



Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2026 – 08:08 PM EDT

PDB ID : 9YBD / pdb_00009ybd
Title : Rana catesbeiana saxiphilin mutant - F561A:STX-C13-OBz (co-crystal)
Authors : Chen, Z.; Zakrzewska, S.; Minor, D.L.
Deposited on : 2025-09-17
Resolution : 2.40 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

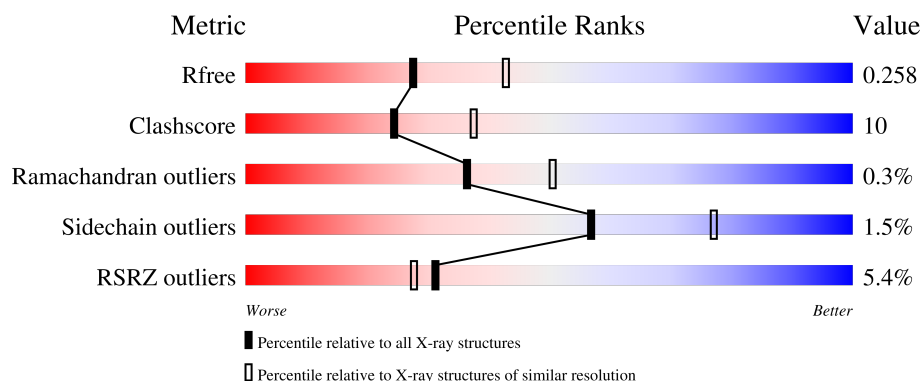
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	 6% 79% 18% .
1	B	853	 5% 75% 20% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12862 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.

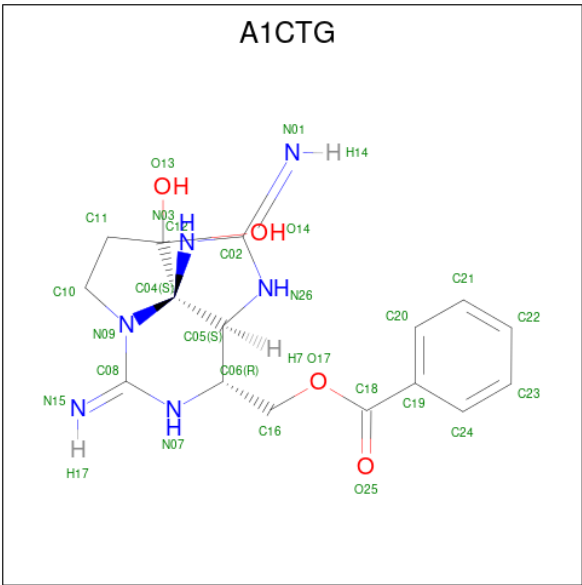
- Molecule 1 is a protein called Saxiphilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	834	Total	C	N	O	S	0	0	0
			6426	4012	1112	1243	59			
1	B	820	Total	C	N	O	S	0	0	0
			6322	3946	1093	1224	59			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	561	ALA	PHE	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	561	ALA	PHE	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		

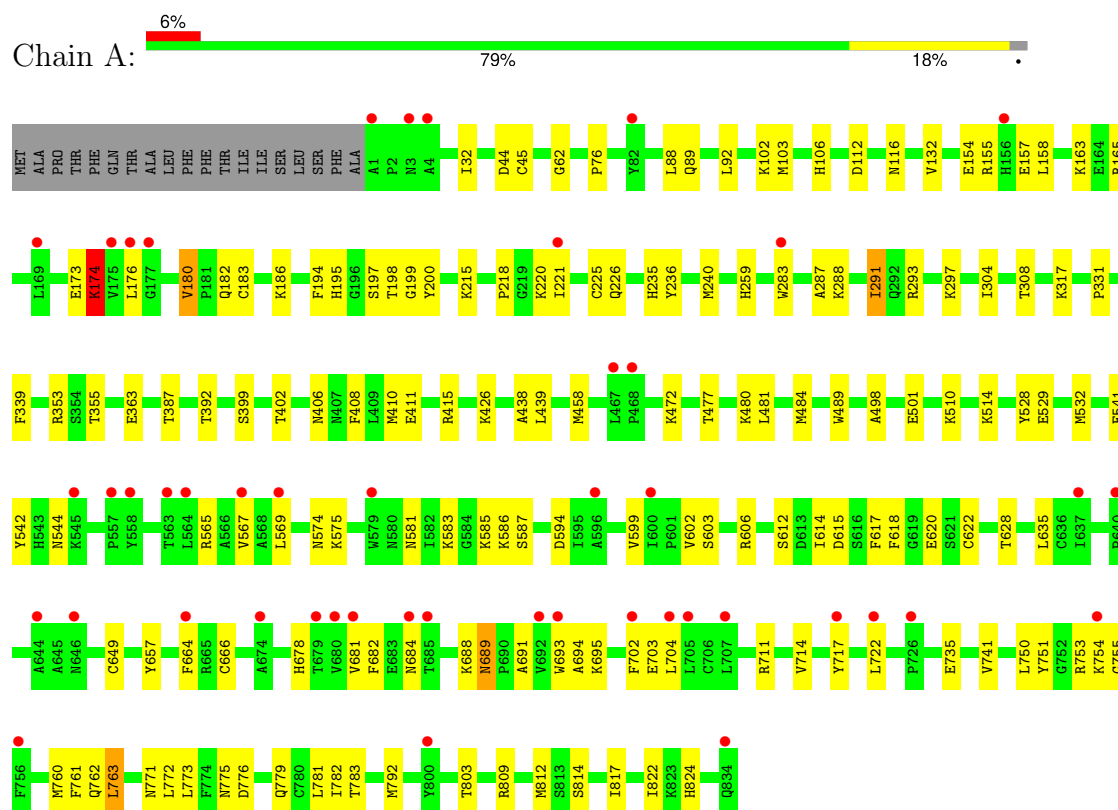
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	23	Total	O	0	0
			23	23		

