



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 01:06 AM UTC

PDB ID : 5A3S / pdb_00005a3s
Title : Crystal structure of the (SR) Calcium ATPase E2-vanadate complex bound to thapsigargin and TNP-ATP
Authors : Clausen, J.D.; Bublitz, M.; Arnou, B.; Olesen, C.; Andersen, J.P.; Moller, J.V.; Nissen, P.
Deposited on : 2015-06-03
Resolution : 3.30 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

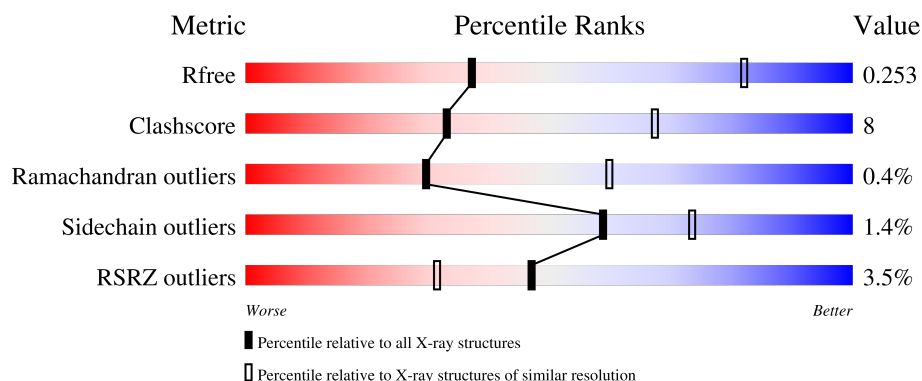
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	995	4% 83% 16% .
1	B	995	3% 82% 17% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15554 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.

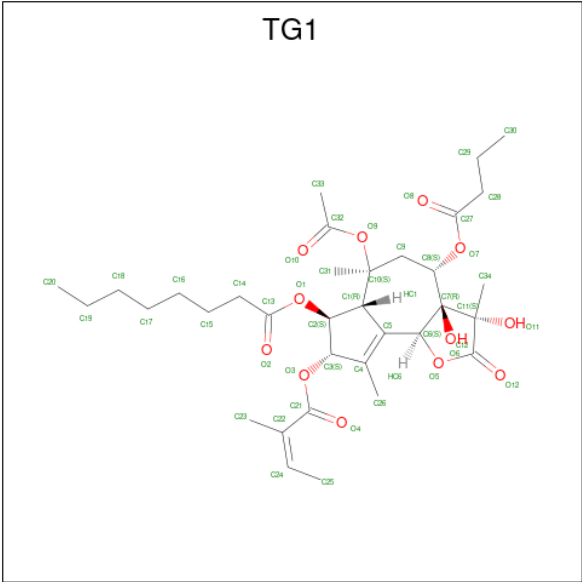
- Molecule 1 is a protein called SARCOPLASMIC RETICULUM CALCIUM ATPASE 1 MOLECULE SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	995	Total	C	N	O	S	0	0	0
			7672	4877	1287	1451	57			
1	B	995	Total	C	N	O	S	0	0	0
			7674	4878	1287	1452	57			

There are 2 discrepancies between the modelled and reference sequences:

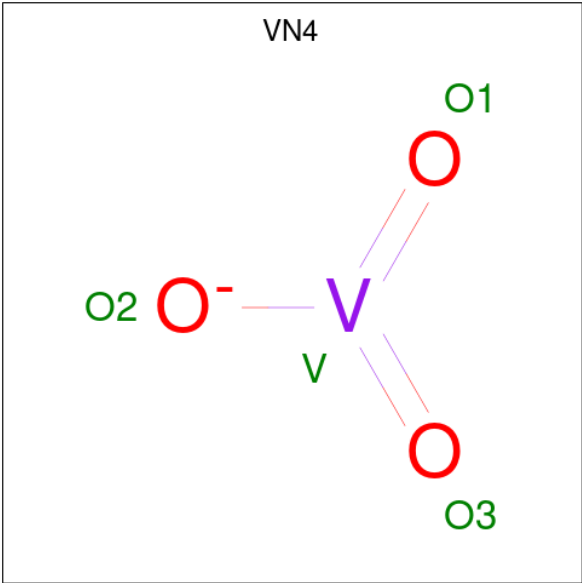
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP PO4191
B	0	ACE	-	acetylation	UNP PO4191

- Molecule 2 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BALPHA]]-6-(ACETYLOXY)-2,3,-3A,4,5,6,6A,7,8,9B-DECAHYDRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (CCD ID: TG1) (formula: C₃₄H₅₀O₁₂).



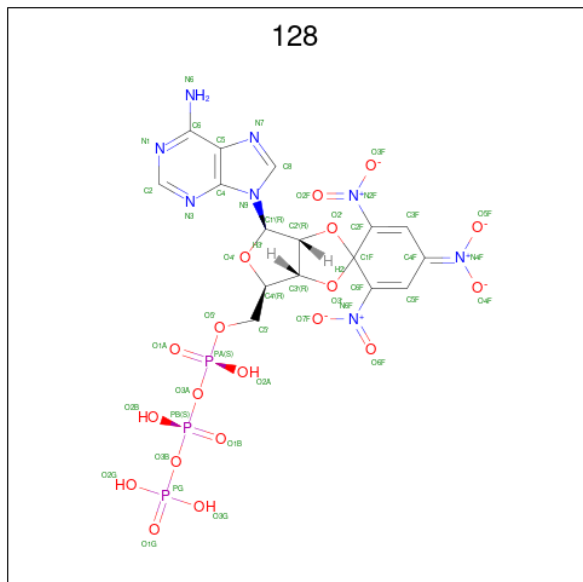
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			46	34	12		
2	B	1	Total	C	O	0	0
			46	34	12		

