



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:50 am BST

PDB ID : 2YFY
Title : SERCA in the HnE2 State Complexed With Debutanoyl Thapsigargin
Authors : Sonntag, Y.; Musgaard, M.; Olesen, C.; Schiott, B.; Moller, J.V.; Nissen, P.;
Thogersen, L.
Deposited on : 2011-04-11
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

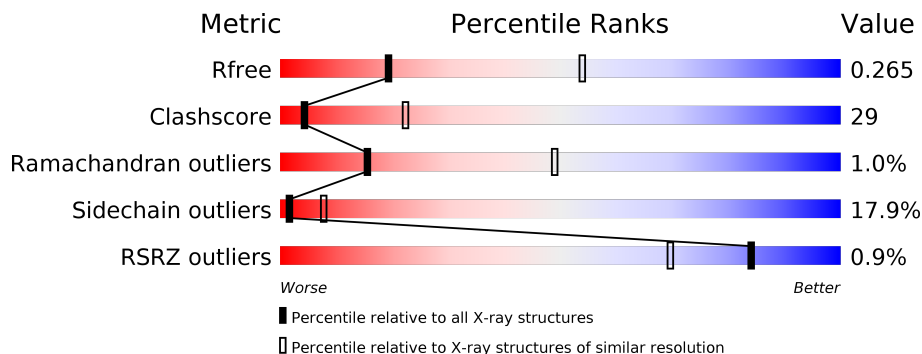
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	994	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	9TN	A	1995	-	-	X	-
3	K	A	1996	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	1997	-	-	-	X

2 Entry composition [i](#)

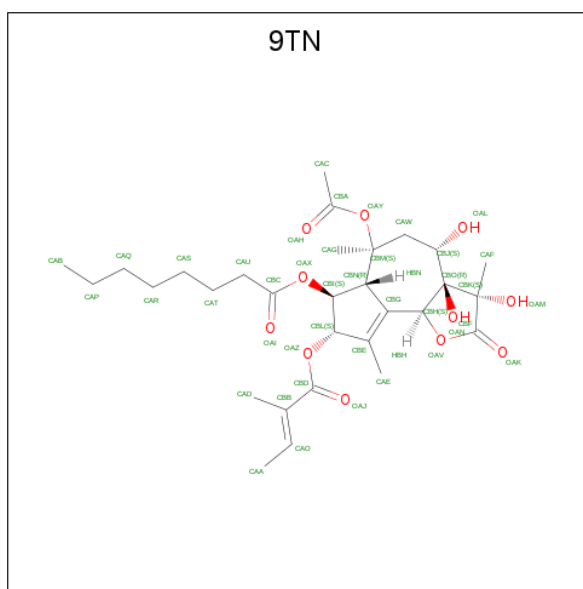
There are 4 unique types of molecules in this entry. The entry contains 7714 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	994	7671	4876	1287	1451	57	0	0	0

- Molecule 2 is DEBUTANOYL THAPSIGARGIN (three-letter code: 9TN) (formula: C₃₀H₄₄O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	41	30	11	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
3	A	1	1	1	0	0

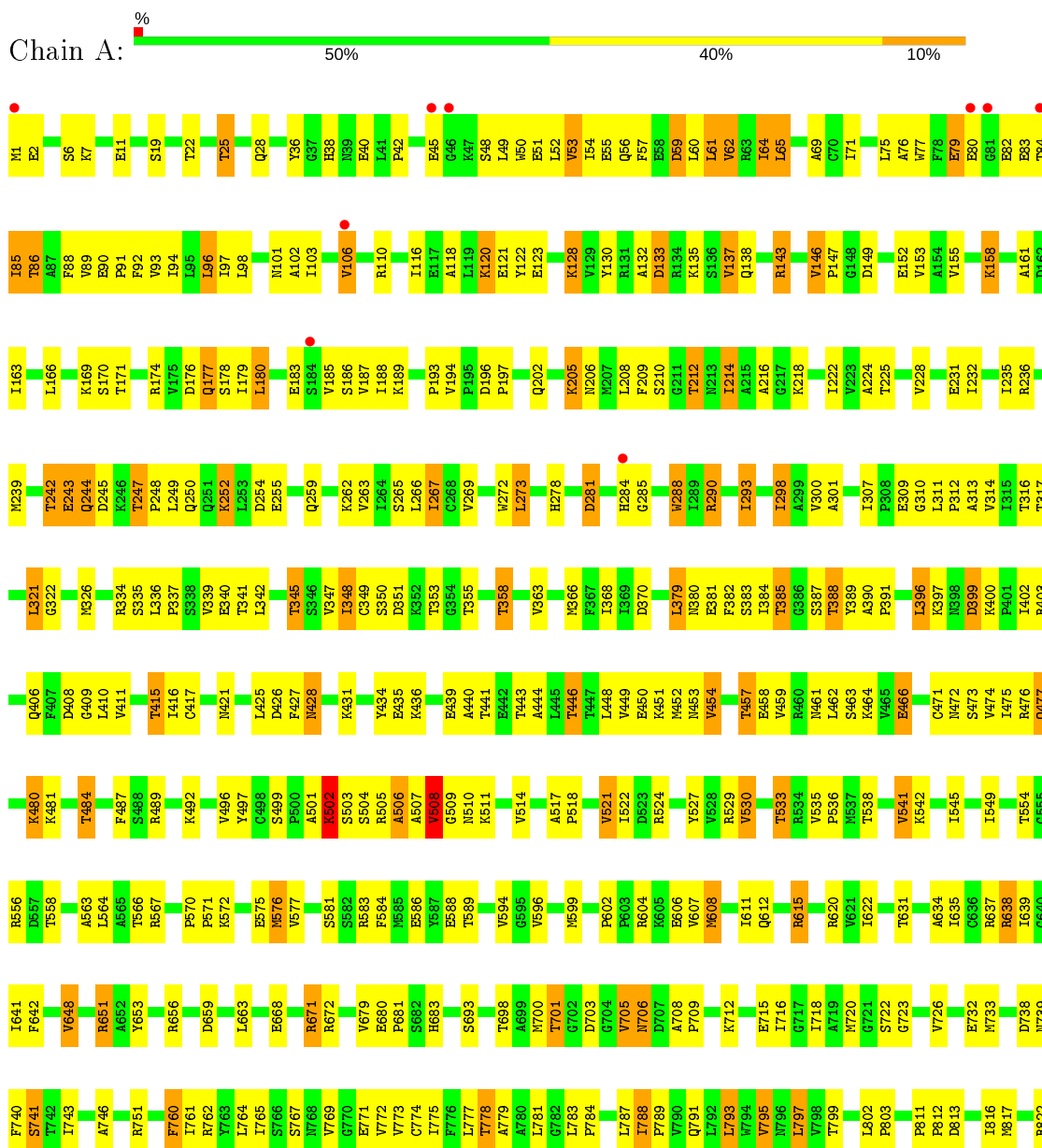
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

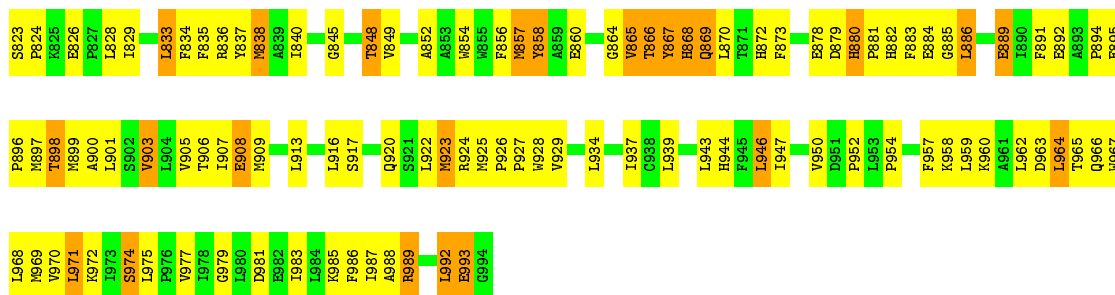
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.36Å 71.36Å 587.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.68 – 3.10 57.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (57.68-3.10) 100.0 (57.68-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.239 , 0.278 0.236 , 0.265	Depositor DCC
R_{free} test set	937 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	90.6	Xtrriage
Anisotropy	0.281	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7714	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: 9TN, K, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/7812	0.44	0/10592

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7671	0	7764	448	0
2	A	41	0	44	21	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
All	All	7714	0	7808	451	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 29.

