



Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2026 – 08:07 PM EDT

PDB ID : 9YBF / pdb_00009ybf
Title : Rana catesbeiana saxiphilin mutant - T563A:STX-C13-OBz (co-crystal)
Authors : Chen, Z.; Zakrzewska, S.; Minor, D.L.
Deposited on : 2025-09-17
Resolution : 2.45 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

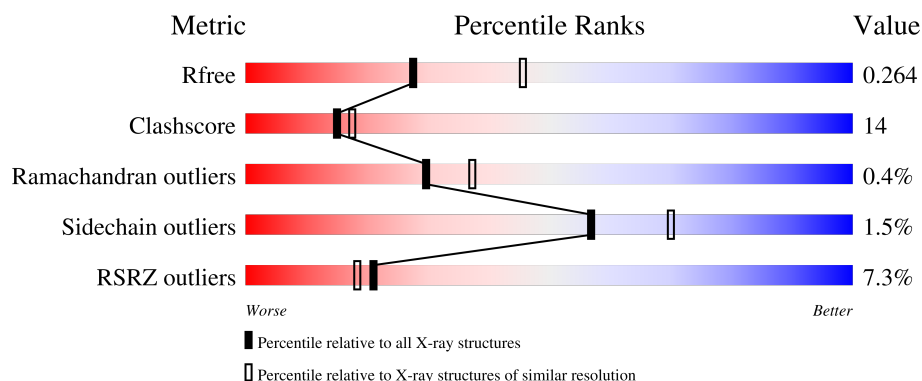
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	853	
1	B	853	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12940 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.

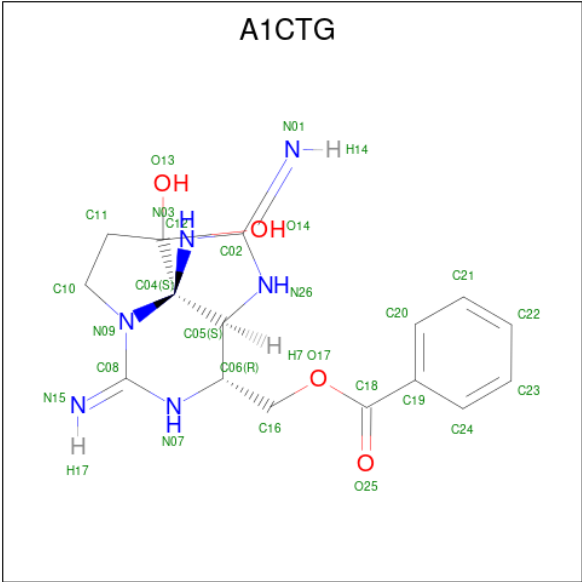
- Molecule 1 is a protein called Saxiphilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	830	Total	C	N	O	S	0	0	0
			6397	3995	1107	1236	59			
1	B	815	Total	C	N	O	S	0	0	0
			6291	3928	1090	1214	59			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	563	ALA	THR	engineered mutation	UNP P31226
A	826	SER	-	expression tag	UNP P31226
A	827	ASN	-	expression tag	UNP P31226
A	828	SER	-	expression tag	UNP P31226
A	829	LEU	-	expression tag	UNP P31226
A	830	GLU	-	expression tag	UNP P31226
A	831	VAL	-	expression tag	UNP P31226
A	832	LEU	-	expression tag	UNP P31226
A	833	PHE	-	expression tag	UNP P31226
A	834	GLN	-	expression tag	UNP P31226
B	563	ALA	THR	engineered mutation	UNP P31226
B	826	SER	-	expression tag	UNP P31226
B	827	ASN	-	expression tag	UNP P31226
B	828	SER	-	expression tag	UNP P31226
B	829	LEU	-	expression tag	UNP P31226
B	830	GLU	-	expression tag	UNP P31226
B	831	VAL	-	expression tag	UNP P31226
B	832	LEU	-	expression tag	UNP P31226
B	833	PHE	-	expression tag	UNP P31226
B	834	GLN	-	expression tag	UNP P31226

- Molecule 2 is [(2Z,3aS,4R,6Z,7R,10aS)-10,10-dihydroxy-2,6-diiminooctahydro-1H,8H-pyrrolo[1,2-c]purin-4-yl]methyl benzoate (CCD ID: A1CTG) (formula: C₁₆H₂₀N₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	16	6	4		
2	B	1	Total	C	N	O	0	0
			26	16	6	4		

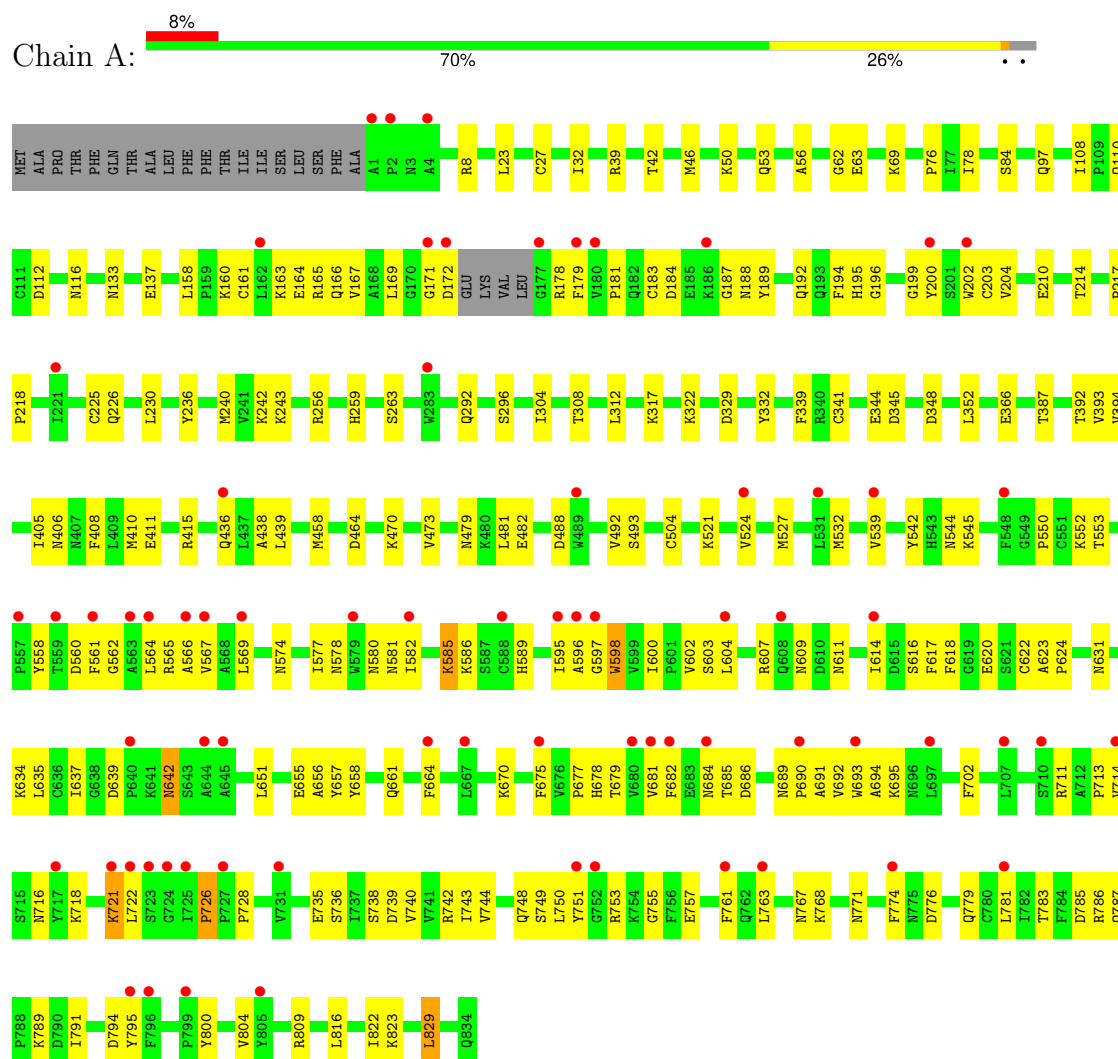
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	0	0
			120	120		
3	B	80	Total	O	0	0
			80	80		

