Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2020 – 05:36 PM BST

PDB ID	:	1L5R
Title	:	Human liver glycogen phosphorylase a complexed with riboflavin, N-Acetyl-beta-D-Glucopyranosylamine and CP-403,700
Authors	:	Ekstrom, J.L.; Pauly, T.A.; Carty, M.D.; Soeller, W.C.; Culp, J.; Danley, D.E.; Hoover, D.J.; Treadway, J.L.; Gibbs, E.M.; Fletterick, R.J.; Day, Y.S.N.; Myszka, D.G.; Rath, V.L.
Deposited on	:	2002-03-07
Resolution	:	2.10 Å(reported)

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

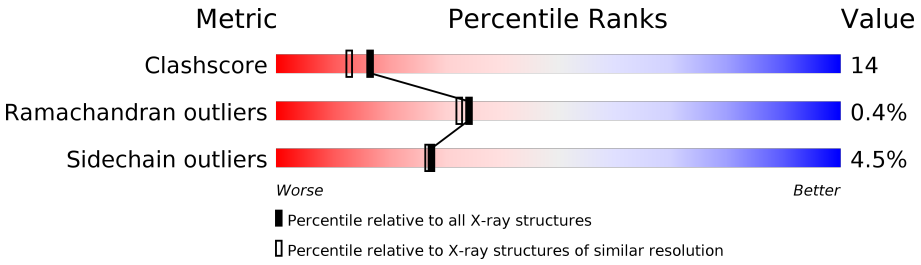
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	847	65% 26% • 7%
1	B	847	65% 27% • 7%

2 Entry composition

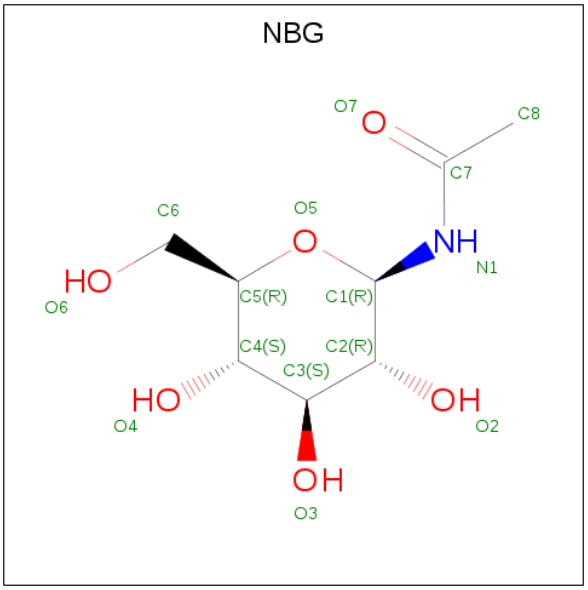
There are 7 unique types of molecules in this entry. The entry contains 13497 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called glycogen phosphorylase, liver form.

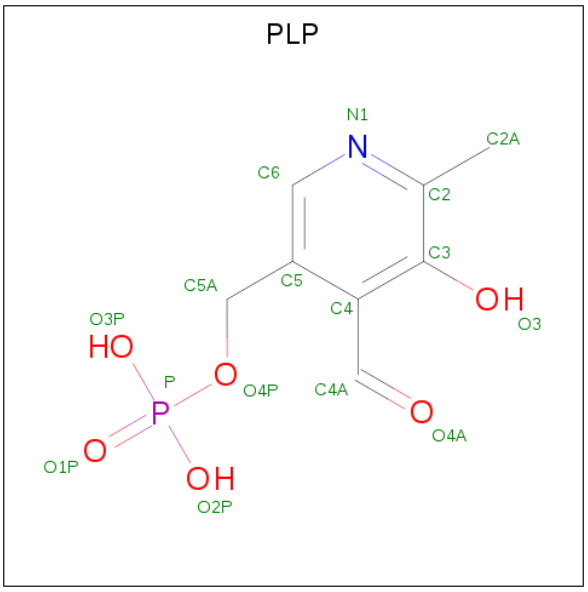
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	790	Total	C	N	O	S	0	0	0
			6417	4125	1089	1174	29			
1	B	791	Total	C	N	O	S	0	0	0
			6423	4128	1090	1176	29			

- Molecule 2 is N-acetyl-beta-D-glucopyranosylamine (three-letter code: NBG) (formula: $C_8H_{15}NO_6$).



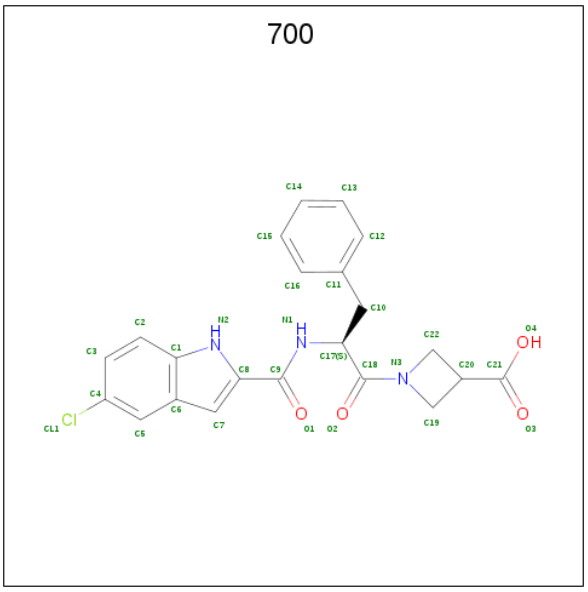
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



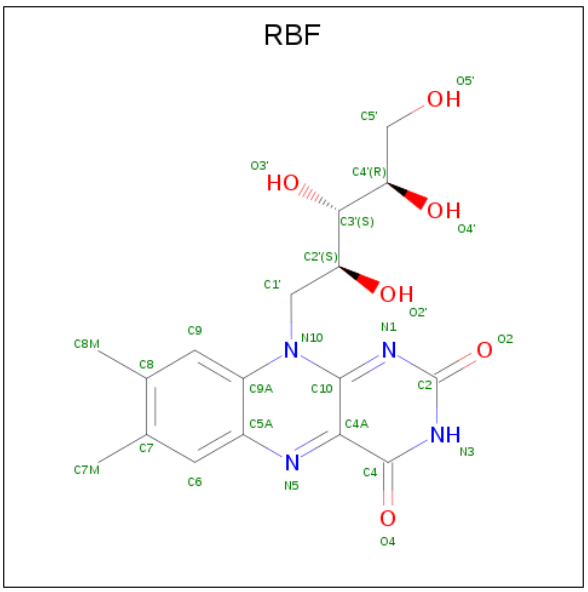
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is [5-CHLORO-1H-INDOL-2-CARBONYL-PHENYLALANINYL]-AZETIDINE -3-CARBOXYLIC ACID (three-letter code: 700) (formula: $C_{22}H_{20}ClN_3O_4$).