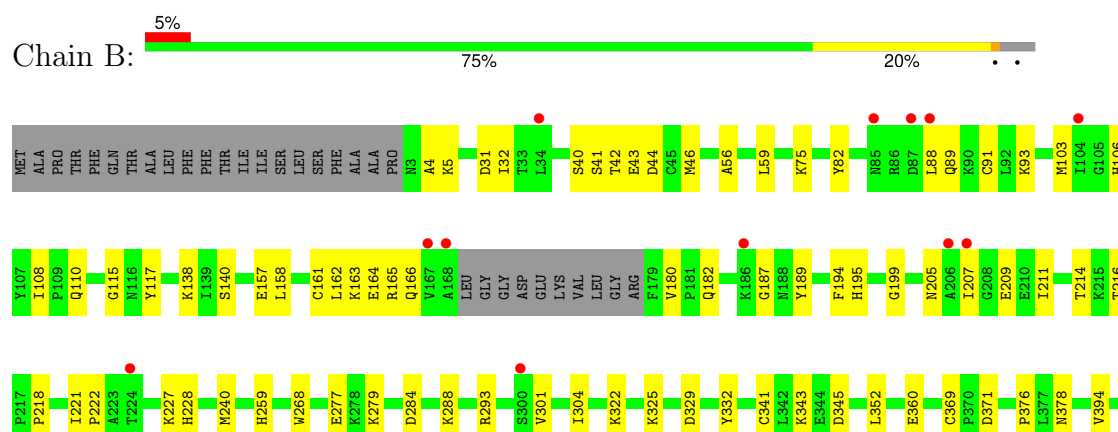
3 Residue-property plots

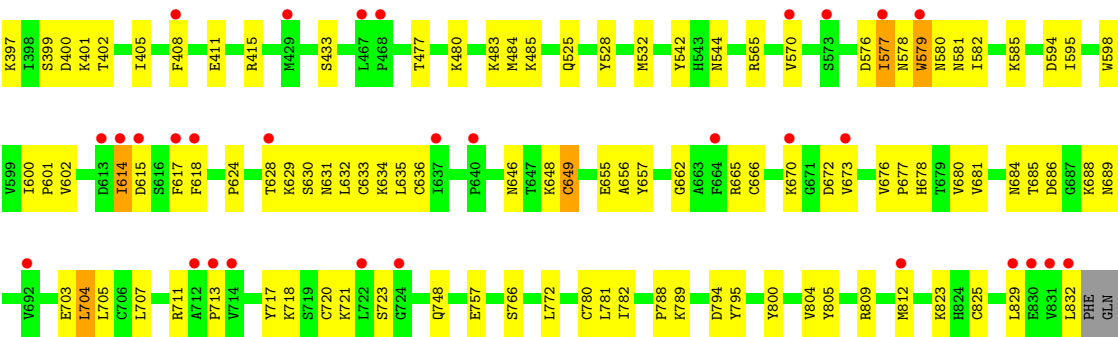
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 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	96.42Å 110.04Å 256.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.21 – 2.40 48.21 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.21-2.40) 99.9 (48.21-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.229 , 0.258 0.229 , 0.258	Depositor DCC
R_{free} test set	5393 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12862	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: 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	0.21	1/6554 (0.0%)	0.40	1/8847 (0.0%)
1	B	0.18	0/6447	0.37	0/8702
All	All	0.20	1/13001 (0.0%)	0.39	1/17549 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	ILE	CG1-CD1	5.18	1.72	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ILE	CA-CB-CG1	-5.53	101.00	110.40

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	6426	0	6297	123	1
1	B	6322	0	6188	129	1
2	A	26	0	0	0	0
2	B	26	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	39	0	0	2	0
3	B	23	0	0	0	0
All	All	12862	0	12485	251	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 10.