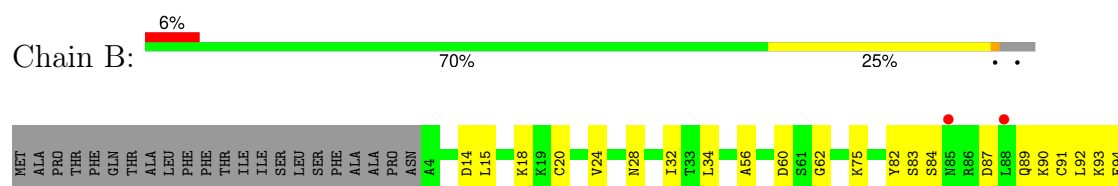
3 Residue-property plots [i](#)

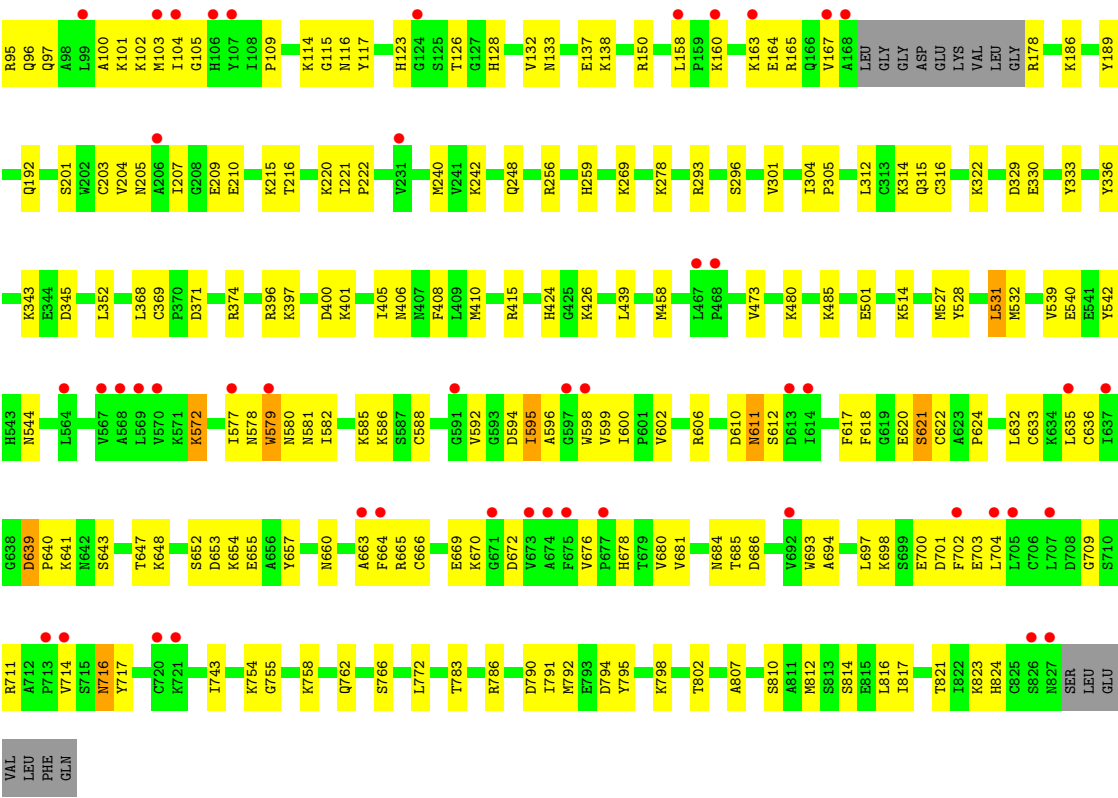
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Saxiphilin



• Molecule 1: Saxiphilin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.12Å 105.71Å 251.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.73 – 2.45 48.73 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.73-2.45) 99.2 (48.73-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.231 , 0.263 0.232 , 0.264	Depositor DCC
R_{free} test set	4735 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.8	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	0.95	EDS
Total number of atoms	12940	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1CTG

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	0.20	1/6525 (0.0%)	0.36	0/8806
1	B	0.20	0/6417	0.40	0/8659
All	All	0.20	1/12942 (0.0%)	0.38	0/17465

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	726	PRO	CA-C	-6.57	1.48	1.51

There are no bond angle outliers.

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	6397	0	6259	170	1
1	B	6291	0	6155	175	1
2	A	26	0	0	1	0
2	B	26	0	0	3	0
3	A	120	0	0	3	0
3	B	80	0	0	5	0
All	All	12940	0	12414	344	1

