



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:48 PM UTC

PDB ID : 4M2S / pdb_00004m2s
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 ⓘ 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

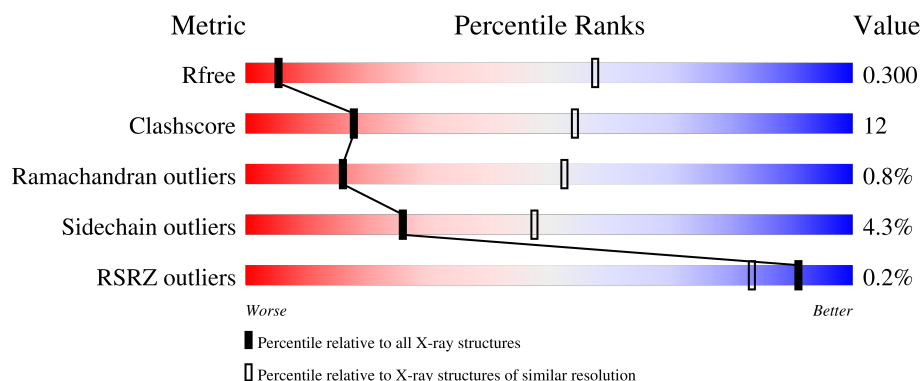
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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	1282	
1	B	1282	

2 Entry composition

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.

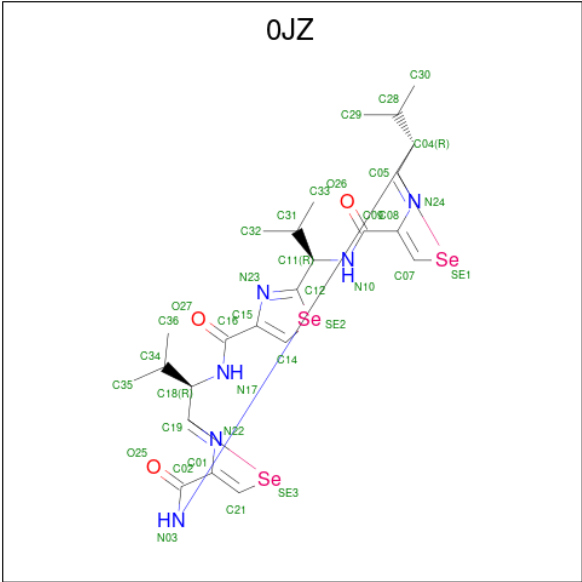
- Molecule 1 is a protein called Multidrug resistance protein 1A.

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

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

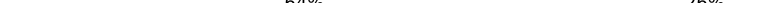
- Molecule 2 is (4R,11R,18R)-4,11,18-tri(propan-2-yl)-6,13,20-triseleno-3,10,17,22,23,24-hexaazatetracyclo[17.2.1.1 5,8 .1 12,15]tetracos-1(21),5(24),7,12(23),14,19(22)-hexaene-2,9,16-trione (CCD ID: 0JZ) (formula: C₂₄H₃₀N₆O₃Se₃).

