Full wwPDB X-ray Structure Validation Report (i)

Feb 20, 2024 – 11:34 AM EST

PDB ID	:	4M2S
Title	:	Corrected Structure of Mouse P-glycoprotein bound to QZ59-RRR
Authors	:	Li, J.; Jaimes, K.F.; Aller, S.G.
Deposited on	:	2013-08-05
Resolution	:	4.40 Å(reported)

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

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

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

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

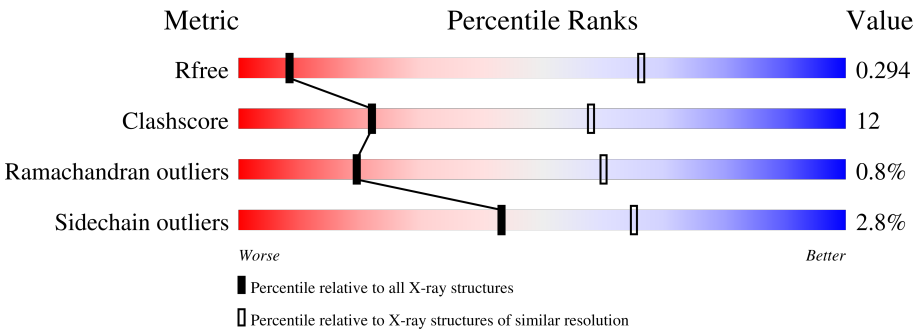
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1282	65% 27% • 7%
1	B	1282	66% 24% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18439 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.

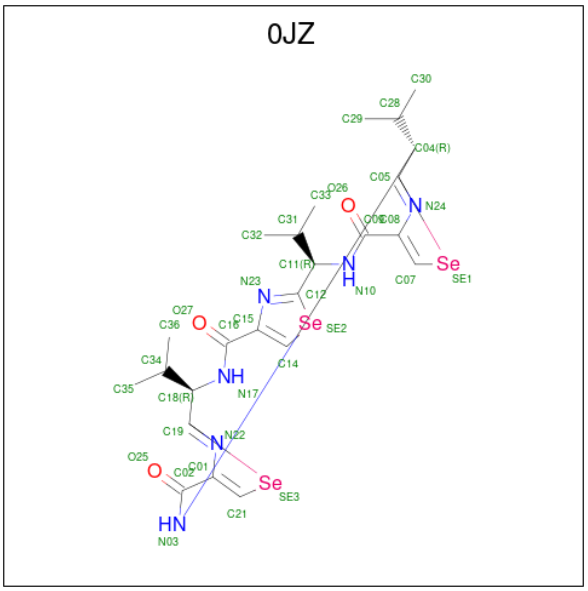
- Molecule 1 is a protein called Multidrug resistance protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1188	9214	5923	1559	1694	38	0	0	0
1	B	1180	9153	5887	1550	1678	38	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLN	ASN	conflict	UNP P21447
A	87	GLN	ASN	conflict	UNP P21447
A	90	GLN	ASN	conflict	UNP P21447
A	1277	HIS	-	expression tag	UNP P21447
A	1278	HIS	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
B	83	GLN	ASN	conflict	UNP P21447
B	87	GLN	ASN	conflict	UNP P21447
B	90	GLN	ASN	conflict	UNP P21447
B	1277	HIS	-	expression tag	UNP P21447
B	1278	HIS	-	expression tag	UNP P21447
B	1279	HIS	-	expression tag	UNP P21447
B	1280	HIS	-	expression tag	UNP P21447
B	1281	HIS	-	expression tag	UNP P21447
B	1282	HIS	-	expression tag	UNP P21447

- Molecule 2 is (4R,11R,18R)-4,11,18-tri(propan-2-yl)-6,13,20-triselena-3,10,17,22,23,24-hexaa zatetracyclo[17.2.1.1 5,8 .1 12,15]tetracosa-1(21),5(24),7,12(23),14,19(22)-hexaene-2,9,16-tri one (three-letter code: 0JZ) (formula: $C_{24}H_{30}N_6O_3Se_3$).



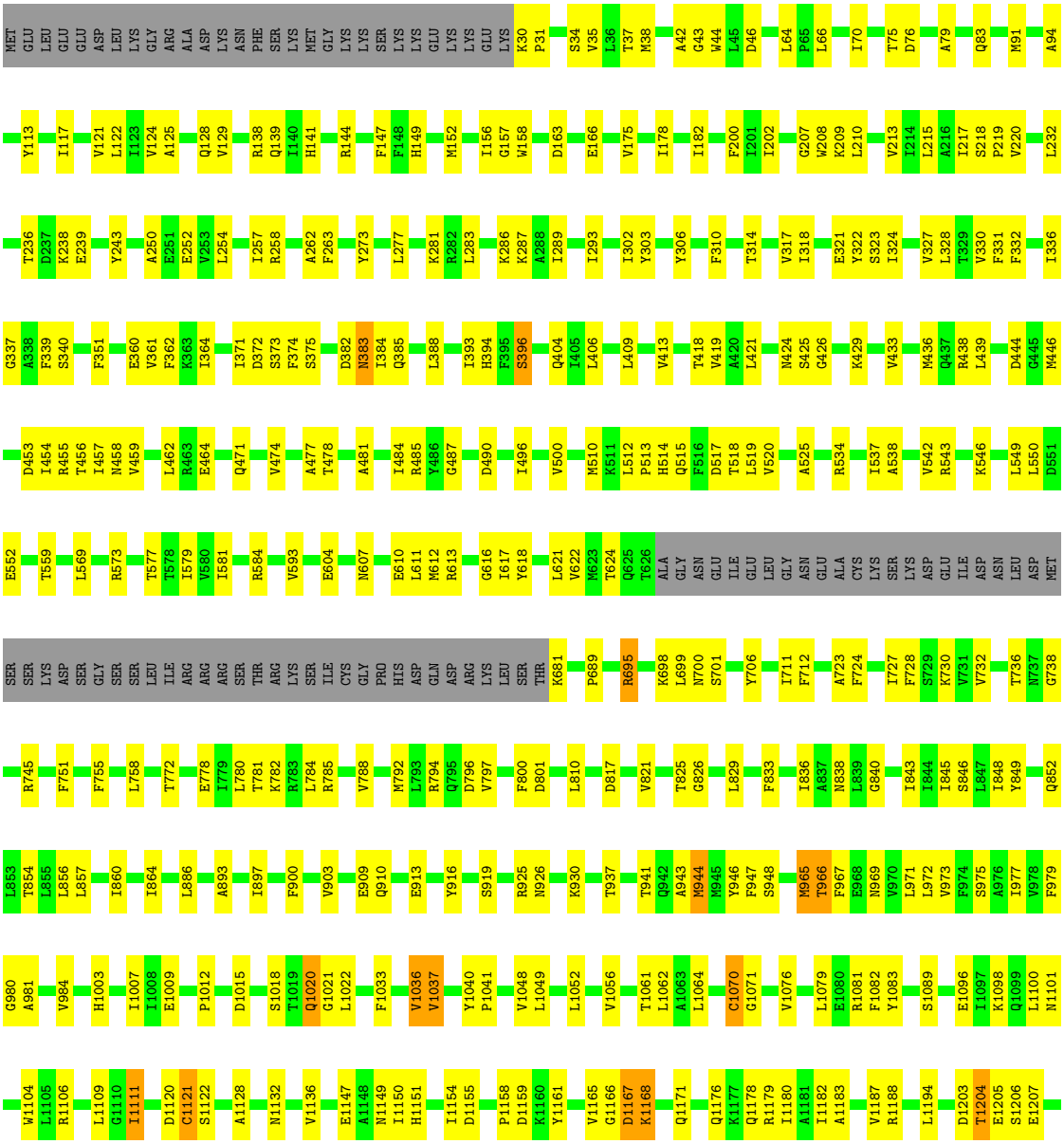
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	Se		
2	A	1	36	24	6	3	3	0	0
			Total	C	N	O	Se		
2	B	1	36	24	6	3	3	0	0

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.

