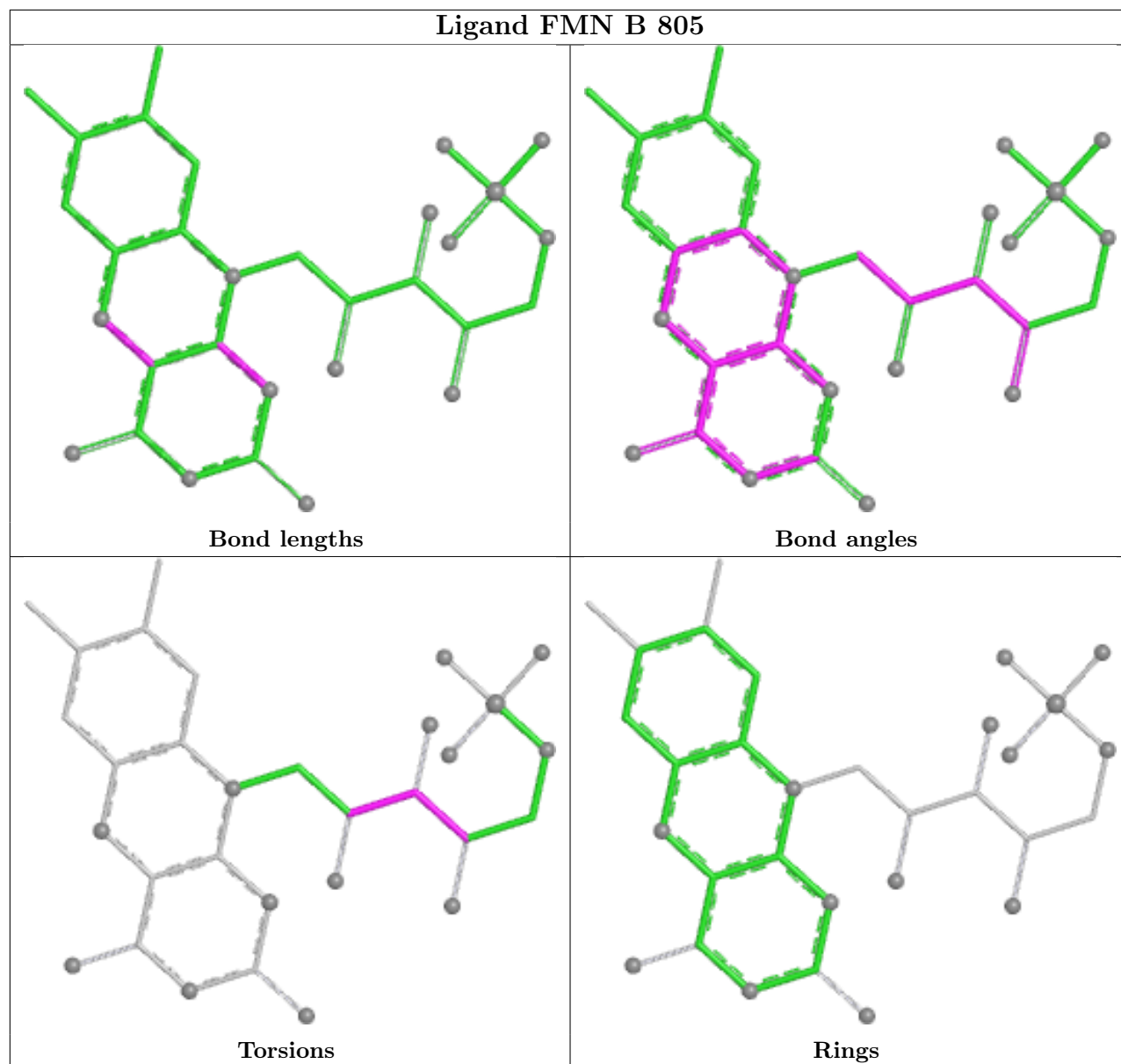
11 monomers are involved in 21 short contacts:

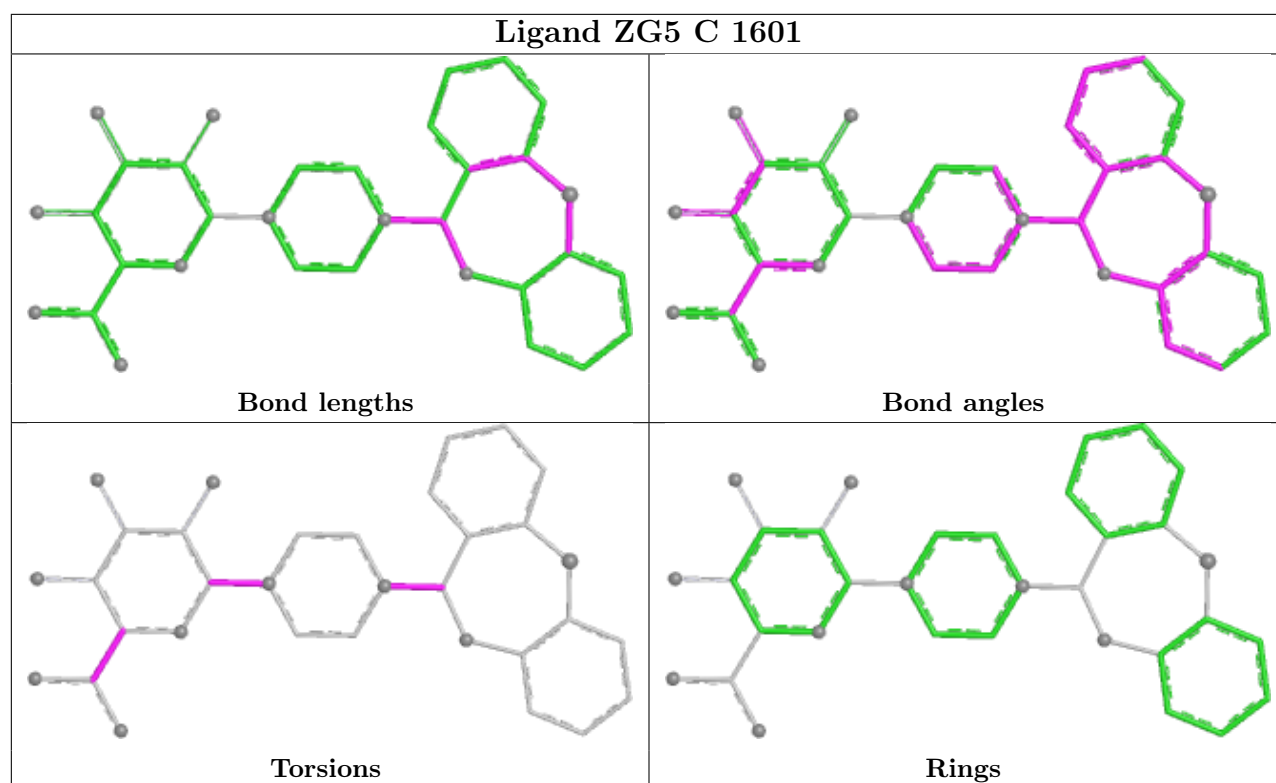
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1604	FMN	2	0
2	C	1603	GOL	3	0
2	B	803	GOL	1	0
2	C	1602	GOL	2	0
4	A	803	FMN	1	0
2	A	801	GOL	1	0
3	D	801	BDP	1	0
4	B	805	FMN	4	0
3	A	802	BDP	2	0
3	B	804	BDP	3	0
5	C	1601	ZG5	1	0