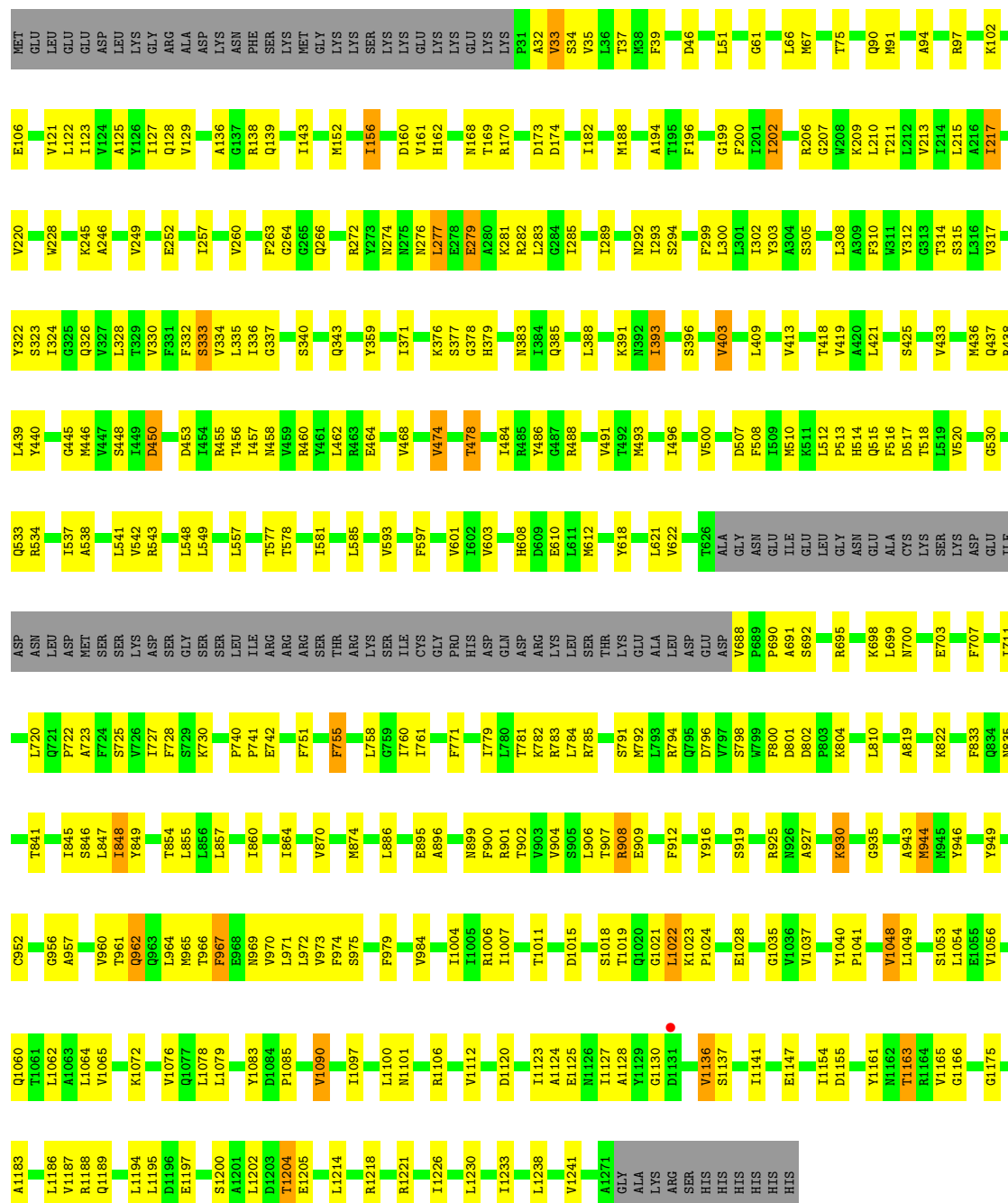


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		
2	B	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		



- Molecule 1: Multidrug resistance protein 1A

Chain B:  64% 26% 8%



4 Data and refinement statistics

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 24.51 – 4.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (24.51-4.40) 87.5 (24.51-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.227 , 0.294 0.236 , 0.300	Depositor DCC
R_{free} test set	2684 reflections (9.54%)	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 , 129.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.34	0/9383	0.77	2/12685 (0.0%)
1	B	0.33	0/9322	0.78	2/12602 (0.0%)
All	All	0.33	0/18705	0.78	4/25287 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	964	LEU	CB-CA-C	-5.78	109.93	116.63
1	A	688	VAL	CA-C-N	-5.47	114.74	120.38
1	A	688	VAL	C-N-CA	-5.47	114.74	120.38
1	B	450	ASP	CB-CA-C	-5.05	110.78	116.63