- Molecule 3 is oxido(dioxo)vanadium (CCD ID: VN4) (formula: O₃V).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			4	3	1		
3	B	1	Total	O	V	0	0
			4	3	1		

- Molecule 4 is SPIRO(2,4,6-TRINITROBENZENE[1,2A]-2O',3O'-METHYLENE-ADENIN E-TRIPHOSPHATE (CCD ID: 128) (formula: $C_{16}H_{16}N_8O_{19}P_3$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Cl 1	0	0
7	B	1	Total 1	Cl 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total 4	O 4	0	0
8	B	4	Total 4	O 4	0	0

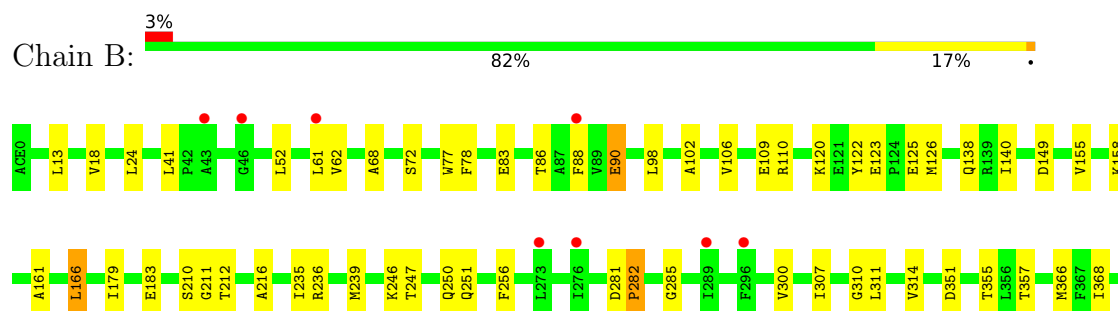
3 Residue-property plots

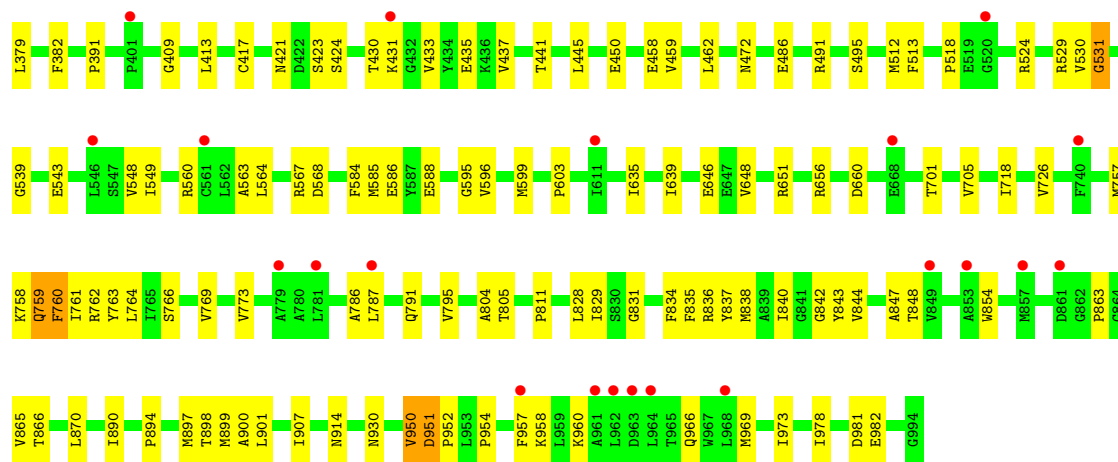
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SARCOPLASMIC RETICULUM CALCIUM ATPASE 1 MOLECULE SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1



- Molecule 1: SARCOPLASMIC RETICULUM CALCIUM ATPASE 1 MOLECULE SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.56Å 93.78Å 135.69Å 90.00° 107.26° 90.00°	Depositor
Resolution (Å)	78.91 – 3.30 78.91 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (78.91-3.30) 99.8 (78.91-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.210 , 0.245 0.214 , 0.253	Depositor DCC
R_{free} test set	783 reflections (1.65%)	wwPDB-VP
Wilson B-factor (Å ²)	97.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 85.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for l,k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15554	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: VN4, MG, 128, TG1, K, CL, ACE

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	0.13	0/7810	0.33	0/10588
1	B	0.14	0/7813	0.32	0/10594
All	All	0.13	0/15623	0.33	0/21182

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

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	7672	0	7765	119	0
1	B	7674	0	7767	112	0
2	A	46	0	50	15	0
2	B	46	0	50	13	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	46	0	13	1	0
4	B	46	0	13	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	4	0	0	0	0
8	B	4	0	0	1	0
All	All	15554	0	15658	243	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 8.