- Molecule 1: Multidrug resistance protein 1A

Chain A: 65% 27% • 7%



K1216 A1217 R1218 I1226 R1229 Q1234 V1241 E1249 H1253 Q1259 Y1263 A1271 GLY ALA LYS ARG SER HIS HIS HIS HIS HIS

• Molecule 1: Multidrug resistance protein 1A

Chain B: 66% 24% • 8%

MET GLU LEU GLU GLU ASP LEU LYS GLY ARG ALA ASP LYS ASN PHE SER LYS MET GLY LYS LYS SER LYS LYS GLU LYS LYS GLU LYS LYS P31 A32 V33 S34 T37 M38 F39 D46 G61 L66 T75 Q90 N91 A94 R97 K102 E106 V121 L122

I123 V124 A125 Y126 I127 Q128 V129 A136 G137 R138 Q139 M152 I156 D160 V161 H162 N168 T169 D173 I182 A194 T195 F196 G199 F200 I201 I202 R206 G207 W208 K209 L210 T211 L212 V213 I214 L215 A216 I217 V220 W228 K245 A246 E252 I257

V260 F263 R272 Y273 N274 N275 N276 L277 E278 E279 A280 K281 R282 L283 C284 I285 I289 N292 I293 S294 F299 L300 L301 I302 Y303 A304 S305 L308 A309 F310 T314 V317 Y322 S323 I324 G325 Q326 V327 L328 T329 V330 F331 F332 S333 V334 L335 I336 G337 S340

Q343 Y359 I371 K376 S377 G378 H379 K380 P381 D382 N383 I384 Q385 L388 K391 N392 I393 S396 V403 L409 V413 T418 L421 S425 V433 M436 Q437 R438 L439 Y440 G445 D450 R455 T456 I457 N458 V459 R460 Y461 L462 R463 E464

V474 T478 I484 R485 Y486 G487 R488 V491 T492 M493 I496 V500 D507 F508 I509 M510 K511 L512 P513 H514 Q515 F516 D517 T518 L519 V520 G530 Q533 R534 I537 A538 L541 V542 R543 L549 L557 T577 T578 I581 L585 F597 V601

H608 D609 E610 Y618 L621 T626 ALA GLY ASN GLU ILE GLU LEU GLY ASN GLU ALA CYS LYS SER LYS ASP GLU ILE ASP ASN LEU ASP MET SER SER SER LYS ASP SER GLY SER SER LEU ILE ARG ARG ARG SER THR ARG LYS SER ILE CYS GLY PRO HIS ASP GLN ASP ARG

LYS LEU SER THR LYS GLU ALA LEU ASP GLU ASP V688 P689 P690 A691 S692 R695 K698 L699 N700 E703 F707 I711 L720 Q721 P722 A723 F724 S725 V726 I727 F728 S729 K730 P740 P741 F751 F755 L758 G759 I760 I761 F771 I779 L780 T781 K782 R783

L784 R785 S791 M792 L793 R794 Q795 D796 V797 S798 W799 F800 D801 D802 P803 K804 L810 D817 A818 A819 K822 R828 F833 Q834 N835 T841 I845 S846 L847 I848 Y849 T854 L857 I860 I864 E895 A896 N899 F900 R901 T902 V903 V904 S905 L906 T907

R908 E909 F912 Y916 S919 R925 N926 A927 K930 G935 A943 M944 M945 Y946 Y949 C952 G956 A957 V960 T961 Q962 M965 T966 F967 E968 N969 V970 L971 L972 V973 F974 S975 F979 V984 I1004 I1005 R1006 I1007 T1011 D1015 S1018 T1019

Q1020 G1021 L1022 K1023 P1024 E1028 G1035 Y1040 P1041 V1048 L1049 S1053 V1056 Q1060 T1061 L1062 A1063 L1064 V1065 K1072 V1076 Q1077 L1078 L1079 Y1083 D1084 P1085 V1090 I1097 L1100 N1101 R1106 V1112 D1120 I1123 A1124 E1125 N1126 I1127 A1128 Y1129 G1130

V1136 S1137 I1141 I1154 D1155 Y1161 N1162 T1163 R1164 V1165 G1166 D1167 G1175 A1183 V1187 R1188 Q1189 L1194 L1195 D1196 E1197 S1200 A1201 L1202 D1203 T1204 E1205 L1214 R1218 R1221 I1226 L1230 I1233 L1238 V1241 A1271 GLY ALA LYS ARG SER HIS HIS

HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.63Å 115.09Å 374.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.51 – 4.40 49.02 – 4.31	Depositor EDS
% Data completeness (in resolution range)	94.7 (24.51-4.40) 87.3 (49.02-4.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.227 , 0.294 0.229 , 0.294	Depositor DCC
R_{free} test set	2633 reflections (9.67%)	wwPDB-VP
Wilson B-factor (Å^2)	202.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 112.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	18439	wwPDB-VP
Average B, all atoms (Å^2)	209.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 0JZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.26	0/9383	0.43	0/12685
1	B	0.26	0/9322	0.44	0/12602
All	All	0.26	0/18705	0.43	0/25287

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9214	0	9388	235	0
1	B	9153	0	9338	212	0
2	A	36	0	27	4	0
2	B	36	0	27	6	0
All	All	18439	0	18780	439	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 12.