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	243	0
1	B	9153	0	9338	225	0
2	A	36	0	27	4	0
2	B	36	0	27	6	0
All	All	18439	0	18780	459	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 (459) 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: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: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:792:MET:HE1	1:B:810:LEU:HB3	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:OJZ:H33	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:930:LYS:HB2	1:A:930:LYS:HZ2	1.63	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:OJZ: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:1035:GLY:H	1:B:1053:SER:HG	1.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OJZ: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:446:MET:HE2	1:A:448:SER:HB2	1.85	0.56
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: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:B:612:MET:HE1	1:B:622:VAL:HG21	1.88	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:199:GLY:O	1:B:333:SER:OG	2.19	0.54
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:446:MET:HE3	1:A:453:ASP:OD2	2.08	0.53
1:A:846:SER:O	1:A:854:THR:OG1	2.24	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:A:612:MET:HE1	1:A:622:VAL:HG11	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:B:446:MET:HE2	1:B:448:SER:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:46:ASP:CG	1:A:138:ARG:HH12	2.18	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:A:930:LYS:NZ	1:A:930:LYS:HB2	2.26	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:OJZ: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:B:870:VAL:HG12	1:B:874:MET:HE2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:446:MET:HE3	1:B:453:ASP:OD2	2.13	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:34:SER:OG	1:B:37:THR:OG1	2.28	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:239:GLU:HB2	1:A:287:LYS:HZ3	1.78	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:A:792:MET:HE3	1:A:810:LEU:HD22	1.95	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:OJZ:H30	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ASN:OD1	1:A:383:ASN:N	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: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:OJZ:H30A	1.81	0.46
1:A:394:HIS:HA	1:A:406:LEU:O	2.15	0.46
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:B:792:MET:HE2	1:B:792:MET:HB3	1.84	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:OJZ:C21	2.47	0.45
1:A:332:PHE:CE1	2:A:6001:OJZ:H36B	2.52	0.45
1:A:371:ILE:O	1:A:373:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:1203:ASP:O	1:A:1206:SER:OG	2.35	0.44
2:B:6002:OJZ:H30B	2:B:6002:OJZ: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
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:39:PHE:CD1	1:A:50:MET:HE1	2.53	0.44
1:B:170:ARG:HG3	1:B:174:ASP:CG	2.42	0.44
1:A:156:ILE:HG12	1:A:439:LEU:HB3	1.98	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:A:792:MET:HE1	1:A:810:LEU:HB3	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:415:SER:C	1:A:417:GLN:H	2.25	0.43
1:A:1056:VAL:HG22	1:A:1062:LEU:HD13	2.00	0.43
1:B:67:MET:HE3	1:B:946:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:232:LEU:O	1:A:236:THR:OG1	2.25	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
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:B:548:LEU:C	1:B:549:LEU:HD12	2.44	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:OJZ: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:312:TYR:O	1:B:315:SER:OG	2.33	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: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: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
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:A:850:GLY:O	1:A:854:THR:OG1	2.37	0.42
1:B:728:PHE:CE2	1:B:971:LEU:HD21	2.55	0.42
1:B:1147:GLU:CD	1:B:1186:LEU:HD21	2.45	0.42
1:A:310:PHE:HD2	1:A:755:PHE:HE2	1.68	0.42
1:A:515:GLN:CD	1:B:138:ARG:HH21	2.28	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:B:264:GLY:C	1:B:266:GLN:H	2.28	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:39:PHE:HD1	1:A:50:MET:HE1	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:188:MET:HE2	1:B:188:MET:HB3	1.95	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:A:62:VAL:C	1:A:65:PRO:HD2	2.45	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: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
1:A:418:THR:HG21	1:A:573:ARG:HH11	1.86	0.41
1:A:719:GLY:C	1:A:722:PRO:HD2	2.46	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:203:GLY:C	1:A:211:THR:HG21	2.46	0.40
1:A:213:VAL:O	1:A:217:ILE:HG12	2.21	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:952:CYS:SG	1:B:974:PHE:HD1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

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	1184/1282 (92%)	1104 (93%)	72 (6%)	8 (1%)	18	55
1	B	1176/1282 (92%)	1083 (92%)	83 (7%)	10 (1%)	14	49
All	All	2360/2564 (92%)	2187 (93%)	155 (7%)	18 (1%)	16	52

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	943 (96%)	36 (4%)	30	51
1	B	973/1063 (92%)	926 (95%)	47 (5%)	23	45
All	All	1952/2126 (92%)	1869 (96%)	83 (4%)	26	47

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	48	LEU
1	A	64	LEU
1	A	121	VAL
1	A	156	ILE
1	A	170	ARG
1	A	374	PHE
1	A	375	SER
1	A	382	ASP
1	A	383	ASN
1	A	385	GLN

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Mol	Chain	Res	Type
1	A	396	SER
1	A	411	LEU
1	A	450	ASP
1	A	474	VAL
1	A	478	THR
1	A	520	VAL
1	A	601	VAL
1	A	681	LYS
1	A	695	ARG
1	A	778	GLU
1	A	852	GLN
1	A	863	ILE
1	A	909	GLU
1	A	930	LYS
1	A	944	MET
1	A	965	MET
1	A	966	THR
1	A	1007	ILE
1	A	1020	GLN
1	A	1037	VAL
1	A	1048	VAL
1	A	1090	VAL
1	A	1111	ILE
1	A	1167	ASP
1	A	1168	LYS
1	B	35	VAL
1	B	51	LEU
1	B	75	THR
1	B	143	ILE
1	B	156	ILE
1	B	202	ILE
1	B	211	THR
1	B	217	ILE
1	B	220	VAL
1	B	249	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

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Mol	Chain	Res	Type
1	B	403	VAL
1	B	409	LEU
1	B	419	VAL
1	B	468	VAL
1	B	474	VAL
1	B	478	THR
1	B	593	VAL
1	B	601	VAL
1	B	603	VAL
1	B	688	VAL
1	B	720	LEU
1	B	725	SER
1	B	742	GLU
1	B	755	PHE
1	B	847	LEU
1	B	848	ILE
1	B	855	LEU
1	B	886	LEU
1	B	908	ARG
1	B	930	LYS
1	B	944	MET
1	B	967	PHE
1	B	970	VAL
1	B	1019	THR
1	B	1022	LEU
1	B	1037	VAL
1	B	1048	VAL
1	B	1054	LEU
1	B	1090	VAL
1	B	1163	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	744	GLN
1	A	834	GLN
1	A	838	ASN
1	A	852	GLN
1	A	910	GLN
1	A	962	GLN
1	A	1103	GLN