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 (344) 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:691:ALA:HA	1:A:695:LYS:HE3	1.45	0.97
1:A:195:HIS:HB2	1:A:202:TRP:HH2	1.26	0.96
1:A:292:GLN:HE22	1:A:308:THR:H	1.16	0.92
1:B:579:TRP:HA	1:B:582:ILE:HD11	1.58	0.84
1:B:572:LYS:HD2	1:B:703:GLU:HG3	1.60	0.83
1:A:550:PRO:HG2	1:A:558:TYR:HB3	1.59	0.82
1:B:527:MET:HE3	1:B:531:LEU:HD21	1.61	0.82
1:B:621:SER:HB2	1:B:632:LEU:HD13	1.62	0.82
1:B:647:THR:HB	1:B:654:LYS:HB3	1.63	0.79
1:A:631:ASN:HA	1:A:634:LYS:HD3	1.62	0.79
1:A:635:LEU:HB2	1:A:670:LYS:HD3	1.65	0.78
1:A:195:HIS:HB2	1:A:202:TRP:CH2	2.18	0.74
1:B:617:PHE:HD2	1:B:618:PHE:CD1	2.06	0.74
1:B:754:LYS:NZ	3:B:1001:HOH:O	2.21	0.73
1:B:103:MET:HG3	1:B:104:ILE:H	1.53	0.73
1:B:160:LYS:H	1:B:160:LYS:HD2	1.54	0.73
1:A:689:ASN:ND2	1:A:690:PRO:O	2.22	0.72
1:B:207:ILE:HD11	1:B:209:GLU:HG3	1.70	0.72
1:B:84:SER:O	1:B:90:LYS:NZ	2.22	0.71
1:A:164:GLU:OE1	1:A:189:TYR:OH	2.08	0.70
1:A:532:MET:HA	1:A:532:MET:HE2	1.74	0.69
1:A:158:LEU:HD23	1:A:163:LYS:HE2	1.75	0.69
1:B:635:LEU:HD12	1:B:635:LEU:H	1.57	0.69
1:B:160:LYS:H	1:B:160:LYS:CD	2.05	0.69
1:B:578:ASN:ND2	1:B:709:GLY:O	2.26	0.69
1:A:761:PHE:HE2	1:A:763:LEU:HD23	1.58	0.68
1:B:703:GLU:OE1	1:B:711:ARG:NE	2.26	0.68
1:B:681:VAL:O	1:B:685:THR:HG22	1.92	0.68
1:A:160:LYS:NZ	1:A:164:GLU:OE1	2.22	0.68
1:A:560:ASP:OD2	1:A:562:GLY:N	2.25	0.68
1:B:248:GLN:HE22	1:B:374:ARG:HG3	1.58	0.68
1:B:105:GLY:O	1:B:123:HIS:NE2	2.26	0.68
1:B:158:LEU:HD13	1:B:163:LYS:HB2	1.76	0.67
1:A:713:PRO:HG2	1:A:716:ASN:HB2	1.77	0.66
1:A:200:TYR:HB3	1:A:202:TRP:CZ3	2.30	0.66
1:A:366:GLU:OE1	3:A:1001:HOH:O	2.14	0.66
1:A:567:VAL:HG12	1:A:721:LYS:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ASN:O	1:A:585:LYS:NZ	2.28	0.65
1:A:689:ASN:O	1:A:695:LYS:NZ	2.28	0.65
1:B:178:ARG:N	3:B:1005:HOH:O	2.29	0.65
1:B:617:PHE:HD2	1:B:618:PHE:HD1	1.45	0.65
1:B:164:GLU:OE1	1:B:189:TYR:OH	2.13	0.65
1:A:695:LYS:HE2	1:A:695:LYS:HA	1.77	0.64
1:A:542:TYR:HD2	1:A:779:GLN:HB2	1.62	0.64
1:B:542:TYR:CZ	1:B:544:ASN:HB3	2.33	0.64
1:A:504:CYS:SG	3:A:1004:HOH:O	2.55	0.64
1:B:401:LYS:NZ	3:B:1004:HOH:O	2.26	0.63
1:B:301:VAL:HG22	1:B:315:GLN:HG2	1.80	0.63
1:B:75:LYS:HG2	1:B:397:LYS:HA	1.80	0.62
1:A:598:TRP:O	1:A:602:VAL:HG22	1.99	0.62
1:A:550:PRO:CG	1:A:558:TYR:HB3	2.27	0.62
1:A:569:LEU:HD11	1:A:702:PHE:HB3	1.82	0.62
1:B:126:THR:HG23	1:B:128:HIS:H	1.64	0.62
1:A:200:TYR:HB3	1:A:202:TRP:HZ3	1.62	0.62
1:B:595:ILE:HD12	1:B:595:ILE:H	1.64	0.62
1:B:242:LYS:NZ	1:B:345:ASP:OD1	2.31	0.61
1:A:595:ILE:O	1:A:600:ILE:HG12	2.00	0.61
1:A:637:ILE:HG22	1:A:657:TYR:CE2	2.36	0.61
1:A:560:ASP:OD1	1:A:565:ARG:NH2	2.34	0.61
1:A:596:ALA:HB3	1:A:677:PRO:HD3	1.82	0.60
1:B:94:GLU:OE1	1:B:117:TYR:OH	2.10	0.60
1:A:539:VAL:HG12	1:A:783:THR:HA	1.84	0.60
1:A:691:ALA:HA	1:A:695:LYS:CE	2.28	0.60
1:A:76:PRO:HB3	1:A:392:THR:HG21	1.84	0.60
1:A:577:ILE:HD12	1:A:585:LYS:HG2	1.84	0.59
1:B:817:ILE:O	1:B:821:THR:HG23	2.01	0.59
1:A:172:ASP:O	1:A:178:ARG:NH2	2.36	0.59
1:A:684:ASN:HA	1:A:689:ASN:HB2	1.83	0.59
1:B:755:GLY:O	1:B:758:LYS:HG2	2.02	0.59
1:A:637:ILE:HG23	1:A:656:ALA:HB3	1.84	0.59
1:B:192:GLN:NE2	1:B:201:SER:HB2	2.19	0.58
1:A:748:GLN:OE1	1:A:781:LEU:N	2.33	0.58
1:A:735:GLU:OE1	1:A:735:GLU:N	2.26	0.58
1:A:488:ASP:OD1	1:A:768:LYS:HE2	2.03	0.58
1:A:578:ASN:HB3	1:A:581:ASN:ND2	2.19	0.58
1:B:635:LEU:HD12	1:B:635:LEU:N	2.19	0.58
1:B:664:PHE:HD2	1:B:693:TRP:HZ3	1.51	0.58
1:B:694:ALA:HA	1:B:697:LEU:HG	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ASN:OD1	1:B:117:TYR:N	2.37	0.57
1:B:617:PHE:CD2	1:B:618:PHE:CD1	2.90	0.57
1:A:171:GLY:O	1:A:178:ARG:NH1	2.38	0.56
1:A:569:LEU:HD22	1:A:681:VAL:HG22	1.88	0.56
1:A:292:GLN:HE22	1:A:308:THR:N	1.95	0.56
1:B:473:VAL:HG23	1:B:743:ILE:HD12	1.85	0.56
1:A:589:HIS:CD2	1:A:623:ALA:HB2	2.41	0.56
1:B:685:THR:OG1	1:B:686:ASP:N	2.39	0.56
1:B:794:ASP:O	2:B:901:A1CTG:N03	2.39	0.56
1:B:14:ASP:O	1:B:18:LYS:HG2	2.05	0.56
1:B:20:CYS:O	1:B:24:VAL:HG23	2.05	0.56
1:B:192:GLN:HE21	1:B:201:SER:HB2	1.71	0.56
1:B:539:VAL:HG12	1:B:783:THR:HA	1.88	0.55
1:B:577:ILE:O	1:B:711:ARG:NH1	2.39	0.55
1:B:657:TYR:CE2	1:B:666:CYS:HA	2.40	0.55
1:B:301:VAL:HG23	1:B:314:LYS:HB3	1.89	0.55
1:B:572:LYS:HG3	1:B:701:ASP:O	2.07	0.55
1:A:789:LYS:HG3	1:A:794:ASP:HB2	1.89	0.55
1:A:56:ALA:HB2	1:A:405:ILE:HD13	1.88	0.55
1:A:603:SER:O	1:A:607:ARG:HG2	2.07	0.55
1:B:203:CYS:O	1:B:210:GLU:HA	2.07	0.54
1:B:606:ARG:NH1	1:B:611:ASN:HD22	2.04	0.54
1:A:97:GLN:HE22	1:A:436:GLN:NE2	2.04	0.54
1:A:236:TYR:CE2	1:A:387:THR:HG22	2.43	0.54
1:B:532:MET:HG2	1:B:817:ILE:HG23	1.90	0.54
1:B:572:LYS:NZ	1:B:700:GLU:O	2.31	0.54
1:B:221:ILE:HD13	1:B:786:ARG:HG2	1.89	0.54
1:A:622:CYS:HB2	1:A:635:LEU:HD12	1.89	0.53
1:B:205:ASN:HB2	1:B:824:HIS:CE1	2.44	0.53
1:B:336:TYR:CZ	1:B:426:LYS:HD2	2.44	0.53
1:B:665:ARG:HH11	1:B:693:TRP:NE1	2.06	0.53
1:A:192:GLN:NE2	1:A:225:CYS:SG	2.81	0.53
1:B:205:ASN:ND2	1:B:209:GLU:HB2	2.24	0.53
1:A:740:VAL:O	1:A:744:VAL:HG23	2.08	0.53
1:A:479:ASN:ND2	1:A:482:GLU:H	2.07	0.53
1:B:617:PHE:CD2	1:B:618:PHE:HD1	2.24	0.53