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 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	639/757 (84%)	-0.02	6 (0%) 81 75	30, 62, 92, 135	0
1	B	644/757 (85%)	0.04	6 (0%) 81 75	30, 65, 92, 119	0
1	C	659/757 (87%)	-0.06	4 (0%) 85 81	41, 60, 94, 127	1 (0%)
1	D	623/757 (82%)	0.50	36 (5%) 29 22	30, 77, 110, 137	0
All	All	2565/3028 (84%)	0.11	52 (2%) 65 56	30, 66, 99, 137	1 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	440	GLY	6.1
1	D	186	ALA	5.0
1	A	210	ALA	4.2
1	C	718	GLY	4.1
1	D	210	ALA	3.8
1	D	375	LEU	3.7
1	D	182	PHE	3.5
1	D	200	GLU	3.5
1	D	243	SER	3.3
1	D	158	TYR	3.3
1	D	211	ALA	3.3
1	D	336	TRP	3.2
1	D	247	ALA	3.2
1	D	199	ALA	3.1
1	D	197	LYS	3.0
1	D	529	GLY	3.0
1	D	195	THR	2.9
1	D	149	VAL	2.8
1	D	163	GLY	2.7
1	D	212	GLY	2.7
1	D	241	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	223	VAL	2.6
1	D	249	ASP	2.6
1	D	222	ALA	2.6
1	A	437	GLY	2.5
1	B	610	PRO	2.5
1	D	374	GLY	2.5
1	D	430	ILE	2.5
1	B	112	GLU	2.5
1	D	431	SER	2.5
1	D	406	THR	2.5
1	D	96	GLY	2.4
1	A	65	PRO	2.4
1	D	126	ARG	2.3
1	D	423	TYR	2.3
1	B	643	LYS	2.3
1	B	512	TRP	2.3
1	D	224	HIS	2.3
1	C	207	THR	2.3
1	C	0	MET	2.3
1	D	194	TYR	2.3
1	D	128	TYR	2.2
1	B	609	VAL	2.2
1	D	348	ASN	2.2
1	D	248	VAL	2.2
1	B	629	HIS	2.1
1	D	198	ASP	2.1
1	A	0	MET	2.1
1	D	376	SER	2.1
1	A	248	VAL	2.1
1	D	237	ALA	2.1
1	D	169	GLU	2.1

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 oligosaccharides in this entry.

6.4 Ligands

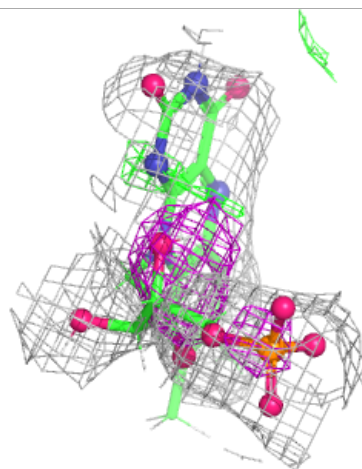
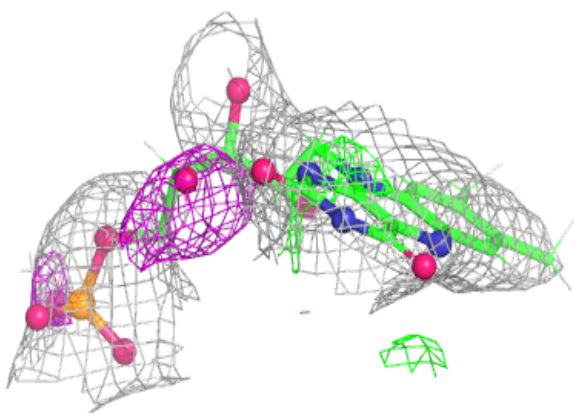
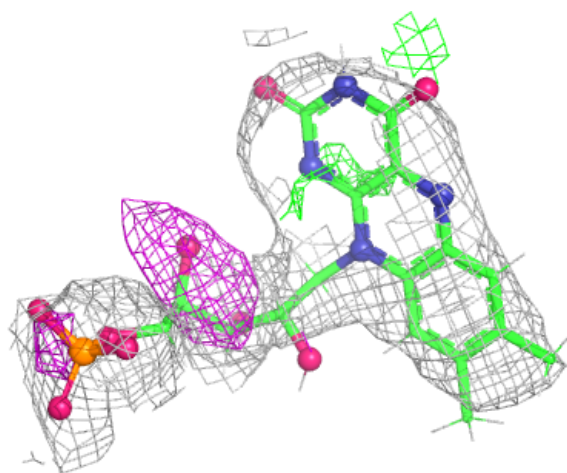
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	803	6/6	0.79	0.12	80,114,125,128	0
4	FMN	C	1604	31/31	0.80	0.13	78,91,104,123	0
3	BDP	B	804	13/13	0.82	0.19	55,67,95,98	22
3	BDP	D	801	13/13	0.83	0.16	83,100,127,142	22
2	GOL	B	801	6/6	0.85	0.12	76,103,117,120	0
2	GOL	A	801	6/6	0.85	0.16	64,91,118,118	0
4	FMN	A	803	31/31	0.85	0.11	77,87,96,111	0
2	GOL	D	802	6/6	0.85	0.16	67,97,115,115	0
2	GOL	C	1602	6/6	0.87	0.12	68,105,116,142	0
2	GOL	C	1603	6/6	0.89	0.15	55,82,102,102	0
3	BDP	A	802	13/13	0.89	0.12	53,67,86,101	22
4	FMN	B	805	31/31	0.90	0.10	63,78,93,102	0
5	ZG5	C	1601	33/33	0.91	0.14	43,67,97,107	0
2	GOL	B	802	6/6	0.95	0.18	55,83,98,101	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.