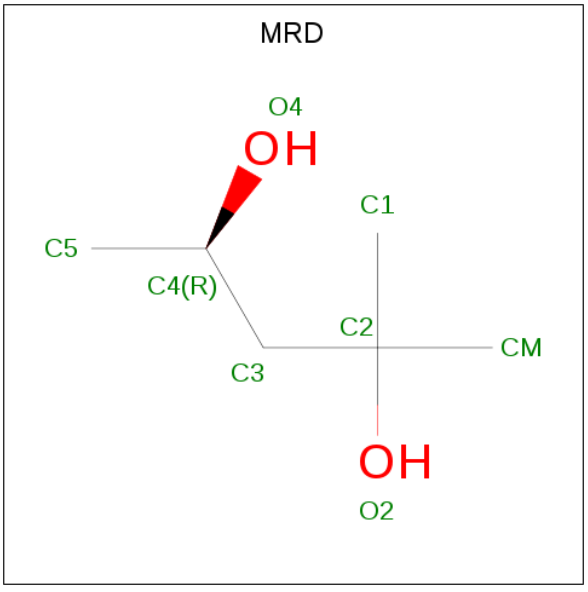
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is RIBOFLAVIN (three-letter code: RBF) (formula: $C_{17}H_{20}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			27	17	4	6		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	307	Total O 307 307	0	0
7	B	240	Total O 240 240	0	0

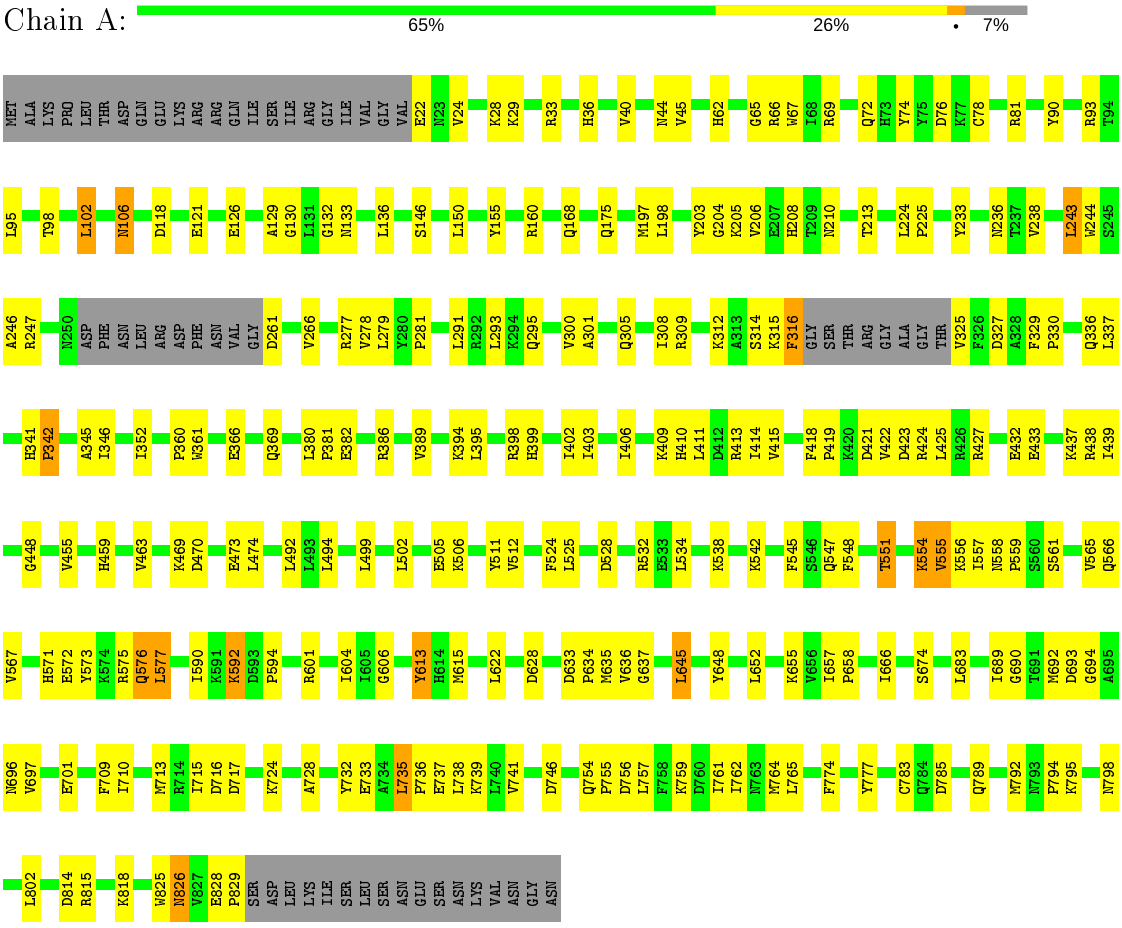
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

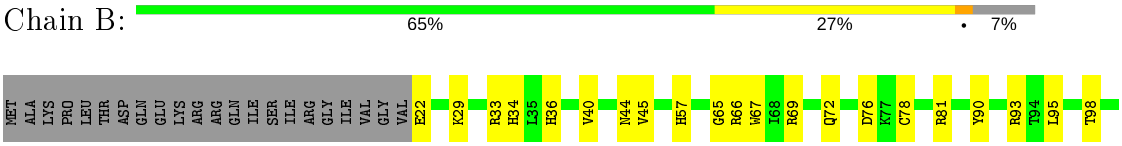
- Molecule 1: glycogen phosphorylase, liver form

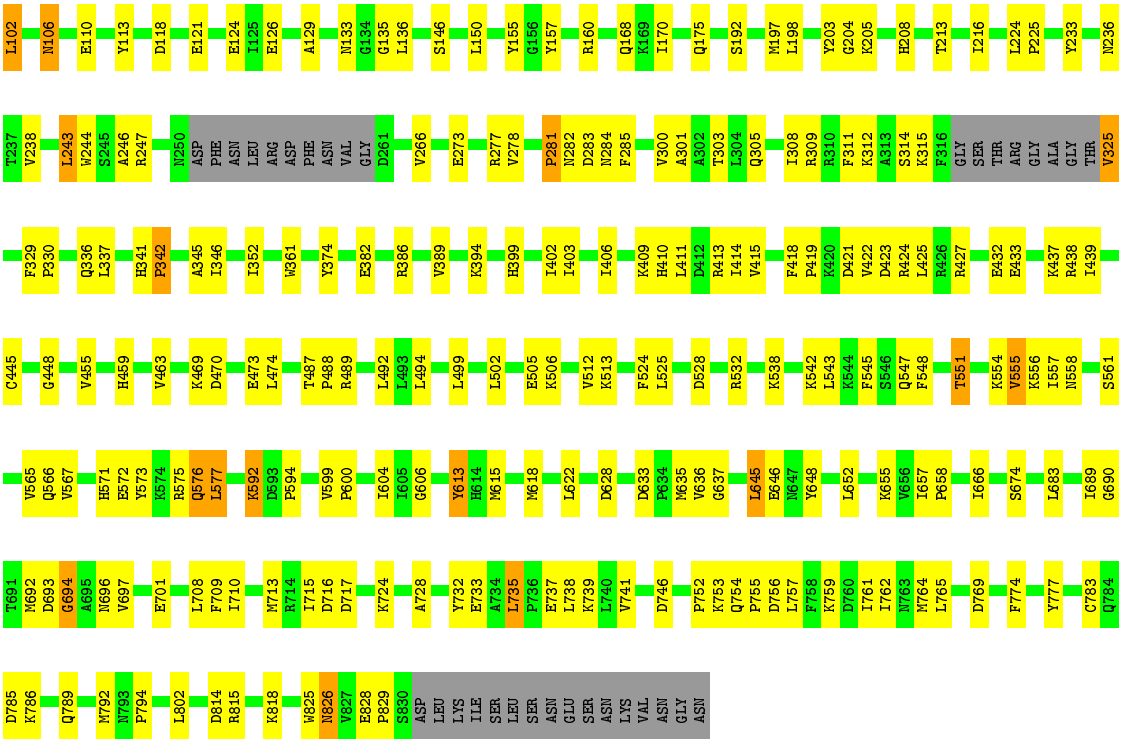
Chain A:



- Molecule 1: glycogen phosphorylase, liver form

Chain B:




L102 N106 E110 Y113 D118 E121 E124 I125 E126 A129 N133 G134 G135 L136 S146 L150 Y155 G156 Y157 R160 Q168 K169 I170 Q175 S192 M197 L198 Y203 G204 K205 H208 T213 I216 L224 P225 Y233 N236
T237 V238 L243 W244 S245 A246 R247 N280 ASP PHE ASN LEU ARG ASP PHE ASN VAL GLY D261 V266 E273 R277 V278 P281 N282 D283 N284 F285 V300 A301 A302 T303 L304 Q305 I308 R309 R310 F311 K312 A313 S314 K315 F316 GLY SER THR ARG GLY ALA GLY THR V325
F329 P330 Q336 L337 H341 P342 A345 I346 I352 W361 Y374 E382 R386 V389 K394 H399 I402 I403 I406 K409 H410 L411 D412 R413 I414 V415 F418 P419 K420 D421 V422 D423 R424 L425 R426 R427 E432 E433 K437 R438 I439
C445 G448 V455 H459 V463 K469 D470 E473 L474 T487 P488 R489 L492 L493 L494 L499 L502 E505 K506 V512 K513 F524 L525 D528 R532 K538 K542 L543 K544 F545 S546 Q547 F548 T551 K554 V555 K556 I557 N558 S561
V565 Q566 V567 H571 E572 Y573 K574 R575 Q576 L577 K592 D593 P594 V599 P600 I604 I605 G606 Y613 H614 M615 M618 L622 D628 D633 P634 M635 V636 G637 L645 E646 N647 Y648 L652 K655 V656 I657 P658 I666 S674 L683 I689 G690
T691 M692 D693 G694 A695 N696 V697 E701 L708 F709 I710 M713 R714 I715 D716 D717 K724 A728 Y732 E733 A734 L736 P736 E737 L738 K739 L740 V741 D746 P752 K753 Q754 P755 D756 L757 F758 K759 D760 I761 I762 N763 M764 L765 D769 F774 Y777 C783 Q784
D785 K786 Q789 M792 N793 P794 L802 D814 R815 K818 W825 N826 V827 E828 P829 S830 ASP LEU LYS ILE SER LEU SER ASN GLU SER ASN LYS VAL ASN GLY ASN

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	124.42Å 124.42Å 124.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.61 – 2.10	Depositor
% Data completeness (in resolution range)	95.5 (55.61-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13497	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, RBF, 700, NBG, PLP

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	0.44	0/6561	0.65	1/8873 (0.0%)
1	B	0.43	0/6567	0.65	1/8881 (0.0%)
All	All	0.43	0/13128	0.65	2/17754 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	129	ALA	N-CA-C	-5.82	95.29	111.00
1	A	129	ALA	N-CA-C	-5.38	96.47	111.00

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	6417	0	6412	191	0
1	B	6423	0	6417	183	0
2	A	15	0	15	0	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
4	A	30	0	18	0	0
5	A	27	0	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	0	14	0	0
7	A	307	0	0	28	0
7	B	240	0	0	18	0
All	All	13497	0	12910	368	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 14.