All (439) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:ARG:NH1	1:A:1015:ASP:OD2	1.91	1.02
1:A:46:ASP:OD1	1:A:138:ARG:NH1	2.07	0.88
1:A:433:VAL:HG13	1:A:549:LEU:HD23	1.62	0.81
1:A:1106:ARG:O	1:A:1188:ARG:NH1	2.14	0.80
1:A:801:ASP:OD2	1:A:1083:TYR:OH	2.01	0.78
1:A:510:MET:SD	1:A:515:GLN:NE2	2.57	0.78
1:B:792:MET:HE1	1:B:810:LEU:HB3	1.65	0.77
1:A:1149:ASN:O	1:A:1179:ARG:NH2	2.17	0.77
1:B:510:MET:SD	1:B:515:GLN:NE2	2.58	0.77
1:A:393:ILE:HB	1:A:409:LEU:HB3	1.68	0.76
1:A:43:GLY:H	1:A:46:ASP:HB2	1.50	0.76
1:A:926:ASN:O	1:A:930:LYS:NZ	2.18	0.76
1:A:281:LYS:NZ	1:A:785:ARG:HD2	2.02	0.75
1:B:206:ARG:HG3	1:B:326:GLN:HG3	1.66	0.75
1:A:66:LEU:HD23	1:A:202:ILE:HD11	1.68	0.75
1:A:388:LEU:HB2	1:A:413:VAL:HB	1.67	0.75
1:B:1021:GLY:HA2	1:B:1101:ASN:HB2	1.67	0.75
1:A:695:ARG:NH1	1:A:1009:GLU:OE2	2.20	0.74
1:B:794:ARG:HH12	1:B:1011:THR:HA	1.54	0.73
1:A:1079:LEU:HG	1:A:1109:LEU:HD21	1.71	0.72
1:A:966:THR:OG1	1:A:967:PHE:N	2.22	0.72
1:B:433:VAL:HG13	1:B:549:LEU:HD23	1.72	0.72
1:B:272:ARG:NH2	1:B:1125:GLU:OE2	2.23	0.72
1:A:396:SER:HB3	1:A:404:GLN:HA	1.72	0.71
1:B:952:CYS:HG	1:B:974:PHE:HD1	1.39	0.70
1:B:695:ARG:HA	1:B:698:LYS:NZ	2.07	0.69
1:A:784:LEU:HD22	1:A:821:VAL:HG11	1.74	0.69
1:A:1021:GLY:HA3	1:A:1101:ASN:HB2	1.74	0.69
1:B:245:LYS:NZ	1:B:279:GLU:OE1	2.25	0.69
1:A:519:LEU:HD21	1:B:925:ARG:HD3	1.74	0.68
1:B:371:ILE:HD13	1:B:438:ARG:HG2	1.75	0.68
1:B:1022:LEU:HD21	1:B:1100:LEU:HA	1.76	0.68
1:A:262:ALA:HB1	1:A:1111:ILE:HG21	1.74	0.68
1:B:690:PRO:HD2	1:B:1006:ARG:NH1	2.09	0.68
1:A:857:LEU:HD12	1:A:973:VAL:HG12	1.75	0.67
1:B:846:SER:HB2	1:B:973:VAL:HG13	1.75	0.67
1:A:421:LEU:HB2	1:A:581:ILE:HG12	1.76	0.66
1:B:335:LEU:HB3	2:B:6002:0JZ:H33	1.77	0.66
1:A:252:GLU:OE2	1:A:1120:ASP:N	2.28	0.66
1:B:206:ARG:O	1:B:326:GLN:NE2	2.28	0.66
1:A:281:LYS:HZ2	1:A:782:LYS:HA	1.60	0.65
1:B:849:TYR:HB3	1:B:969:ASN:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:HZ3	1:A:785:ARG:HD2	1.61	0.65
1:A:1079:LEU:HD23	1:A:1194:LEU:HD21	1.77	0.65
1:B:1035:GLY:N	1:B:1053:SER:OG	2.24	0.65
1:A:559:THR:HG22	1:A:584:ARG:HH12	1.62	0.64
1:A:792:MET:HE1	1:A:810:LEU:HB3	1.78	0.64
1:B:257:ILE:HG12	1:B:800:PHE:CE2	2.32	0.64
1:B:484:ILE:HG21	1:B:496:ILE:HG23	1.79	0.64
1:A:281:LYS:NZ	1:A:782:LYS:HA	2.11	0.64
1:A:281:LYS:NZ	1:A:781:THR:HG22	2.13	0.64
1:A:209:LYS:NZ	1:A:321:GLU:OE1	2.28	0.63
1:B:122:LEU:HB3	1:B:943:ALA:HB2	1.81	0.63
1:B:722:PRO:HG2	1:B:841:THR:HB	1.80	0.63
1:B:949:TYR:OH	2:B:6002:0JZ:O27	2.13	0.63
1:B:379:HIS:HB2	1:B:457:ILE:HG22	1.81	0.63
1:B:393:ILE:H	1:B:445:GLY:HA3	1.64	0.63
1:B:801:ASP:OD2	1:B:1083:TYR:OH	2.16	0.62
1:B:129:VAL:HG13	1:B:935:GLY:HA2	1.80	0.62
1:A:464:GLU:HA	1:A:543:ARG:HH21	1.63	0.62
1:A:794:ARG:HG2	1:A:1012:PRO:HG3	1.81	0.62
1:A:406:LEU:HD13	1:A:409:LEU:HD22	1.80	0.62
1:B:39:PHE:HA	1:B:139:GLN:HE22	1.65	0.62
1:A:394:HIS:HB2	1:A:444:ASP:HB3	1.82	0.61
1:B:1175:GLY:HA2	1:B:1202:LEU:HD11	1.82	0.61
1:A:1121:CYS:SG	1:A:1122:SER:N	2.69	0.61
1:B:1106:ARG:O	1:B:1188:ARG:NH1	2.33	0.61
1:B:1214:LEU:HB3	1:B:1218:ARG:HH21	1.65	0.61
1:A:699:LEU:HD23	1:A:784:LEU:HD11	1.81	0.61
1:B:217:ILE:HG21	1:B:305:SER:HB2	1.83	0.61
1:B:585:LEU:HD11	1:B:621:LEU:HB3	1.83	0.60
1:B:421:LEU:HB2	1:B:581:ILE:HG12	1.83	0.60
1:A:318:ILE:HD12	1:A:745:ARG:HE	1.65	0.60
1:B:94:ALA:HB1	1:B:97:ARG:HE	1.67	0.60
1:A:152:MET:HA	1:A:900:PHE:HE2	1.65	0.60
1:B:210:LEU:HD23	1:B:330:VAL:HB	1.82	0.60
1:B:314:THR:HA	1:B:317:VAL:HG12	1.84	0.60
1:A:208:TRP:N	1:A:322:TYR:OH	2.35	0.60
1:A:604:GLU:OE2	1:A:616:GLY:HA3	2.02	0.59
1:B:396:SER:OG	1:B:403:VAL:O	2.20	0.59
1:A:144:ARG:HB3	1:A:175:VAL:HG11	1.83	0.59
1:B:160:ASP:OD2	1:B:440:TYR:OH	2.13	0.59
1:B:802:ASP:OD2	1:B:804:LYS:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:THR:H	1:B:967:PHE:HA	1.67	0.59
1:A:424:ASN:HB2	1:A:621:LEU:HD21	1.85	0.59
1:B:328:LEU:HD22	1:B:332:PHE:HE2	1.68	0.59
1:A:339:PHE:CG	2:A:6001:0JZ:H32	2.38	0.59
1:B:1076:VAL:HG13	1:B:1194:LEU:HD13	1.85	0.59
1:A:1151:HIS:HA	1:A:1154:ILE:HD12	1.84	0.58
1:B:436:MET:HB3	1:B:549:LEU:HD21	1.85	0.58
1:A:780:LEU:O	1:A:784:LEU:HB2	2.03	0.58
1:B:252:GLU:OE2	1:B:1120:ASP:N	2.37	0.58
1:A:384:ILE:HD11	1:A:546:LYS:HB2	1.86	0.58
1:B:784:LEU:HD21	1:B:1004:ILE:HG21	1.85	0.58
1:B:965:MET:HB3	1:B:966:THR:OG1	2.04	0.58
1:A:1081:ARG:HG2	1:A:1081:ARG:HH11	1.69	0.58
1:B:388:LEU:HB2	1:B:413:VAL:HB	1.86	0.58
1:A:419:VAL:HG22	1:A:593:VAL:HB	1.87	0.57
1:B:156:ILE:HD11	1:B:439:LEU:HB3	1.86	0.57
1:B:857:LEU:HD12	1:B:973:VAL:HG12	1.85	0.57
1:B:758:LEU:HD12	1:B:761:ILE:HD12	1.86	0.57
1:B:796:ASP:OD2	1:B:798:SER:OG	2.11	0.57
1:A:175:VAL:HA	1:A:178:ILE:HG22	1.87	0.57
1:B:711:ILE:HG12	1:B:833:PHE:HE2	1.70	0.57
1:A:382:ASP:OD1	1:A:382:ASP:N	2.37	0.56
1:A:1064:LEU:HB2	1:A:1226:ILE:HG13	1.86	0.56
1:B:957:ALA:O	1:B:961:THR:HG23	2.06	0.56
1:A:846:SER:O	1:A:854:THR:OG1	2.24	0.56
1:A:91:MET:HB3	1:A:94:ALA:HB3	1.87	0.56
1:A:421:LEU:HD11	1:A:579:ILE:HD11	1.86	0.56
1:B:274:ASN:HA	1:B:277:LEU:HB2	1.87	0.56
1:A:1101:ASN:HB3	1:A:1104:TRP:HB3	1.88	0.56
1:A:1096:GLU:OE1	1:A:1098:LYS:N	2.36	0.55
1:A:484:ILE:HG23	1:A:542:VAL:HG21	1.87	0.55
1:B:695:ARG:HA	1:B:698:LYS:HZ3	1.69	0.55
1:A:75:THR:HG22	1:A:967:PHE:HZ	1.71	0.55
1:A:1061:THR:HG21	1:A:1218:ARG:HD3	1.89	0.55
1:B:438:ARG:NH1	1:B:455:ARG:HA	2.22	0.55
1:B:507:ASP:OD1	1:B:508:PHE:N	2.39	0.55
1:A:406:LEU:HD22	1:A:409:LEU:HD13	1.88	0.55
1:A:833:PHE:HA	1:A:836:ILE:HG22	1.89	0.55
1:A:1076:VAL:HG13	1:A:1194:LEU:HB3	1.89	0.55
1:B:1189:GLN:OE1	1:B:1221:ARG:NH2	2.40	0.55
1:A:1207:GLU:OE1	1:A:1229:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:TRP:HB3	1:B:294:SER:HB2	1.89	0.55
1:B:207:GLY:HA3	1:B:330:VAL:HG21	1.88	0.55
1:B:727:ILE:HG21	1:B:755:PHE:HB3	1.88	0.54
1:A:141:HIS:NE2	1:B:517:ASP:OD1	2.41	0.54
1:A:286:LYS:HA	1:A:289:ILE:HD12	1.90	0.54
1:A:324:ILE:HD11	1:A:732:VAL:HG12	1.89	0.54
1:A:429:LYS:HB3	1:A:581:ILE:HD13	1.90	0.54
1:A:512:LEU:HD13	1:A:518:THR:HG21	1.90	0.54
1:A:607:ASN:HB3	1:A:610:GLU:OE2	2.08	0.54
1:B:794:ARG:NE	1:B:1015:ASP:OD2	2.41	0.54
1:B:322:TYR:O	1:B:326:GLN:HB3	2.08	0.53
1:A:612:MET:HE1	1:A:622:VAL:HG11	1.90	0.53
1:A:79:ALA:HA	1:A:736:THR:HA	1.91	0.53
1:B:66:LEU:HD23	1:B:202:ILE:HD11	1.90	0.53
1:A:200:PHE:HE2	1:A:215:LEU:HD12	1.74	0.53
1:B:930:LYS:NZ	1:B:930:LYS:HB2	2.24	0.53
1:A:76:ASP:OD1	1:A:323:SER:OG	2.14	0.53
1:B:484:ILE:HG23	1:B:542:VAL:HG21	1.91	0.53
1:A:289:ILE:O	1:A:293:ILE:HG12	2.08	0.53
1:A:490:ASP:HB2	1:B:460:ARG:HH12	1.74	0.52
1:B:385:GLN:HB2	1:B:450:ASP:OD2	2.09	0.52
1:B:1136:VAL:HG22	1:B:1137:SER:H	1.74	0.52
1:A:825:THR:OG1	1:A:826:GLY:N	2.41	0.52
1:B:845:ILE:HG22	1:B:972:LEU:HD11	1.91	0.52
1:A:149:HIS:HA	1:A:913:GLU:OE2	2.09	0.52
1:A:550:LEU:HD21	1:A:569:LEU:HD22	1.92	0.52
1:B:160:ASP:OD1	1:B:901:ARG:NH2	2.42	0.52
1:B:457:ILE:HD11	1:B:462:LEU:HD13	1.90	0.52
1:B:538:ALA:O	1:B:542:VAL:HG23	2.08	0.52
1:A:1033:PHE:HD1	1:A:1036:VAL:HG11	1.74	0.52
1:A:846:SER:HB2	1:A:973:VAL:HG13	1.92	0.52
1:A:621:LEU:HA	1:A:624:THR:HG22	1.91	0.52
1:A:372:ASP:HA	1:A:373:SER:HB3	1.91	0.51
1:A:517:ASP:O	1:B:925:ARG:NH1	2.40	0.51
1:A:930:LYS:NZ	1:A:930:LYS:HB2	2.26	0.51
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.42	0.51
1:A:1168:LYS:HB2	1:A:1168:LYS:NZ	2.25	0.51
1:B:956:GLY:O	1:B:960:VAL:HG23	2.10	0.51
1:B:276:ASN:HA	1:B:279:GLU:HG3	1.92	0.51
1:A:239:GLU:HB2	1:A:287:LYS:NZ	2.25	0.51
1:A:689:PRO:HG3	1:A:1003:HIS:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:944:MET:HA	1:A:947:PHE:HB2	1.93	0.51
1:A:257:ILE:HG12	1:A:800:PHE:CE2	2.45	0.51
1:B:102:LYS:HE3	1:B:106:GLU:OE2	2.10	0.51
1:B:207:GLY:HA2	1:B:326:GLN:HE21	1.76	0.51
1:A:43:GLY:N	1:A:46:ASP:HB2	2.23	0.51
1:A:453:ASP:OD1	1:A:454:ILE:N	2.44	0.51
1:A:1176:GLN:O	1:A:1180:ILE:HG13	2.11	0.51
1:B:388:LEU:HD13	1:B:577:THR:HG21	1.92	0.51
1:B:794:ARG:NH1	1:B:1011:THR:HA	2.25	0.51
1:B:257:ILE:HG12	1:B:800:PHE:HE2	1.73	0.51
1:B:695:ARG:HD2	1:B:698:LYS:HE2	1.92	0.51
1:B:979:PHE:HE2	2:B:6002:0JZ:N22	2.09	0.50
1:A:388:LEU:HD13	1:A:577:THR:HG21	1.92	0.50
1:B:61:GLY:HA3	1:B:194:ALA:HB3	1.93	0.50
1:A:481:ALA:O	1:A:485:ARG:HG2	2.11	0.50
1:B:281:LYS:HG3	1:B:782:LYS:HB2	1.92	0.50
1:A:158:TRP:HZ2	1:A:364:ILE:HD12	1.76	0.50
1:A:281:LYS:HZ2	1:A:781:THR:HG22	1.74	0.50
1:B:846:SER:O	1:B:854:THR:OG1	2.30	0.50
1:A:239:GLU:HB2	1:A:287:LYS:HZ3	1.76	0.50
1:A:38:MET:HA	1:A:362:PHE:HE2	1.77	0.49
1:A:538:ALA:O	1:A:542:VAL:HG23	2.12	0.49
1:A:122:LEU:HB3	1:A:943:ALA:HB2	1.95	0.49
1:A:937:THR:O	1:A:941:THR:HG23	2.12	0.49
1:B:257:ILE:HD12	1:B:260:VAL:HB	1.93	0.49
1:B:317:VAL:HG23	1:B:323:SER:HA	1.94	0.49
1:B:1128:ALA:HB2	1:B:1141:ILE:HD11	1.94	0.49
1:A:925:ARG:HA	1:B:514:HIS:CD2	2.47	0.49
1:A:163:ASP:HB3	1:A:166:GLU:HG2	1.95	0.49
1:B:608:HIS:HD2	1:B:618:TYR:HE2	1.59	0.49
1:B:700:ASN:ND2	1:B:703:GLU:OE1	2.46	0.49
1:B:534:ARG:HA	1:B:537:ILE:HD12	1.95	0.49
1:B:200:PHE:CZ	1:B:334:VAL:HG13	2.48	0.49
1:B:210:LEU:HB3	1:B:330:VAL:HG11	1.95	0.49
1:B:94:ALA:HB1	1:B:97:ARG:NE	2.28	0.49
1:A:1101:ASN:OD1	1:A:1104:TRP:N	2.23	0.48
1:A:730:LYS:HB3	1:A:751:PHE:CE2	2.47	0.48
1:B:1078:LEU:HD22	1:B:1085:PRO:HD3	1.95	0.48
1:A:215:LEU:O	1:A:219:PRO:HD3	2.13	0.48
1:A:273:TYR:CE2	1:A:277:LEU:HD11	2.48	0.48
1:A:425:SER:OG	1:A:426:GLY:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:LEU:HD21	1:A:1071:GLY:HA3	1.95	0.48
1:B:1065:VAL:HG23	1:B:1241:VAL:HA	1.95	0.48
1:A:281:LYS:HE2	1:A:785:ARG:NH1	2.29	0.48
1:B:1230:LEU:HD23	1:B:1233:ILE:HD12	1.96	0.48
1:A:303:TYR:HE1	1:A:758:LEU:HD23	1.79	0.48
1:A:925:ARG:HA	1:B:514:HIS:HD2	1.77	0.48
1:B:425:SER:HB3	1:B:597:PHE:O	2.13	0.48
1:A:125:ALA:O	1:A:129:VAL:HG12	2.13	0.48
1:B:1204:THR:OG1	1:B:1205:GLU:N	2.46	0.48
1:B:337:GLY:O	1:B:340:SER:OG	2.30	0.48
1:A:1015:ASP:OD1	1:A:1018:SER:N	2.46	0.48
1:A:1022:LEU:HB2	1:A:1100:LEU:HD23	1.96	0.48
1:A:1167:ASP:HA	1:A:1171:GLN:HE22	1.79	0.48
1:B:169:THR:O	1:B:173:ASP:HB2	2.14	0.48
1:B:1197:GLU:HB3	1:B:1200:SER:HB3	1.96	0.47