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Mol	Chain	Res	Type
1	A	1114	GLN
1	A	1151	HIS
1	A	1171	GLN
1	A	1243	GLN
1	A	1244	ASN
1	B	60	HIS
1	B	139	GLN
1	B	141	HIS
1	B	191	GLN
1	B	292	ASN
1	B	326	GLN
1	B	387	ASN
1	B	625	GLN
1	B	700	ASN
1	B	838	ASN
1	B	910	GLN
1	B	1108	GLN

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 oligosaccharides 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	OJZ	B	6002	-	33,39,39	2.77	11 (33%)	51,57,57	3.03	18 (35%)
2	OJZ	A	6001	-	33,39,39	2.73	13 (39%)	51,57,57	2.75	17 (33%)

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	OJZ	B	6002	-	-	12/42/48/48	0/4/4/4
2	OJZ	A	6001	-	-	5/42/48/48	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6001	OJZ	C02-N03	6.81	1.48	1.34
2	B	6002	OJZ	C14-C15	6.70	1.46	1.35
2	B	6002	OJZ	C09-N10	6.46	1.47	1.34
2	A	6001	OJZ	C14-C15	6.20	1.45	1.35
2	A	6001	OJZ	C09-N10	6.05	1.46	1.34
2	B	6002	OJZ	C02-N03	5.73	1.46	1.34
2	A	6001	OJZ	C21-C01	5.37	1.44	1.35
2	B	6002	OJZ	C16-N17	5.06	1.44	1.34
2	B	6002	OJZ	C07-C08	4.87	1.43	1.35
2	B	6002	OJZ	C21-C01	4.85	1.43	1.35
2	A	6001	OJZ	C16-N17	4.76	1.44	1.34
2	A	6001	OJZ	C07-C08	4.59	1.42	1.35
2	B	6002	OJZ	C08-C09	3.21	1.54	1.48
2	B	6002	OJZ	SE1-C07	3.18	1.95	1.86
2	A	6001	OJZ	C08-C09	3.08	1.54	1.48
2	A	6001	OJZ	SE1-C07	2.63	1.93	1.86
2	B	6002	OJZ	SE2-C12	2.60	1.93	1.88
2	B	6002	OJZ	C01-C02	2.41	1.53	1.48
2	B	6002	OJZ	SE2-C14	2.37	1.92	1.86
2	A	6001	OJZ	C01-C02	2.36	1.53	1.48
2	A	6001	OJZ	SE3-C21	2.23	1.92	1.86
2	A	6001	OJZ	C08-N24	2.18	1.43	1.38
2	A	6001	OJZ	SE2-C12	2.13	1.92	1.88
2	A	6001	OJZ	SE2-C14	2.05	1.91	1.86

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6002	OJZ	C15-N23-C12	8.22	121.63	113.49
2	B	6002	OJZ	C15-C16-N17	7.88	126.42	115.22
2	B	6002	OJZ	C01-N22-C19	7.68	121.10	113.49
2	A	6001	OJZ	C15-N23-C12	7.15	120.57	113.49
2	A	6001	OJZ	C14-SE2-C12	6.92	93.62	84.61
2	B	6002	OJZ	C08-N24-C05	6.31	119.74	113.49
2	A	6001	OJZ	C01-N22-C19	5.91	119.34	113.49
2	B	6002	OJZ	C07-SE1-C05	5.79	92.15	84.61
2	B	6002	OJZ	C14-SE2-C12	5.74	92.09	84.61
2	A	6001	OJZ	C21-SE3-C19	5.43	91.69	84.61
2	A	6001	OJZ	C07-SE1-C05	5.37	91.61	84.61
2	A	6001	OJZ	SE2-C14-C15	-5.18	103.63	111.07
2	B	6002	OJZ	C21-SE3-C19	5.13	91.30	84.61
2	A	6001	OJZ	C08-N24-C05	4.91	118.36	113.49
2	A	6001	OJZ	SE3-C21-C01	-4.73	104.28	111.07
2	B	6002	OJZ	SE1-C07-C08	-4.31	104.87	111.07
2	A	6001	OJZ	SE1-C07-C08	-3.94	105.42	111.07
2	B	6002	OJZ	SE2-C14-C15	-3.88	105.50	111.07
2	A	6001	OJZ	SE2-C12-N23	-3.81	104.50	113.38
2	B	6002	OJZ	SE3-C21-C01	-3.67	105.79	111.07
2	B	6002	OJZ	SE2-C12-N23	-3.59	105.02	113.38
2	B	6002	OJZ	O27-C16-N17	-3.46	117.00	123.09
2	B	6002	OJZ	SE3-C19-N22	-3.34	105.61	113.38
2	A	6001	OJZ	C08-C09-N10	3.27	119.87	115.22
2	B	6002	OJZ	SE1-C05-N24	-3.16	106.01	113.38
2	A	6001	OJZ	C01-C02-N03	3.14	119.69	115.22
2	A	6001	OJZ	C18-N17-C16	3.02	127.71	121.57
2	B	6002	OJZ	C09-C08-N24	-2.86	115.25	120.67
2	A	6001	OJZ	SE3-C19-N22	-2.85	106.75	113.38
2	A	6001	OJZ	SE1-C05-N24	-2.76	106.94	113.38
2	B	6002	OJZ	C04-N03-C02	2.29	126.23	121.57
2	B	6002	OJZ	C11-N10-C09	2.16	125.96	121.57
2	A	6001	OJZ	C36-C34-C35	2.13	116.43	110.58
2	A	6001	OJZ	C35-C34-C18	2.13	116.99	111.16
2	B	6002	OJZ	C16-C15-N23	2.09	124.62	120.67