All (243) 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:848:THR:HG23	1:B:900:ALA:HB1	1.58	0.86
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.60	0.83
1:A:82:GLU:CA	1:A:83:GLU:N	2.43	0.82
1:A:260:LEU:HD13	2:A:1000:TG1:H232	1.61	0.80
2:A:1000:TG1:H313	2:A:1000:TG1:H332	1.63	0.80
1:B:769:VAL:HG21	2:B:1000:TG1:H333	1.62	0.80
1:A:894:PRO:HB3	1:A:959:LEU:H	1.50	0.76
1:B:646:GLU:OE2	1:B:651:ARG:NH1	2.19	0.74
1:B:786:ALA:HA	1:B:897:MET:HA	1.70	0.73
1:A:790:VAL:HB	1:A:957:PHE:HE1	1.54	0.72
1:A:848:THR:HG23	1:A:900:ALA:HB1	1.71	0.72
1:A:947:ILE:HD13	1:A:953:LEU:HD13	1.70	0.71
1:A:829:ILE:HG21	2:A:1000:TG1:H333	1.72	0.70
1:B:811:PRO:HD3	1:B:930:ASN:HD21	1.57	0.69
1:A:23:GLY:HA3	1:A:131:ARG:HA	1.74	0.69
1:A:85:ILE:O	1:A:88:PHE:HB3	1.91	0.69
1:A:829:ILE:HA	1:A:833:LEU:HD23	1.75	0.68
1:A:773:VAL:HG11	1:A:842:GLY:HA2	1.77	0.66
1:A:773:VAL:HG22	2:A:1000:TG1:H202	1.76	0.66
1:A:894:PRO:HA	1:A:958:LYS:HD2	1.75	0.66
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.77	0.66
1:A:651:ARG:NH2	1:A:674:CYS:SG	2.69	0.66
1:A:769:VAL:HA	2:A:1000:TG1:H251	1.79	0.65
1:A:897:MET:HB2	1:A:958:LYS:HG3	1.81	0.63
1:B:829:ILE:HD12	2:B:1000:TG1:HC91	1.80	0.62
1:B:835:PHE:HA	1:B:838:MET:HB3	1.81	0.62
1:B:125:GLU:HG3	1:B:126:MET:HG2	1.81	0.62
1:A:790:VAL:HB	1:A:957:PHE:CE1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:SER:HB3	1:A:22:THR:HG22	1.82	0.62
2:B:1000:TG1:O10	2:B:1000:TG1:HC92	1.99	0.62
1:B:866:THR:CG2	1:B:870:LEU:HB2	2.29	0.61
1:A:76:ALA:HB1	1:A:88:PHE:CD2	2.35	0.61
1:A:786:ALA:HA	1:A:897:MET:HG2	1.83	0.61
1:A:155:VAL:HG12	1:A:216:ALA:HA	1.81	0.61
1:A:665:GLU:O	1:A:669:ALA:HB2	2.01	0.60
1:B:648:VAL:HG13	1:B:651:ARG:HB2	1.83	0.60
1:A:90:GLU:HG3	1:A:91:PRO:HD3	1.83	0.60
1:B:368:ILE:HG21	1:B:409:GLY:HA3	1.83	0.60
1:A:603:PRO:HB3	1:A:639:ILE:HD11	1.84	0.59
1:A:836:ARG:NH1	1:A:981:ASP:OD1	2.35	0.59
1:A:834:PHE:CZ	2:A:1000:TG1:H142	2.38	0.58
1:B:109:GLU:HG2	1:B:110:ARG:H	1.69	0.58
1:A:91:PRO:O	1:A:95:LEU:N	2.34	0.57
1:B:183:GLU:OE2	8:B:2002:HOH:O	2.16	0.57
1:B:155:VAL:HG12	1:B:216:ALA:HA	1.86	0.57
1:A:948:LEU:HD13	1:A:960:LYS:HG3	1.86	0.57
1:B:424:SER:O	1:B:437:VAL:HB	2.05	0.57
1:B:486:GLU:O	1:B:491:ARG:NH2	2.36	0.57
1:B:529:ARG:NH2	1:B:568:ASP:OD1	2.37	0.57
1:A:459:VAL:HA	1:A:462:LEU:HG	1.87	0.56
2:B:1000:TG1:C24	2:B:1000:TG1:H311	2.36	0.56
1:A:757:MET:HA	1:A:760:PHE:CE2	2.41	0.56
1:B:763:TYR:O	1:B:766:SER:OG	2.23	0.56
1:B:705:VAL:HG22	1:B:726:VAL:HG11	1.88	0.55
1:A:837:TYR:HA	1:A:840:ILE:HG22	1.89	0.55
2:B:1000:TG1:H262	2:B:1000:TG1:H233	1.88	0.55
1:A:529:ARG:NH2	1:A:568:ASP:OD1	2.40	0.55
1:A:758:LYS:HG2	1:A:828:LEU:HD23	1.89	0.55
1:B:491:ARG:NH1	1:B:588:GLU:OE2	2.40	0.55
1:A:512:MET:HB2	1:A:567:ARG:HB3	1.89	0.54
1:B:512:MET:HB2	1:B:567:ARG:HB3	1.88	0.54
1:A:611:ILE:HG13	1:A:639:ILE:HG22	1.90	0.54
1:B:41:LEU:HB3	1:B:236:ARG:HD2	1.90	0.54
1:A:301:ALA:HB2	1:A:789:PRO:HG3	1.88	0.54
1:A:762:ARG:NH2	1:A:828:LEU:O	2.39	0.54
1:A:828:LEU:HD13	2:A:1000:TG1:H303	1.89	0.54
1:A:107:TRP:HA	1:A:110:ARG:HG2	1.89	0.53
1:B:757:MET:O	1:B:758:LYS:C	2.52	0.53
1:B:246:LYS:HE2	1:B:251:GLN:HG2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:VAL:HG11	1:B:842:GLY:HA2	1.89	0.53
1:B:914:ASN:HD21	1:B:978:ILE:HA	1.73	0.53
1:B:524:ARG:HH11	1:B:585:MET:HE3	1.74	0.53
1:B:837:TYR:HA	1:B:840:ILE:HG22	1.89	0.53
1:A:560:ARG:HG3	4:A:1002:128:C2	2.39	0.53
1:B:357:THR:HA	1:B:603:PRO:HA	1.91	0.53
1:B:256:PHE:CE1	2:B:1000:TG1:H24	2.45	0.52
1:B:701:THR:HA	1:B:718:ILE:O	2.09	0.52
1:A:829:ILE:HG12	2:A:1000:TG1:HC8	1.92	0.52
1:A:59:ASP:HB3	1:A:62:VAL:HG12	1.92	0.52
1:A:943:LEU:O	1:A:947:ILE:HG12	2.11	0.51
1:A:72:SER:HB3	1:A:91:PRO:HB3	1.91	0.51
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.46	0.51