1:A:156:ILE:HD12	1:A:157:GLY:N	2.29	0.47
1:A:337:GLY:O	1:A:340:SER:OG	2.33	0.47
1:A:1253:HIS:ND1	1:A:1263:TYR:OH	2.38	0.47
1:A:360:GLU:O	1:A:364:ILE:HG12	2.15	0.47
1:B:460:ARG:HG3	1:B:907:THR:HG21	1.96	0.47
1:B:488:ARG:CZ	1:B:491:VAL:HG12	2.45	0.47
1:A:436:MET:HB3	1:A:549:LEU:HD21	1.96	0.47
1:A:496:ILE:O	1:A:500:VAL:HG23	2.14	0.47
1:B:199:GLY:O	1:B:333:SER:OG	2.19	0.47
1:B:1097:ILE:HA	1:B:1100:LEU:HD12	1.97	0.47
1:A:238:LYS:HG2	1:A:283:LEU:HD11	1.97	0.47
1:A:302:ILE:HD12	2:A:6001:0JZ:H30	1.97	0.47
1:A:383:ASN:N	1:A:383:ASN:OD1	2.48	0.47
1:B:379:HIS:ND1	1:B:456:THR:O	2.37	0.47
1:A:1234:GLN:HG2	1:A:1253:HIS:CE1	2.50	0.47
1:B:200:PHE:CE2	1:B:215:LEU:HD12	2.50	0.47
1:B:34:SER:OG	1:B:37:THR:OG1	2.28	0.47
1:B:418:THR:HG23	1:B:578:THR:HB	1.96	0.47
1:B:1183:ALA:O	1:B:1187:VAL:HG23	2.15	0.47
1:B:513:PRO:HB2	1:B:514:HIS:ND1	2.29	0.46
1:B:691:ALA:HB1	1:B:692:SER:HB2	1.97	0.46
1:B:707:PHE:O	1:B:711:ILE:HG13	2.15	0.46
1:B:711:ILE:HG12	1:B:833:PHE:CE2	2.49	0.46
1:B:332:PHE:HE1	2:B:6002:0JZ:H30A	1.81	0.46
1:A:394:HIS:HA	1:A:406:LEU:O	2.15	0.46
1:A:46:ASP:CG	1:A:138:ARG:HH12	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:TYR:O	1:A:772:THR:HB	2.15	0.46
1:A:893:ALA:O	1:A:897:ILE:HG12	2.15	0.46
1:A:1020:GLN:HG2	1:A:1021:GLY:N	2.31	0.46
1:A:1178:GLN:O	1:A:1182:ILE:HG12	2.16	0.46
1:A:1207:GLU:HB2	1:A:1229:ARG:HH22	1.80	0.46
1:B:1018:SER:O	1:B:1101:ASN:ND2	2.48	0.46
1:A:513:PRO:HB2	1:A:514:HIS:CD2	2.50	0.46
1:A:64:LEU:HD12	1:A:336:ILE:HG21	1.97	0.46
1:A:1070:CYS:HA	1:A:1071:GLY:HA2	1.51	0.46
1:A:121:VAL:HG21	1:A:946:TYR:CE2	2.51	0.46
1:A:446:MET:HB2	1:A:453:ASP:OD2	2.15	0.46
1:B:530:GLY:HA2	1:B:557:LEU:HD21	1.99	0.46
1:A:1040:TYR:HA	1:A:1041:PRO:HD3	1.85	0.45
1:B:610:GLU:N	1:B:610:GLU:OE1	2.48	0.45
1:B:437:GLN:HG3	1:B:439:LEU:HG	1.98	0.45
1:A:147:PHE:CE1	1:A:361:VAL:HG22	2.51	0.45
1:A:860:ILE:O	1:A:864:ILE:HG13	2.17	0.45
1:B:895:GLU:O	1:B:899:ASN:ND2	2.39	0.45
1:B:1064:LEU:HB2	1:B:1226:ILE:HG13	1.97	0.45
1:A:210:LEU:HD21	1:A:327:VAL:HG13	1.98	0.45
1:A:534:ARG:HA	1:A:537:ILE:HD12	1.98	0.45
1:A:35:VAL:HG23	1:A:351:PHE:HZ	1.82	0.45
1:A:200:PHE:CE2	1:A:215:LEU:HD12	2.51	0.45
1:A:250:ALA:O	1:A:254:LEU:HG	2.16	0.45
1:B:478:THR:O	1:B:520:VAL:HG12	2.16	0.45
1:B:975:SER:HB3	2:B:6002:0JZ:C21	2.47	0.45
1:A:332:PHE:CE1	2:A:6001:0JZ:H36B	2.52	0.45
1:A:371:ILE:O	1:A:373:SER:HB3	2.16	0.45
1:B:168:ASN:OD1	1:B:169:THR:N	2.50	0.45
1:B:1040:TYR:HA	1:B:1041:PRO:HD3	1.85	0.45
1:A:1165:VAL:HA	1:A:1166:GLY:HA2	1.62	0.45
1:A:215:LEU:O	1:A:218:SER:OG	2.28	0.45
1:B:488:ARG:NH1	1:B:542:VAL:O	2.50	0.45
1:B:156:ILE:H	1:B:156:ILE:HG13	1.66	0.45
1:B:281:LYS:O	1:B:285:ILE:HG12	2.17	0.45
2:B:6002:0JZ:H30B	2:B:6002:0JZ:N24	2.32	0.44
1:B:1165:VAL:HA	1:B:1166:GLY:HA2	1.68	0.44
1:B:122:LEU:HB3	1:B:943:ALA:CB	2.44	0.44
1:A:243:TYR:CD1	1:A:785:ARG:NH1	2.85	0.44
1:A:487:GLY:O	1:A:543:ARG:NH1	2.50	0.44
1:A:1049:LEU:HD22	1:A:1052:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:MET:HA	1:B:900:PHE:HE2	1.83	0.44
1:B:156:ILE:CD1	1:B:439:LEU:HB3	2.46	0.44
1:A:156:ILE:HG12	1:A:439:LEU:HB3	1.98	0.44
1:A:930:LYS:HB2	1:A:930:LYS:HZ2	1.83	0.44
1:A:1150:ILE:HG22	1:A:1179:ARG:HB3	2.00	0.44
1:A:845:ILE:HG22	1:A:972:LEU:HD21	1.99	0.44
1:B:302:ILE:HG13	1:B:303:TYR:N	2.33	0.44
1:B:758:LEU:HA	1:B:761:ILE:HD12	2.00	0.44
1:A:30:LYS:HA	1:A:31:PRO:HD3	1.74	0.44
1:B:281:LYS:HE3	1:B:785:ARG:NH2	2.32	0.44
1:B:289:ILE:O	1:B:293:ILE:HG12	2.17	0.44
1:B:378:GLY:H	1:B:458:ASN:HB2	1.83	0.44
1:A:421:LEU:HD12	1:A:581:ILE:HD11	2.00	0.44
1:B:90:GLN:HG2	1:B:91:MET:H	1.82	0.44
1:B:902:THR:O	1:B:906:LEU:HD12	2.18	0.44
1:A:70:ILE:HD13	1:A:113:TYR:HB3	2.00	0.43
1:A:490:ASP:OD2	1:B:460:ARG:NH1	2.50	0.43
1:B:1154:ILE:HG13	1:B:1155:ASP:OD2	2.18	0.43
1:A:314:THR:HA	1:A:317:VAL:HG12	2.00	0.43
1:B:289:ILE:HD13	1:B:771:PHE:HE1	1.83	0.43
1:A:916:TYR:O	1:A:919:SER:OG	2.30	0.43
1:A:1154:ILE:HD13	1:A:1161:TYR:CZ	2.53	0.43
1:B:695:ARG:HA	1:B:698:LYS:HZ1	1.79	0.43
1:A:1056:VAL:HG22	1:A:1062:LEU:HD13	2.00	0.43
1:B:263:PHE:CD1	1:B:1130:GLY:HA2	2.53	0.43
1:B:864:ILE:HG12	1:B:944:MET:SD	2.59	0.43
1:B:961:THR:OG1	1:B:962:GLN:N	2.51	0.43
1:A:1089:SER:HB3	1:A:1096:GLU:OE2	2.19	0.43
1:B:161:VAL:HG23	1:B:162:HIS:CD2	2.53	0.43
1:B:1062:LEU:HD12	1:B:1238:LEU:O	2.19	0.43
1:B:1127:ILE:HG21	1:B:1141:ILE:HG23	2.01	0.43
1:B:281:LYS:NZ	1:B:781:THR:HG21	2.34	0.43
1:B:1090:VAL:O	1:B:1097:ILE:HG13	2.19	0.43
1:A:121:VAL:HA	1:A:124:VAL:HG22	2.01	0.43
1:A:457:ILE:HD11	1:A:462:LEU:HD13	2.00	0.43
1:B:376:LYS:HA	1:B:377:SER:HA	1.58	0.43
1:B:699:LEU:O	1:B:783:ARG:NH2	2.43	0.43
1:A:42:ALA:HB2	1:A:139:GLN:OE1	2.17	0.43
1:A:75:THR:HG22	1:A:967:PHE:CZ	2.53	0.43
1:A:840:GLY:O	1:A:843:ILE:HG22	2.19	0.43
1:A:860:ILE:HG21	1:A:948:SER:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:ALA:O	1:A:984:VAL:HG22	2.19	0.43
1:B:960:VAL:HG21	1:B:967:PHE:CB	2.48	0.43
1:A:281:LYS:HZ3	1:A:785:ARG:CD	2.31	0.43
1:A:611:LEU:HB3	1:A:618:TYR:HD2	1.84	0.43
1:B:196:PHE:HD1	1:B:337:GLY:O	2.02	0.43
1:A:158:TRP:CZ2	1:A:364:ILE:HD12	2.54	0.43
1:A:711:ILE:HG13	1:A:712:PHE:N	2.34	0.43
1:A:854:THR:HG23	1:A:977:ILE:HD11	2.00	0.43
1:B:33:VAL:HG22	1:B:359:TYR:HD1	1.82	0.43
1:B:908:ARG:HE	1:B:908:ARG:HA	1.83	0.43
1:B:1123:ILE:HG12	1:B:1163:THR:HG23	2.01	0.43
1:A:723:ALA:O	1:A:727:ILE:HG12	2.19	0.42
1:A:975:SER:HA	1:A:979:PHE:CD2	2.53	0.42
1:A:83:GLN:HA	1:A:738:GLY:HA3	2.00	0.42
1:A:331:PHE:CE2	2:A:6001:0JZ:H36	2.55	0.42
1:A:689:PRO:HG3	1:A:1003:HIS:NE2	2.35	0.42
1:B:791:SER:OG	1:B:1007:ILE:O	2.30	0.42
1:A:796:ASP:OD1	1:A:1012:PRO:HB2	2.19	0.42
1:B:340:SER:O	1:B:343:GLN:HG2	2.20	0.42
1:B:1124:ALA:HB2	1:B:1161:TYR:HB2	2.01	0.42
1:A:453:ASP:HB3	1:A:456:THR:HG23	2.01	0.42
1:A:838:ASN:ND2	1:A:980:GLY:O	2.52	0.42
1:A:910:GLN:NE2	1:B:491:VAL:O	2.51	0.42
1:A:965:MET:HA	1:A:966:THR:HA	1.72	0.42
1:A:1081:ARG:HG2	1:A:1081:ARG:NH1	2.32	0.42
1:B:533:GLN:O	1:B:537:ILE:HG13	2.19	0.42
1:A:438:ARG:NH1	1:A:455:ARG:HA	2.34	0.42
1:A:113:TYR:O	1:A:117:ILE:HG13	2.20	0.42
1:A:232:LEU:O	1:A:236:THR:OG1	2.25	0.42
1:A:1158:PRO:HA	1:A:1159:ASP:HA	1.49	0.42
1:B:916:TYR:O	1:B:919:SER:OG	2.26	0.42
1:A:617:ILE:HD12	1:A:617:ILE:H	1.84	0.42
1:A:698:LYS:O	1:A:701:SER:OG	2.34	0.42
1:B:46:ASP:OD1	1:B:138:ARG:NH1	2.53	0.42
1:B:512:LEU:HD13	1:B:518:THR:HG21	2.01	0.42
1:A:458:ASN:OD1	1:A:459:VAL:N	2.53	0.42
1:A:471:GLN:HB3	1:A:552:GLU:HB2	2.01	0.42
1:A:797:VAL:HG21	1:A:1082:PHE:CD1	2.54	0.42
1:B:474:VAL:HG13	1:B:902:THR:HG21	2.00	0.42
1:B:723:ALA:O	1:B:727:ILE:HG12	2.19	0.42
1:A:306:TYR:CD1	1:A:724:PHE:HZ	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:LEU:HD23	1:A:829:LEU:HA	1.86	0.42
1:A:849:TYR:O	1:A:969:ASN:HB3	2.20	0.42
1:B:728:PHE:CE2	1:B:971:LEU:HD21	2.55	0.42
1:A:310:PHE:HD2	1:A:755:PHE:HE2	1.68	0.42
1:A:515:GLN:OE1	1:B:138:ARG:NH2	2.52	0.42
1:B:217:ILE:HD11	1:B:308:LEU:HD22	2.01	0.42
1:B:496:ILE:O	1:B:500:VAL:HG23	2.19	0.42
1:A:484:ILE:HG21	1:A:496:ILE:HG23	2.02	0.41
1:A:1128:ALA:HB1	1:A:1136:VAL:HG21	2.02	0.41
1:A:263:PHE:O	1:A:1132:ASN:ND2	2.53	0.41
1:A:610:GLU:HG3	1:A:613:ARG:HH21	1.84	0.41
1:A:328:LEU:HD11	1:A:732:VAL:HG11	2.02	0.41
1:A:788:VAL:HG13	1:A:1007:ILE:HG21	2.02	0.41
1:A:886:LEU:HD12	1:A:886:LEU:HA	1.96	0.41
1:A:1037:VAL:HG23	1:A:1049:LEU:O	2.21	0.41
1:B:121:VAL:HG21	1:B:946:TYR:CE1	2.56	0.41
1:B:136:ALA:HB1	1:B:182:ILE:HG13	2.01	0.41
1:B:730:LYS:HB3	1:B:751:PHE:CE2	2.55	0.41
1:B:1072:LYS:HD3	1:B:1226:ILE:HG23	2.02	0.41
1:A:147:PHE:CG	1:A:361:VAL:HG13	2.56	0.41
1:A:306:TYR:CE1	1:A:724:PHE:HZ	2.38	0.41
1:B:246:ALA:HB2	1:B:276:ASN:O	2.20	0.41
1:B:299:PHE:HA	1:B:302:ILE:HG12	2.03	0.41
1:B:323:SER:OG	1:B:324:ILE:N	2.53	0.41
1:B:486:TYR:O	1:B:906:LEU:HD22	2.20	0.41
1:B:835:ASN:OD1	1:B:984:VAL:HA	2.21	0.41
1:B:209:LYS:O	1:B:213:VAL:HG23	2.20	0.41
1:B:1079:LEU:HD23	1:B:1194:LEU:HD21	2.02	0.41
1:A:1147:GLU:O	1:A:1216:LYS:HD2	2.20	0.41
1:B:960:VAL:HG21	1:B:967:PHE:HB2	2.02	0.41
1:A:207:GLY:HA3	1:A:330:VAL:HG11	2.03	0.41
1:A:1203:ASP:O	1:A:1206:SER:OG	2.35	0.41
1:B:500:VAL:HG21	1:B:516:PHE:HE1	1.85	0.41
1:B:740:PRO:HA	1:B:741:PRO:HD3	1.88	0.41
1:B:860:ILE:O	1:B:864:ILE:HG13	2.21	0.41
1:A:217:ILE:O	1:A:220:VAL:HG12	2.21	0.41
1:A:1120:ASP:HB3	1:A:1168:LYS:HD2	2.03	0.41
1:B:300:LEU:HD11	1:B:760:ILE:HD13	2.03	0.41
1:B:896:ALA:HB2	1:B:912:PHE:CD2	2.56	0.41
1:B:904:VAL:HG23	1:B:909:GLU:OE2	2.20	0.41
1:B:1048:VAL:HG22	1:B:1049:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:THR:HG21	1:A:573:ARG:HH11	1.86	0.41
1:A:728:PHE:CE1	1:A:971:LEU:HD21	2.56	0.41
1:B:819:ALA:O	1:B:822:LYS:HG2	2.21	0.41
1:A:139:GLN:NE2	1:A:182:ILE:HD12	2.36	0.40
1:A:213:VAL:O	1:A:217:ILE:HG12	2.21	0.40
1:A:239:GLU:OE1	1:A:287:LYS:NZ	2.50	0.40
1:A:784:LEU:CD2	1:A:821:VAL:HG11	2.49	0.40
1:A:1183:ALA:O	1:A:1187:VAL:HG23	2.20	0.40
1:B:1056:VAL:HG23	1:B:1060:GLN:HG3	2.02	0.40
1:A:34:SER:OG	1:A:37:THR:OG1	2.36	0.40
1:B:608:HIS:HD2	1:B:618:TYR:CE2	2.38	0.40
1:B:927:ALA:HA	1:B:930:LYS:HB3	2.02	0.40
1:A:856:LEU:O	1:A:860:ILE:HG13	2.21	0.40
1:A:1241:VAL:HB	1:A:1249:GLU:HB2	2.03	0.40
1:B:125:ALA:O	1:B:129:VAL:HG12	2.21	0.40
1:B:282:ARG:HH22	1:B:779:ILE:HA	1.86	0.40
1:B:493:MET:HA	1:B:496:ILE:HD12	2.03	0.40
1:B:541:LEU:HD23	1:B:541:LEU:HA	1.93	0.40
1:B:1023:LYS:HA	1:B:1024:PRO:HD3	1.71	0.40
1:A:848:ILE:HG13	1:A:849:TYR:CD1	2.57	0.40
1:A:1154:ILE:HD13	1:A:1161:TYR:CE2	2.56	0.40
1:B:123:ILE:O	1:B:127:ILE:HG12	2.21	0.40
1:B:381:PRO:O	1:B:461:TYR:OH	2.30	0.40
1:B:464:GLU:HA	1:B:543:ARG:HH21	1.84	0.40
1:B:848:ILE:HG22	1:B:849:TYR:CD2	2.57	0.40
1:A:900:PHE:HA	1:A:903:VAL:HG12	2.04	0.40
1:A:1249:GLU:HG2	1:A:1259:GLN:NE2	2.36	0.40
1:B:1112:VAL:HB	1:B:1195:LEU:HD13	2.04	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	1184/1282 (92%)	1104 (93%)	72 (6%)	8 (1%)	22	62
1	B	1176/1282 (92%)	1083 (92%)	83 (7%)	10 (1%)	17	56
All	All	2360/2564 (92%)	2187 (93%)	155 (7%)	18 (1%)	19	60