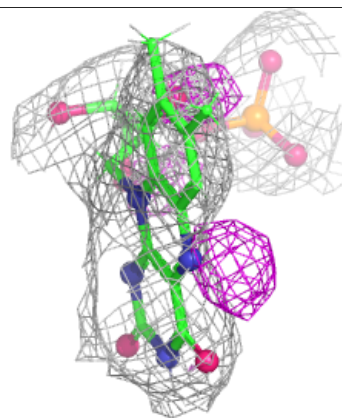
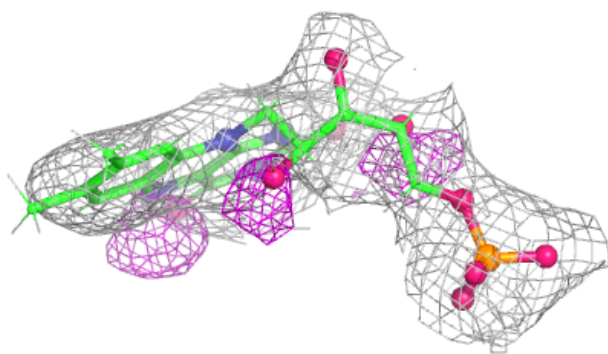
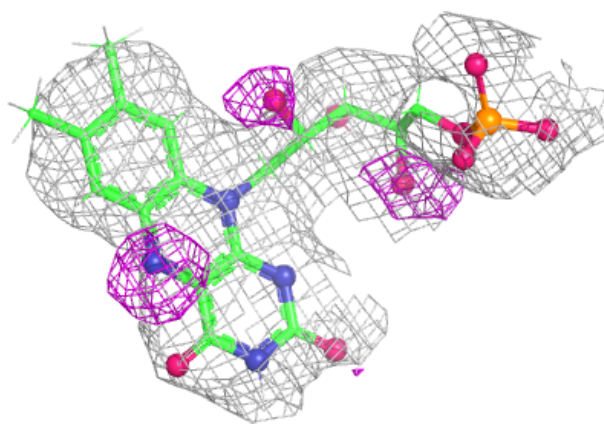
Electron density around FMN C 1604:

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



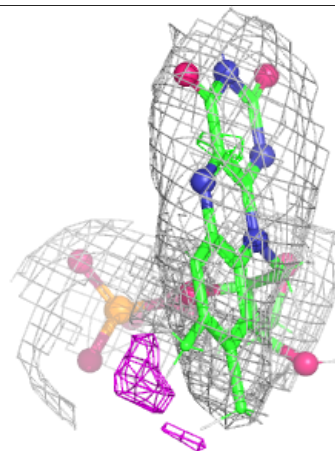
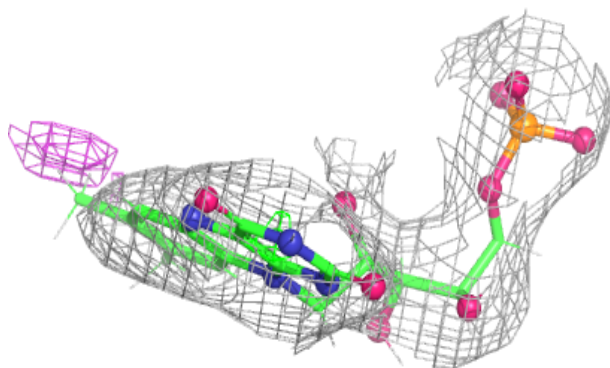
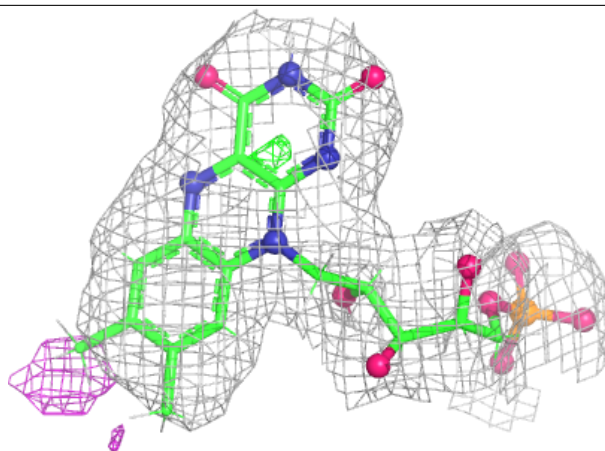
Electron density around FMN A 803:

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

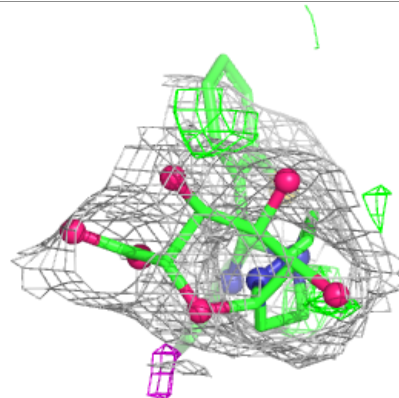
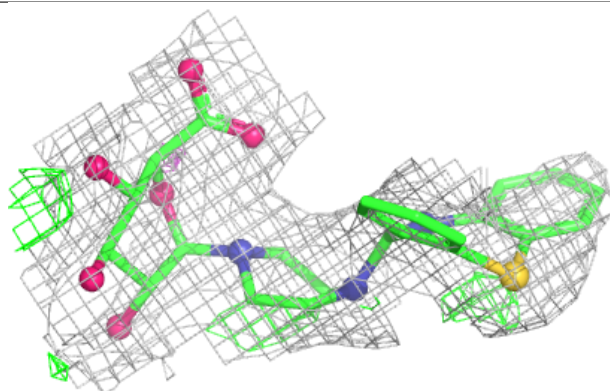
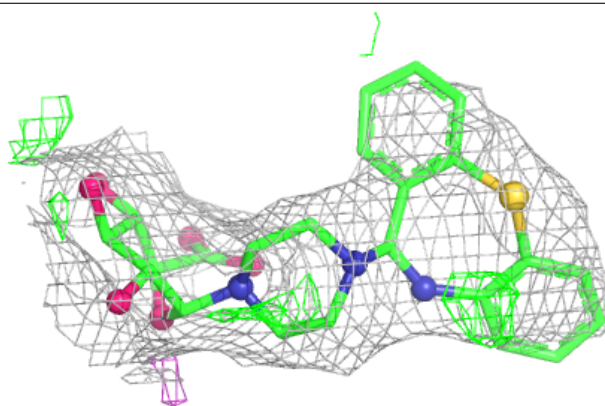


Electron density around FMN B 805:

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

**Electron density around ZG5 C 1601:**

$2mF_o-DF_c$ (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.