All (451) 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:834:PHE:HD1	2:A:1995:9TN:OAH	0.89	1.24
1:A:772:VAL:HG21	2:A:1995:9TN:CAA	1.73	1.17
1:A:772:VAL:CG2	2:A:1995:9TN:HAA3	1.79	1.12
1:A:651:ARG:HH11	1:A:651:ARG:HG3	1.06	1.10
1:A:249:LEU:HB2	1:A:340:GLU:OE1	1.67	0.95
1:A:772:VAL:CG2	2:A:1995:9TN:CAA	2.40	0.94
1:A:61:LEU:HA	1:A:64:ILE:HD11	1.50	0.93
1:A:957:PHE:HB3	1:A:959:LEU:HD13	1.51	0.92
1:A:772:VAL:HG21	2:A:1995:9TN:HAA3	0.91	0.89
1:A:459:VAL:HA	1:A:462:LEU:HD13	1.56	0.88
1:A:869:GLN:HB2	1:A:872:HIS:CD2	2.09	0.87
1:A:987:ILE:C	1:A:989:ARG:HH12	1.78	0.87
1:A:391:PRO:HD2	1:A:434:TYR:CD2	2.10	0.86
1:A:390:ALA:HA	1:A:434:TYR:HD2	1.40	0.86
1:A:311:LEU:HD13	1:A:764:LEU:HD12	1.59	0.85
1:A:651:ARG:HG3	1:A:651:ARG:NH1	1.85	0.84
1:A:497:TYR:HE1	1:A:510:ASN:HD22	1.26	0.84
1:A:834:PHE:CD1	2:A:1995:9TN:CBA	2.61	0.83
1:A:502:LYS:HZ2	1:A:504:SER:H	1.22	0.83
1:A:680:GLU:H	1:A:683:HIS:HD2	1.27	0.82
1:A:964:LEU:HD22	1:A:964:LEU:H	1.45	0.82
1:A:901:LEU:HD13	1:A:959:LEU:HD21	1.62	0.82
1:A:638:ARG:HH11	1:A:638:ARG:HG3	1.47	0.80
1:A:869:GLN:HB2	1:A:872:HIS:HD2	1.49	0.78
1:A:989:ARG:CZ	1:A:989:ARG:H	1.96	0.77
1:A:288:TRP:CE3	1:A:288:TRP:HA	2.19	0.76
1:A:130:TYR:CZ	1:A:137:VAL:HG23	2.22	0.75
1:A:473:SER:O	1:A:477:GLN:HG2	1.87	0.74
1:A:193:PRO:HA	1:A:206:ASN:HD22	1.53	0.74
1:A:288:TRP:HE3	1:A:288:TRP:HA	1.53	0.73
1:A:988:ALA:N	1:A:989:ARG:HH12	1.86	0.73
1:A:463:SER:HB3	1:A:466:GLU:HG2	1.71	0.73
1:A:64:ILE:HD13	1:A:307:ILE:HD11	1.70	0.73
1:A:380:ASN:HB3	1:A:382:PHE:HE1	1.52	0.72
1:A:988:ALA:H	1:A:989:ARG:HH22	1.34	0.72
1:A:880:HIS:HA	1:A:884:GLU:HB2	1.71	0.71
1:A:865:VAL:HG21	1:A:870:LEU:HB2	1.73	0.71
1:A:988:ALA:HA	1:A:992:LEU:HB3	1.72	0.71
1:A:899:MET:O	1:A:903:VAL:HG12	1.90	0.71
1:A:760:PHE:C	1:A:760:PHE:HD1	1.94	0.71
1:A:873:PHE:HB2	1:A:891:PHE:CE2	2.26	0.70
1:A:680:GLU:H	1:A:683:HIS:CD2	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:OE1	1:A:84:THR:HB	1.93	0.69
1:A:898:THR:HG21	1:A:960:LYS:H	1.58	0.69
1:A:350:SER:HA	1:A:701:THR:OG1	1.93	0.69
1:A:61:LEU:HD13	1:A:307:ILE:HG23	1.75	0.69
1:A:856:PHE:O	1:A:864:GLY:HA2	1.94	0.69
1:A:6:SER:HA	1:A:194:VAL:O	1.93	0.68
1:A:963:ASP:H	1:A:966:GLN:HE21	1.39	0.68
1:A:396:LEU:HD12	1:A:399:ASP:HA	1.76	0.68
1:A:963:ASP:H	1:A:966:GLN:NE2	1.91	0.67
1:A:865:VAL:HB	1:A:868:HIS:CB	2.24	0.67
1:A:889:GLU:HG3	1:A:889:GLU:O	1.94	0.67
1:A:829:ILE:HB	2:A:1995:9TN:HBJ	1.77	0.67
1:A:89:VAL:O	1:A:93:VAL:HG23	1.94	0.67
1:A:232:ILE:H	1:A:232:ILE:HD12	1.60	0.66
1:A:232:ILE:HD12	1:A:232:ILE:N	2.11	0.66
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.77	0.66
1:A:122:TYR:HE2	1:A:726:VAL:HG21	1.60	0.66
1:A:59:ASP:O	1:A:62:VAL:HG13	1.94	0.66
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.77	0.66
1:A:348:ILE:HD11	1:A:740:PHE:CE2	2.30	0.66
1:A:313:ALA:O	1:A:317:THR:HG23	1.96	0.66
1:A:415:THR:HG22	1:A:475:ILE:HG23	1.76	0.66
1:A:989:ARG:CZ	1:A:989:ARG:N	2.59	0.66
1:A:252:LYS:O	1:A:255:GLU:HG2	1.96	0.66
1:A:77:TRP:CE3	1:A:88:PHE:HZ	2.14	0.66
1:A:572:LYS:HB2	1:A:575:GLU:HG2	1.77	0.66
1:A:760:PHE:C	1:A:760:PHE:CD1	2.67	0.66
1:A:845:GLY:O	1:A:849:VAL:HG22	1.95	0.66
1:A:120:LYS:HA	1:A:123:GLU:HG3	1.78	0.65
1:A:480:LYS:HB2	1:A:501:ALA:HB2	1.77	0.65
1:A:502:LYS:O	1:A:506:ALA:HB2	1.97	0.65
1:A:567:ARG:NH1	1:A:571:PRO:HD3	2.11	0.65
1:A:857:MET:HA	1:A:864:GLY:HA3	1.79	0.65
1:A:278:HIS:O	1:A:281:ASP:HB2	1.97	0.64
1:A:453:ASN:HB3	1:A:471:CYS:SG	2.36	0.64
1:A:86:THR:O	1:A:89:VAL:HG22	1.96	0.64
1:A:321:LEU:HD13	1:A:321:LEU:N	2.13	0.64
1:A:638:ARG:HG3	1:A:638:ARG:NH1	2.07	0.64
1:A:822:ARG:HH11	1:A:826:GLU:HG2	1.63	0.64
1:A:834:PHE:CE1	2:A:1995:9TN:CBA	2.80	0.64
1:A:703:ASP:OD1	1:A:723:GLY:HA2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:ILE:HG23	1:A:977:VAL:HG21	1.79	0.64
1:A:927:PRO:HB2	1:A:934:LEU:HD21	1.78	0.64
1:A:989:ARG:N	1:A:989:ARG:NH1	2.46	0.64
1:A:986:PHE:C	1:A:989:ARG:NH1	2.52	0.64
1:A:950:VAL:O	1:A:954:PRO:HD3	1.98	0.63
1:A:98:LEU:HA	1:A:101:ASN:OD1	1.98	0.63
1:A:262:LYS:O	1:A:266:LEU:HG	1.99	0.63