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	VAL
1	B	1136	VAL
1	A	1036	VAL
1	A	1204	THR
1	B	32	ALA
1	A	44	TRP
1	A	477	ALA
1	A	1070	CYS
1	B	128	GLN
1	B	383	ASN
1	B	962	GLN
1	A	128	GLN
1	A	1121	CYS
1	B	391	LYS
1	B	1204	THR
1	B	1028	GLU
1	A	525	ALA
1	B	393	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	979/1063 (92%)	953 (97%)	26 (3%)	44	66
1	B	973/1063 (92%)	944 (97%)	29 (3%)	41	63
All	All	1952/2126 (92%)	1897 (97%)	55 (3%)	43	65

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	ARG
1	A	374	PHE
1	A	375	SER
1	A	383	ASN
1	A	385	GLN
1	A	396	SER
1	A	474	VAL
1	A	478	THR
1	A	520	VAL
1	A	681	LYS
1	A	695	ARG
1	A	700	ASN
1	A	778	GLU
1	A	817	ASP
1	A	852	GLN
1	A	909	GLU
1	A	944	MET
1	A	965	MET
1	A	966	THR
1	A	1020	GLN
1	A	1037	VAL
1	A	1048	VAL
1	A	1111	ILE
1	A	1155	ASP
1	A	1167	ASP
1	A	1168	LYS
1	B	75	THR
1	B	90	GLN
1	B	211	THR
1	B	220	VAL
1	B	277	LEU
1	B	279	GLU
1	B	283	LEU
1	B	292	ASN
1	B	310	PHE
1	B	333	SER
1	B	336	ILE
1	B	409	LEU
1	B	474	VAL
1	B	478	THR
1	B	601	VAL
1	B	700	ASN
1	B	720	LEU