All (368) 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:110:GLU:HA	7:B:2505:HOH:O	1.65	0.93
1:B:113:TYR:HB3	7:B:2505:HOH:O	1.69	0.93
1:A:213:THR:HB	7:A:2504:HOH:O	1.70	0.91
1:A:710:ILE:HD13	7:A:2205:HOH:O	1.72	0.89
1:A:798:ASN:HB3	7:A:2061:HOH:O	1.72	0.87
1:A:247:ARG:HD3	7:A:2472:HOH:O	1.76	0.85
1:A:547:GLN:O	1:A:551:THR:HG23	1.76	0.85
1:B:547:GLN:O	1:B:551:THR:HG23	1.77	0.84
1:B:308:ILE:CD1	1:B:352:ILE:HG21	2.10	0.82
1:A:645:LEU:HD13	1:A:652:LEU:HD11	1.61	0.81
1:A:469:LYS:HG3	7:A:2489:HOH:O	1.81	0.79
1:B:645:LEU:HD13	1:B:652:LEU:HD11	1.62	0.79
1:A:645:LEU:CD1	1:A:652:LEU:HD11	2.13	0.79
1:A:308:ILE:CD1	1:A:352:ILE:HG21	2.13	0.78
1:B:645:LEU:CD1	1:B:652:LEU:HD11	2.15	0.76
1:A:278:VAL:HG21	1:B:266:VAL:HG11	1.69	0.74
1:A:279:LEU:HD22	7:A:2498:HOH:O	1.89	0.72
1:A:198:LEU:HD21	1:A:309:ARG:NH2	2.05	0.71
1:A:615:MET:CE	1:A:761:ILE:HG12	2.20	0.71
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.72	0.70
1:B:599:VAL:HB	7:B:2328:HOH:O	1.91	0.70
1:A:205:LYS:HB2	7:A:2292:HOH:O	1.91	0.70
1:B:615:MET:CE	1:B:761:ILE:HG12	2.21	0.69
1:A:279:LEU:CD2	7:A:2498:HOH:O	2.41	0.69
1:B:198:LEU:HD21	1:B:309:ARG:NH2	2.08	0.69
1:A:615:MET:HE1	1:A:761:ILE:HG12	1.73	0.68
1:A:130:GLY:O	7:A:2498:HOH:O	2.11	0.68
1:A:146:SER:O	1:A:150:LEU:HD13	1.92	0.68
1:B:433:GLU:HG2	1:B:437:LYS:HE2	1.76	0.68
1:A:433:GLU:HG2	1:A:437:LYS:HE2	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LYS:HG2	1:B:33:ARG:NH2	2.08	0.67
1:A:266:VAL:HG11	1:B:278:VAL:HG21	1.76	0.67
1:A:29:LYS:HG2	1:A:33:ARG:NH2	2.09	0.67
1:B:455:VAL:HG23	1:B:674:SER:HB2	1.76	0.67
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.77	0.67
1:A:532:ARG:HH11	1:A:532:ARG:HB2	1.60	0.67
1:B:532:ARG:HB2	1:B:532:ARG:HH11	1.58	0.67
1:B:455:VAL:H	1:B:459:HIS:HD2	1.43	0.66
1:A:594:PRO:HG3	1:A:635:MET:SD	2.34	0.66
1:B:146:SER:O	1:B:150:LEU:HD13	1.95	0.66
1:B:81:ARG:NH1	1:B:155:TYR:OH	2.29	0.66
1:A:325:VAL:HG12	1:A:327:ASP:H	1.62	0.65
1:A:534:LEU:HD23	7:A:2061:HOH:O	1.94	0.65
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.77	0.65
1:B:192:SER:HB3	7:B:2004:HOH:O	1.96	0.65
1:B:415:VAL:HG22	1:B:425:LEU:HD11	1.79	0.65
1:B:594:PRO:HG3	1:B:635:MET:SD	2.37	0.65
1:A:278:VAL:HG21	1:B:266:VAL:CG1	2.26	0.64
1:A:81:ARG:NH1	1:A:155:TYR:OH	2.30	0.64
1:A:415:VAL:HG22	1:A:425:LEU:HD11	1.79	0.64
1:A:409:LYS:O	1:A:413:ARG:HG2	1.97	0.64
1:A:455:VAL:H	1:A:459:HIS:HD2	1.43	0.64
1:B:469:LYS:O	1:B:473:GLU:HG3	1.97	0.63
1:A:278:VAL:CG2	1:B:266:VAL:HG11	2.28	0.63
1:B:828:GLU:HG3	1:B:829:PRO:HD2	1.80	0.63
1:A:386:ARG:NH2	1:A:438:ARG:HD2	2.14	0.63
1:A:455:VAL:HG23	1:A:674:SER:HB2	1.81	0.62
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.80	0.62
1:B:386:ARG:NH2	1:B:438:ARG:HD2	2.15	0.62
1:A:118:ASP:OD1	1:A:121:GLU:HG3	2.00	0.62
1:A:366:GLU:HA	7:A:2453:HOH:O	2.00	0.61
1:B:409:LYS:O	1:B:413:ARG:HG2	1.99	0.61
1:A:764:MET:SD	1:A:765:LEU:HD12	2.41	0.61
1:A:469:LYS:O	1:A:473:GLU:HG3	2.00	0.60
1:B:118:ASP:OD1	1:B:121:GLU:HG3	2.02	0.60
1:B:308:ILE:HD12	1:B:352:ILE:HG21	1.84	0.60
1:A:615:MET:HE3	1:A:615:MET:O	2.01	0.60
1:A:316:PHE:CD2	1:A:316:PHE:N	2.67	0.60
1:A:421:ASP:OD1	1:A:424:ARG:HD2	2.02	0.59
1:B:814:ASP:O	1:B:818:LYS:HG3	2.03	0.59
1:A:93:ARG:HG2	1:A:126:GLU:HG2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ILE:HD13	1:A:448:GLY:HA3	1.85	0.59
1:A:399:HIS:O	1:A:403:ILE:HG13	2.01	0.59
1:B:124:GLU:OE2	7:B:2413:HOH:O	2.16	0.58
1:B:470:ASP:O	1:B:474:LEU:HD13	2.03	0.58
1:B:615:MET:O	1:B:615:MET:HE3	2.02	0.58
1:A:369:GLN:HB2	7:A:2453:HOH:O	2.02	0.58
1:A:423:ASP:O	1:A:427:ARG:HG3	2.03	0.58
1:B:204:GLY:C	1:B:205:LYS:HD2	2.24	0.58
1:B:543:LEU:HB3	7:B:2406:HOH:O	2.04	0.58
1:A:233:TYR:CZ	1:A:512:VAL:HG11	2.39	0.58
1:A:814:ASP:O	1:A:818:LYS:HG3	2.04	0.57
1:B:399:HIS:O	1:B:403:ILE:HG13	2.03	0.57
1:B:386:ARG:HB3	1:B:438:ARG:HD3	1.85	0.57
1:B:422:VAL:HG23	1:B:423:ASP:N	2.19	0.57
1:B:433:GLU:CG	1:B:437:LYS:HE2	2.34	0.57
1:A:386:ARG:HB3	1:A:438:ARG:HD3	1.86	0.57
1:A:433:GLU:CG	1:A:437:LYS:HE2	2.35	0.57
1:B:785:ASP:O	1:B:789:GLN:HG2	2.05	0.57
1:A:266:VAL:CG1	1:B:278:VAL:HG21	2.34	0.56
1:A:325:VAL:HA	7:A:2508:HOH:O	2.04	0.56
1:A:330:PRO:HB2	7:A:2416:HOH:O	2.05	0.56
1:A:735:LEU:HD23	1:A:777:TYR:HD2	1.70	0.56
1:B:592:LYS:O	1:B:594:PRO:HD3	2.06	0.56
1:B:81:ARG:NH2	7:B:2240:HOH:O	2.35	0.56
1:A:470:ASP:O	1:A:474:LEU:HD13	2.05	0.56
1:B:752:PRO:HG2	7:B:2354:HOH:O	2.05	0.56
1:B:753:LYS:HG2	7:B:2354:HOH:O	2.06	0.56
1:A:421:ASP:CG	1:A:424:ARG:HB2	2.26	0.56
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.46	0.56
1:A:266:VAL:HG11	1:B:278:VAL:CG2	2.37	0.56
1:A:204:GLY:C	1:A:205:LYS:HD2	2.27	0.55
1:A:422:VAL:HG23	1:A:423:ASP:N	2.21	0.55
1:B:538:LYS:O	1:B:542:LYS:HG3	2.07	0.55
1:B:421:ASP:CG	1:B:424:ARG:HB2	2.27	0.55
1:B:309:ARG:NH2	7:B:2450:HOH:O	2.33	0.55
1:B:422:VAL:CG2	1:B:423:ASP:N	2.71	0.54
1:A:592:LYS:O	1:A:594:PRO:HD3	2.07	0.54
1:A:785:ASP:O	1:A:789:GLN:HG2	2.08	0.54
1:B:423:ASP:O	1:B:427:ARG:HG3	2.07	0.54
1:A:314:SER:O	1:A:315:LYS:HB3	2.07	0.54
1:B:421:ASP:OD1	1:B:424:ARG:HD2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:ARG:NH1	1:B:532:ARG:HB2	2.22	0.53
1:A:572:GLU:HG3	1:A:613:TYR:OH	2.08	0.53
1:B:118:ASP:HA	7:B:2363:HOH:O	2.07	0.53
1:A:132:GLY:N	7:A:2498:HOH:O	2.42	0.53
1:B:314:SER:O	1:B:315:LYS:HB3	2.07	0.53
1:A:106:ASN:HD22	1:A:106:ASN:N	2.06	0.53
1:A:532:ARG:NH1	1:A:532:ARG:HB2	2.23	0.53
1:A:538:LYS:O	1:A:542:LYS:HG3	2.08	0.53
1:B:106:ASN:N	1:B:106:ASN:HD22	2.07	0.53
1:A:422:VAL:CG2	1:A:423:ASP:N	2.71	0.53
1:B:565:VAL:HG22	1:B:604:ILE:HB	1.91	0.53
1:B:735:LEU:HD23	1:B:777:TYR:HD2	1.73	0.53
1:A:316:PHE:HD2	1:A:316:PHE:N	2.05	0.52
1:A:459:HIS:O	1:A:463:VAL:HG23	2.10	0.52
1:A:206:VAL:HG13	7:A:2504:HOH:O	2.08	0.52
1:B:93:ARG:HG2	1:B:126:GLU:HG2	1.92	0.52
1:B:697:VAL:O	1:B:701:GLU:HG3	2.10	0.52
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.50	0.52
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.40	0.52
1:B:308:ILE:HD12	1:B:352:ILE:HD13	1.92	0.52
1:A:565:VAL:HG22	1:A:604:ILE:HB	1.91	0.51
1:A:308:ILE:HD12	1:A:352:ILE:HG21	1.91	0.51
1:A:233:TYR:CE2	1:A:512:VAL:HG11	2.46	0.51
1:B:459:HIS:O	1:B:463:VAL:HG23	2.10	0.51
1:B:410:HIS:O	1:B:414:ILE:HD13	2.09	0.51
1:A:208:HIS:ND1	1:A:213:THR:HG22	2.26	0.51
1:A:22:GLU:HB3	1:A:62:HIS:HE1	1.76	0.51
1:A:735:LEU:CD1	1:A:735:LEU:N	2.73	0.51
1:B:208:HIS:ND1	1:B:213:THR:HG22	2.25	0.51
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.93	0.51
1:B:735:LEU:CD1	1:B:735:LEU:N	2.74	0.51
1:B:246:ALA:O	1:B:247:ARG:HD2	2.11	0.51
1:B:300:VAL:CG1	1:B:345:ALA:HA	2.41	0.50
1:A:410:HIS:O	1:A:414:ILE:HD13	2.10	0.50
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.92	0.50
1:B:67:TRP:HA	1:B:238:VAL:HB	1.93	0.50
1:A:693:ASP:O	1:A:696:ASN:HB2	2.12	0.50
1:B:66:ARG:HD2	1:B:236:ASN:HA	1.93	0.50
1:B:45:VAL:HG12	1:B:45:VAL:O	2.11	0.50
1:B:693:ASP:O	1:B:696:ASN:HB2	2.10	0.50
1:B:764:MET:SD	1:B:765:LEU:HD12	2.52	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:GLU:HG3	1:B:613:TYR:OH	2.11	0.50
1:A:795:LYS:HB2	7:A:2122:HOH:O	2.11	0.50
1:A:411:LEU:O	1:A:415:VAL:HG23	2.12	0.50
1:A:697:VAL:O	1:A:701:GLU:HG3	2.12	0.50
1:A:308:ILE:O	1:A:312:LYS:HG3	2.12	0.49
1:A:66:ARG:HD2	1:A:236:ASN:HA	1.94	0.49
1:B:300:VAL:HG13	1:B:345:ALA:HA	1.94	0.49
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.93	0.49
1:B:826:ASN:HD22	1:B:826:ASN:C	2.14	0.49
1:B:577:LEU:CD1	1:B:765:LEU:HD11	2.42	0.49
1:A:198:LEU:HD21	1:A:309:ARG:CZ	2.42	0.49
1:B:411:LEU:O	1:B:415:VAL:HG23	2.12	0.49
1:A:66:ARG:CD	1:A:236:ASN:HA	2.42	0.49
1:A:828:GLU:HG3	1:A:829:PRO:HD2	1.94	0.49
1:B:826:ASN:O	1:B:826:ASN:ND2	2.38	0.49
1:A:737:GLU:O	1:A:741:VAL:HG23	2.12	0.49
1:B:737:GLU:O	1:B:741:VAL:HG23	2.12	0.49
1:A:246:ALA:O	1:A:247:ARG:HD2	2.12	0.48
1:A:615:MET:HE2	1:A:761:ILE:HG12	1.93	0.48
1:A:645:LEU:HD11	1:A:652:LEU:HD11	1.90	0.48
1:B:157:TYR:HD2	1:B:303:THR:HG1	1.58	0.48
1:A:369:GLN:NE2	7:A:2453:HOH:O	2.46	0.48
1:A:67:TRP:HA	1:A:238:VAL:HB	1.95	0.48
1:B:66:ARG:CD	1:B:236:ASN:HA	2.43	0.48
1:B:724:LYS:O	1:B:724:LYS:HD3	2.13	0.48
1:A:197:MET:HE2	1:A:224:LEU:HD13	1.95	0.48
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.49	0.48
1:A:494:LEU:HD23	1:A:494:LEU:C	2.34	0.48
1:B:198:LEU:HD21	1:B:309:ARG:CZ	2.44	0.48
1:B:652:LEU:HD13	1:B:652:LEU:O	2.14	0.48
1:A:556:LYS:HD3	1:A:557:ILE:N	2.28	0.48
1:A:133:ASN:OD1	1:A:281:PRO:HA	2.14	0.48
1:A:689:ILE:O	1:A:689:ILE:HG23	2.14	0.48
1:A:65:GLY:O	1:A:69:ARG:HG3	2.14	0.48