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	6001	OJZ	C21-C01-C02-N03
2	A	6001	OJZ	C21-C01-C02-O25
2	A	6001	OJZ	N22-C01-C02-N03

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Mol	Chain	Res	Type	Atoms
2	A	6001	OJZ	N22-C01-C02-O25
2	B	6002	OJZ	C12-C11-C31-C33
2	B	6002	OJZ	N23-C15-C16-N17
2	B	6002	OJZ	N17-C18-C19-N22
2	B	6002	OJZ	C34-C18-C19-N22
2	B	6002	OJZ	C19-C18-C34-C36
2	B	6002	OJZ	N17-C18-C34-C36
2	B	6002	OJZ	N23-C15-C16-O27
2	B	6002	OJZ	N17-C18-C34-C35
2	B	6002	OJZ	C19-C18-C34-C35
2	B	6002	OJZ	C14-C15-C16-N17
2	B	6002	OJZ	C14-C15-C16-O27
2	B	6002	OJZ	N10-C11-C31-C33
2	A	6001	OJZ	C05-C04-N03-C02

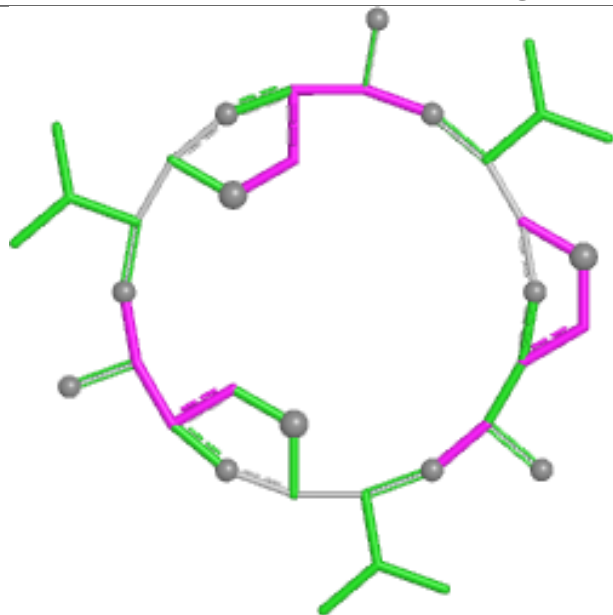
There are no ring outliers.

2 monomers are involved in 10 short contacts:

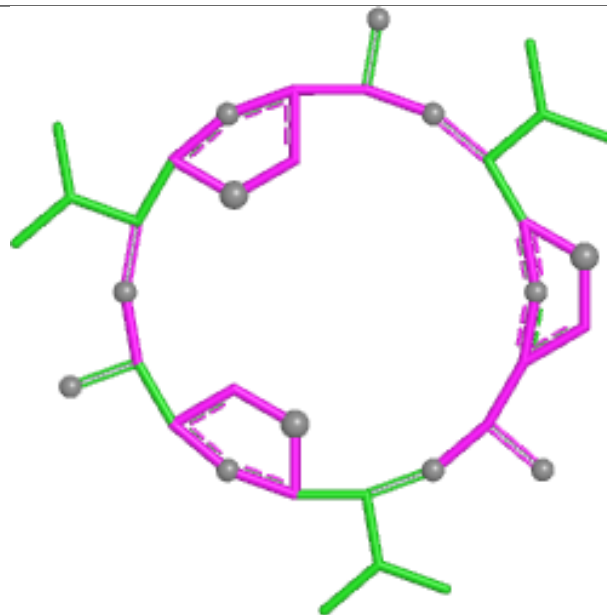
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6002	OJZ	6	0
2	A	6001	OJZ	4	0

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 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.