1:A:834:PHE:HZ	2:A:1000:TG1:H142	1.74	0.51
1:A:179:ILE:HD13	1:A:212:THR:HA	1.91	0.51
1:A:68:ALA:HB1	1:A:300:VAL:HG23	1.93	0.51
1:A:120:LYS:O	1:A:123:GLU:HG2	2.10	0.51
1:B:256:PHE:HE1	2:B:1000:TG1:H24	1.77	0.50
1:B:656:ARG:NH1	1:B:660:ASP:OD1	2.45	0.50
1:B:836:ARG:NH1	1:B:981:ASP:OD1	2.45	0.50
1:B:68:ALA:HB1	1:B:300:VAL:HG23	1.93	0.50
1:B:844:VAL:HB	1:B:907:ILE:HG21	1.93	0.50
1:A:278:HIS:ND1	1:A:295:TYR:OH	2.35	0.50
1:B:950:VAL:HG22	1:B:951:ASP:H	1.76	0.49
2:B:1000:TG1:H233	2:B:1000:TG1:C4	2.43	0.49
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.94	0.49
1:B:247:THR:O	1:B:250:GLN:HG2	2.13	0.49
1:B:757:MET:O	1:B:760:PHE:HD1	1.95	0.49
1:B:431:LYS:HG3	1:B:435:GLU:OE2	2.12	0.49
2:B:1000:TG1:H332	2:B:1000:TG1:H142	1.93	0.49
1:B:281:ASP:HB2	1:B:282:PRO:HD3	1.95	0.49
1:A:795:VAL:HA	1:A:799:THR:HG22	1.95	0.48
2:A:1000:TG1:H333	2:A:1000:TG1:HC91	1.94	0.48
1:B:866:THR:HG23	1:B:870:LEU:HB2	1.94	0.48
1:B:950:VAL:HG13	1:B:954:PRO:HD3	1.95	0.48
1:B:847:ALA:HB2	1:B:973:ILE:HG21	1.95	0.48
1:B:901:LEU:HD23	1:B:957:PHE:CZ	2.48	0.48
1:B:539:GLY:O	1:B:543:GLU:HG2	2.13	0.48
1:B:898:THR:HG21	1:B:960:LYS:HB3	1.96	0.48
1:A:844:VAL:HB	1:A:907:ILE:HG21	1.95	0.48
1:A:907:ILE:O	1:A:911:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:THR:HG23	1:A:333:VAL:HB	1.95	0.47
1:A:436:LYS:HB2	1:A:443:THR:HG21	1.96	0.47
2:B:1000:TG1:H233	2:B:1000:TG1:C26	2.43	0.47
1:A:94:ILE:HG12	1:A:793:LEU:HD21	1.95	0.47
1:B:762:ARG:NH2	1:B:828:LEU:O	2.46	0.47
1:A:357:THR:HA	1:A:603:PRO:HA	1.96	0.47
1:A:829:ILE:HG12	2:A:1000:TG1:C9	2.45	0.47
1:B:72:SER:HB3	1:B:90:GLU:OE1	2.14	0.47
1:B:179:ILE:HD13	1:B:212:THR:HA	1.96	0.47
1:B:282:PRO:HB2	1:B:285:GLY:HA3	1.97	0.47
1:B:795:VAL:HG21	1:B:901:LEU:HD11	1.96	0.47
1:A:950:VAL:HG12	1:A:951:ASP:N	2.29	0.47
1:A:950:VAL:O	1:A:954:PRO:HG2	2.14	0.47
1:A:84:THR:OG1	1:A:87:ALA:HB3	2.14	0.46
1:B:757:MET:O	1:B:760:PHE:CD1	2.69	0.46
1:A:611:ILE:HG13	1:A:639:ILE:CG2	2.46	0.46
1:A:837:TYR:HD2	2:A:1000:TG1:H331	1.81	0.46
1:B:391:PRO:HB3	1:B:450:GLU:HB3	1.96	0.46
1:A:950:VAL:CG1	1:A:952:PRO:HD2	2.39	0.46
1:B:366:MET:HG3	1:B:382:PHE:HB2	1.96	0.46
1:A:424:SER:O	1:A:437:VAL:HB	2.16	0.46
1:B:957:PHE:O	1:B:958:LYS:HB2	2.15	0.46
1:A:609:GLY:O	1:A:613:LEU:HG	2.16	0.46
1:A:951:ASP:HB3	1:A:952:PRO:HD3	1.98	0.46
1:B:61:LEU:HB2	1:B:307:ILE:HD12	1.96	0.46
1:B:459:VAL:HA	1:B:462:LEU:HG	1.97	0.46
1:A:78:PHE:CE2	1:A:293:ILE:HG21	2.50	0.46
1:B:758:LYS:HG2	1:B:828:LEU:HD22	1.97	0.46
1:A:76:ALA:HB1	1:A:88:PHE:HD2	1.78	0.46
1:A:512:MET:O	1:A:566:THR:HA	2.16	0.45
1:A:352:LYS:HD2	1:A:635:ILE:HG13	1.97	0.45
1:A:868:HIS:ND1	1:A:869:GLN:HG3	2.32	0.45
2:A:1000:TG1:HC91	2:A:1000:TG1:C33	2.46	0.45
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.98	0.45
1:A:312:PRO:HA	1:A:315:ILE:HG12	1.99	0.45
1:A:441:THR:HG23	1:A:599:MET:HE1	1.99	0.45
1:B:978:ILE:O	1:B:982:GLU:HB2	2.16	0.45
1:A:379:LEU:HD12	1:A:548:VAL:HG21	1.99	0.45
1:A:985:LYS:HG2	1:A:989:ARG:HH12	1.82	0.45
1:B:368:ILE:HD13	1:B:595:GLY:HA3	1.99	0.45
1:A:78:PHE:CG	1:A:80:GLU:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PRO:HD2	1:A:341:THR:HG22	1.99	0.44
1:A:624:ILE:HG22	1:A:684:LYS:HE2	1.98	0.44
1:B:413:LEU:HD12	1:B:564:LEU:HD22	2.00	0.44
1:B:635:ILE:O	1:B:639:ILE:HG12	2.17	0.44
1:B:829:ILE:O	2:B:1000:TG1:H343	2.17	0.44
2:B:1000:TG1:H332	2:B:1000:TG1:C14	2.47	0.44
1:A:599:MET:HE3	1:A:599:MET:HB2	1.86	0.44
1:B:441:THR:HG23	1:B:599:MET:HE1	1.99	0.44
2:B:1000:TG1:H261	2:B:1000:TG1:O5	2.18	0.44
1:A:618:GLY:HA3	1:A:821:PRO:HD3	1.99	0.44
1:A:78:PHE:CZ	1:A:293:ILE:HG13	2.53	0.44
1:A:843:TYR:CE2	1:A:973:ILE:HG23	2.52	0.44
1:B:314:VAL:HG12	1:B:760:PHE:CE2	2.52	0.44
1:B:843:TYR:CE2	1:B:973:ILE:HG23	2.53	0.44