1:B:640:PRO:HA	1:B:643:SER:OG	2.09	0.53
1:B:92:LEU:O	1:B:96:GLN:HG3	2.10	0.53
1:B:15:LEU:H	1:B:15:LEU:HD12	1.73	0.52
1:B:697:LEU:HD13	1:B:702:PHE:HZ	1.74	0.52
1:A:240:MET:HE1	1:A:339:PHE:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:THR:HG21	1:B:222:PRO:HA	1.92	0.52
1:A:317:LYS:HD3	1:A:332:TYR:CZ	2.46	0.51
1:A:545:LYS:O	1:A:545:LYS:NZ	2.26	0.51
1:B:680:VAL:O	1:B:684:ASN:ND2	2.35	0.51
1:A:595:ILE:HG23	1:A:600:ILE:HD11	1.92	0.51
1:A:681:VAL:HG11	1:A:714:VAL:HG11	1.92	0.51
1:B:606:ARG:HH11	1:B:611:ASN:HD22	1.58	0.51
1:B:248:GLN:HA	1:B:368:LEU:HD11	1.93	0.51
1:A:243:LYS:HA	1:A:366:GLU:OE1	2.10	0.51
1:B:34:LEU:HB2	1:B:408:PHE:CZ	2.46	0.51
1:A:199:GLY:HA3	1:A:218:PRO:HG3	1.93	0.50
1:B:56:ALA:HB2	1:B:405:ILE:HD13	1.93	0.50
1:A:137:GLU:OE2	1:A:829:LEU:N	2.32	0.50
1:B:595:ILE:HG22	1:B:600:ILE:HD11	1.92	0.50
1:A:292:GLN:NE2	1:A:308:THR:H	1.97	0.50
1:A:560:ASP:OD1	1:A:718:LYS:HE2	2.11	0.50
1:A:479:ASN:HD22	1:A:481:LEU:H	1.57	0.50
1:A:597:GLY:HA2	1:A:675:PHE:O	2.11	0.50
1:A:226:GLN:NE2	1:A:822:ILE:HD11	2.27	0.50
1:B:95:ARG:HA	1:B:109:PRO:HD2	1.94	0.49
1:A:63:GLU:HG2	1:A:263:SER:HB3	1.94	0.49
1:B:582:ILE:HB	1:B:617:PHE:CZ	2.46	0.49
1:A:664:PHE:HD2	1:A:693:TRP:HZ3	1.61	0.49
1:A:256:ARG:O	1:A:348:ASP:N	2.34	0.49
1:A:410:MET:HE1	1:A:438:ALA:HA	1.94	0.49
1:A:738:SER:O	1:A:742:ARG:HG2	2.12	0.49
1:B:205:ASN:HD21	1:B:209:GLU:HB2	1.78	0.49
1:B:606:ARG:HD2	1:B:611:ASN:HB3	1.94	0.49
1:B:663:ALA:O	1:B:666:CYS:HB3	2.12	0.49
1:A:558:TYR:HH	1:A:561:PHE:HD2	1.60	0.49
1:A:786:ARG:NH1	1:A:787:GLN:O	2.46	0.49
1:B:32:ILE:HG21	1:B:408:PHE:HB2	1.95	0.49
1:B:606:ARG:HH11	1:B:606:ARG:HB3	1.78	0.49
1:B:89:GLN:NE2	1:B:114:LYS:O	2.46	0.48
1:B:639:ASP:OD1	1:B:641:LYS:HB3	2.12	0.48
1:A:406:ASN:OD1	1:A:439:LEU:HB2	2.13	0.48
1:A:609:ASN:HB2	1:A:611:ASN:ND2	2.28	0.48
1:B:678:HIS:CG	1:B:717:TYR:CD2	3.01	0.48
1:A:42:THR:O	1:A:46:MET:HG3	2.14	0.48
1:A:664:PHE:HD2	1:A:693:TRP:CZ3	2.32	0.48
1:B:794:ASP:OD1	2:B:901:A1CTG:N01	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:VAL:HG12	1:B:624:PRO:O	2.14	0.48
1:A:296:SER:HA	1:A:312:LEU:HD21	1.96	0.48
1:B:83:SER:OG	1:B:93:LYS:NZ	2.47	0.48
1:B:485:LYS:HD3	1:B:772:LEU:HB2	1.96	0.48
1:B:240:MET:HE2	1:B:352:LEU:HD21	1.96	0.48
1:B:133:ASN:ND2	1:B:137:GLU:HB2	2.29	0.48
1:B:259:HIS:CD2	1:B:304:ILE:HG12	2.48	0.48
1:B:665:ARG:HD3	1:B:693:TRP:CE2	2.49	0.48
1:A:479:ASN:HD22	1:A:481:LEU:N	2.12	0.47
1:A:567:VAL:HA	1:A:722:LEU:HD13	1.97	0.47
1:A:322:LYS:HD2	1:A:329:ASP:HB3	1.96	0.47
1:B:296:SER:HA	1:B:312:LEU:HD21	1.97	0.47
1:B:572:LYS:HG3	1:B:701:ASP:C	2.39	0.47
1:B:698:LYS:O	1:B:701:ASP:HB2	2.14	0.47
1:A:179:PHE:O	1:A:181:PRO:HD3	2.15	0.47
1:A:774:PHE:CE1	1:A:781:LEU:HD11	2.49	0.47
1:A:785:ASP:OD1	1:A:785:ASP:N	2.44	0.47
1:B:322:LYS:HD2	1:B:329:ASP:HB3	1.97	0.47
1:B:617:PHE:CD2	1:B:618:PHE:CE1	3.03	0.47
1:B:703:GLU:OE1	1:B:711:ARG:NH2	2.48	0.47
1:A:166:GLN:HG3	1:A:167:VAL:N	2.28	0.46
1:A:661:GLN:HG2	1:A:693:TRP:HZ2	1.80	0.46
1:A:750:LEU:HB2	1:A:751:TYR:CE2	2.50	0.46
1:B:636:CYS:HB3	1:B:655:GLU:OE1	2.16	0.46
1:B:15:LEU:HD23	1:B:424:HIS:O	2.14	0.46
1:A:786:ARG:NE	1:A:791:ILE:HD13	2.30	0.46
1:B:396:ARG:HH21	1:B:400:ASP:CG	2.23	0.46
1:B:635:LEU:HD23	1:B:670:LYS:HB2	1.97	0.46
1:A:84:SER:HA	1:A:230:LEU:O	2.15	0.46
1:A:240:MET:HE1	1:A:339:PHE:CE1	2.50	0.46
1:A:771:ASN:H	1:A:776:ASP:CG	2.21	0.46
1:A:411:GLU:OE1	1:A:415:ARG:NH1	2.49	0.45
1:A:635:LEU:HD22	1:A:670:LYS:HB3	1.99	0.45
1:B:256:ARG:HG2	1:B:301:VAL:HG12	1.98	0.45
1:B:369:CYS:HB2	1:B:371:ASP:OD1	2.15	0.45
1:B:704:LEU:HD13	1:B:714:VAL:HA	1.97	0.45
1:A:578:ASN:ND2	1:A:580:ASN:H	2.14	0.45
1:B:100:ALA:O	1:B:101:LYS:HD2	2.17	0.45
1:A:550:PRO:HG2	1:A:558:TYR:CB	2.40	0.45
1:A:564:LEU:HD23	1:A:678:HIS:HE1	1.81	0.45
1:A:651:LEU:HD23	1:A:658:TYR:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ASP:OD1	1:B:62:GLY:N	2.40	0.45
1:B:657:TYR:OH	1:B:669:GLU:OE1	2.15	0.45
1:A:308:THR:HB	1:B:293:ARG:HD3	1.99	0.45
1:B:158:LEU:HD12	1:B:158:LEU:O	2.16	0.45
1:B:210:GLU:OE1	1:B:215:LYS:HE3	2.16	0.45
1:B:594:ASP:O	1:B:599:VAL:HG23	2.17	0.45
1:A:527:MET:HG3	1:A:795:TYR:CZ	2.52	0.45
1:B:578:ASN:HB3	1:B:581:ASN:ND2	2.32	0.45
1:B:595:ILE:HD12	1:B:595:ILE:N	2.31	0.45
1:B:617:PHE:HD2	1:B:618:PHE:CE1	2.35	0.45
1:B:685:THR:HG1	1:B:686:ASP:N	2.14	0.45
1:B:802:THR:HG22	1:B:807:ALA:HB2	1.98	0.45
1:A:655:GLU:HG3	1:A:657:TYR:H	1.81	0.45
1:A:736:SER:O	1:A:740:VAL:HG23	2.17	0.45
1:A:753:ARG:HE	1:A:779:GLN:HA	1.82	0.45
1:B:103:MET:HE3	1:B:103:MET:HA	1.98	0.45
1:B:528:TYR:CE2	1:B:812:MET:HB3	2.51	0.45
1:A:492:VAL:HG12	1:A:751:TYR:CZ	2.52	0.44
1:A:194:PHE:CZ	1:A:196:GLY:HA2	2.52	0.44
1:A:642:ASN:OD1	1:A:642:ASN:N	2.50	0.44
1:B:527:MET:HG3	1:B:795:TYR:CZ	2.53	0.44
1:A:32:ILE:HG21	1:A:408:PHE:HB2	1.99	0.44
1:B:28:ASN:O	1:B:415:ARG:NE	2.51	0.44
1:B:269:LYS:HD3	1:B:458:MET:HE1	1.99	0.44
1:B:716:ASN:OD1	1:B:716:ASN:N	2.51	0.44
1:A:332:TYR:OH	1:A:344:GLU:OE1	2.29	0.44
1:A:582:ILE:HG13	1:A:617:PHE:HZ	1.82	0.44
1:B:652:SER:OG	1:B:653:ASP:N	2.50	0.44
1:B:664:PHE:CD2	1:B:693:TRP:HZ3	2.33	0.44