1:A:102:ALA:O	1:A:106:VAL:HG12	1.98	0.63
1:A:957:PHE:O	1:A:958:LYS:HB2	1.99	0.62
1:A:380:ASN:HB3	1:A:382:PHE:CE1	2.33	0.62
1:A:193:PRO:HA	1:A:206:ASN:ND2	2.13	0.62
1:A:907:ILE:HG13	1:A:974:SER:HB3	1.82	0.62
1:A:391:PRO:HD2	1:A:434:TYR:HD2	1.64	0.62
1:A:403:ARG:HD3	1:A:406:GLN:HE21	1.64	0.62
1:A:788:ILE:CD1	1:A:789:PRO:HD2	2.29	0.62
1:A:608:MET:HE2	1:A:608:MET:H	1.64	0.62
1:A:408:ASP:O	1:A:411:VAL:HG22	2.00	0.61
1:A:481:LYS:O	1:A:481:LYS:HG3	2.00	0.61
1:A:834:PHE:CE1	2:A:1995:9TN:OAH	2.48	0.61
1:A:155:VAL:HA	1:A:214:ILE:HG22	1.81	0.61
1:A:379:LEU:H	1:A:379:LEU:HD12	1.64	0.61
1:A:571:PRO:HG2	1:A:576:MET:SD	2.40	0.61
1:A:146:VAL:HG22	1:A:147:PRO:HD2	1.83	0.61
1:A:259:GLN:O	1:A:263:VAL:HG23	2.01	0.61
1:A:397:LYS:HB3	1:A:402:ILE:HD11	1.81	0.61
1:A:522:ILE:HG22	1:A:542:LYS:HE3	1.81	0.61
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.83	0.60
1:A:505:ARG:HG3	1:A:505:ARG:O	1.98	0.60
1:A:298:ILE:HD12	1:A:779:ALA:HB2	1.84	0.60
1:A:174:ARG:HG2	1:A:188:ILE:HD13	1.84	0.60
1:A:950:VAL:CG1	1:A:952:PRO:HD2	2.32	0.60
1:A:80:GLU:HB2	1:A:83:GLU:HB3	1.83	0.59
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.84	0.59
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.84	0.59
1:A:355:THR:HG22	1:A:738:ASP:O	2.03	0.59
1:A:235:ILE:O	1:A:239:MET:HG3	2.03	0.59
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.85	0.59
1:A:40:GLU:OE1	1:A:143:ARG:HD2	2.02	0.59
1:A:761:ILE:O	1:A:765:ILE:HG12	2.02	0.59
1:A:981:ASP:O	1:A:985:LYS:HB2	2.03	0.58
1:A:668:GLU:HG3	1:A:672:ARG:NH1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:LEU:HD11	1:A:891:PHE:CE1	2.39	0.58
1:A:411:VAL:HA	1:A:454:VAL:HG21	1.86	0.58
1:A:583:ARG:O	1:A:586:GLU:HG2	2.04	0.58
1:A:968:LEU:O	1:A:972:LYS:HG3	2.04	0.58
1:A:272:TRP:HE3	1:A:273:LEU:HD23	1.69	0.58
1:A:50:TRP:CZ3	1:A:54:ILE:HD11	2.38	0.58
1:A:71:ILE:O	1:A:75:LEU:HG	2.03	0.58
1:A:848:THR:HG22	1:A:900:ALA:O	2.04	0.58
1:A:391:PRO:HD2	1:A:434:TYR:CE2	2.40	0.57
1:A:248:PRO:O	1:A:252:LYS:HD2	2.04	0.57
1:A:322:GLY:O	1:A:326:MET:HG3	2.04	0.57
1:A:50:TRP:O	1:A:54:ILE:HG12	2.05	0.57
1:A:321:LEU:H	1:A:321:LEU:HD13	1.70	0.57
1:A:49:LEU:O	1:A:53:VAL:HG22	2.04	0.57
1:A:615:ARG:HH11	1:A:615:ARG:HB3	1.70	0.57
1:A:177:GLN:HA	1:A:212:THR:HG22	1.86	0.56
2:A:1995:9TN:OAL	2:A:1995:9TN:HAG2	2.05	0.56
1:A:979:GLY:O	1:A:983:ILE:HG13	2.04	0.56
1:A:436:LYS:CB	1:A:443:THR:HG21	2.36	0.56
1:A:988:ALA:N	1:A:989:ARG:HH22	2.02	0.56
1:A:385:THR:O	1:A:451:LYS:HE2	2.05	0.56
1:A:57:PHE:HA	1:A:62:VAL:HG21	1.88	0.56
1:A:870:LEU:O	1:A:873:PHE:HB3	2.06	0.56
1:A:1:MET:HA	1:A:224:ALA:O	2.05	0.56
1:A:988:ALA:N	1:A:989:ARG:NH1	2.53	0.56
1:A:950:VAL:O	1:A:954:PRO:CD	2.54	0.56
1:A:285:GLY:O	1:A:288:TRP:HB2	2.05	0.56
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.46	0.56
1:A:963:ASP:N	1:A:966:GLN:HE21	2.03	0.56
1:A:471:CYS:O	1:A:474:VAL:HG22	2.06	0.55
1:A:659:ASP:OD1	1:A:683:HIS:HE1	1.89	0.55
1:A:767:SER:HB3	1:A:908:GLU:OE2	2.06	0.55
1:A:92:PHE:O	1:A:96:LEU:HG	2.06	0.55
1:A:502:LYS:HD3	1:A:504:SER:OG	2.07	0.55
1:A:854:TRP:O	1:A:857:MET:O	2.25	0.55
2:A:1995:9TN:OAH	2:A:1995:9TN:CAW	2.55	0.55
1:A:789:PRO:O	1:A:793:LEU:HD23	2.07	0.55
1:A:242:THR:HG21	1:A:712:LYS:HG2	1.89	0.55
1:A:249:LEU:CB	1:A:340:GLU:OE1	2.49	0.55
1:A:80:GLU:OE1	1:A:83:GLU:HB3	2.07	0.55
1:A:7:LYS:HD3	1:A:11:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:SER:HB3	1:A:218:LYS:H	1.72	0.54
1:A:866:THR:HG22	1:A:867:TYR:N	2.22	0.54
1:A:122:TYR:O	1:A:158:LYS:HD3	2.07	0.54
1:A:312:PRO:O	1:A:316:THR:HG23	2.08	0.54
1:A:427:PHE:CE2	1:A:464:LYS:HB3	2.43	0.54
1:A:381:GLU:O	1:A:397:LYS:HD2	2.07	0.54
1:A:795:VAL:HA	1:A:799:THR:HB	1.89	0.54
1:A:811:PRO:HG3	1:A:929:VAL:HG12	1.88	0.54
1:A:894:PRO:O	1:A:898:THR:HG23	2.07	0.54
1:A:769:VAL:HA	2:A:1995:9TN:CAA	2.38	0.54
1:A:788:ILE:HD12	1:A:789:PRO:HD2	1.89	0.54
1:A:209:PHE:CD1	1:A:231:GLU:HG3	2.42	0.54
1:A:760:PHE:HD1	1:A:761:ILE:N	2.04	0.54
1:A:75:LEU:HD22	1:A:293:ILE:HG23	1.90	0.54
1:A:865:VAL:O	1:A:868:HIS:HB2	2.08	0.54
1:A:25:THR:HG23	1:A:28:GLN:HG3	1.89	0.54