1:A:45:VAL:O	1:A:45:VAL:HG12	2.14	0.48
1:B:205:LYS:HG3	7:B:2302:HOH:O	2.13	0.47
1:B:689:ILE:HG23	1:B:689:ILE:O	2.14	0.47
1:A:301:ALA:O	1:A:305:GLN:HG3	2.13	0.47
1:A:386:ARG:HA	1:A:439:ILE:O	2.14	0.47
1:A:724:LYS:O	1:A:724:LYS:HD3	2.14	0.47
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:LEU:HD11	1:B:652:LEU:HD11	1.94	0.47
1:B:65:GLY:O	1:B:69:ARG:HG3	2.15	0.47
1:A:545:PHE:O	1:A:548:PHE:HB3	2.14	0.47
1:A:577:LEU:CD1	1:A:765:LEU:HD11	2.44	0.47
1:A:261:ASP:N	7:A:2495:HOH:O	2.47	0.47
1:A:414:ILE:CG2	1:A:425:LEU:HD23	2.45	0.47
1:B:532:ARG:CB	1:B:532:ARG:NH1	2.78	0.47
1:B:655:LYS:O	1:B:658:PRO:HD2	2.15	0.47
1:B:746:ASP:HB2	1:B:762:ILE:HG13	1.97	0.47
1:A:203:TYR:HE2	1:A:394:LYS:HD2	1.80	0.47
1:A:511:TYR:N	7:A:2148:HOH:O	2.47	0.47
1:A:746:ASP:HB2	1:A:762:ILE:HG13	1.97	0.47
1:A:132:GLY:O	7:A:2498:HOH:O	2.20	0.47
1:A:532:ARG:NH1	1:A:532:ARG:CB	2.78	0.47
1:B:506:LYS:HD2	1:B:524:PHE:CE2	2.50	0.47
1:A:424:ARG:HH22	1:A:474:LEU:CD1	2.28	0.46
1:A:738:LEU:HB2	1:A:777:TYR:CE2	2.49	0.46
1:A:293:LEU:HG	1:A:395:LEU:HD23	1.96	0.46
1:A:571:HIS:H	1:A:576:GLN:NE2	2.12	0.46
1:B:301:ALA:O	1:B:305:GLN:HG3	2.15	0.46
1:A:506:LYS:HD2	1:A:524:PHE:CE2	2.50	0.46
1:A:402:ILE:O	1:A:406:ILE:HG13	2.15	0.46
1:A:576:GLN:NE2	1:A:576:GLN:H	2.13	0.46
1:B:732:TYR:CE1	1:B:739:LYS:HA	2.51	0.46
1:A:398:ARG:O	1:A:402:ILE:HG13	2.16	0.46
1:A:592:LYS:HE2	1:A:592:LYS:O	2.15	0.46
1:A:633:ASP:O	1:A:636:VAL:HG22	2.15	0.46
1:B:225:PRO:HB3	1:B:244:TRP:CZ3	2.51	0.46
1:A:732:TYR:CE1	1:A:739:LYS:HA	2.51	0.46
1:A:826:ASN:O	1:A:826:ASN:ND2	2.39	0.46
1:B:754:GLN:HB3	1:B:757:LEU:HB2	1.96	0.46
1:B:402:ILE:O	1:B:406:ILE:HG13	2.16	0.46
1:B:566:GLN:HA	7:B:2012:HOH:O	2.15	0.46
1:A:575:ARG:HD3	1:A:666:ILE:O	2.15	0.46
1:B:576:GLN:H	1:B:576:GLN:NE2	2.13	0.46
1:B:693:ASP:O	1:B:694:GLY:C	2.54	0.46
1:A:136:LEU:C	1:A:136:LEU:HD23	2.36	0.46
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.98	0.45
1:A:826:ASN:C	1:A:826:ASN:HD22	2.19	0.45
1:B:432:GLU:O	1:B:437:LYS:HA	2.17	0.45
1:B:738:LEU:HB2	1:B:777:TYR:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:ILE:HG23	1:A:716:ASP:N	2.30	0.45
1:B:133:ASN:OD1	1:B:281:PRO:HA	2.16	0.45
1:B:216:ILE:HB	7:B:2168:HOH:O	2.16	0.45
1:B:648:TYR:HD1	1:B:652:LEU:HD12	1.81	0.45
1:B:728:ALA:HB1	1:B:774:PHE:CD1	2.51	0.45
1:B:633:ASP:O	1:B:636:VAL:HG22	2.16	0.45
1:A:754:GLN:HB3	1:A:757:LEU:HB2	1.97	0.45
1:B:414:ILE:CG2	1:B:425:LEU:HD23	2.45	0.45
1:B:433:GLU:HG3	1:B:437:LYS:HG2	1.99	0.45
1:B:715:ILE:HG23	1:B:716:ASP:N	2.31	0.45
1:B:72:GLN:HE21	1:B:76:ASP:CG	2.19	0.45
1:A:693:ASP:O	1:A:694:GLY:C	2.54	0.45
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.98	0.45
1:B:592:LYS:O	1:B:592:LYS:HE2	2.15	0.45
1:B:636:VAL:HG23	1:B:637:GLY:N	2.32	0.45
1:A:389:VAL:HG22	1:A:437:LYS:O	2.16	0.45
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.99	0.45
1:B:545:PHE:O	1:B:548:PHE:HB3	2.16	0.45
1:B:81:ARG:HD3	1:B:155:TYR:HE2	1.82	0.45
1:A:648:TYR:HD1	1:A:652:LEU:HD12	1.82	0.45
1:A:525:LEU:HD23	1:A:802:LEU:HD23	1.99	0.45
1:B:571:HIS:H	1:B:576:GLN:NE2	2.15	0.45
1:A:732:TYR:CD1	1:A:739:LYS:HA	2.52	0.45
1:B:308:ILE:HD13	1:B:352:ILE:HG21	1.92	0.45
1:B:438:ARG:HB3	1:B:438:ARG:HE	1.60	0.45
1:A:380:LEU:HA	1:A:381:PRO:HD3	1.82	0.44
1:A:592:LYS:C	1:A:592:LYS:HE2	2.38	0.44
1:B:81:ARG:HD3	1:B:155:TYR:CE2	2.52	0.44
1:B:315:LYS:HG3	1:B:315:LYS:O	2.17	0.44
1:B:592:LYS:C	1:B:592:LYS:HE2	2.38	0.44
1:B:341:HIS:HB2	1:B:342:PRO:HD3	1.99	0.44
1:A:316:PHE:HD2	1:A:316:PHE:H	1.64	0.44
1:B:732:TYR:CD1	1:B:739:LYS:HA	2.52	0.44
1:B:615:MET:HE2	1:B:761:ILE:HG12	1.96	0.44
1:A:415:VAL:HG22	1:A:425:LEU:CD1	2.48	0.44
1:A:728:ALA:HB1	1:A:774:PHE:CD1	2.52	0.44
1:B:308:ILE:O	1:B:312:LYS:HG3	2.17	0.44
1:B:106:ASN:HB3	7:B:2216:HOH:O	2.17	0.44
1:B:556:LYS:HD3	1:B:557:ILE:N	2.32	0.44
1:B:487:THR:HA	1:B:488:PRO:HD3	1.88	0.44
1:A:336:GLN:OE1	1:A:825:TRP:NE1	2.45	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ASN:HB3	1:A:561:SER:HB3	2.00	0.43
1:B:98:THR:O	1:B:102:LEU:HB2	2.18	0.43
1:B:424:ARG:HH22	1:B:474:LEU:CD1	2.30	0.43
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.99	0.43
1:A:308:ILE:HD12	1:A:352:ILE:HD13	2.00	0.43
1:A:555:VAL:HG12	1:A:556:LYS:N	2.33	0.43
1:A:81:ARG:HD3	1:A:155:TYR:CE2	2.53	0.43
1:B:567:VAL:HA	1:B:606:GLY:O	2.18	0.43
1:B:575:ARG:HD3	1:B:666:ILE:O	2.18	0.43
1:B:36:HIS:O	1:B:40:VAL:HA	2.19	0.43
1:B:386:ARG:HA	1:B:439:ILE:O	2.17	0.43
1:A:438:ARG:HE	1:A:438:ARG:HB3	1.62	0.43
1:B:135:GLY:HA3	7:B:2008:HOH:O	2.18	0.43
1:B:615:MET:CE	1:B:618:MET:HB2	2.48	0.43
1:A:566:GLN:HA	7:A:2057:HOH:O	2.18	0.43
1:B:389:VAL:HG22	1:B:437:LYS:O	2.17	0.43
1:B:415:VAL:HG22	1:B:425:LEU:CD1	2.47	0.43
1:B:555:VAL:HG12	1:B:556:LYS:N	2.33	0.43
1:A:432:GLU:O	1:A:437:LYS:HA	2.19	0.43
1:A:756:ASP:O	1:A:759:LYS:HB2	2.18	0.43
1:B:756:ASP:O	1:B:759:LYS:HB2	2.18	0.43
1:A:198:LEU:CD2	1:A:309:ARG:NH2	2.78	0.43
1:B:311:PHE:CE1	1:B:329:PHE:HA	2.54	0.43
1:B:708:LEU:HG	7:B:2209:HOH:O	2.18	0.43
1:A:636:VAL:HG23	1:A:637:GLY:N	2.33	0.43
1:B:336:GLN:OE1	1:B:825:TRP:NE1	2.47	0.43
1:B:170:ILE:HG12	1:B:646:GLU:HB3	2.01	0.43
1:B:792:MET:O	1:B:794:PRO:HD3	2.18	0.43
1:B:828:GLU:CG	1:B:829:PRO:HD2	2.47	0.43
1:A:567:VAL:HA	1:A:606:GLY:O	2.19	0.42
1:B:197:MET:HE2	1:B:224:LEU:HD13	2.01	0.42
1:B:374:TYR:CG	1:B:445:CYS:HB3	2.54	0.42
1:A:24:VAL:O	1:A:28:LYS:HG3	2.18	0.42
1:B:754:GLN:N	1:B:755:PRO:HD3	2.34	0.42
1:A:360:PRO:HB2	7:A:2441:HOH:O	2.19	0.42
1:A:382:GLU:H	1:A:382:GLU:CD	2.23	0.42
1:A:792:MET:O	1:A:794:PRO:HD3	2.19	0.42
1:B:325:VAL:HA	7:B:2535:HOH:O	2.19	0.42
1:A:818:LYS:HD3	7:A:2547:HOH:O	2.20	0.42
1:A:761:ILE:O	1:A:765:LEU:HD13	2.20	0.42
1:A:74:TYR:HB3	1:A:81:ARG:NH1	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:ASN:HB3	1:B:561:SER:HB3	2.01	0.42
1:A:713:MET:HB3	1:A:717:ASP:HB2	2.01	0.42
1:A:735:LEU:HD23	1:A:777:TYR:CD2	2.52	0.42
1:A:210:ASN:ND2	7:A:2270:HOH:O	2.53	0.42
1:A:36:HIS:O	1:A:40:VAL:HA	2.19	0.42
1:A:554:LYS:O	1:A:555:VAL:O	2.38	0.42
1:A:735:LEU:N	1:A:735:LEU:HD12	2.35	0.42
1:B:233:TYR:CD2	1:B:513:LYS:HE3	2.55	0.42
1:B:382:GLU:CD	1:B:382:GLU:H	2.22	0.42
1:B:713:MET:HB3	1:B:717:ASP:HB2	2.02	0.42
1:A:557:ILE:O	1:A:559:PRO:HD3	2.20	0.42
1:A:690:GLY:O	1:A:710:ILE:HA	2.20	0.42
1:A:72:GLN:HE21	1:A:76:ASP:CG	2.23	0.42
1:A:98:THR:O	1:A:102:LEU:HB2	2.18	0.41
1:B:657:ILE:HB	1:B:658:PRO:HD3	2.02	0.41
1:A:300:VAL:HG13	1:A:345:ALA:HA	2.02	0.41
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.86	0.41
1:B:761:ILE:O	1:B:765:LEU:HD13	2.19	0.41
1:A:433:GLU:HG3	1:A:437:LYS:HG2	2.01	0.41
1:B:136:LEU:HD23	1:B:136:LEU:C	2.40	0.41
1:B:283:ASP:O	1:B:284:ASN:HB2	2.20	0.41
1:A:590:ILE:HA	7:A:2392:HOH:O	2.21	0.41
1:A:81:ARG:HD3	1:A:155:TYR:HE2	1.86	0.41
1:B:22:GLU:OE1	1:B:22:GLU:HA	2.20	0.41
1:A:315:LYS:O	1:A:316:PHE:C	2.58	0.41
1:A:754:GLN:N	1:A:755:PRO:HD3	2.36	0.41
1:B:735:LEU:HD23	1:B:777:TYR:CD2	2.54	0.41
1:A:315:LYS:O	1:A:315:LYS:HG3	2.21	0.41
1:B:786:LYS:HB3	1:B:786:LYS:HE2	1.72	0.41
1:A:633:ASP:HA	1:A:634:PRO:HD3	1.91	0.41
1:B:494:LEU:HD23	1:B:494:LEU:C	2.40	0.41
1:B:525:LEU:HD23	1:B:802:LEU:HD23	2.03	0.41
1:B:233:TYR:CZ	1:B:512:VAL:HG11	2.56	0.41
1:B:636:VAL:CG2	1:B:637:GLY:N	2.84	0.41
1:A:300:VAL:CG1	1:A:345:ALA:HA	2.51	0.41
1:B:246:ALA:O	1:B:273:GLU:HG2	2.21	0.41
1:A:281:PRO:HD2	7:A:2410:HOH:O	2.20	0.40
1:A:291:LEU:O	1:A:295:GLN:HG3	2.21	0.40
1:A:601:ARG:HG3	7:A:2212:HOH:O	2.21	0.40
1:B:203:TYR:HE2	1:B:394:LYS:HD2	1.86	0.40
1:B:561:SER:HA	1:B:600:PRO:HG2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:ASP:C	1:B:769:ASP:OD1	2.58	0.40
1:A:418:PHE:N	1:A:419:PRO:HD3	2.36	0.40
1:A:655:LYS:O	1:A:658:PRO:HD2	2.21	0.40
1:B:282:ASN:HB3	1:B:285:PHE:HB3	2.04	0.40
1:B:555:VAL:CG1	1:B:556:LYS:N	2.84	0.40
1:B:34:HIS:CE1	1:B:57:HIS:HB3	2.56	0.40
1:B:692:MET:HG3	1:B:697:VAL:HG22	2.03	0.40
1:B:197:MET:HB2	1:B:197:MET:HE2	1.83	0.40
1:B:418:PHE:N	1:B:419:PRO:HD3	2.36	0.40
1:B:690:GLY:O	1:B:710:ILE:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	784/847 (93%)	742 (95%)	39 (5%)	3 (0%)	34	32
1	B	785/847 (93%)	742 (94%)	39 (5%)	4 (0%)	29	26
All	All	1569/1694 (93%)	1484 (95%)	78 (5%)	7 (0%)	34	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	555	VAL
1	B	555	VAL
1	A	554	LYS
1	B	554	LYS
1	A	342	PRO
1	B	342	PRO
1	B	694	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	692/740 (94%)	662 (96%)	30 (4%)	29	29
1	B	693/740 (94%)	661 (95%)	32 (5%)	27	26
All	All	1385/1480 (94%)	1323 (96%)	62 (4%)	27	27