All (251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:GLN:HE22	1:B:781:LEU:H	1.03	0.97
1:A:664:PHE:HE1	1:A:693:TRP:HZ3	1.22	0.83
1:B:748:GLN:NE2	1:B:781:LEU:H	1.79	0.81
1:A:664:PHE:CE1	1:A:693:TRP:HZ3	1.99	0.80
1:A:88:LEU:HD11	1:A:186:LYS:HE3	1.64	0.79
1:A:529:GLU:HG2	1:A:817:ILE:HD11	1.64	0.79
1:B:164:GLU:OE1	1:B:189:TYR:OH	2.04	0.76
1:B:578:ASN:H	1:B:581:ASN:HB3	1.52	0.74
1:B:525:GLN:OE1	1:B:525:GLN:N	2.14	0.74
1:A:587:SER:HB3	1:A:618:PHE:HE2	1.54	0.73
1:A:410:MET:HE1	1:A:438:ALA:HA	1.70	0.73
1:A:617:PHE:HD2	1:A:618:PHE:HD1	1.36	0.72
1:A:703:GLU:OE1	1:A:711:ARG:NH2	2.24	0.71
1:B:582:ILE:HG22	1:B:618:PHE:HE1	1.56	0.71
1:B:582:ILE:HB	1:B:617:PHE:HE2	1.58	0.69
1:B:42:THR:HG22	1:B:46:MET:HE2	1.75	0.69
1:B:684:ASN:HA	1:B:689:ASN:OD1	1.94	0.68
1:A:542:TYR:HB2	1:A:782:ILE:HD13	1.75	0.68
1:A:569:LEU:HD11	1:A:702:PHE:HB3	1.76	0.68
1:B:56:ALA:HB2	1:B:405:ILE:HD13	1.76	0.68
1:A:481:LEU:HB3	1:A:772:LEU:HD21	1.74	0.67
1:B:43:GLU:HA	1:B:46:MET:HE3	1.76	0.66
1:B:676:VAL:HB	1:B:680:VAL:HG11	1.78	0.65
1:A:587:SER:HB3	1:A:618:PHE:CE2	2.32	0.65
1:A:472:LYS:HE3	1:A:498:ALA:HB2	1.79	0.64
1:B:194:PHE:HE2	1:B:199:GLY:HA2	1.63	0.64
1:B:216:THR:HG21	1:B:222:PRO:HA	1.78	0.64
1:A:283:TRP:CH2	1:A:291:ILE:HD11	2.33	0.62
1:B:628:THR:HG23	1:B:629:LYS:HG3	1.80	0.62
1:A:751:TYR:HB2	1:A:763:LEU:HD13	1.80	0.62
1:A:154:GLU:O	3:A:1001:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ASN:O	1:A:585:LYS:NZ	2.27	0.62
1:A:411:GLU:OE1	1:A:415:ARG:NH1	2.33	0.61
1:A:664:PHE:HE1	1:A:693:TRP:CZ3	2.13	0.61
1:A:240:MET:HE1	1:A:339:PHE:CD1	2.36	0.61
1:A:587:SER:CB	1:A:618:PHE:HE2	2.14	0.61
1:A:174:LYS:HE2	1:A:176:LEU:HB2	1.82	0.60
1:B:800:TYR:O	1:B:804:VAL:HG12	2.01	0.60
1:A:735:GLU:OE2	1:A:735:GLU:N	2.25	0.60
1:B:685:THR:OG1	1:B:686:ASP:OD1	2.19	0.60
1:A:353:ARG:HG2	1:A:355:THR:HG23	1.82	0.60
1:B:577:ILE:HG22	1:B:585:LYS:HG2	1.85	0.59
1:B:138:LYS:HE3	1:B:140:SER:HA	1.85	0.59
1:A:283:TRP:CZ3	1:A:291:ILE:HD11	2.37	0.59
1:B:525:GLN:H	1:B:525:GLN:CD	2.10	0.58
1:B:199:GLY:HA3	1:B:218:PRO:HG3	1.84	0.58
1:A:689:ASN:ND2	1:A:694:ALA:O	2.37	0.58
1:A:221:ILE:HD12	1:A:221:ILE:O	2.04	0.58
1:A:617:PHE:HD2	1:A:618:PHE:CD1	2.19	0.57
1:A:287:ALA:H	1:A:288:LYS:HZ3	1.52	0.56
1:A:182:GLN:N	1:A:182:GLN:OE1	2.38	0.56
1:B:75:LYS:HG2	1:B:397:LYS:HA	1.87	0.56
1:B:636:CYS:O	1:B:648:LYS:HD3	2.06	0.56
1:B:748:GLN:NE2	1:B:780:CYS:HB2	2.20	0.56
1:A:617:PHE:CD2	1:A:618:PHE:HD1	2.20	0.56
1:B:158:LEU:O	1:B:163:LYS:HD2	2.05	0.55
1:B:635:LEU:HD12	1:B:670:LYS:HB3	1.87	0.55
1:A:317:LYS:HB3	1:A:331:PRO:HG2	1.88	0.55
1:A:76:PRO:HB3	1:A:392:THR:HG21	1.88	0.55
1:B:636:CYS:HB2	1:B:648:LYS:HG3	1.89	0.55
1:A:684:ASN:C	1:A:689:ASN:HB3	2.32	0.55
1:B:182:GLN:N	1:B:182:GLN:OE1	2.40	0.55
1:B:525:GLN:HG3	1:B:595:ILE:HD11	1.88	0.55
1:A:62:GLY:O	1:A:458:MET:HE1	2.07	0.54
1:B:211:ILE:HB	1:B:214:THR:HG21	1.88	0.54
1:A:704:LEU:HG	1:A:714:VAL:HA	1.89	0.54
1:A:308:THR:HB	1:B:293:ARG:HD2	1.90	0.54
1:A:567:VAL:HA	1:A:722:LEU:HD13	1.90	0.54
1:B:600:ILE:HD11	1:B:800:TYR:CE2	2.43	0.54
1:A:240:MET:HE1	1:A:339:PHE:HD1	1.72	0.53
1:B:657:TYR:HD2	1:B:666:CYS:HB2	1.74	0.53
1:B:240:MET:HE2	1:B:352:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLN:HE22	1:A:194:PHE:H	1.55	0.53
1:A:165:ARG:HG2	1:A:180:VAL:HG23	1.90	0.53
1:A:235:HIS:CD2	1:A:355:THR:HG22	2.43	0.52
1:A:617:PHE:CD2	1:A:618:PHE:CD1	2.96	0.52
1:B:582:ILE:HG22	1:B:618:PHE:CE1	2.42	0.52
1:B:677:PRO:O	1:B:680:VAL:HG12	2.09	0.52
1:B:582:ILE:HD12	1:B:582:ILE:H	1.74	0.52
1:A:664:PHE:CE1	1:A:693:TRP:CZ3	2.90	0.52
1:B:485:LYS:HD3	1:B:772:LEU:HB2	1.90	0.52
1:B:322:LYS:HD3	1:B:329:ASP:HB3	1.91	0.52
1:A:155:ARG:HB3	1:A:157:GLU:CD	2.36	0.51