1:A:358:THR:OG1	1:A:602:PRO:HG2	2.08	0.54
1:A:898:THR:HG22	1:A:959:LEU:HA	1.89	0.54
1:A:351:ASP:OD2	1:A:701:THR:HB	2.08	0.53
1:A:873:PHE:HB2	1:A:891:PHE:CD2	2.42	0.53
1:A:146:VAL:O	1:A:149:ASP:HB2	2.08	0.53
1:A:363:VAL:HG11	1:A:448:LEU:HD22	1.90	0.53
1:A:656:ARG:HA	1:A:656:ARG:NE	2.23	0.53
1:A:235:ILE:HD13	1:A:705:VAL:HG13	1.89	0.53
1:A:637:ARG:HG2	1:A:642:PHE:HB2	1.91	0.53
1:A:79:GLU:OE1	1:A:83:GLU:HG3	2.07	0.53
1:A:651:ARG:CG	1:A:651:ARG:NH1	2.64	0.53
1:A:762:ARG:HB3	1:A:837:TYR:CE2	2.44	0.53
1:A:84:THR:HG22	1:A:86:THR:N	2.24	0.53
1:A:336:LEU:N	1:A:337:PRO:CD	2.72	0.53
1:A:310:GLY:O	1:A:314:VAL:HG23	2.09	0.53
1:A:502:LYS:NZ	1:A:504:SER:H	2.02	0.53
1:A:235:ILE:HG23	1:A:709:PRO:HG3	1.91	0.53
1:A:880:HIS:N	1:A:881:PRO:HD2	2.24	0.53
1:A:348:ILE:HD12	1:A:743:ILE:HG21	1.91	0.53
1:A:769:VAL:O	1:A:773:VAL:HG23	2.09	0.53
1:A:969:MET:HA	1:A:969:MET:HE3	1.91	0.53
1:A:232:ILE:H	1:A:232:ILE:CD1	2.23	0.52
1:A:774:CYS:SG	1:A:849:VAL:HG13	2.49	0.52
1:A:751:ARG:HD2	1:A:817:MET:CE	2.40	0.52
1:A:865:VAL:HB	1:A:868:HIS:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLN:OE1	1:A:489:ARG:HD3	2.09	0.52
1:A:762:ARG:HB3	1:A:837:TYR:HE2	1.74	0.52
1:A:895:GLU:N	1:A:896:PRO:HD2	2.25	0.52
1:A:901:LEU:C	1:A:901:LEU:HD23	2.29	0.52
1:A:909:MET:HE3	1:A:937:ILE:HG12	1.92	0.52
1:A:981:ASP:O	1:A:985:LYS:N	2.40	0.52
1:A:983:ILE:O	1:A:987:ILE:HG13	2.10	0.52
1:A:307:ILE:HB	1:A:309:GLU:OE2	2.09	0.52
1:A:348:ILE:HG12	1:A:348:ILE:O	2.10	0.52
1:A:389:TYR:CE2	1:A:436:LYS:HB3	2.45	0.52
1:A:865:VAL:O	1:A:868:HIS:N	2.43	0.51
1:A:900:ALA:O	1:A:903:VAL:HG13	2.10	0.51
1:A:950:VAL:HG13	1:A:952:PRO:HD2	1.92	0.51
1:A:985:LYS:C	1:A:989:ARG:NH2	2.64	0.51
1:A:52:LEU:HD21	1:A:106:VAL:HB	1.92	0.51
1:A:946:LEU:C	1:A:946:LEU:HD12	2.31	0.51
1:A:247:THR:HG22	1:A:250:GLN:H	1.75	0.51
1:A:349:CYS:HA	1:A:622:ILE:O	2.10	0.51
1:A:52:LEU:CD2	1:A:106:VAL:HB	2.41	0.51
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.92	0.51
1:A:852:ALA:HB2	1:A:900:ALA:HB2	1.93	0.51
1:A:342:LEU:O	1:A:345:THR:HG23	2.11	0.50
1:A:612:GLN:HA	1:A:615:ARG:HG3	1.92	0.50
1:A:865:VAL:CG2	1:A:870:LEU:HB2	2.40	0.50
1:A:535:VAL:HG13	1:A:536:PRO:HD2	1.92	0.50
1:A:355:THR:HG23	1:A:720:MET:CE	2.41	0.50
1:A:85:ILE:HG13	1:A:86:THR:N	2.25	0.50
1:A:517:ALA:O	1:A:521:VAL:HG13	2.11	0.50
1:A:926:PRO:O	1:A:929:VAL:HG23	2.12	0.50
1:A:783:LEU:HG	1:A:784:PRO:HD2	1.94	0.50
1:A:239:MET:O	1:A:242:THR:HG22	2.11	0.50
1:A:760:PHE:CD1	1:A:761:ILE:N	2.80	0.50
1:A:992:LEU:HG	1:A:993:GLU:H	1.77	0.50
1:A:518:PRO:HA	1:A:563:ALA:HB2	1.93	0.50
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.93	0.50
1:A:379:LEU:HD12	1:A:379:LEU:N	2.27	0.50
1:A:484:THR:HB	1:A:496:VAL:HG12	1.94	0.50
1:A:700:MET:HE3	1:A:701:THR:N	2.26	0.50
1:A:248:PRO:HB2	1:A:340:GLU:OE2	2.11	0.50
1:A:428:ASN:HD21	1:A:431:LYS:H	1.59	0.50
1:A:607:VAL:O	1:A:611:ILE:HG12	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:ILE:HG12	1:A:897:MET:HE1	1.92	0.49
1:A:680:GLU:N	1:A:683:HIS:HD2	2.05	0.49
1:A:835:PHE:O	1:A:838:MET:HB3	2.12	0.49
1:A:298:ILE:HD11	1:A:778:THR:HG22	1.94	0.49
1:A:507:ALA:C	1:A:509:GLY:H	2.16	0.49
1:A:958:LYS:C	1:A:959:LEU:HD12	2.32	0.49
1:A:272:TRP:CE3	1:A:273:LEU:HD23	2.47	0.49
1:A:309:GLU:O	1:A:312:PRO:HD2	2.13	0.49
1:A:368:ILE:HD12	1:A:409:GLY:HA3	1.94	0.49
1:A:449:VAL:HG13	1:A:472:ASN:HD21	1.77	0.49
1:A:909:MET:CE	1:A:937:ILE:HA	2.43	0.49
1:A:444:ALA:HB3	1:A:599:MET:CE	2.43	0.49
1:A:267:ILE:HD13	2:A:1995:9TN:HAP2	1.95	0.48
1:A:880:HIS:ND1	1:A:881:PRO:HD3	2.28	0.48
1:A:342:LEU:HD21	1:A:746:ALA:HB1	1.95	0.48
1:A:52:LEU:C	1:A:52:LEU:HD23	2.34	0.48
1:A:817:MET:HE2	1:A:817:MET:HA	1.95	0.48
1:A:923:MET:CE	1:A:924:ARG:HH11	2.25	0.48
1:A:639:ILE:HG13	1:A:641:ILE:HG13	1.95	0.48
1:A:103:ILE:O	1:A:106:VAL:HG13	2.14	0.48
1:A:161:ALA:HA	1:A:210:SER:HB2	1.95	0.48
1:A:93:VAL:O	1:A:97:ILE:HD13	2.14	0.48
1:A:116:ILE:HG23	1:A:236:ARG:HG3	1.95	0.48
1:A:946:LEU:O	1:A:946:LEU:HD12	2.13	0.48
1:A:901:LEU:HD22	1:A:944:HIS:HE1	1.79	0.48
1:A:341:THR:O	1:A:716:ILE:HD11	2.14	0.47