1:A:112:ASP:OD1	1:A:116:ASN:N	2.51	0.44
1:A:553:THR:O	1:A:553:THR:OG1	2.33	0.44
1:A:586:LYS:HG2	1:A:620:GLU:HB2	1.99	0.44
1:B:485:LYS:HD2	1:B:766:SER:HB2	2.00	0.44
1:A:617:PHE:HE2	1:A:618:PHE:CE1	2.36	0.44
1:B:186:LYS:H	1:B:186:LYS:HG3	1.59	0.44
1:B:582:ILE:O	1:B:585:LYS:HG2	2.18	0.44
1:A:62:GLY:O	1:A:458:MET:HE1	2.18	0.44
1:A:200:TYR:CZ	1:A:217:PRO:HG3	2.53	0.44
1:B:693:TRP:H	1:B:693:TRP:CD1	2.36	0.44
1:A:566:ALA:O	1:A:722:LEU:HB2	2.18	0.44
1:B:648:LYS:HA	1:B:655:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:ASP:OD1	1:B:654:LYS:NZ	2.50	0.43
1:A:682:PHE:CD1	1:A:682:PHE:N	2.86	0.43
1:A:684:ASN:CA	1:A:689:ASN:HB2	2.47	0.43
1:B:640:PRO:HA	1:B:643:SER:HG	1.83	0.43
1:A:133:ASN:ND2	1:A:137:GLU:HB2	2.33	0.43
1:A:750:LEU:HB2	1:A:751:TYR:CD2	2.53	0.43
1:B:100:ALA:HA	1:B:102:LYS:NZ	2.33	0.43
1:B:578:ASN:O	1:B:580:ASN:N	2.51	0.43
1:A:574:ASN:O	1:A:711:ARG:NH1	2.51	0.43
1:B:514:LYS:NZ	3:B:1011:HOH:O	2.51	0.43
1:B:762:GLN:N	1:B:762:GLN:OE1	2.52	0.43
1:A:479:ASN:ND2	1:A:481:LEU:HB2	2.34	0.43
1:A:823:LYS:NZ	3:A:1003:HOH:O	2.31	0.43
1:B:301:VAL:CG2	1:B:314:LYS:HB3	2.48	0.43
1:B:406:ASN:OD1	1:B:439:LEU:HB2	2.18	0.43
1:A:242:LYS:NZ	1:A:345:ASP:OD1	2.39	0.43
1:A:492:VAL:HG12	1:A:492:VAL:O	2.19	0.43
1:B:82:TYR:OH	1:B:823:LYS:NZ	2.30	0.43
1:B:621:SER:HB2	1:B:632:LEU:CD1	2.41	0.43
1:A:8:ARG:HE	1:A:8:ARG:HB2	1.59	0.43
1:A:200:TYR:CB	1:A:202:TRP:HZ3	2.28	0.43
1:B:91:CYS:HB3	1:B:115:GLY:O	2.19	0.43
1:B:138:LYS:NZ	3:B:1002:HOH:O	2.22	0.43
1:A:78:ILE:HB	1:A:393:VAL:HB	2.01	0.43
1:A:204:VAL:HG12	1:A:210:GLU:HA	2.00	0.43
1:A:602:VAL:HG12	1:A:614:ILE:HG21	1.99	0.43
1:A:735:GLU:CD	1:A:735:GLU:H	2.09	0.43
1:B:582:ILE:HB	1:B:617:PHE:HZ	1.83	0.43
1:A:76:PRO:HA	1:A:394:VAL:HG12	2.01	0.43
1:A:203:CYS:HB2	1:A:214:THR:HG21	2.00	0.43
1:A:604:LEU:HD23	1:A:604:LEU:HA	1.81	0.43
1:B:204:VAL:HA	1:B:209:GLU:O	2.18	0.43
1:B:540:GLU:OE1	2:B:901:A1CTG:N07	2.52	0.43
1:A:259:HIS:CD2	1:A:304:ILE:HG12	2.54	0.42
1:B:104:ILE:HD13	1:B:104:ILE:HA	1.84	0.42
1:B:595:ILE:H	1:B:595:ILE:CD1	2.32	0.42
1:B:602:VAL:O	1:B:606:ARG:HG3	2.19	0.42
1:A:542:TYR:CE2	1:A:544:ASN:HB3	2.54	0.42
1:B:102:LYS:N	1:B:102:LYS:HE2	2.34	0.42
1:B:660:ASN:HB3	1:B:680:VAL:HG22	2.00	0.42
1:B:87:ASP:O	1:B:90:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LYS:HG2	1:B:97:GLN:NE2	2.34	0.42
1:A:524:VAL:HG21	1:A:726:PRO:HG2	2.02	0.42
1:A:767:ASN:HD21	1:A:768:LYS:NZ	2.17	0.42
1:B:598:TRP:O	1:B:602:VAL:HG22	2.20	0.42
1:A:97:GLN:HE22	1:A:436:GLN:CD	2.28	0.42
1:A:794:ASP:O	2:A:901:A1CTG:N03	2.52	0.42
1:B:588:CYS:HB3	1:B:666:CYS:HB3	1.92	0.42
1:B:620:GLU:C	1:B:635:LEU:HD11	2.44	0.42
1:A:761:PHE:CE2	1:A:763:LEU:HD23	2.46	0.42
1:A:39:ARG:HH21	1:A:53:GLN:NE2	2.17	0.42
1:A:158:LEU:HD23	1:A:163:LYS:CE	2.47	0.42
1:A:521:LYS:HD3	1:A:728:PRO:HB3	2.01	0.42
1:B:480:LYS:HD2	1:B:501:GLU:OE2	2.19	0.42
1:B:798:LYS:O	1:B:802:THR:HG23	2.20	0.42
1:A:473:VAL:HG23	1:A:743:ILE:HD12	2.01	0.41
1:B:790:ASP:OD2	1:B:792:MET:HB2	2.20	0.41
1:B:814:SER:OG	1:B:817:ILE:HG13	2.19	0.41
1:A:542:TYR:CZ	1:A:544:ASN:HB3	2.56	0.41
1:B:165:ARG:HA	1:B:165:ARG:HD2	1.81	0.41
1:A:69:LYS:NZ	1:A:464:ASP:OD2	2.34	0.41
1:A:161:CYS:HB3	1:A:187:GLY:O	2.21	0.41
1:A:552:LYS:HB3	1:A:552:LYS:HE2	1.86	0.41
1:A:624:PRO:HG3	1:A:655:GLU:HG2	2.01	0.41
1:A:678:HIS:CE1	1:A:679:THR:HG23	2.55	0.41
1:B:220:LYS:HE3	1:B:220:LYS:HB2	1.92	0.41
1:B:622:CYS:HB2	1:B:635:LEU:HB2	2.02	0.41
1:B:665:ARG:HD3	1:B:693:TRP:CD2	2.55	0.41
1:A:184:ASP:OD1	1:A:188:ASN:N	2.52	0.41
1:A:681:VAL:O	1:A:685:THR:HG22	2.19	0.41
1:A:685:THR:HG23	1:A:686:ASP:N	2.35	0.41
1:A:689:ASN:ND2	1:A:694:ALA:HB3	2.35	0.41
1:A:165:ARG:O	1:A:169:LEU:HG	2.21	0.41
1:B:305:PRO:HG2	1:B:333:TYR:HA	2.02	0.41
1:B:406:ASN:O	1:B:410:MET:HG2	2.21	0.41
1:A:524:VAL:CG2	1:A:726:PRO:HG2	2.51	0.41
1:A:749:SER:O	1:A:755:GLY:HA2	2.20	0.41
1:A:194:PHE:CE2	1:A:196:GLY:HA2	2.56	0.41
1:B:133:ASN:HD21	1:B:137:GLU:HB2	1.86	0.41
1:B:278:LYS:HD3	1:B:278:LYS:HA	1.75	0.41
1:A:532:MET:HE1	1:A:809:ARG:CD	2.51	0.41
1:A:558:TYR:N	1:A:558:TYR:CD1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:TYR:O	1:A:804:VAL:HG23	2.21	0.41
1:B:93:LYS:HB2	1:B:93:LYS:HE3	1.82	0.41
1:B:123:HIS:HB3	1:B:126:THR:CG2	2.51	0.41
1:A:332:TYR:CG	1:A:341:CYS:HB2	2.56	0.41
1:B:316:CYS:HB3	1:B:330:GLU:OE1	2.21	0.41
1:B:586:LYS:HB2	1:B:672:ASP:OD1	2.21	0.41
1:B:676:VAL:HB	1:B:680:VAL:HG21	2.03	0.41
1:B:92:LEU:HA	1:B:92:LEU:HD23	1.88	0.40
1:B:186:LYS:HE3	1:B:810:SER:HB3	2.02	0.40
1:B:596:ALA:HA	1:B:600:ILE:HD12	2.03	0.40
1:B:654:LYS:HD2	1:B:654:LYS:HA	1.92	0.40
1:A:589:HIS:HD2	1:A:623:ALA:HB2	1.83	0.40
1:B:786:ARG:CZ	1:B:791:ILE:HD13	2.51	0.40
1:A:50:LYS:HE3	1:A:50:LYS:HB3	1.83	0.40
1:A:532:MET:HA	1:A:532:MET:CE	2.48	0.40
1:B:207:ILE:CD1	1:B:209:GLU:HG3	2.46	0.40
1:A:23:LEU:HD13	1:A:27:CYS:HB2	2.04	0.40
1:A:108:ILE:O	1:A:110:GLN:NE2	2.50	0.40
1:A:470:LYS:HB3	1:A:739:ASP:OD1	2.21	0.40
1:B:694:ALA:HA	1:B:697:LEU:CG	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:GLU:OE1	1:B:102:LYS:NZ[3_544]	2.00	0.20