1:A:106:VAL:O	1:A:110:ARG:HG2	2.17	0.44
1:B:560:ARG:HG3	4:B:1002:128:N1	2.33	0.44
1:A:198:ARG:NH2	1:A:660:ASP:OD1	2.51	0.43
1:A:275:ASN:HB2	1:A:278:HIS:HB2	2.00	0.43
1:A:760:PHE:HB2	1:A:804:ALA:HB1	2.00	0.43
1:B:760:PHE:HD1	1:B:761:ILE:N	2.16	0.43
1:A:391:PRO:HB3	1:A:450:GLU:HB3	1.99	0.43
1:B:311:LEU:HD13	1:B:764:LEU:HD12	2.01	0.43
1:B:379:LEU:HD12	1:B:548:VAL:HG21	1.99	0.43
1:B:897:MET:HB2	1:B:958:LYS:HE3	2.00	0.43
1:B:899:MET:HE1	1:B:966:GLN:O	2.17	0.43
1:A:78:PHE:HE2	1:A:293:ILE:HG21	1.84	0.43
1:A:753:ILE:O	1:A:757:MET:HG3	2.18	0.43
1:B:894:PRO:HA	1:B:958:LYS:HD2	2.01	0.43
1:A:502:LYS:HG3	1:A:503:SER:H	1.83	0.43
1:B:417:CYS:HB3	1:B:445:LEU:HB3	1.99	0.43
1:A:648:VAL:HG13	1:A:651:ARG:HB2	2.01	0.43
1:B:759:GLN:OE1	1:B:762:ARG:NH1	2.43	0.43
1:A:90:GLU:O	1:A:94:ILE:HG13	2.18	0.42
1:A:347:VAL:HG11	1:A:691:LEU:HD13	2.01	0.42
1:A:883:PHE:HB3	1:A:886:LEU:HD11	2.01	0.42
1:B:13:LEU:HD21	1:B:166:LEU:HD21	2.01	0.42
1:B:62:VAL:HG23	1:B:98:LEU:HD22	2.01	0.42
1:B:122:TYR:O	1:B:211:GLY:HA2	2.19	0.42
1:B:235:ILE:O	1:B:239:MET:HG3	2.19	0.42
1:B:549:ILE:HD11	1:B:596:VAL:HG21	1.99	0.42
1:A:51:GLU:HA	1:A:54:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ASP:OD1	1:A:427:PHE:N	2.52	0.42
1:A:161:ALA:HA	1:A:210:SER:HB2	2.01	0.42
1:A:511:LYS:CD	1:A:568:ASP:HA	2.50	0.42
1:B:310:GLY:O	1:B:314:VAL:HG23	2.20	0.42
1:A:199:ALA:HB1	1:A:203:ASP:HB2	2.01	0.42
1:B:83:GLU:HB2	1:B:86:THR:HB	2.02	0.42
1:A:611:ILE:HD12	1:A:621:VAL:HG11	2.02	0.42
1:B:52:LEU:HD23	1:B:52:LEU:O	2.20	0.42
1:B:760:PHE:CD1	1:B:761:ILE:N	2.88	0.42
1:B:760:PHE:O	1:B:763:TYR:HB3	2.20	0.42
1:B:760:PHE:HD2	1:B:804:ALA:O	2.01	0.42
1:B:865:VAL:O	1:B:866:THR:HB	2.20	0.42
1:A:122:TYR:O	1:A:211:GLY:HA2	2.20	0.42
1:A:950:VAL:HG12	1:A:951:ASP:H	1.85	0.42
2:A:1000:TG1:H203	2:A:1000:TG1:H172	1.77	0.42
1:B:495:SER:HA	1:B:513:PHE:O	2.19	0.42
1:B:950:VAL:CG1	1:B:954:PRO:HD3	2.50	0.42
1:A:93:VAL:HA	1:A:96:LEU:HG	2.02	0.42
1:A:389:TYR:HB3	1:A:425:LEU:HD11	2.01	0.41
1:A:88:PHE:O	1:A:91:PRO:HD2	2.20	0.41
1:B:138:GLN:HB3	1:B:140:ILE:HG23	2.02	0.41
1:A:90:GLU:OE1	1:A:789:PRO:HB2	2.18	0.41
1:B:834:PHE:O	1:B:838:MET:HB2	2.20	0.41
1:A:367:PHE:CD1	1:A:379:LEU:HD13	2.56	0.41
1:B:102:ALA:O	1:B:106:VAL:HG23	2.21	0.41
1:A:713:LYS:HD2	1:A:713:LYS:HA	1.88	0.41
1:A:829:ILE:CG1	2:A:1000:TG1:HC8	2.50	0.41
1:B:491:ARG:NH1	1:B:584:PHE:HB3	2.35	0.41
1:B:158:LYS:HB2	1:B:158:LYS:HE3	1.92	0.41
1:B:314:VAL:HG13	1:B:805:THR:OG1	2.21	0.41
1:B:530:VAL:O	1:B:531:GLY:C	2.63	0.41
1:B:854:TRP:CD1	1:B:969:MET:HE2	2.55	0.41
1:A:202:GLN:N	1:A:202:GLN:OE1	2.53	0.41
1:A:321:LEU:HD13	1:A:809:PHE:HZ	1.85	0.41
1:A:420:CYS:HA	1:A:496:VAL:HG21	2.03	0.41
1:B:24:LEU:HG	1:B:149:ASP:HA	2.03	0.41
1:B:120:LYS:O	1:B:123:GLU:HG2	2.21	0.41
1:B:787:LEU:HD21	1:B:848:THR:HG21	2.03	0.41
1:B:907:ILE:HD11	1:B:973:ILE:HG22	2.03	0.41
1:A:443:THR:O	1:A:447:THR:HG22	2.21	0.41
1:B:351:ASP:O	1:B:355:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:TRP:HD1	1:B:78:PHE:CE1	2.38	0.40
1:B:314:VAL:HG12	1:B:760:PHE:HE2	1.85	0.40
1:B:791:GLN:HG2	1:B:957:PHE:CE1	2.56	0.40
1:A:482:GLU:OE2	1:A:573:ARG:NH1	2.54	0.40
1:B:423:SER:HB2	1:B:437:VAL:O	2.20	0.40
1:B:431:LYS:HB3	1:B:433:VAL:HG12	2.03	0.40
1:B:863:PRO:HG2	1:B:890:ILE:HG21	2.02	0.40
1:B:518:PRO:HA	1:B:563:ALA:HB2	2.03	0.40
1:B:161:ALA:HA	1:B:210:SER:HB2	2.04	0.40
1:B:958:LYS:HB2	1:B:958:LYS:HE2	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	991/995 (100%)	925 (93%)	66 (7%)	0	100	100
1	B	993/995 (100%)	931 (94%)	55 (6%)	7 (1%)	18	49
All	All	1984/1990 (100%)	1856 (94%)	121 (6%)	7 (0%)	30	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	531	GLY
1	B	831	GLY
1	B	950	VAL
1	B	282	PRO
1	B	458	GLU
1	B	951	ASP
1	B	952	PRO