1:A:355:THR:HA	1:A:738:ASP:O	2.14	0.47
1:A:88:PHE:O	1:A:92:PHE:HD2	1.97	0.47
1:A:923:MET:HG2	1:A:924:ARG:N	2.29	0.47
1:A:760:PHE:CE1	1:A:761:ILE:HG13	2.49	0.47
1:A:76:ALA:HB1	1:A:88:PHE:HD1	1.79	0.47
1:A:772:VAL:HG23	2:A:1995:9TN:CAA	2.42	0.47
1:A:439:GLU:HG3	1:A:440:ALA:N	2.28	0.47
1:A:263:VAL:HG11	2:A:1995:9TN:HAD1	1.96	0.47
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.45	0.47
1:A:169:LYS:HD2	1:A:169:LYS:N	2.29	0.47
1:A:384:ILE:HD12	1:A:384:ILE:N	2.29	0.47
1:A:417:CYS:O	1:A:421:ASN:HB2	2.14	0.47
1:A:427:PHE:CD1	1:A:428:ASN:N	2.83	0.47
1:A:793:LEU:O	1:A:797:LEU:HB2	2.14	0.47
1:A:905:VAL:O	1:A:909:MET:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:TRP:O	1:A:971:LEU:HD23	2.15	0.47
1:A:507:ALA:O	1:A:509:GLY:N	2.47	0.47
1:A:581:SER:HA	1:A:584:PHE:CD2	2.49	0.47
1:A:428:ASN:OD1	1:A:431:LYS:HB2	2.15	0.47
1:A:885:GLY:O	1:A:886:LEU:HG	2.15	0.47
1:A:300:VAL:HG23	1:A:301:ALA:N	2.30	0.47
1:A:524:ARG:HD3	1:A:588:GLU:O	2.15	0.47
1:A:788:ILE:HG12	1:A:897:MET:CE	2.45	0.47
1:A:133:ASP:N	1:A:133:ASP:OD1	2.49	0.46
1:A:421:ASN:ND2	1:A:446:THR:HG22	2.30	0.46
1:A:700:MET:HE3	1:A:701:THR:H	1.80	0.46
1:A:781:LEU:HD23	1:A:781:LEU:N	2.31	0.46
1:A:901:LEU:HD22	1:A:944:HIS:CE1	2.50	0.46
1:A:267:ILE:HD13	2:A:1995:9TN:CAP	2.45	0.46
1:A:606:GLU:HB2	1:A:741:SER:OG	2.15	0.46
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.98	0.46
1:A:170:SER:CB	1:A:218:LYS:H	2.29	0.46
1:A:943:LEU:O	1:A:947:ILE:HG23	2.15	0.46
1:A:992:LEU:CG	1:A:993:GLU:H	2.28	0.46
1:A:80:GLU:HB2	1:A:83:GLU:CB	2.46	0.46
1:A:88:PHE:O	1:A:92:PHE:CD2	2.68	0.46
1:A:249:LEU:HA	1:A:252:LYS:HD3	1.98	0.46
1:A:765:ILE:O	1:A:769:VAL:HG23	2.15	0.46
1:A:706:ASN:O	1:A:709:PRO:HD2	2.16	0.46
1:A:118:ALA:CB	1:A:726:VAL:HG22	2.46	0.46
1:A:928:TRP:HA	1:A:934:LEU:CD1	2.45	0.46
1:A:473:SER:HA	1:A:476:ARG:HG3	1.98	0.46
1:A:530:VAL:CG2	1:A:530:VAL:O	2.64	0.46
1:A:84:THR:HG22	1:A:86:THR:H	1.79	0.46
1:A:903:VAL:HA	1:A:970:VAL:HG13	1.98	0.46
1:A:964:LEU:O	1:A:968:LEU:HD12	2.15	0.46
1:A:879:ASP:O	1:A:879:ASP:CG	2.55	0.46
1:A:77:TRP:HE3	1:A:88:PHE:HZ	1.63	0.46
1:A:122:TYR:CE2	1:A:726:VAL:HG21	2.46	0.45
1:A:80:GLU:N	1:A:83:GLU:HG2	2.31	0.45
1:A:505:ARG:O	1:A:507:ALA:N	2.50	0.45
1:A:244:GLN:H	1:A:244:GLN:HG2	1.67	0.45
1:A:50:TRP:CE3	1:A:54:ILE:HD11	2.51	0.45
1:A:668:GLU:OE1	1:A:671:ARG:HD3	2.16	0.45
1:A:90:GLU:N	1:A:91:PRO:HD2	2.30	0.45
1:A:965:THR:HA	1:A:968:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLN:HA	1:A:212:THR:CG2	2.46	0.45
1:A:310:GLY:HA2	1:A:797:LEU:HD22	1.98	0.45
1:A:80:GLU:CD	1:A:83:GLU:OE1	2.55	0.45
1:A:829:ILE:HD13	1:A:837:TYR:HD2	1.81	0.45
1:A:265:SER:O	1:A:269:VAL:HG23	2.16	0.45
1:A:427:PHE:CD2	1:A:464:LYS:HB3	2.51	0.45
1:A:659:ASP:OD1	1:A:683:HIS:CE1	2.69	0.45
1:A:128:LYS:HG3	1:A:152:GLU:O	2.16	0.45
1:A:45:GLU:HG3	1:A:45:GLU:O	2.17	0.45
1:A:701:THR:HA	1:A:718:ILE:O	2.17	0.45
1:A:988:ALA:N	1:A:989:ARG:NH2	2.65	0.45
1:A:436:LYS:HB3	1:A:443:THR:HG21	1.98	0.45
1:A:858:TYR:CE1	1:A:866:THR:O	2.70	0.45
1:A:769:VAL:HA	2:A:1995:9TN:HAA1	1.99	0.45
1:A:788:ILE:HD13	1:A:789:PRO:HD2	2.00	0.45
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.98	0.44
1:A:988:ALA:HA	1:A:992:LEU:CB	2.45	0.44
1:A:163:ILE:HB	1:A:208:LEU:HB2	1.99	0.44
1:A:390:ALA:HA	1:A:434:TYR:CD2	2.32	0.44
1:A:416:ILE:HD11	1:A:566:THR:HG22	2.00	0.44
1:A:541:VAL:O	1:A:545:ILE:HG13	2.18	0.44
1:A:799:THR:HG21	1:A:905:VAL:HG13	1.99	0.44
1:A:913:LEU:HB3	1:A:922:LEU:HD21	1.99	0.44
1:A:391:PRO:HB3	1:A:450:GLU:CB	2.47	0.44
1:A:564:LEU:N	1:A:564:LEU:HD23	2.32	0.44
1:A:80:GLU:H	1:A:83:GLU:CD	2.21	0.44
1:A:25:THR:HA	1:A:132:ALA:HB3	1.99	0.44
1:A:811:PRO:HA	1:A:812:PRO:HD3	1.73	0.44
1:A:38:HIS:CG	1:A:143:ARG:NH1	2.86	0.44
1:A:53:VAL:HA	1:A:56:GLN:CG	2.48	0.44
1:A:89:VAL:HG23	1:A:90:GLU:N	2.33	0.44
1:A:577:VAL:HB	1:A:583:ARG:HH21	1.83	0.44
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.76	0.44
1:A:527:TYR:HD1	1:A:536:PRO:HA	1.82	0.44
1:A:823:SER:HA	1:A:824:PRO:HD2	1.82	0.44
1:A:487:PHE:C	1:A:487:PHE:CD1	2.91	0.43
1:A:642:PHE:CD2	1:A:648:VAL:HG21	2.53	0.43