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	826/853 (97%)	791 (96%)	33 (4%)	2 (0%)	43 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	811/853 (95%)	766 (94%)	40 (5%)	5 (1%)	21	27
All	All	1637/1706 (96%)	1557 (95%)	73 (4%)	7 (0%)	30	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	610	ASP
1	B	633	CYS
1	B	595	ILE
1	B	612	SER
1	A	598	TRP
1	A	692	VAL
1	B	579	TRP

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	710/730 (97%)	700 (99%)	10 (1%)	59	72
1	B	699/730 (96%)	688 (98%)	11 (2%)	55	69
All	All	1409/1460 (96%)	1388 (98%)	21 (2%)	57	70

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	CYS
1	A	352	LEU
1	A	493	SER
1	A	585	LYS
1	A	616	SER
1	A	639	ASP
1	A	642	ASN
1	A	721	LYS
1	A	816	LEU

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Mol	Chain	Res	Type
1	A	829	LEU
1	B	132	VAL
1	B	150	ARG
1	B	167	VAL
1	B	343	LYS
1	B	531	LEU
1	B	572	LYS
1	B	611	ASN
1	B	621	SER
1	B	639	ASP
1	B	716	ASN
1	B	816	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	97	GLN
1	A	116	ASN
1	A	248	GLN
1	A	292	GLN
1	A	315	GLN
1	A	479	ASN
1	A	678	HIS
1	A	684	ASN
1	A	824	HIS
1	B	143	ASN
1	B	192	GLN
1	B	248	GLN
1	B	471	ASN
1	B	511	GLN
1	B	574	ASN

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 [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	A1CTG	B	901	-	23,29,29	0.50	0	22,45,45	1.06	1 (4%)
2	A1CTG	A	901	-	23,29,29	0.41	0	22,45,45	1.12	1 (4%)

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	A1CTG	B	901	-	-	1/9/57/57	0/4/4/4
2	A1CTG	A	901	-	-	1/9/57/57	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	A1CTG	N03-C04-N09	-4.10	105.36	112.45
2	B	901	A1CTG	N03-C04-N09	-3.04	107.20	112.45

There are no chirality outliers.