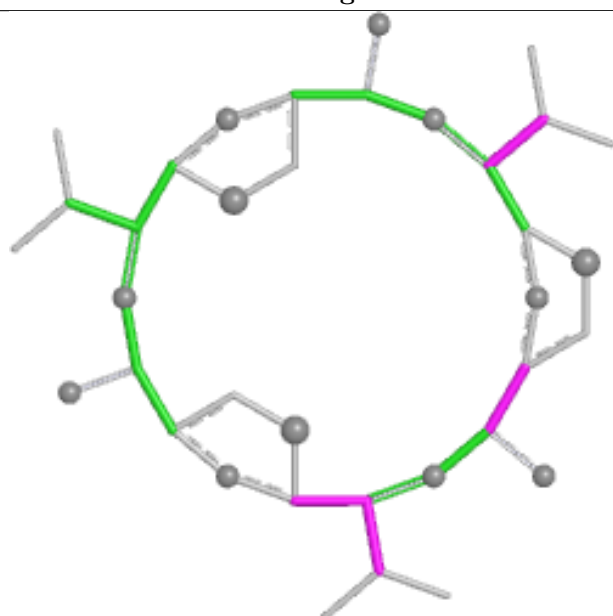
Ligand 0JZ B 6002



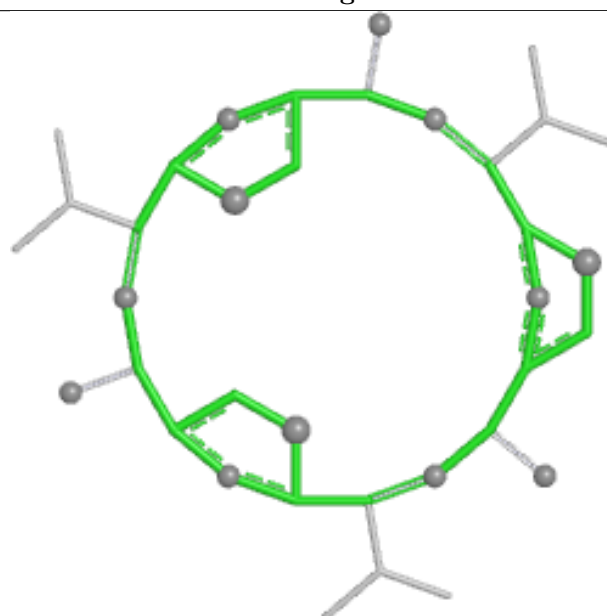
Bond lengths



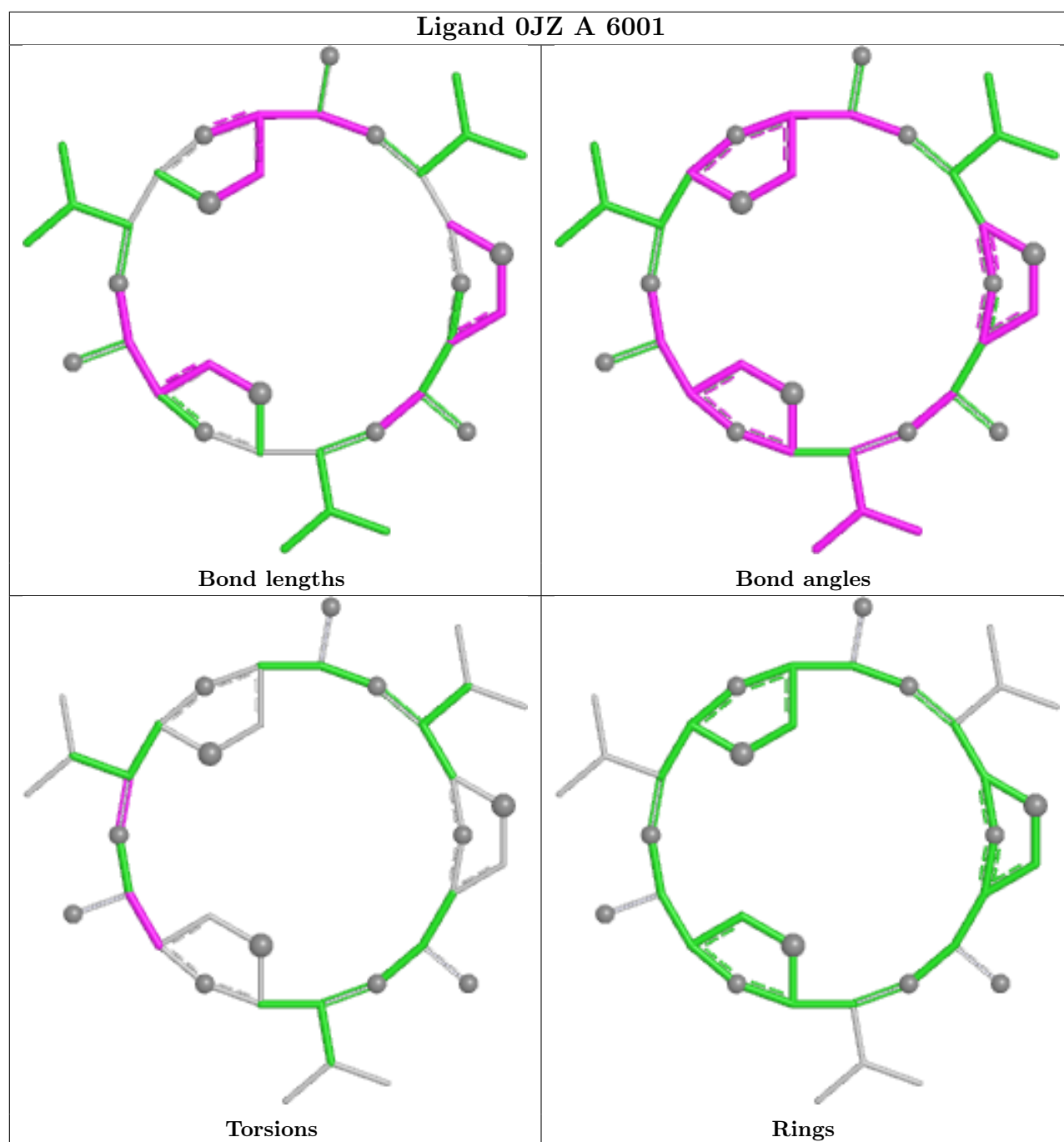
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1188/1282 (92%)	-0.49	3 (0%) 90 80	117, 200, 297, 422	0
1	B	1180/1282 (92%)	-0.49	1 (0%) 92 87	123, 198, 304, 458	0
All	All	2368/2564 (92%)	-0.49	4 (0%) 91 83	117, 198, 303, 458	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	987	VAL	5.6
1	B	1131	ASP	2.5
1	A	1084	ASP	2.4
1	A	984	VAL	2.4