1:A:772:VAL:CG2	2:A:1995:9TN:HAA1	2.44	0.43
1:A:457:THR:HG21	1:A:474:VAL:HG11	2.00	0.43
1:A:964:LEU:H	1:A:964:LEU:CD2	2.20	0.43
1:A:196:ASP:HA	1:A:197:PRO:HD3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:OD1	1:A:61:LEU:N	2.51	0.43
1:A:608:MET:HB2	1:A:608:MET:HE3	1.73	0.43
1:A:155:VAL:HG22	1:A:216:ALA:HA	1.99	0.43
1:A:501:ALA:O	1:A:502:LYS:HG2	2.18	0.43
1:A:558:THR:HG22	1:A:634:ALA:HB1	2.00	0.43
1:A:69:ALA:HB2	1:A:94:ILE:CG2	2.48	0.43
1:A:235:ILE:HG23	1:A:709:PRO:CG	2.48	0.43
1:A:882:HIS:O	1:A:882:HIS:CD2	2.72	0.43
1:A:390:ALA:CA	1:A:434:TYR:HD2	2.22	0.43
1:A:813:ASP:O	1:A:816:ILE:HG13	2.19	0.43
1:A:93:VAL:HA	1:A:96:LEU:HD11	2.01	0.43
1:A:166:LEU:HD11	1:A:222:ILE:HB	2.01	0.43
1:A:189:LYS:HD2	1:A:205:LYS:O	2.18	0.43
1:A:290:ARG:HD3	1:A:290:ARG:O	2.18	0.43
1:A:425:LEU:CD1	1:A:443:THR:HG23	2.48	0.43
1:A:69:ALA:HB2	1:A:94:ILE:HG21	2.01	0.43
1:A:538:THR:O	1:A:541:VAL:HG23	2.17	0.43
1:A:174:ARG:CZ	1:A:188:ILE:HD11	2.49	0.43
1:A:388:THR:HB	1:A:390:ALA:H	1.84	0.43
1:A:837:TYR:CB	2:A:1995:9TN:HAC2	2.49	0.42
1:A:209:PHE:O	1:A:212:THR:OG1	2.36	0.42
1:A:249:LEU:O	1:A:250:GLN:C	2.57	0.42
1:A:567:ARG:O	1:A:570:PRO:HD3	2.19	0.42
1:A:250:GLN:O	1:A:254:ASP:OD1	2.38	0.42
1:A:606:GLU:OE2	1:A:739:ASN:ND2	2.51	0.42
1:A:243:GLU:HA	1:A:243:GLU:OE1	2.20	0.42
1:A:51:GLU:O	1:A:55:GLU:HG3	2.20	0.42
1:A:715:GLU:C	1:A:716:ILE:HG13	2.39	0.42
1:A:178:SER:HB3	1:A:183:GLU:O	2.19	0.42
1:A:400:LYS:O	1:A:402:ILE:HG13	2.19	0.42
1:A:679:VAL:HG13	1:A:680:GLU:O	2.19	0.42
1:A:174:ARG:HB3	1:A:186:SER:HB2	2.02	0.42
1:A:760:PHE:HE1	1:A:761:ILE:HG13	1.83	0.42
1:A:530:VAL:O	1:A:533:THR:HG23	2.20	0.42
1:A:788:ILE:HB	1:A:791:GLN:NE2	2.35	0.42
1:A:176:ASP:O	1:A:212:THR:HG22	2.20	0.42
1:A:837:TYR:HB3	2:A:1995:9TN:HAC2	2.01	0.42
1:A:883:PHE:N	1:A:883:PHE:CD1	2.87	0.42
1:A:986:PHE:CD1	1:A:986:PHE:O	2.73	0.42
1:A:777:LEU:O	1:A:781:LEU:HG	2.20	0.42
1:A:833:LEU:O	1:A:836:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:TYR:HD1	1:A:840:ILE:HD12	1.85	0.42
1:A:339:VAL:O	1:A:342:LEU:HB3	2.20	0.42
1:A:791:GLN:HB3	1:A:901:LEU:HD12	2.02	0.42
1:A:345:THR:HG22	1:A:716:ILE:CD1	2.50	0.41
1:A:461:ASN:ND2	1:A:462:LEU:HD12	2.35	0.41
1:A:668:GLU:HA	1:A:668:GLU:OE1	2.20	0.41
1:A:788:ILE:HG23	1:A:789:PRO:HD2	2.01	0.41
1:A:209:PHE:CE1	1:A:231:GLU:HG3	2.55	0.41
2:A:1995:9TN:OAL	2:A:1995:9TN:CAG	2.68	0.41
1:A:368:ILE:HD13	1:A:410:LEU:HD23	2.01	0.41
1:A:872:HIS:H	1:A:872:HIS:CD2	2.38	0.41
1:A:917:SER:OG	1:A:920:GLN:HB2	2.20	0.41
1:A:939:LEU:O	1:A:943:LEU:HG	2.20	0.41
1:A:366:MET:HE2	1:A:382:PHE:CG	2.55	0.41
1:A:606:GLU:OE1	1:A:606:GLU:N	2.54	0.41
1:A:826:GLU:O	1:A:826:GLU:HG3	2.20	0.41
1:A:836:ARG:O	1:A:840:ILE:HG13	2.20	0.41
1:A:988:ALA:HB3	1:A:989:ARG:NH2	2.35	0.41
1:A:36:TYR:CG	1:A:147:PRO:HG2	2.55	0.41
1:A:382:PHE:CD1	1:A:382:PHE:N	2.88	0.41
1:A:857:MET:HA	1:A:864:GLY:CA	2.49	0.41
1:A:501:ALA:O	1:A:502:LYS:CB	2.67	0.41
1:A:347:VAL:HA	1:A:620:ARG:O	2.20	0.41
1:A:452:MET:O	1:A:453:ASN:C	2.58	0.41
1:A:64:ILE:HG13	1:A:64:ILE:H	1.53	0.41
1:A:638:ARG:CG	1:A:638:ARG:HH11	2.23	0.41
1:A:857:MET:SD	1:A:865:VAL:HG23	2.60	0.41
1:A:180:LEU:HA	1:A:180:LEU:HD12	1.85	0.41
1:A:508:VAL:HB	1:A:511:LYS:HE2	2.03	0.41
1:A:518:PRO:HB3	1:A:549:ILE:CD1	2.50	0.41
1:A:487:PHE:CZ	1:A:492:LYS:HA	2.56	0.41
1:A:653:TYR:OH	1:A:672:ARG:NH2	2.54	0.41
1:A:879:ASP:OD2	1:A:882:HIS:CD2	2.74	0.41
1:A:883:PHE:N	1:A:883:PHE:HD1	2.19	0.41
1:A:118:ALA:HB1	1:A:726:VAL:HG22	2.03	0.40
1:A:923:MET:HE2	1:A:924:ARG:HH11	1.85	0.40
1:A:668:GLU:O	1:A:671:ARG:HG2	2.21	0.40
1:A:771:GLU:O	1:A:775:ILE:HG12	2.22	0.40
1:A:50:TRP:CE3	1:A:50:TRP:HA	2.57	0.40
1:A:620:ARG:NH1	1:A:622:ILE:HD11	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	992/994 (100%)	935 (94%)	47 (5%)	10 (1%)	15	49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	866	THR
1	A	506	ALA
1	A	508	VAL
1	A	993	GLU
1	A	992	LEU
1	A	502	LYS
1	A	2	GLU
1	A	335	SER
1	A	865	VAL
1	A	42	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	840/840 (100%)	690 (82%)	150 (18%)	2	8