All (2) torsion outliers are listed below:

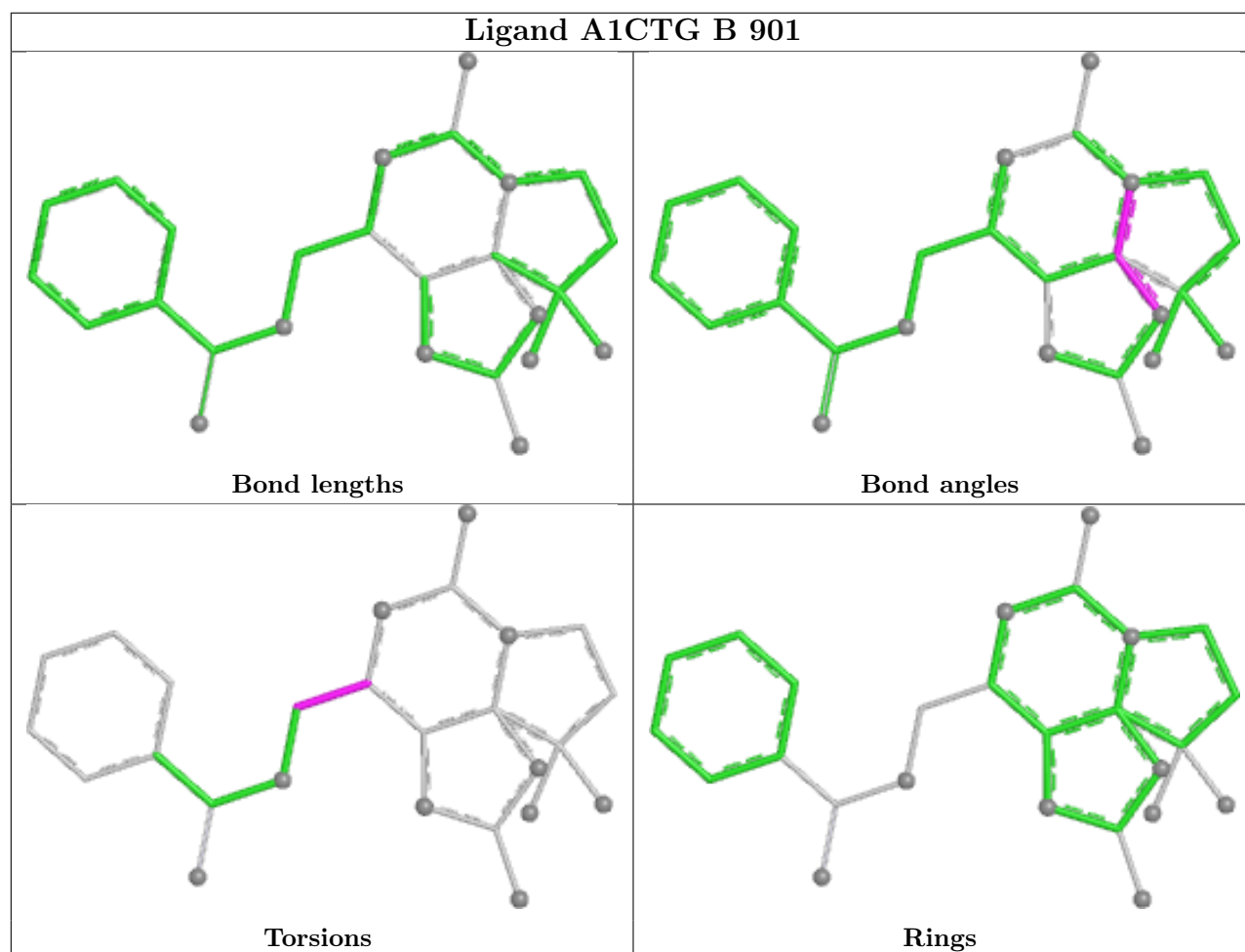
Mol	Chain	Res	Type	Atoms
2	A	901	A1CTG	C05-C06-C16-O17
2	B	901	A1CTG	C05-C06-C16-O17

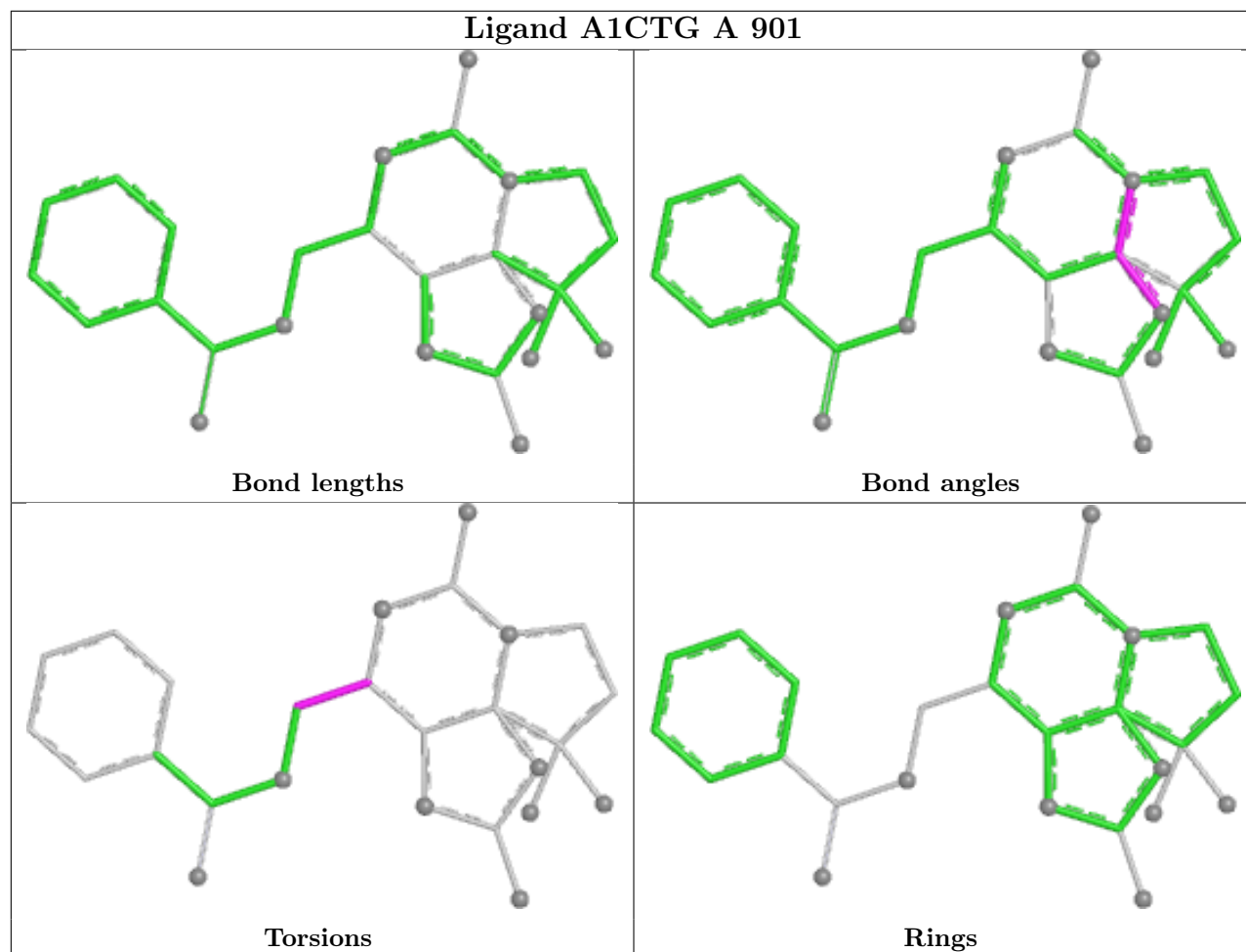
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	A1CTG	3	0
2	A	901	A1CTG	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	830/853 (97%)	0.59	71 (8%) 16 14	48, 82, 170, 230	0
1	B	815/853 (95%)	0.58	49 (6%) 27 24	50, 84, 152, 197	0
All	All	1645/1706 (96%)	0.59	120 (7%) 21 18	48, 83, 166, 230	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	4.7
1	A	645	ALA	4.4
1	A	569	LEU	4.2
1	B	568	ALA	4.1
1	B	674	ALA	4.0
1	B	569	LEU	4.0
1	A	664	PHE	3.9
1	B	614	ILE	3.8
1	B	713	PRO	3.8
1	B	613	ASP	3.7
1	B	99	LEU	3.7
1	A	675	PHE	3.7
1	A	721	LYS	3.6
1	B	167	VAL	3.6
1	A	725	ILE	3.6
1	B	827	ASN	3.5
1	B	673	VAL	3.5
1	B	664	PHE	3.3
1	A	724	GLY	3.2
1	B	104	ILE	3.2
1	A	727	PRO	3.2
1	B	88	LEU	3.2
1	A	644	ALA	3.2
1	B	106	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	684	ASN	3.2
1	A	579	TRP	3.1
1	B	468	PRO	3.1
1	A	588	CYS	3.1
1	A	781	LEU	3.0
1	B	567	VAL	3.0
1	A	186	LYS	3.0
1	A	2	PRO	3.0
1	A	681	VAL	2.9
1	A	559	THR	2.9
1	A	171	GLY	2.9
1	B	85	ASN	2.9
1	A	563	ALA	2.9
1	A	162	LEU	2.9
1	B	702	PHE	2.9
1	B	714	VAL	2.8
1	B	467	LEU	2.8
1	A	717	TYR	2.7
1	A	283	TRP	2.7
1	A	180	VAL	2.7
1	B	721	LYS	2.7
1	A	608	GLN	2.7
1	A	200	TYR	2.7
1	A	564	LEU	2.7
1	A	763	LEU	2.7
1	B	677	PRO	2.6
1	B	168	ALA	2.6
1	A	179	PHE	2.6
1	B	107	TYR	2.6
1	A	723	SER	2.6
1	A	582	ILE	2.5
1	A	722	LEU	2.5
1	A	567	VAL	2.5
1	B	720	CYS	2.5
1	A	177	GLY	2.5
1	A	796	PHE	2.5
1	B	707	LEU	2.5
1	A	680	VAL	2.5
1	B	692	VAL	2.5
1	A	752	GLY	2.5
1	A	172	ASP	2.5
1	A	682	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	103	MET	2.5
1	A	707	LEU	2.5
1	A	531	LEU	2.4
1	B	675	PHE	2.4
1	A	561	PHE	2.4
1	A	799	PRO	2.4
1	B	577	ILE	2.4
1	A	640	PRO	2.3
1	B	705	LEU	2.3
1	A	690	PRO	2.3
1	A	710	SER	2.3
1	B	564	LEU	2.3
1	A	202	TRP	2.3
1	B	158	LEU	2.3
1	A	557	PRO	2.3
1	A	436	GLN	2.3
1	B	124	GLY	2.3
1	B	597	GLY	2.3
1	A	221	ILE	2.3
1	A	604	LEU	2.3
1	B	704	LEU	2.3
1	B	206	ALA	2.2
1	A	597	GLY	2.2
1	B	160	LYS	2.2
1	A	524	VAL	2.2
1	B	598	TRP	2.2
1	A	693	TRP	2.2
1	A	731	VAL	2.2
1	B	570	VAL	2.2
1	B	163	LYS	2.2
1	A	795	TYR	2.2
1	A	614	ILE	2.2
1	A	761	PHE	2.2
1	A	714	VAL	2.1
1	B	231	VAL	2.1
1	B	826	SER	2.1
1	A	774	PHE	2.1
1	A	566	ALA	2.1
1	A	697	LEU	2.1
1	B	591	GLY	2.1
1	A	539	VAL	2.1
1	B	663	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	667	LEU	2.1
1	B	671	GLY	2.1
1	A	751	TYR	2.1
1	B	579	TRP	2.1
1	B	635	LEU	2.1
1	A	595	ILE	2.1
1	A	548	PHE	2.0
1	A	489	TRP	2.0
1	A	4	ALA	2.0
1	A	596	ALA	2.0
1	B	637	ILE	2.0
1	A	805	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