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 [i](#)

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

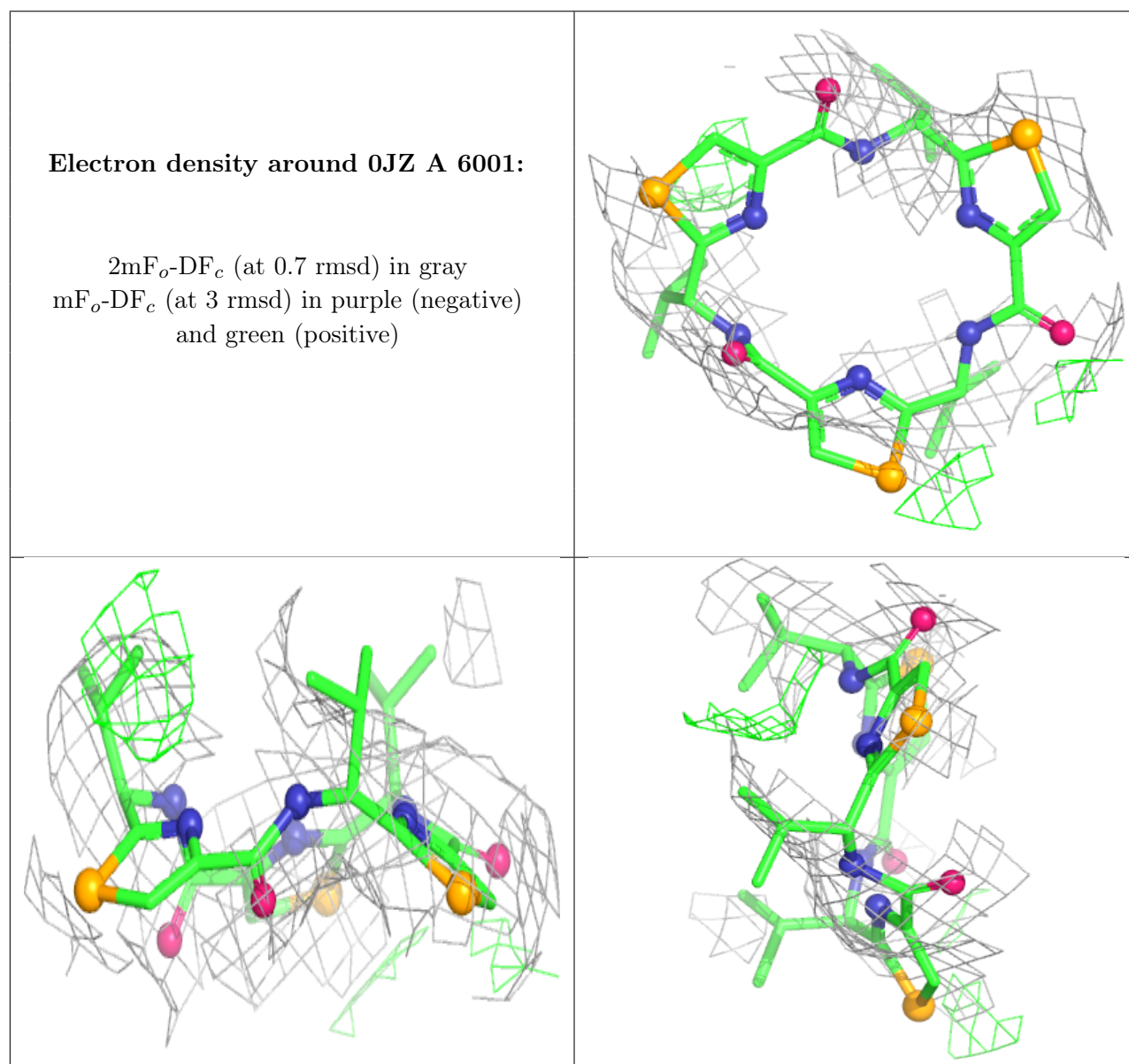
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OJZ	A	6001	36/36	0.72	0.10	180,230,476,517	0