1:A:735:GLU:H	1:A:735:GLU:CD	2.13	0.51
1:A:363:GLU:OE2	1:A:363:GLU:HA	2.10	0.51
1:A:760:MET:HA	1:A:760:MET:HE2	1.90	0.51
1:A:574:ASN:O	1:A:711:ARG:NH1	2.39	0.51
1:B:615:ASP:CG	1:B:631:ASN:HB2	2.36	0.51
1:A:89:GLN:HE21	1:A:92:LEU:HD12	1.76	0.51
1:A:406:ASN:OD1	1:A:439:LEU:HB2	2.11	0.51
1:A:691:ALA:HA	1:A:695:LYS:HD3	1.93	0.51
1:B:376:PRO:HB2	1:B:378:ASN:OD1	2.11	0.51
1:B:360:GLU:OE2	1:B:360:GLU:N	2.41	0.51
1:A:567:VAL:HG21	1:A:704:LEU:HD13	1.93	0.50
1:B:795:TYR:O	2:B:901:A1CTG:N15	2.44	0.50
1:A:741:VAL:HG21	1:A:783:THR:HG23	1.92	0.50
1:B:4:ALA:HB1	1:B:31:ASP:O	2.10	0.50
1:B:630:SER:OG	1:B:631:ASN:N	2.44	0.50
1:B:277:GLU:O	1:B:279:LYS:HG2	2.11	0.50
1:A:586:LYS:HG3	1:A:620:GLU:H	1.77	0.50
1:B:635:LEU:N	1:B:635:LEU:HD22	2.27	0.50
1:B:581:ASN:OD1	1:B:581:ASN:O	2.30	0.50
1:A:200:TYR:HD2	1:A:215:LYS:HG2	1.77	0.50
1:A:575:LYS:HA	1:A:711:ARG:NH1	2.27	0.49
1:A:762:GLN:N	1:A:762:GLN:OE1	2.45	0.49
1:A:606:ARG:CZ	1:A:612:SER:HB3	2.42	0.49
1:B:205:ASN:HD21	1:B:209:GLU:HB2	1.77	0.49
1:B:598:TRP:O	1:B:602:VAL:HG22	2.12	0.49
1:A:682:PHE:O	1:A:688:LYS:NZ	2.43	0.49
1:B:681:VAL:O	1:B:685:THR:HG23	2.13	0.49
1:A:541:GLU:OE1	1:A:775:ASN:ND2	2.40	0.49
1:B:182:GLN:HE22	1:B:194:PHE:H	1.61	0.49
1:B:633:CYS:O	1:B:648:LYS:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:800:TYR:CE1	1:B:804:VAL:HG11	2.48	0.49
1:B:332:TYR:CG	1:B:341:CYS:HB2	2.48	0.48
1:A:681:VAL:HG21	1:A:714:VAL:CG1	2.43	0.48
1:B:528:TYR:CD2	1:B:812:MET:HE3	2.48	0.48
1:B:579:TRP:O	1:B:582:ILE:HD11	2.13	0.48
1:A:575:LYS:HA	1:A:711:ARG:HH12	1.79	0.48
1:A:480:LYS:O	1:A:484:MET:HG3	2.13	0.48
1:A:532:MET:HE1	1:A:809:ARG:HD3	1.95	0.48
1:B:194:PHE:HD2	1:B:195:HIS:N	2.11	0.48
1:A:565:ARG:HG3	1:A:717:TYR:HD1	1.79	0.48
1:A:622:CYS:HB2	1:A:635:LEU:HD12	1.95	0.48
1:B:704:LEU:HD13	1:B:720:CYS:SG	2.54	0.48
1:A:761:PHE:HE2	1:A:763:LEU:HD12	1.79	0.48
1:A:220:LYS:HG3	1:A:221:ILE:N	2.27	0.47
1:A:594:ASP:O	1:A:599:VAL:HG23	2.15	0.47
1:B:157:GLU:OE1	1:B:157:GLU:N	2.37	0.47
1:B:194:PHE:CE2	1:B:199:GLY:HA2	2.47	0.47
1:B:565:ARG:HH11	1:B:565:ARG:HG2	1.80	0.47
1:A:771:ASN:H	1:A:776:ASP:CG	2.22	0.47
1:B:91:CYS:HB3	1:B:115:GLY:O	2.14	0.47
1:A:681:VAL:HG21	1:A:714:VAL:HG11	1.96	0.47
1:B:542:TYR:CZ	1:B:544:ASN:HB3	2.49	0.47
1:B:284:ASP:HB3	1:B:288:LYS:HD2	1.97	0.47
1:A:480:LYS:HE2	1:A:501:GLU:OE1	2.15	0.46
1:B:703:GLU:HG2	1:B:713:PRO:HA	1.97	0.46
1:B:703:GLU:OE2	1:B:711:ARG:NH1	2.47	0.46
1:A:158:LEU:HD12	1:A:163:LYS:HB2	1.96	0.46
1:B:480:LYS:O	1:B:484:MET:HG3	2.14	0.46
1:B:579:TRP:C	1:B:582:ILE:HD11	2.40	0.46
1:A:477:THR:HG22	1:A:773:LEU:HD21	1.98	0.46
1:A:399:SER:HB2	1:A:402:THR:OG1	2.16	0.46
1:B:82:TYR:OH	1:B:823:LYS:HE2	2.15	0.46
1:B:717:TYR:CE2	1:B:718:LYS:HG3	2.51	0.46
1:A:199:GLY:HA3	1:A:218:PRO:HG3	1.97	0.46
1:A:510:LYS:O	1:A:514:LYS:HG3	2.15	0.46
1:A:195:HIS:HB3	1:A:198:THR:O	2.15	0.46
1:A:615:ASP:OD1	1:A:615:ASP:N	2.49	0.46
1:B:360:GLU:H	1:B:360:GLU:CD	2.23	0.46
1:A:103:MET:HE3	1:A:106:HIS:CG	2.51	0.46
1:B:59:LEU:HD12	1:B:394:VAL:HG11	1.97	0.46
1:B:91:CYS:HB2	1:B:117:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:VAL:HG12	1:B:673:VAL:HG22	1.98	0.46
1:B:108:ILE:O	1:B:110:GLN:NE2	2.47	0.45
1:A:614:ILE:HA	1:A:614:ILE:HD12	1.83	0.45
1:B:40:SER:HB2	1:B:325:LYS:HE2	1.98	0.45
1:B:161:CYS:HB3	1:B:187:GLY:O	2.16	0.45
1:A:542:TYR:CZ	1:A:544:ASN:HB3	2.51	0.45
1:A:259:HIS:CD2	1:A:304:ILE:HG12	2.52	0.45
1:B:32:ILE:HG21	1:B:408:PHE:HB2	1.98	0.45
1:B:194:PHE:HE2	1:B:199:GLY:CA	2.29	0.45
1:A:586:LYS:HG2	1:A:620:GLU:O	2.17	0.45
1:B:41:SER:OG	1:B:44:ASP:OD2	2.35	0.44
1:A:750:LEU:HB3	1:A:751:TYR:CE1	2.53	0.44
1:B:369:CYS:HB2	1:B:371:ASP:OD1	2.18	0.44
1:B:542:TYR:CD1	1:B:782:ILE:HD11	2.53	0.44
1:B:570:VAL:HG11	1:B:705:LEU:HD21	1.98	0.44