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	840/840 (100%)	826 (98%)	14 (2%)	53	71
1	B	840/840 (100%)	830 (99%)	10 (1%)	63	75
All	All	1680/1680 (100%)	1656 (99%)	24 (1%)	59	73

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	PHE
1	A	79	GLU
1	A	80	GLU
1	A	82	GLU
1	A	88	PHE
1	A	298	ILE
1	A	462	LEU
1	A	679	VAL
1	A	788	ILE
1	A	790	VAL
1	A	799	THR
1	A	829	ILE
1	A	882	HIS
1	A	886	LEU
1	B	18	VAL
1	B	88	PHE
1	B	90	GLU
1	B	166	LEU
1	B	421	ASN
1	B	430	THR
1	B	472	ASN
1	B	586	GLU
1	B	759	GLN
1	B	760	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	330	ASN
1	A	510	ASN
1	A	920	GLN
1	B	250	GLN
1	B	330	ASN
1	B	768	ASN
1	B	810	ASN
1	B	930	ASN

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](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	TG1	B	1000	-	44,48,48	0.88	1 (2%)	47,72,72	0.91	1 (2%)
3	VN4	B	1001	8,5,1	0,3,3	-	-	-		
3	VN4	A	1001	8,5,1	0,3,3	-	-	-		
4	128	B	1002	5	42,50,50	1.52	7 (16%)	55,80,80	1.22	8 (14%)
2	TG1	A	1000	-	44,48,48	0.93	1 (2%)	47,72,72	1.35	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	128	A	1002	5	42,50,50	1.51	7 (16%)	55,80,80	1.14	3 (5%)