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Mol	Chain	Res	Type
1	B	725	SER
1	B	755	PHE
1	B	817	ASP
1	B	828	ARG
1	B	848	ILE
1	B	908	ARG
1	B	944	MET
1	B	967	PHE
1	B	1019	THR
1	B	1022	LEU
1	B	1163	THR
1	B	1167	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	608	HIS
1	A	852	GLN
1	A	1103	GLN
1	A	1114	GLN
1	B	60	HIS
1	B	139	GLN
1	B	292	ASN
1	B	326	GLN
1	B	608	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
2	0JZ	B	6002	-	21,39,39	2.25	3 (14%)	24,57,57	2.02	9 (37%)
2	0JZ	A	6001	-	21,39,39	2.31	3 (14%)	24,57,57	2.32	9 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0JZ	B	6002	-	-	5/24/48/48	0/3/4/4
2	0JZ	A	6001	-	-	0/24/48/48	0/3/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6001	0JZ	C02-N03	6.55	1.48	1.34
2	B	6002	0JZ	C09-N10	6.21	1.47	1.34
2	A	6001	0JZ	C09-N10	5.81	1.46	1.34
2	B	6002	0JZ	C02-N03	5.51	1.46	1.34
2	B	6002	0JZ	C16-N17	4.86	1.44	1.34
2	A	6001	0JZ	C16-N17	4.58	1.44	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6002	0JZ	C15-C16-N17	6.04	126.42	115.20
2	A	6001	0JZ	C35-C34-C18	5.98	116.99	111.24
2	A	6001	0JZ	C36-C34-C18	4.89	115.94	111.24
2	A	6001	0JZ	C29-C28-C04	3.53	114.63	111.24
2	A	6001	0JZ	C18-N17-C16	3.39	127.71	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6002	0JZ	C30-C28-C04	3.31	114.42	111.24
2	A	6001	0JZ	C30-C28-C04	3.19	114.31	111.24
2	B	6002	0JZ	O27-C16-N17	-2.96	117.00	122.45
2	B	6002	0JZ	C18-N17-C16	-2.59	118.12	122.28
2	A	6001	0JZ	C08-C09-N10	2.51	119.87	115.20
2	B	6002	0JZ	C36-C34-C18	2.47	113.61	111.24
2	B	6002	0JZ	C04-N03-C02	2.47	126.23	122.28
2	A	6001	0JZ	C01-C02-N03	2.42	119.69	115.20
2	B	6002	0JZ	C11-N10-C09	2.30	125.96	122.28
2	A	6001	0JZ	C32-C31-C11	-2.29	109.03	111.24
2	B	6002	0JZ	C29-C28-C04	2.22	113.37	111.24
2	A	6001	0JZ	C36-C34-C35	2.09	116.43	110.59
2	B	6002	0JZ	O27-C16-C15	-2.07	116.58	121.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	6002	0JZ	N17-C18-C34-C36
2	B	6002	0JZ	N17-C18-C34-C35
2	B	6002	0JZ	C19-C18-C34-C36
2	B	6002	0JZ	C19-C18-C34-C35
2	B	6002	0JZ	N10-C11-C31-C33