1:A:569:LEU:HD13	1:A:681:VAL:HG11	1.99	0.44
1:B:676:VAL:CB	1:B:680:VAL:HG11	2.47	0.44
1:A:532:MET:HA	1:A:532:MET:HE2	1.99	0.44
1:A:182:GLN:NE2	1:A:194:PHE:H	2.16	0.44
1:B:480:LYS:HD3	1:B:480:LYS:N	2.33	0.44
1:B:576:ASP:O	1:B:581:ASN:ND2	2.48	0.44
1:B:579:TRP:O	1:B:579:TRP:CD1	2.71	0.44
1:B:662:GLY:HA2	1:B:665:ARG:HG2	2.00	0.43
1:A:112:ASP:OD1	1:A:116:ASN:N	2.51	0.43
1:A:532:MET:HE3	1:A:792:MET:HE3	2.00	0.43
1:B:614:ILE:HA	1:B:632:LEU:HD11	2.00	0.43
1:A:291:ILE:HD13	1:A:291:ILE:HA	1.67	0.43
1:B:411:GLU:OE1	1:B:415:ARG:HG3	2.19	0.43
1:A:44:ASP:OD2	3:A:1002:HOH:O	2.21	0.43
1:B:162:LEU:O	1:B:166:GLN:HG2	2.18	0.43
1:B:717:TYR:O	1:B:721:LYS:HB3	2.18	0.43
1:A:174:LYS:HG2	1:A:176:LEU:HB2	2.00	0.43
1:A:753:ARG:HG3	1:A:779:GLN:O	2.19	0.43
1:B:565:ARG:HD2	1:B:678:HIS:CE1	2.54	0.43
1:A:293:ARG:O	1:A:297:LYS:HG3	2.18	0.43
1:A:603:SER:OG	1:A:803:THR:O	2.37	0.43
1:B:259:HIS:CD2	1:B:304:ILE:HG12	2.54	0.43
1:B:656:ALA:O	1:B:665:ARG:NE	2.52	0.43
1:B:648:LYS:HA	1:B:655:GLU:OE1	2.19	0.42
1:A:602:VAL:HG22	1:A:614:ILE:HG12	2.01	0.42
1:B:89:GLN:O	1:B:93:LYS:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:MET:HB2	1:B:106:HIS:HB2	2.01	0.42
1:A:781:LEU:C	1:A:782:ILE:HD12	2.44	0.42
1:B:221:ILE:HA	1:B:788:PRO:HA	2.01	0.42
1:A:583:LYS:HA	1:A:617:PHE:CE2	2.54	0.42
1:B:165:ARG:HG3	1:B:180:VAL:HG13	2.01	0.42
1:B:485:LYS:HD2	1:B:766:SER:HB2	2.01	0.42
1:B:532:MET:SD	1:B:809:ARG:HD2	2.59	0.42
1:B:577:ILE:H	1:B:577:ILE:HG12	1.65	0.42
1:A:824:HIS:CD2	1:A:824:HIS:C	2.97	0.42
1:B:477:THR:HG21	1:B:483:LYS:HA	2.01	0.42
1:A:226:GLN:HG2	1:A:822:ILE:HG13	2.01	0.42
1:A:689:ASN:ND2	1:A:695:LYS:O	2.52	0.42
1:B:789:LYS:HG3	1:B:794:ASP:HB2	2.02	0.42
1:A:155:ARG:HD3	1:A:157:GLU:OE2	2.19	0.42
1:A:236:TYR:CE2	1:A:387:THR:HG22	2.55	0.42
1:A:606:ARG:NH1	1:A:612:SER:O	2.52	0.42
1:A:426:LYS:HE3	1:A:426:LYS:HB3	1.85	0.42
1:B:158:LEU:HB3	1:B:163:LYS:HG3	2.01	0.42
1:A:89:GLN:CG	1:A:92:LEU:HD12	2.50	0.41
1:A:489:TRP:HB2	1:A:761:PHE:CZ	2.54	0.41
1:B:227:LYS:O	1:B:228:HIS:ND1	2.53	0.41
1:B:646:ASN:C	1:B:648:LYS:N	2.78	0.41
1:A:195:HIS:NE2	1:A:197:SER:OG	2.50	0.41
1:A:541:GLU:CD	1:A:775:ASN:HD22	2.25	0.41
1:B:214:THR:O	1:B:216:THR:HG23	2.21	0.41
1:B:399:SER:HB2	1:B:402:THR:OG1	2.20	0.41
1:B:585:LYS:HG3	1:B:672:ASP:OD2	2.21	0.41
1:B:804:VAL:HG13	1:B:805:TYR:CD2	2.54	0.41
1:A:528:TYR:CE2	1:A:812:MET:HB3	2.55	0.41
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.84	0.41
1:B:207:ILE:O	1:B:207:ILE:HG13	2.20	0.41
1:B:600:ILE:HD12	1:B:723:SER:HB3	2.03	0.41
1:A:565:ARG:CG	1:A:678:HIS:HD2	2.33	0.41
1:B:259:HIS:CG	1:B:304:ILE:HG12	2.55	0.41
1:B:685:THR:O	1:B:688:LYS:HE3	2.21	0.41
1:A:32:ILE:HG21	1:A:408:PHE:HB2	2.03	0.41
1:A:283:TRP:CZ2	1:A:291:ILE:HD11	2.55	0.41
1:B:598:TRP:O	1:B:601:PRO:HD2	2.21	0.41
1:B:578:ASN:C	1:B:580:ASN:H	2.28	0.41
1:A:173:GLU:C	1:A:174:LYS:HD3	2.46	0.41
1:B:579:TRP:O	1:B:579:TRP:CG	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:ASP:OD2	1:B:594:ASP:N	2.48	0.41
1:B:624:PRO:HA	1:B:649:CYS:HA	2.03	0.41
1:A:215:LYS:HB2	1:A:215:LYS:HE2	1.83	0.40
1:A:617:PHE:CD2	1:A:617:PHE:C	2.99	0.40
1:B:5:LYS:HE2	1:B:5:LYS:HB2	1.84	0.40
1:B:400:ASP:OD1	1:B:400:ASP:N	2.54	0.40
1:A:657:TYR:CG	1:A:666:CYS:HB2	2.56	0.40
1:A:681:VAL:HG23	1:A:682:PHE:CD2	2.56	0.40
1:B:401:LYS:O	1:B:405:ILE:HG13	2.22	0.40
1:A:225:CYS:HB2	1:A:809:ARG:HH12	1.85	0.40
1:A:565:ARG:HG3	1:A:717:TYR:CD1	2.56	0.40
1:A:703:GLU:OE1	1:A:711:ARG:NE	2.54	0.40
1:B:268:TRP:HZ3	1:B:304:ILE:HD13	1.86	0.40
1:B:397:LYS:HB3	1:B:397:LYS:HE2	1.83	0.40
1:B:631:ASN:HA	1:B:634:LYS:HE2	2.04	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:102:LYS:NZ	1:B:757:GLU:OE1[4_455]	2.18	0.02