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER

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Mol	Chain	Res	Type
1	A	22	THR
1	A	25	THR
1	A	48	SER
1	A	53	VAL
1	A	59	ASP
1	A	60	LEU
1	A	61	LEU
1	A	62	VAL
1	A	64	ILE
1	A	65	LEU
1	A	79	GLU
1	A	82	GLU
1	A	85	ILE
1	A	86	THR
1	A	96	LEU
1	A	106	VAL
1	A	110	ARG
1	A	120	LYS
1	A	121	GLU
1	A	128	LYS
1	A	133	ASP
1	A	135	LYS
1	A	137	VAL
1	A	138	GLN
1	A	143	ARG
1	A	146	VAL
1	A	153	VAL
1	A	158	LYS
1	A	171	THR
1	A	177	GLN
1	A	179	ILE
1	A	180	LEU
1	A	185	VAL
1	A	187	VAL
1	A	205	LYS
1	A	212	THR
1	A	214	ILE
1	A	225	THR
1	A	228	VAL
1	A	242	THR
1	A	243	GLU
1	A	244	GLN

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Mol	Chain	Res	Type
1	A	245	ASP
1	A	247	THR
1	A	252	LYS
1	A	267	ILE
1	A	273	LEU
1	A	281	ASP
1	A	284	HIS
1	A	288	TRP
1	A	290	ARG
1	A	293	ILE
1	A	298	ILE
1	A	321	LEU
1	A	334	ARG
1	A	345	THR
1	A	348	ILE
1	A	353	THR
1	A	358	THR
1	A	370	ASP
1	A	379	LEU
1	A	383	SER
1	A	385	THR
1	A	387	SER
1	A	388	THR
1	A	396	LEU
1	A	399	ASP
1	A	415	THR
1	A	426	ASP
1	A	428	ASN
1	A	435	GLU
1	A	441	THR
1	A	446	THR
1	A	454	VAL
1	A	457	THR
1	A	458	GLU
1	A	466	GLU
1	A	477	GLN
1	A	480	LYS
1	A	484	THR
1	A	499	SER
1	A	502	LYS
1	A	503	SER
1	A	508	VAL

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Mol	Chain	Res	Type
1	A	514	VAL
1	A	521	VAL
1	A	529	ARG
1	A	530	VAL
1	A	533	THR
1	A	541	VAL
1	A	554	THR
1	A	556	ARG
1	A	576	MET
1	A	589	THR
1	A	594	VAL
1	A	596	VAL
1	A	608	MET
1	A	615	ARG
1	A	631	THR
1	A	635	ILE
1	A	638	ARG
1	A	648	VAL
1	A	651	ARG
1	A	663	LEU
1	A	671	ARG
1	A	693	SER
1	A	698	THR
1	A	701	THR
1	A	705	VAL
1	A	706	ASN
1	A	722	SER
1	A	732	GLU
1	A	733	MET
1	A	741	SER
1	A	760	PHE
1	A	778	THR
1	A	788	ILE
1	A	793	LEU
1	A	795	VAL
1	A	797	LEU
1	A	828	LEU
1	A	833	LEU
1	A	838	MET
1	A	848	THR
1	A	857	MET
1	A	858	TYR

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Mol	Chain	Res	Type
1	A	860	GLU
1	A	867	TYR
1	A	868	HIS
1	A	869	GLN
1	A	878	GLU
1	A	880	HIS
1	A	886	LEU
1	A	889	GLU
1	A	892	GLU
1	A	898	THR
1	A	903	VAL
1	A	906	THR
1	A	908	GLU
1	A	916	LEU
1	A	923	MET
1	A	925	MET
1	A	946	LEU
1	A	962	LEU
1	A	964	LEU
1	A	971	LEU
1	A	974	SER
1	A	975	LEU
1	A	989	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	213	ASN
1	A	398	ASN
1	A	406	GLN
1	A	472	ASN
1	A	683	HIS
1	A	759	GLN
1	A	872	HIS
1	A	882	HIS
1	A	944	HIS
1	A	966	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	9TN	A	1995	1	39,43,43	2.20	9 (23%)	42,66,66	1.67	6 (14%)

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	9TN	A	1995	1	-	10/26/92/92	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1995	9TN	OAV-CBF	8.84	1.48	1.35
2	A	1995	9TN	OAV-CBH	6.72	1.57	1.46
2	A	1995	9TN	CAW-CBM	-2.73	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1995	9TN	CBO-CBJ	2.70	1.57	1.53
2	A	1995	9TN	OAY-CBM	-2.61	1.43	1.48
2	A	1995	9TN	CBN-CBI	2.58	1.58	1.54
2	A	1995	9TN	OAZ-CBL	-2.52	1.40	1.44
2	A	1995	9TN	OAX-CBC	2.21	1.40	1.34
2	A	1995	9TN	OAN-CBO	-2.15	1.39	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1995	9TN	OAY-CBA-OAH	-5.03	114.37	123.61
2	A	1995	9TN	OAY-CBA-CAC	4.38	118.65	110.68
2	A	1995	9TN	OAK-CBF-CBK	-4.05	124.21	128.28
2	A	1995	9TN	OAV-CBF-OAK	3.17	125.83	121.62
2	A	1995	9TN	CAT-CAU-CBC	-2.83	103.34	113.62
2	A	1995	9TN	CBL-OAZ-CBD	2.05	121.44	117.07

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1995	9TN	CAA-CAO-CBB-CBD
2	A	1995	9TN	CAC-CBA-OAY-CBM
2	A	1995	9TN	CAG-CBM-OAY-CBA
2	A	1995	9TN	CAW-CBM-OAY-CBA
2	A	1995	9TN	CBN-CBM-OAY-CBA
2	A	1995	9TN	CBE-CBL-OAZ-CBD
2	A	1995	9TN	OAH-CBA-OAY-CBM
2	A	1995	9TN	CAU-CBC-OAX-CBI
2	A	1995	9TN	OAI-CBC-OAX-CBI
2	A	1995	9TN	CAP-CAQ-CAR-CAS