There are no ring outliers.

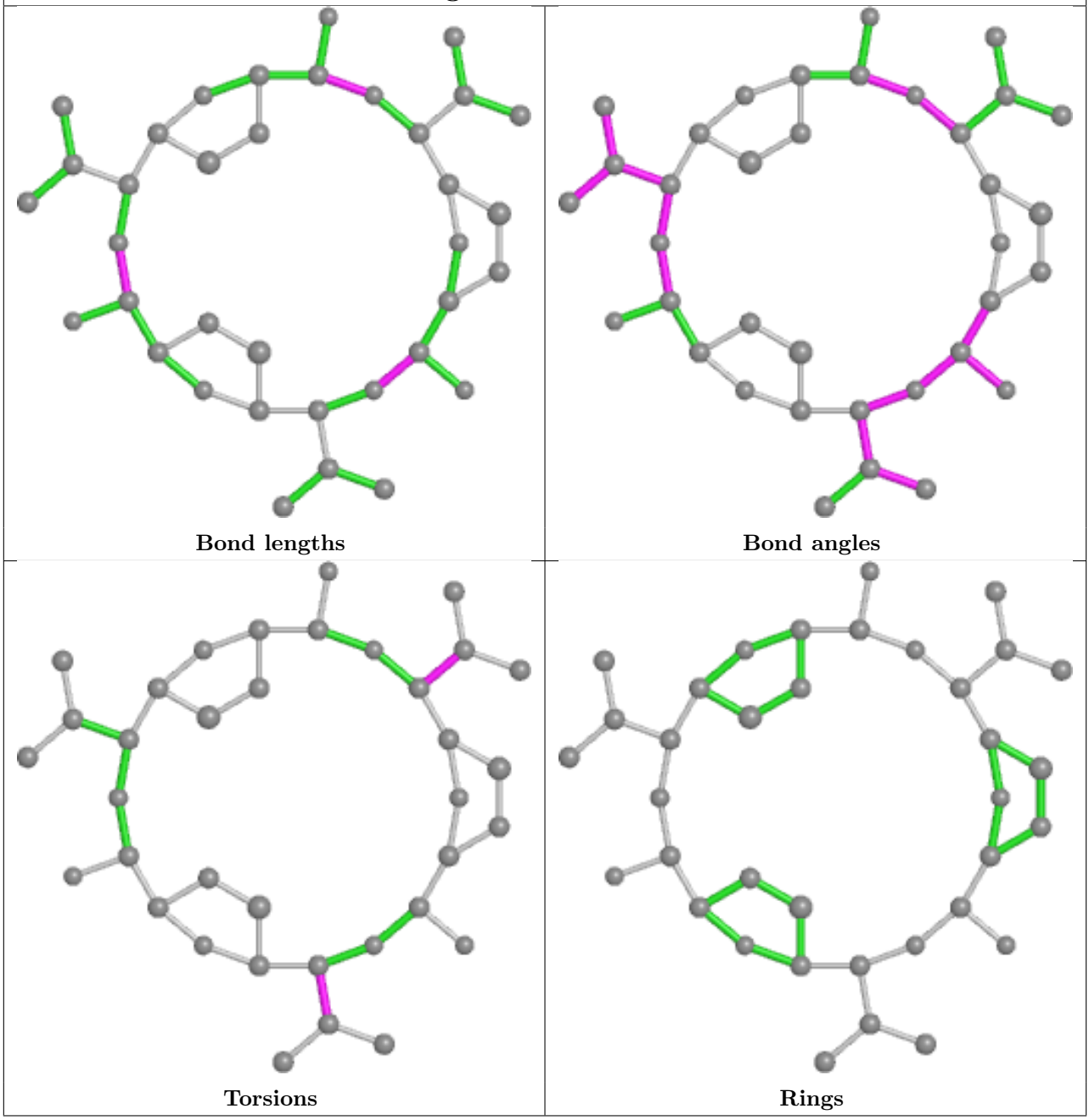
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6002	0JZ	6	0
2	A	6001	0JZ	4	0