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	832/853 (98%)	789 (95%)	41 (5%)	2 (0%)	43 58
1	B	816/853 (96%)	775 (95%)	38 (5%)	3 (0%)	30 43
All	All	1648/1706 (97%)	1564 (95%)	79 (5%)	5 (0%)	36 50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	755	GLY
1	B	301	VAL
1	A	174	LYS
1	B	579	TRP
1	B	829	LEU

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	714/730 (98%)	703 (98%)	11 (2%)	57	77
1	B	704/730 (96%)	694 (99%)	10 (1%)	59	79
All	All	1418/1460 (97%)	1397 (98%)	21 (2%)	57	77

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

Mol	Chain	Res	Type
1	A	45	CYS
1	A	132	VAL
1	A	174	LYS
1	A	180	VAL
1	A	183	CYS
1	A	628	THR
1	A	649	CYS
1	A	689	ASN
1	A	754	LYS
1	A	763	LEU
1	A	814	SER
1	B	343	LYS
1	B	345	ASP
1	B	433	SER
1	B	577	ILE
1	B	614	ILE
1	B	649	CYS
1	B	704	LEU
1	B	707	LEU

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Mol	Chain	Res	Type
1	B	825	CYS
1	B	832	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	97	GLN
1	A	120	GLN
1	A	226	GLN
1	A	235	HIS
1	A	580	ASN
1	A	678	HIS
1	B	188	ASN
1	B	251	GLN
1	B	479	ASN
1	B	578	ASN
1	B	696	ASN
1	B	748	GLN
1	B	787	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	A1CTG	A	901	-	23,29,29	0.59	0	22,45,45	1.11	3 (13%)
2	A1CTG	B	901	-	23,29,29	0.43	0	22,45,45	1.12	3 (13%)

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	A1CTG	N03-C04-N09	-3.16	106.99	112.45
2	A	901	A1CTG	N03-C04-N09	-3.04	107.19	112.45
2	A	901	A1CTG	O13-C12-C11	-2.44	105.41	113.09
2	B	901	A1CTG	O14-C12-C11	-2.12	106.41	113.09
2	B	901	A1CTG	N03-C02-N26	2.10	111.35	109.21
2	A	901	A1CTG	N03-C02-N26	2.04	111.29	109.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

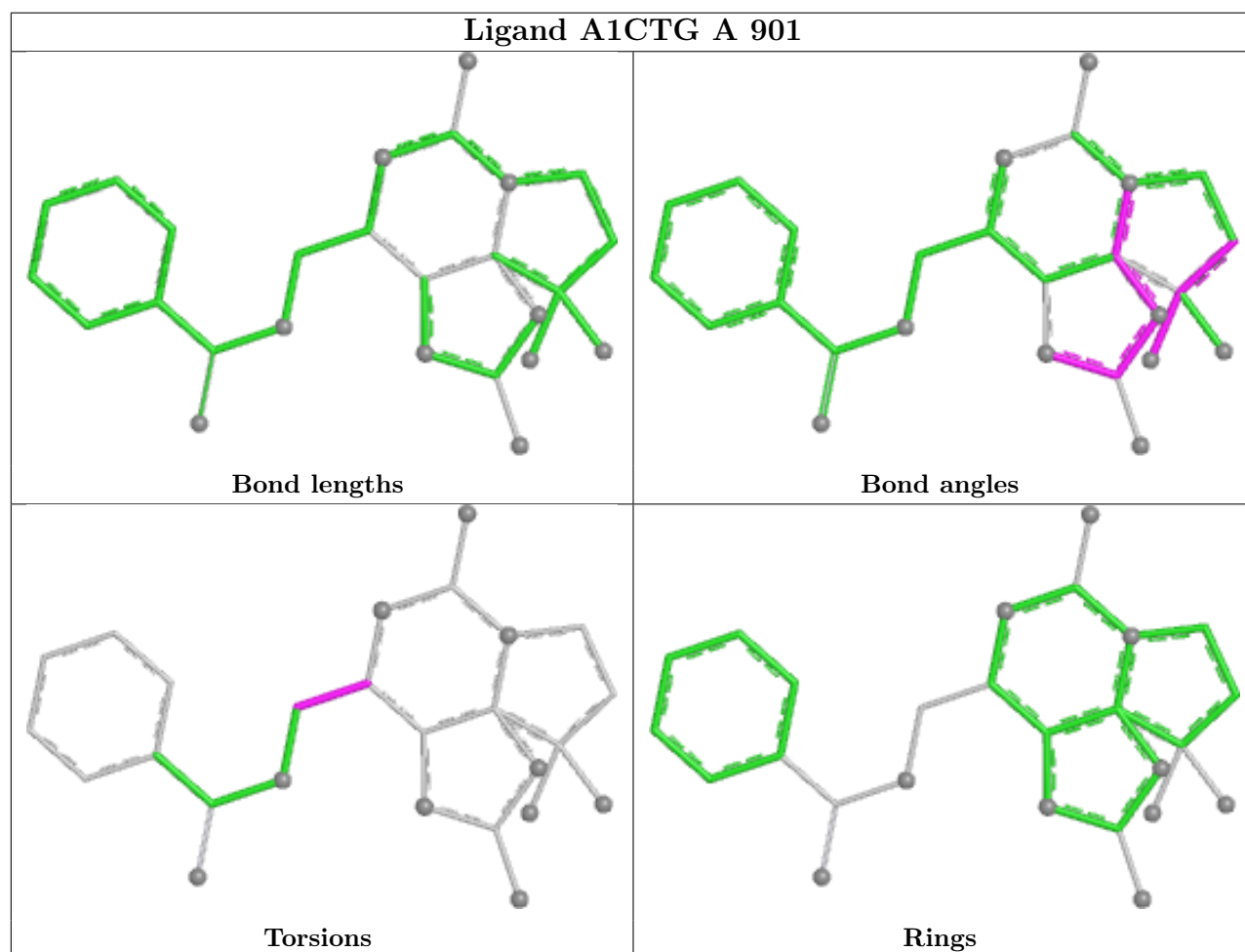
Mol	Chain	Res	Type	Atoms
2	A	901	A1CTG	C05-C06-C16-O17
2	A	901	A1CTG	N07-C06-C16-O17