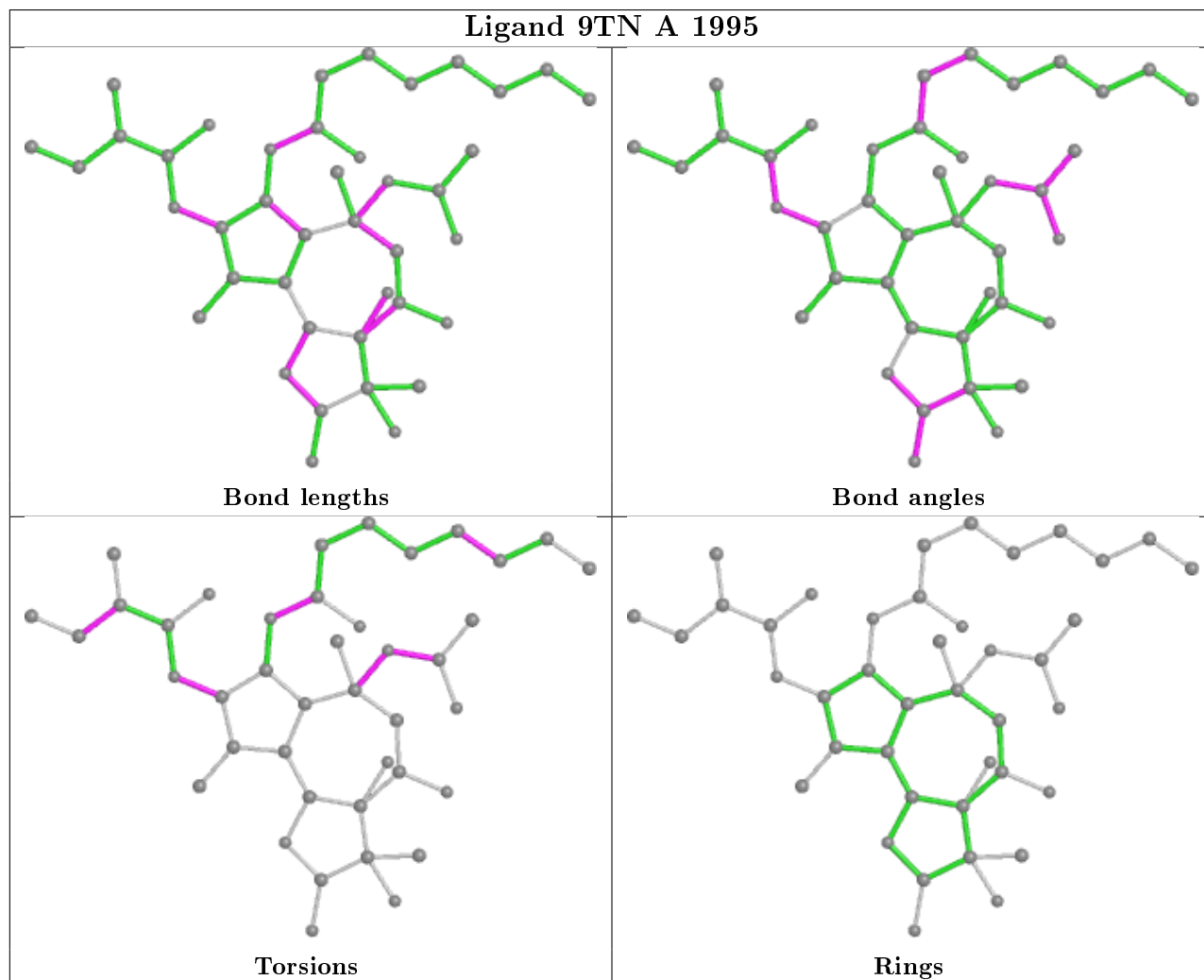
There are no ring outliers.

1 monomer is involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1995	9TN	21	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 [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	994/994 (100%)	-0.15	9 (0%) 84 69	67, 89, 158, 319	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	GLY	3.9
1	A	184	SER	3.0
1	A	45	GLU	3.0
1	A	46	GLY	2.9
1	A	80	GLU	2.9
1	A	106	VAL	2.8
1	A	284	HIS	2.7
1	A	1	MET	2.5
1	A	84	THR	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](#)

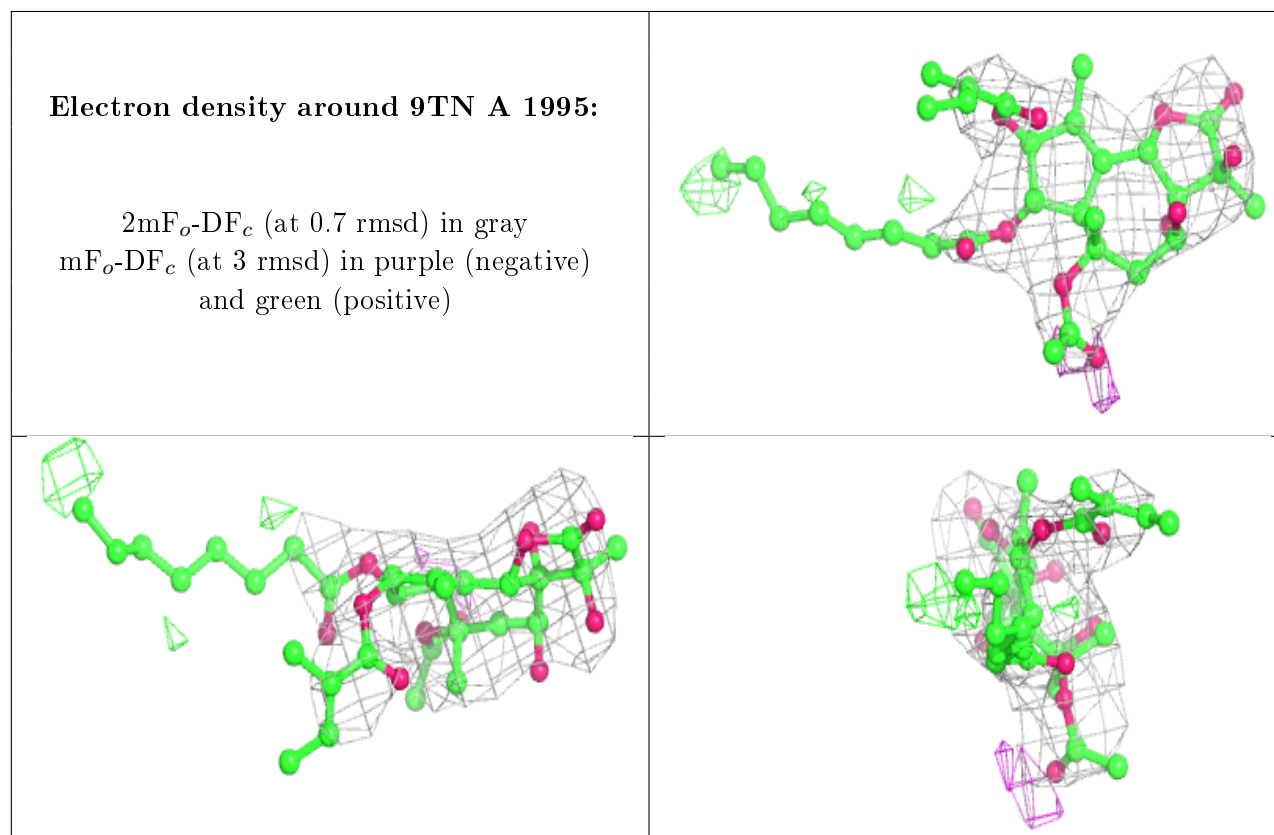
There are no carbohydrates in this entry.

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
4	MG	A	1997	1/1	0.53	0.45	82,82,82,82	0
3	K	A	1996	1/1	0.59	0.61	166,166,166,166	0
2	9TN	A	1995	41/41	0.88	0.39	92,114,135,164	41

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.