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	78	CYS
1	A	90	TYR
1	A	95	LEU
1	A	102	LEU
1	A	106	ASN
1	A	243	LEU
1	A	277	ARG
1	A	316	PHE
1	A	337	LEU
1	A	361	TRP
1	A	492	LEU
1	A	499	LEU
1	A	502	LEU
1	A	505	GLU
1	A	528	ASP
1	A	551	THR
1	A	573	TYR
1	A	576	GLN
1	A	577	LEU
1	A	592	LYS
1	A	613	TYR
1	A	622	LEU
1	A	628	ASP
1	A	645	LEU
1	A	683	LEU
1	A	733	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	735	LEU
1	A	815	ARG
1	A	826	ASN
1	B	44	ASN
1	B	78	CYS
1	B	90	TYR
1	B	95	LEU
1	B	102	LEU
1	B	106	ASN
1	B	243	LEU
1	B	277	ARG
1	B	281	PRO
1	B	325	VAL
1	B	337	LEU
1	B	361	TRP
1	B	489	ARG
1	B	492	LEU
1	B	499	LEU
1	B	502	LEU
1	B	505	GLU
1	B	528	ASP
1	B	551	THR
1	B	573	TYR
1	B	576	GLN
1	B	577	LEU
1	B	592	LYS
1	B	613	TYR
1	B	622	LEU
1	B	628	ASP
1	B	645	LEU
1	B	683	LEU
1	B	733	GLU
1	B	735	LEU
1	B	815	ARG
1	B	826	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	72	GLN
1	A	97	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	106	ASN
1	A	250	ASN
1	A	369	GLN
1	A	459	HIS
1	A	576	GLN
1	B	96	GLN
1	B	105	GLN
1	B	106	ASN
1	B	250	ASN
1	B	369	GLN
1	B	459	HIS
1	B	576	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