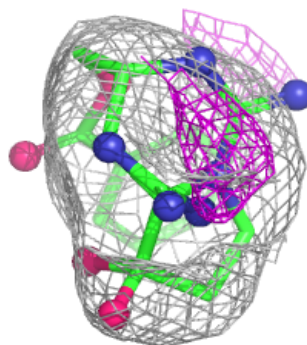
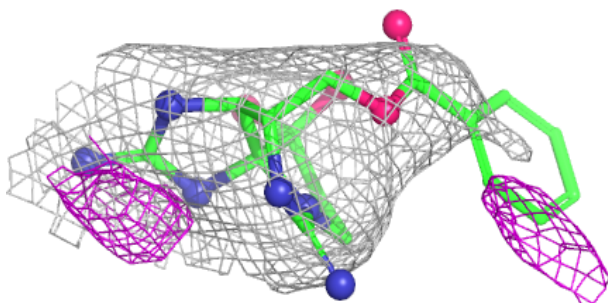
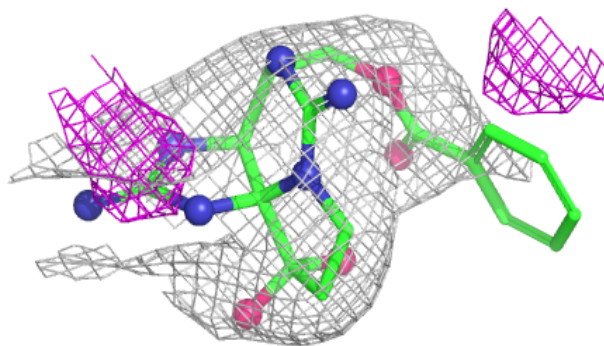
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1CTG	A	901	26/26	0.83	0.14	121,130,139,154	0
2	A1CTG	B	901	26/26	0.87	0.12	78,99,105,112	0

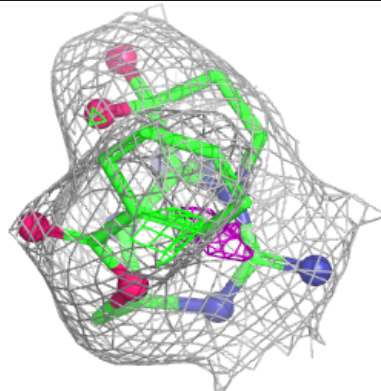
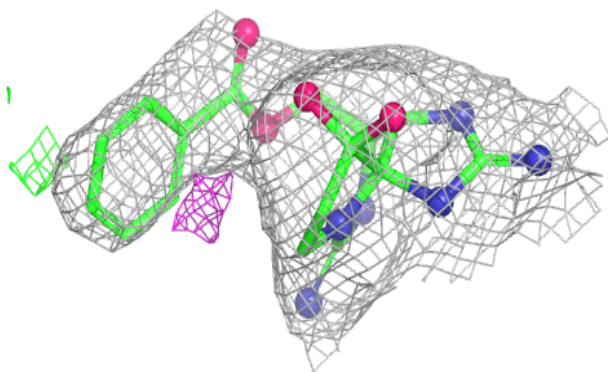
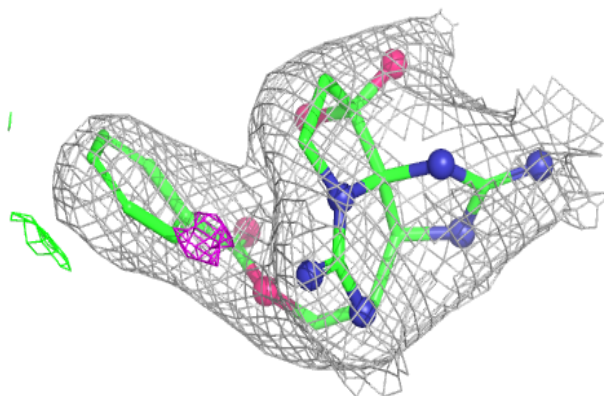
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CTG A 901:

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

**Electron density around A1CTG B 901:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.