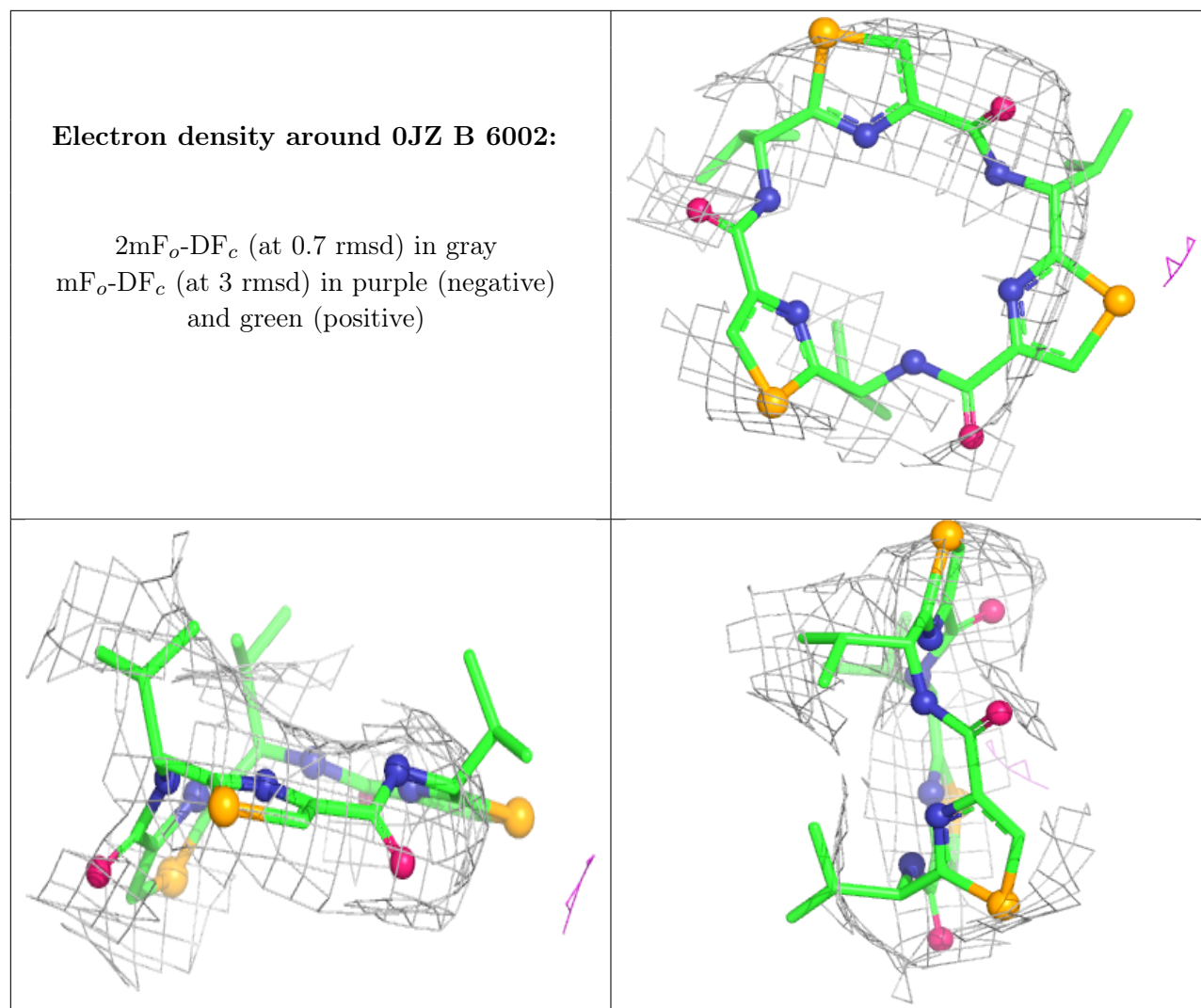
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OJZ	B	6002	36/36	0.87	0.08	159,210,345,550	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.