6 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	$\#\|Z\| > 2$
3	PLP	A	860	1	15,15,16	2.11	4 (26%)	20,22,23	1.34	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PLP	B	860	1	15,15,16	2.00	3 (20%)	20,22,23	0.91	0
2	NBG	A	861	-	15,15,15	1.32	3 (20%)	21,21,21	1.24	2 (9%)
6	MRD	B	902	-	7,7,7	0.71	0	9,10,10	0.72	0
5	RBF	A	859	-	27,29,29	2.48	12 (44%)	33,43,43	3.01	11 (33%)
4	700	A	862	-	28,33,33	1.91	9 (32%)	32,47,47	1.52	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	860	1	-	0/6/6/8	0/1/1/1
3	PLP	B	860	1	-	2/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
6	MRD	B	902	-	-	2/5/5/5	-
5	RBF	A	859	-	-	1/14/14/14	0/3/3/3
4	700	A	862	-	-	0/15/32/32	0/4/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	859	RBF	C4-C4A	6.33	1.52	1.41
3	B	860	PLP	C4A-C4	-5.49	1.40	1.51
3	A	860	PLP	C4A-C4	-5.05	1.41	1.51
5	A	859	RBF	C1'-N10	5.00	1.53	1.48
5	A	859	RBF	C4A-C10	4.37	1.43	1.38
4	A	862	700	C22-C20	4.27	1.59	1.55
4	A	862	700	C5-C4	3.90	1.44	1.36
5	A	859	RBF	C4-N3	3.67	1.39	1.33
3	B	860	PLP	C3-C2	-3.65	1.37	1.40
5	A	859	RBF	C5A-N5	3.42	1.41	1.35
3	A	860	PLP	C5A-C5	3.32	1.59	1.50
4	A	862	700	C3-C4	3.16	1.44	1.38
4	A	862	700	C2-C3	2.95	1.42	1.36
4	A	862	700	C7-C6	2.94	1.52	1.41
5	A	859	RBF	C8M-C8	2.92	1.56	1.51
5	A	859	RBF	C8-C7	2.79	1.47	1.40
5	A	859	RBF	C9A-N10	2.78	1.42	1.38
2	A	861	NBG	C2-C1	2.76	1.55	1.52
4	A	862	700	C16-C11	2.65	1.44	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	859	RBF	C4A-N5	-2.39	1.30	1.33
5	A	859	RBF	C5'-C4'	2.37	1.58	1.52
4	A	862	700	C12-C11	2.33	1.43	1.38
4	A	862	700	C13-C12	2.28	1.43	1.38
4	A	862	700	C15-C14	2.24	1.43	1.38
2	A	861	NBG	C1-N1	2.22	1.46	1.43
5	A	859	RBF	C10-N1	2.21	1.36	1.33
3	A	860	PLP	C2-N1	2.20	1.38	1.33
3	A	860	PLP	P-O3P	-2.13	1.46	1.54
5	A	859	RBF	C4'-C3'	-2.12	1.49	1.53
2	A	861	NBG	C3-C2	2.09	1.57	1.52
3	B	860	PLP	P-O3P	-2.01	1.47	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	859	RBF	C4-N3-C2	8.15	122.03	115.14
5	A	859	RBF	C4-C4A-C10	-6.80	115.45	119.95
5	A	859	RBF	C10-C4A-N5	6.44	125.71	121.26
5	A	859	RBF	O5'-C5'-C4'	-5.76	98.52	111.07
5	A	859	RBF	O4'-C4'-C3'	4.96	121.16	109.10
4	A	862	700	C7-C6-C1	-4.40	102.44	106.27
5	A	859	RBF	C5A-C9A-N10	-4.21	114.67	117.72
5	A	859	RBF	C4A-C10-N10	-4.17	116.02	120.30
2	A	861	NBG	C5-O5-C1	3.98	117.92	112.52
4	A	862	700	C8-C9-N1	3.85	122.36	115.20
4	A	862	700	C8-N2-C1	3.67	112.10	104.45
5	A	859	RBF	C1'-N10-C9A	3.02	120.67	118.29
3	A	860	PLP	O3P-P-O4P	-2.86	99.13	106.73
3	A	860	PLP	O3P-P-O2P	2.81	118.38	107.64
5	A	859	RBF	C1'-N10-C10	-2.57	116.11	118.41
5	A	859	RBF	O4'-C4'-C5'	-2.49	103.29	109.14
5	A	859	RBF	C4A-C4-N3	-2.37	120.19	123.43
4	A	862	700	C3-C2-C1	-2.22	118.05	120.84
2	A	861	NBG	C2-C1-N1	-2.20	108.72	111.30
3	A	860	PLP	C2A-C2-C3	2.12	123.51	120.89