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
4	128	B	1002	5	-	5/26/80/80	0/5/5/5
2	TG1	A	1000	-	-	19/33/99/99	0/3/3/3
4	128	A	1002	5	-	5/26/80/80	0/5/5/5
2	TG1	B	1000	-	-	10/33/99/99	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1002	128	C5F-C6F	4.93	1.51	1.37
4	A	1002	128	C5F-C6F	4.81	1.50	1.37
4	A	1002	128	PA-O3A	3.81	1.63	1.59
4	B	1002	128	PA-O3A	3.75	1.63	1.59
4	B	1002	128	PG-O1G	3.16	1.60	1.50
4	A	1002	128	PG-O1G	3.14	1.60	1.50
4	B	1002	128	PG-O3G	-2.43	1.45	1.54
4	A	1002	128	PG-O3G	-2.38	1.46	1.54
4	B	1002	128	PA-O1A	2.36	1.59	1.50
4	A	1002	128	PA-O1A	2.35	1.59	1.50
4	A	1002	128	C5F-C4F	-2.27	1.32	1.40
4	B	1002	128	C5F-C4F	-2.19	1.32	1.40
4	A	1002	128	O7F-N6F	-2.10	1.21	1.35
4	B	1002	128	O7F-N6F	-2.07	1.21	1.35
2	B	1000	TG1	C1-C5	2.02	1.54	1.51
2	A	1000	TG1	C1-C5	2.01	1.54	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	TG1	C10-O9-C32	4.22	131.25	121.36
4	B	1002	128	O3G-PG-O3B	3.42	116.12	104.64
4	A	1002	128	O3G-PG-O3B	3.27	115.62	104.64
4	A	1002	128	O2B-PB-O3A	3.13	115.74	107.27
4	B	1002	128	O2'-C1F-C2F	-3.12	106.20	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1002	128	O2B-PB-O3A	3.02	115.42	107.27
2	A	1000	TG1	C11-C7-C8	2.76	118.12	114.44
2	B	1000	TG1	C10-O9-C32	2.47	127.15	121.36
4	B	1002	128	O2'-C1F-C6F	2.46	113.83	110.47
4	A	1002	128	O3'-C1F-C6F	-2.44	107.13	110.47
2	A	1000	TG1	O7-C8-C9	2.40	110.92	106.63
2	A	1000	TG1	O1-C13-O2	-2.24	118.47	123.70
2	A	1000	TG1	O1-C13-C14	2.19	116.21	111.48
4	B	1002	128	O3'-C1F-C6F	-2.15	107.53	110.47
4	B	1002	128	C5'-C4'-C3'	2.13	121.47	114.38
4	B	1002	128	O3A-PB-O1B	-2.03	104.59	110.70
4	B	1002	128	O3'-C3'-C2'	2.01	106.83	103.63

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	TG1	O3-C21-C22-C23
2	A	1000	TG1	O3-C21-C22-C24
2	A	1000	TG1	O10-C32-O9-C10
2	A	1000	TG1	C33-C32-O9-C10
2	A	1000	TG1	O8-C27-O7-C8
2	A	1000	TG1	C28-C27-O7-C8
2	B	1000	TG1	C9-C10-O9-C32
2	B	1000	TG1	C1-C10-O9-C32
2	B	1000	TG1	C14-C13-O1-C2
2	B	1000	TG1	C2-C3-O3-C21
2	B	1000	TG1	C22-C21-O3-C3
4	A	1002	128	C5'-O5'-PA-O2A
4	A	1002	128	O4'-C4'-C5'-O5'
4	B	1002	128	C5'-O5'-PA-O1A
4	B	1002	128	C5'-O5'-PA-O2A
4	B	1002	128	C5'-O5'-PA-O3A
2	B	1000	TG1	O2-C13-O1-C2
4	A	1002	128	C3'-C4'-C5'-O5'
2	B	1000	TG1	O4-C21-O3-C3
2	A	1000	TG1	C13-C14-C15-C16
4	B	1002	128	O4'-C4'-C5'-O5'
4	B	1002	128	C3'-C4'-C5'-O5'
2	A	1000	TG1	O4-C21-C22-C23
2	B	1000	TG1	C14-C15-C16-C17
2	A	1000	TG1	C17-C18-C19-C20

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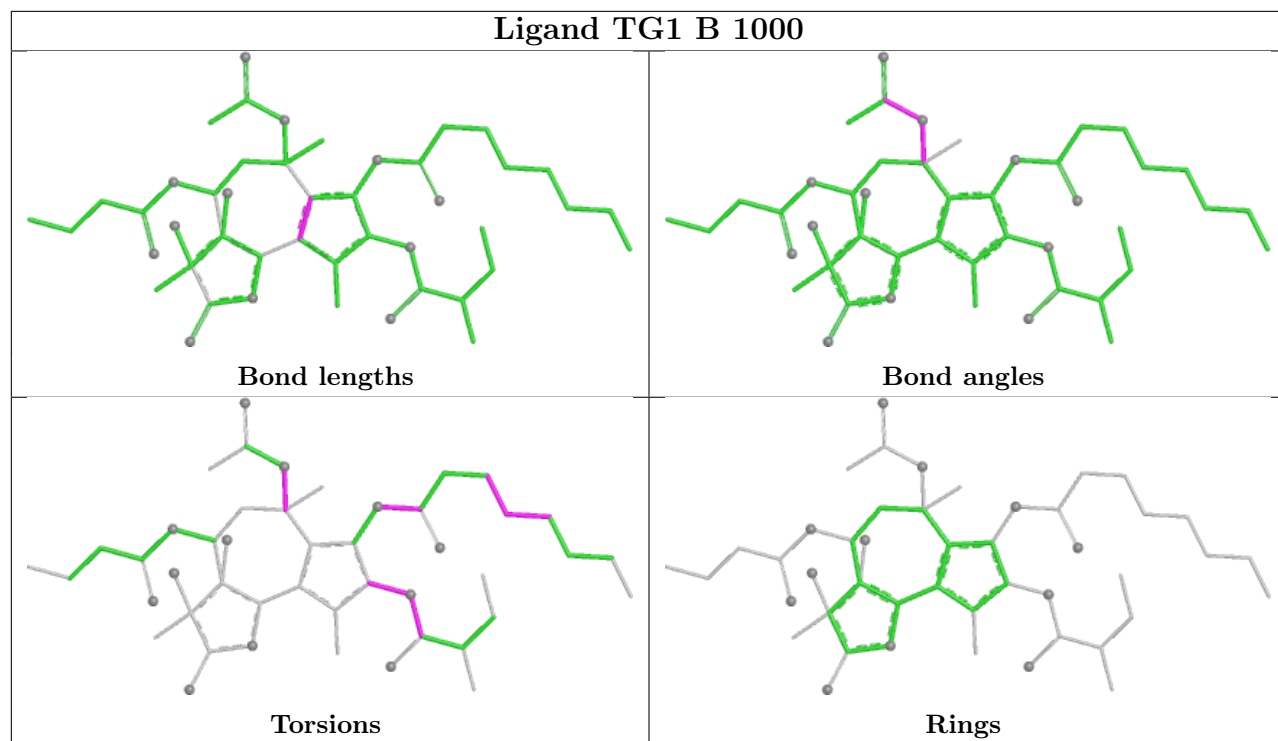
Mol	Chain	Res	Type	Atoms
2	A	1000	TG1	C16-C17-C18-C19
2	A	1000	TG1	C14-C13-O1-C2
2	A	1000	TG1	O4-C21-C22-C24
2	B	1000	TG1	C15-C16-C17-C18
2	A	1000	TG1	O2-C13-O1-C2
2	A	1000	TG1	C21-C22-C24-C25
4	A	1002	128	C5'-O5'-PA-O1A
4	A	1002	128	C5'-O5'-PA-O3A
2	A	1000	TG1	C14-C15-C16-C17
2	A	1000	TG1	C27-C28-C29-C30
2	A	1000	TG1	O7-C27-C28-C29
2	A	1000	TG1	C31-C10-O9-C32
2	B	1000	TG1	C31-C10-O9-C32
2	A	1000	TG1	O8-C27-C28-C29