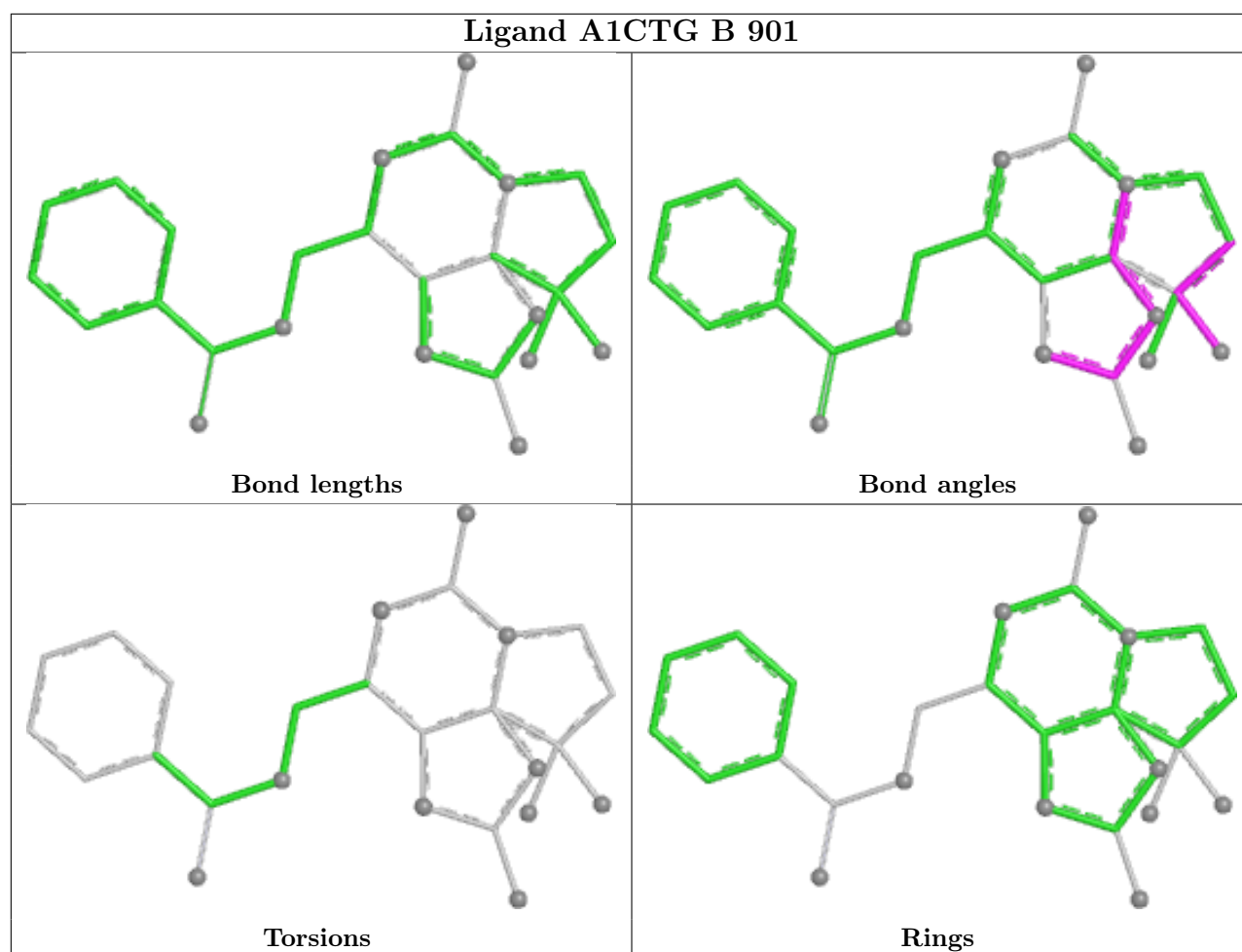
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	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	834/853 (97%)	0.47	47 (5%)	30 26	51, 86, 168, 199	0
1	B	820/853 (96%)	0.55	42 (5%)	33 30	52, 89, 154, 208	0
All	All	1654/1706 (96%)	0.51	89 (5%)	31 28	51, 88, 162, 208	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	832	LEU	6.2
1	A	1	ALA	6.2
1	B	829	LEU	5.6
1	B	831	VAL	5.2
1	B	168	ALA	4.9
1	B	830	GLU	4.5
1	B	88	LEU	4.3
1	A	664	PHE	4.3
1	A	834	GLN	3.8
1	A	564	LEU	3.8
1	B	167	VAL	3.4
1	A	176	LEU	3.4
1	B	640	PRO	3.0
1	B	408	PHE	3.0
1	A	644	ALA	2.9
1	A	467	LEU	2.9
1	A	800	TYR	2.9
1	A	596	ALA	2.8
1	B	614	ILE	2.8
1	B	712	ALA	2.8
1	A	557	PRO	2.7
1	A	177	GLY	2.7
1	A	283	TRP	2.7
1	B	85	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	685	THR	2.7
1	B	467	LEU	2.7
1	A	175	VAL	2.6
1	A	707	LEU	2.6
1	B	34	LEU	2.6
1	B	207	ILE	2.6
1	A	705	LEU	2.5
1	B	637	ILE	2.5
1	A	637	ILE	2.5
1	B	104	ILE	2.5
1	A	3	ASN	2.5
1	B	673	VAL	2.5
1	A	156	HIS	2.5
1	B	613	ASP	2.4
1	B	692	VAL	2.4
1	B	300	SER	2.4
1	B	618	PHE	2.4
1	B	615	ASP	2.4
1	A	558	TYR	2.4
1	A	704	LEU	2.4
1	A	702	PHE	2.4
1	A	579	TRP	2.4
1	B	468	PRO	2.3
1	B	579	TRP	2.4
1	B	722	LEU	2.3
1	A	684	ASN	2.3
1	A	754	LYS	2.3
1	A	717	TYR	2.3
1	A	4	ALA	2.3
1	A	640	PRO	2.3
1	A	722	LEU	2.3
1	B	664	PHE	2.3
1	A	681	VAL	2.3
1	A	674	ALA	2.3
1	B	724	GLY	2.3
1	A	600	ILE	2.3
1	B	617	PHE	2.3
1	B	206	ALA	2.2
1	A	569	LEU	2.2
1	B	577	ILE	2.2
1	A	693	TRP	2.2
1	A	756	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	82	TYR	2.2
1	B	573	SER	2.2
1	A	468	PRO	2.2
1	B	570	VAL	2.2
1	B	224	THR	2.2
1	B	87	ASP	2.2
1	A	692	VAL	2.1
1	A	646	ASN	2.1
1	A	169	LEU	2.1
1	A	563	THR	2.1
1	B	713	PRO	2.1
1	A	680	VAL	2.1
1	B	670	LYS	2.1
1	B	628	THR	2.1
1	A	221	ILE	2.1
1	B	429	MET	2.1
1	A	545	LYS	2.0
1	A	679	THR	2.0
1	B	812	MET	2.0
1	A	567	VAL	2.0
1	B	714	VAL	2.0
1	B	186	LYS	2.0
1	A	726	PRO	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.