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	860	PLP	C6-C5-C5A-O4P

Continued on next page...

Continued from previous page...

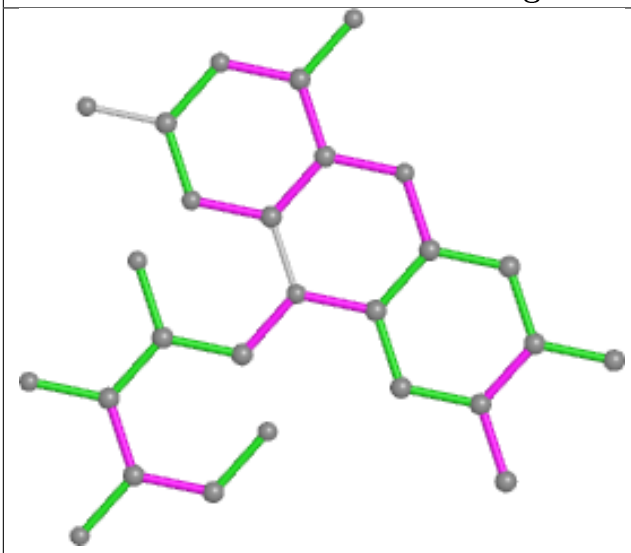
Mol	Chain	Res	Type	Atoms
3	B	860	PLP	C4-C5-C5A-O4P
6	B	902	MRD	C2-C3-C4-C5
6	B	902	MRD	C2-C3-C4-O4
5	A	859	RBF	O3'-C3'-C4'-C5'

There are no ring outliers.

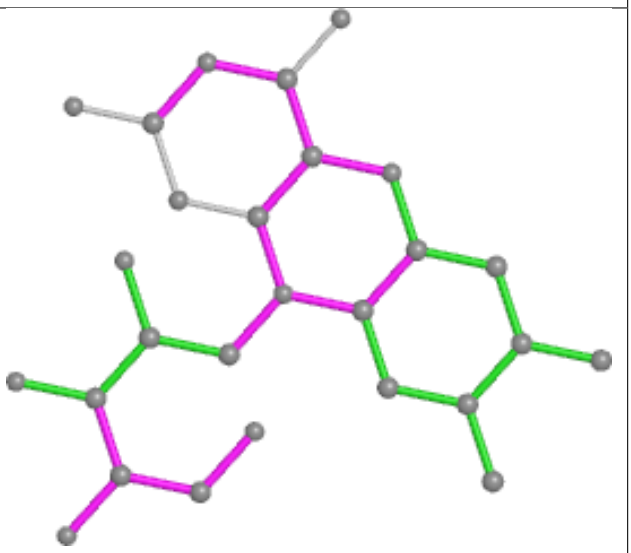
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

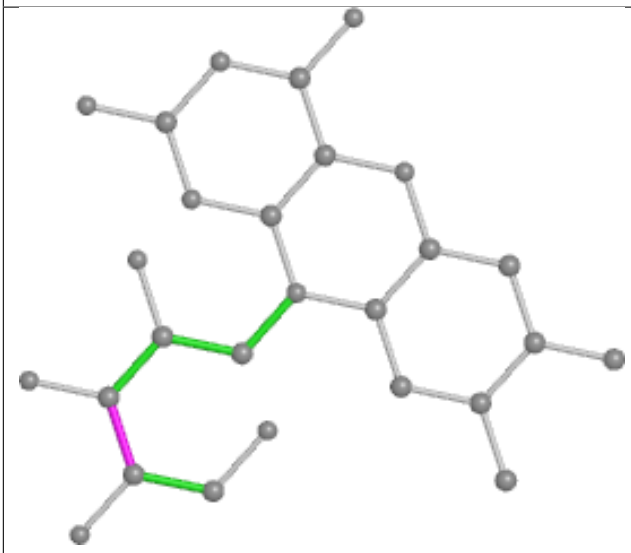
Ligand RBF A 859



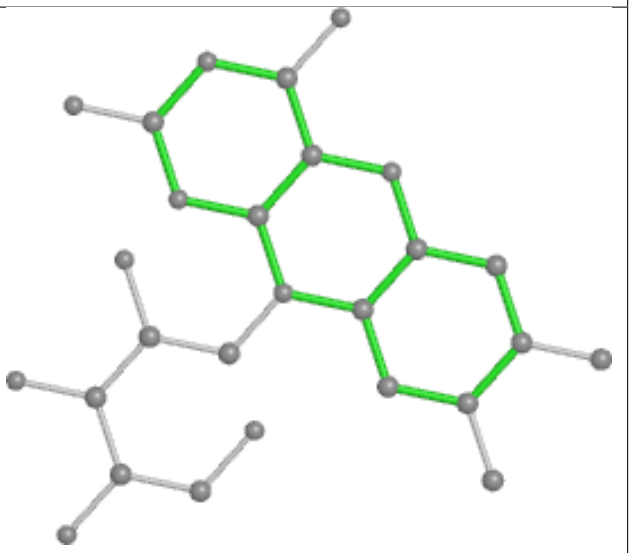
Bond lengths



Bond angles

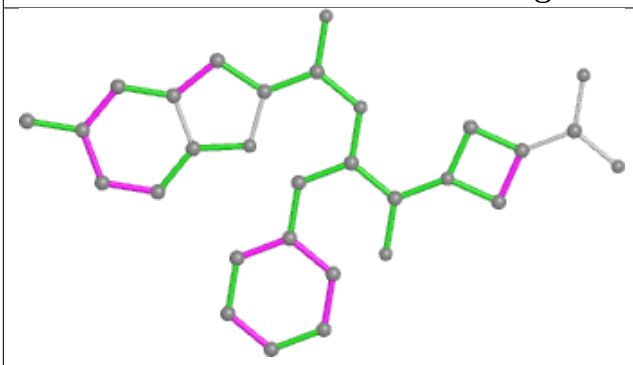


Torsions

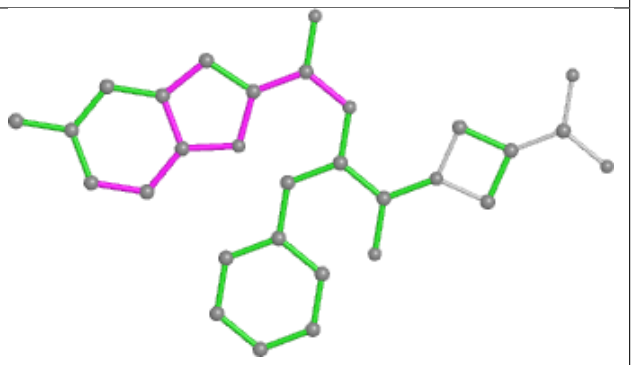


Rings

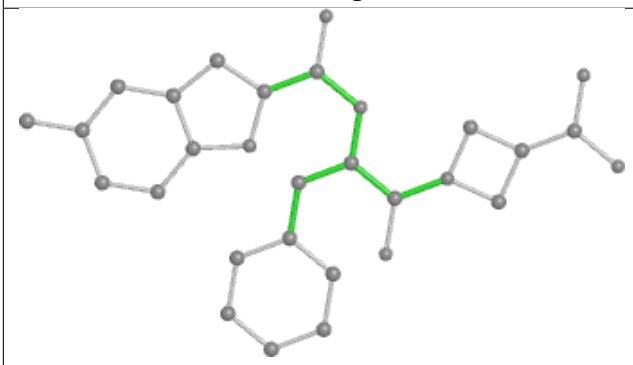
Ligand 700 A 862



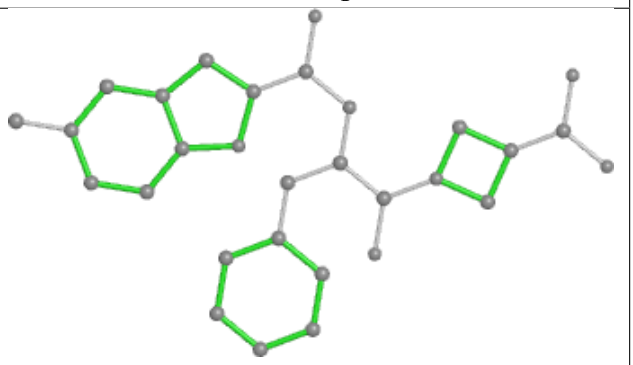
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.