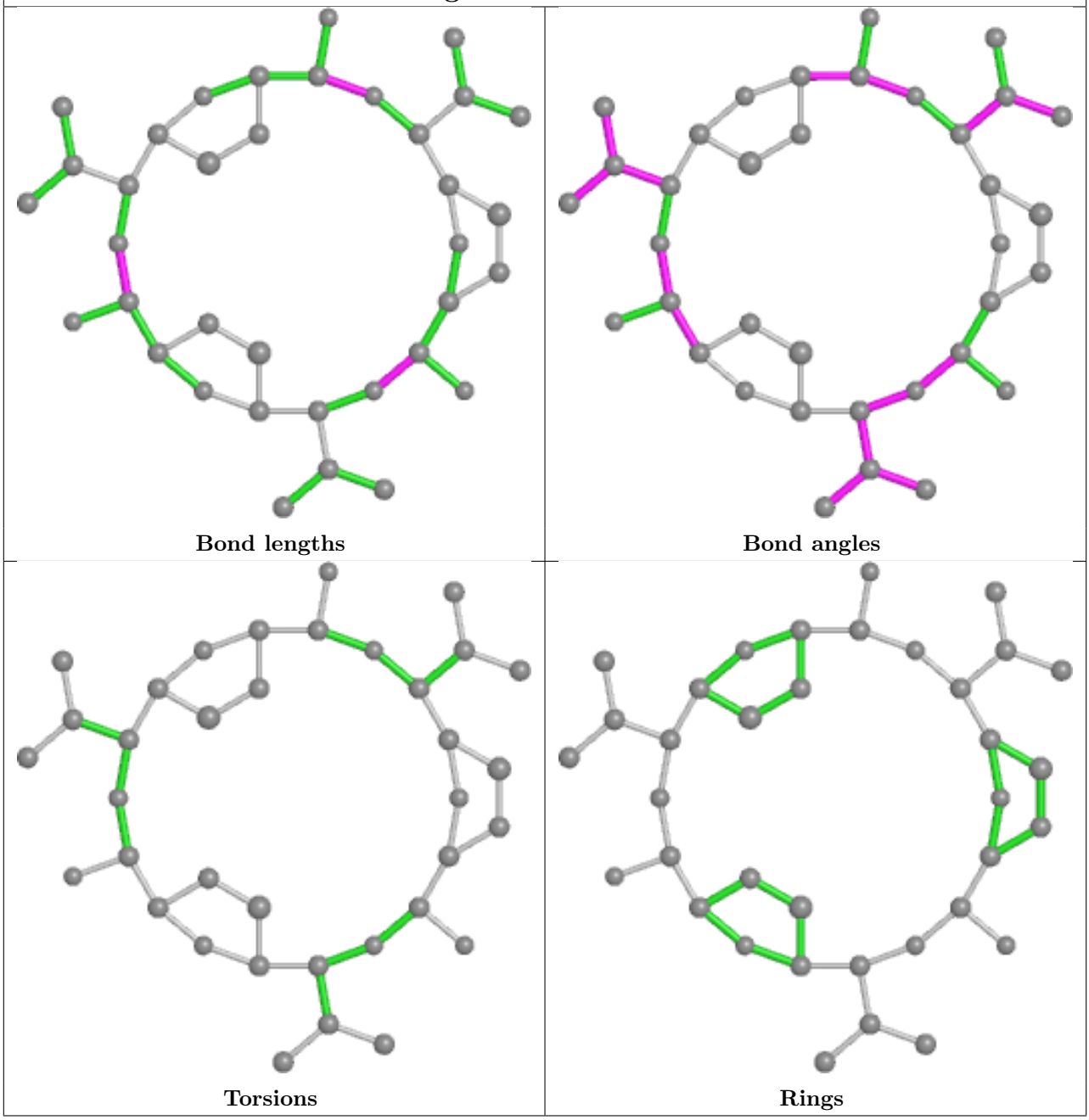
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

Ligand 0JZ B 6002



Ligand 0JZ A 6001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

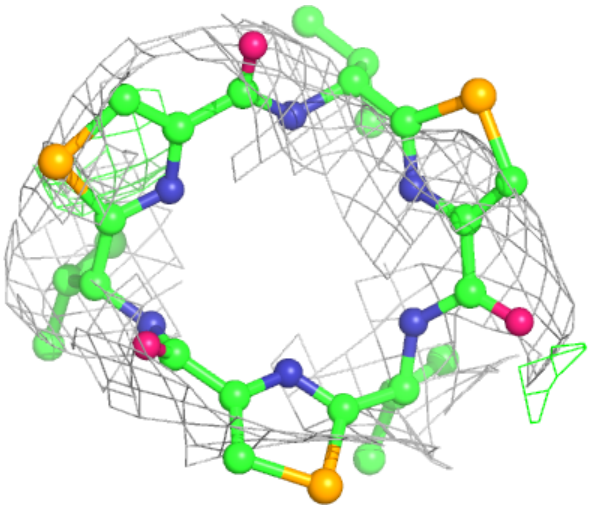
6.4 Ligands (i)

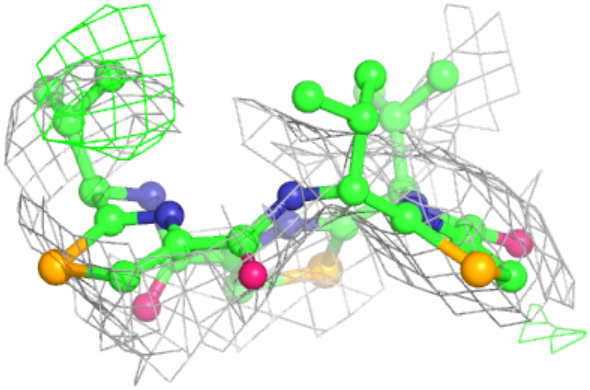
Unable to reproduce the depositors R factor - this section is therefore empty.

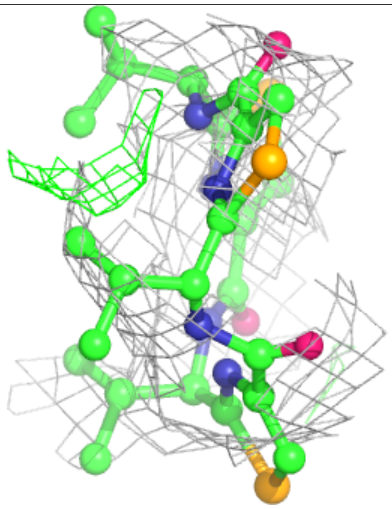
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 0JZ A 6001:

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

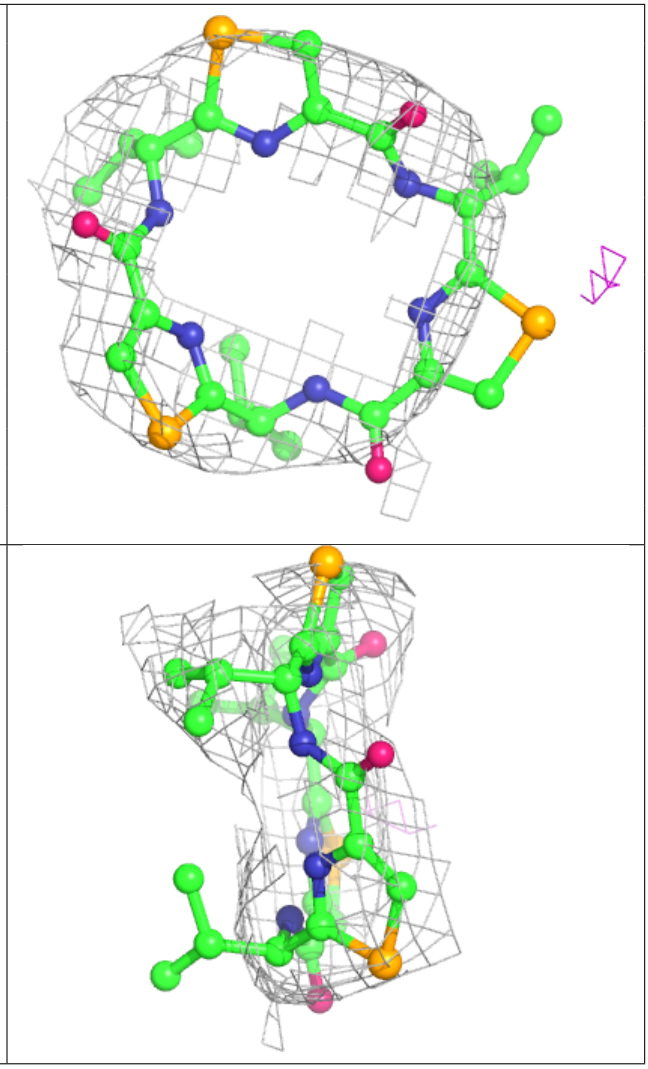






Electron density around 0JZ B 6002:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.