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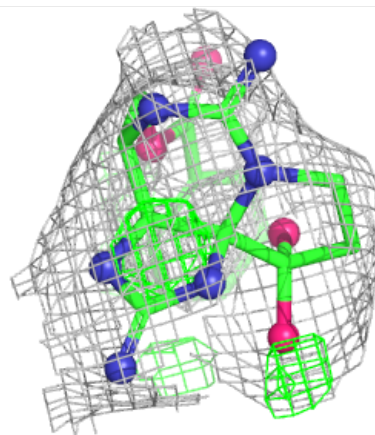
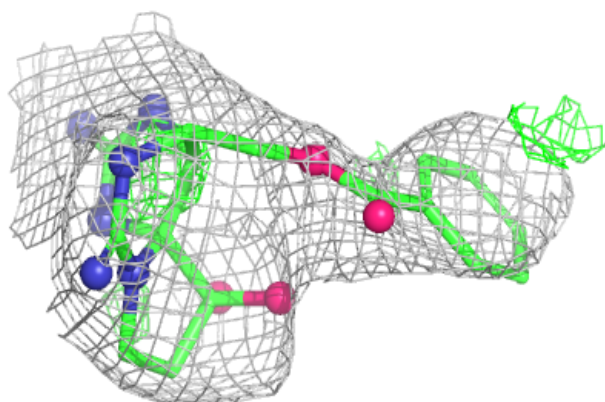
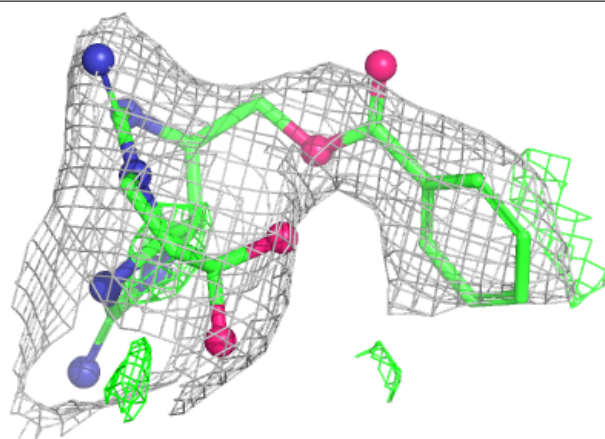
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1CTG	A	901	26/26	0.86	0.17	110,121,145,187	0
2	A1CTG	B	901	26/26	0.90	0.12	69,86,100,108	0

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.

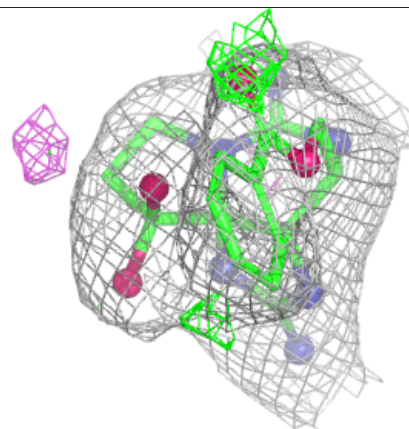
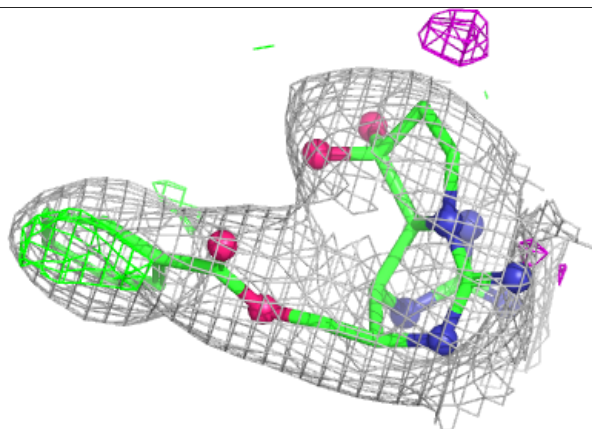
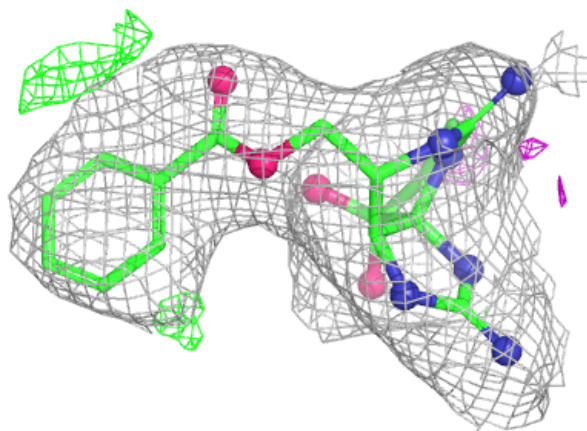
Electron density around A1CTG A 901:

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 ⓘ

There are no such residues in this entry.