There are no ring outliers.

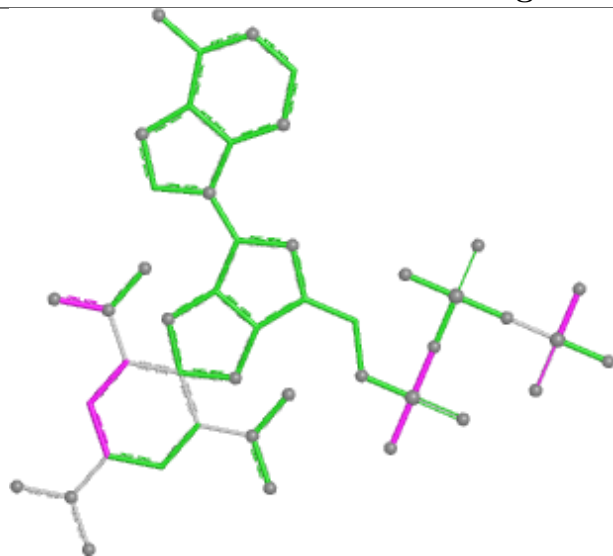
4 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	TG1	13	0
4	B	1002	128	1	0
2	A	1000	TG1	15	0
4	A	1002	128	1	0

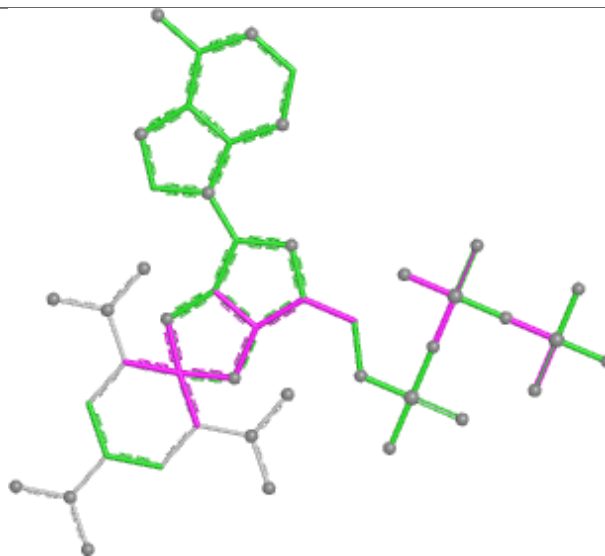
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



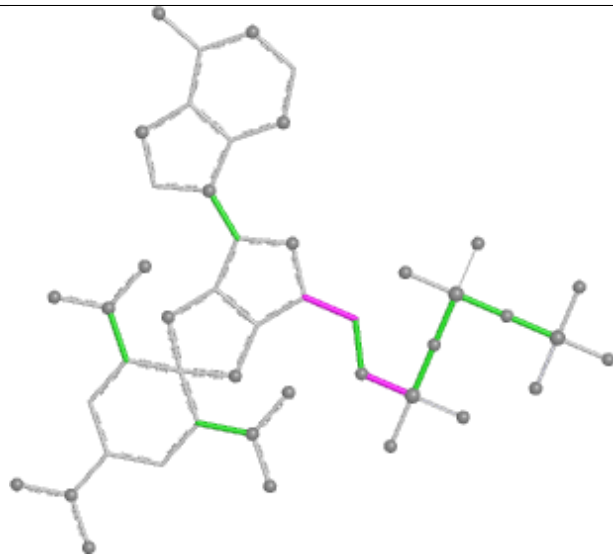
Ligand 128 B 1002



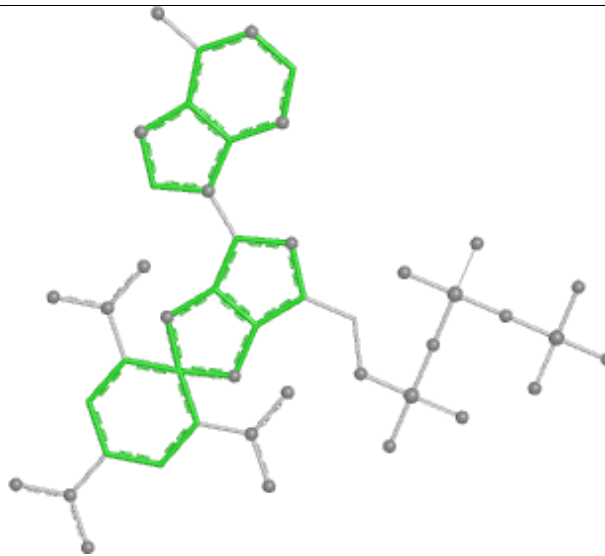
Bond lengths



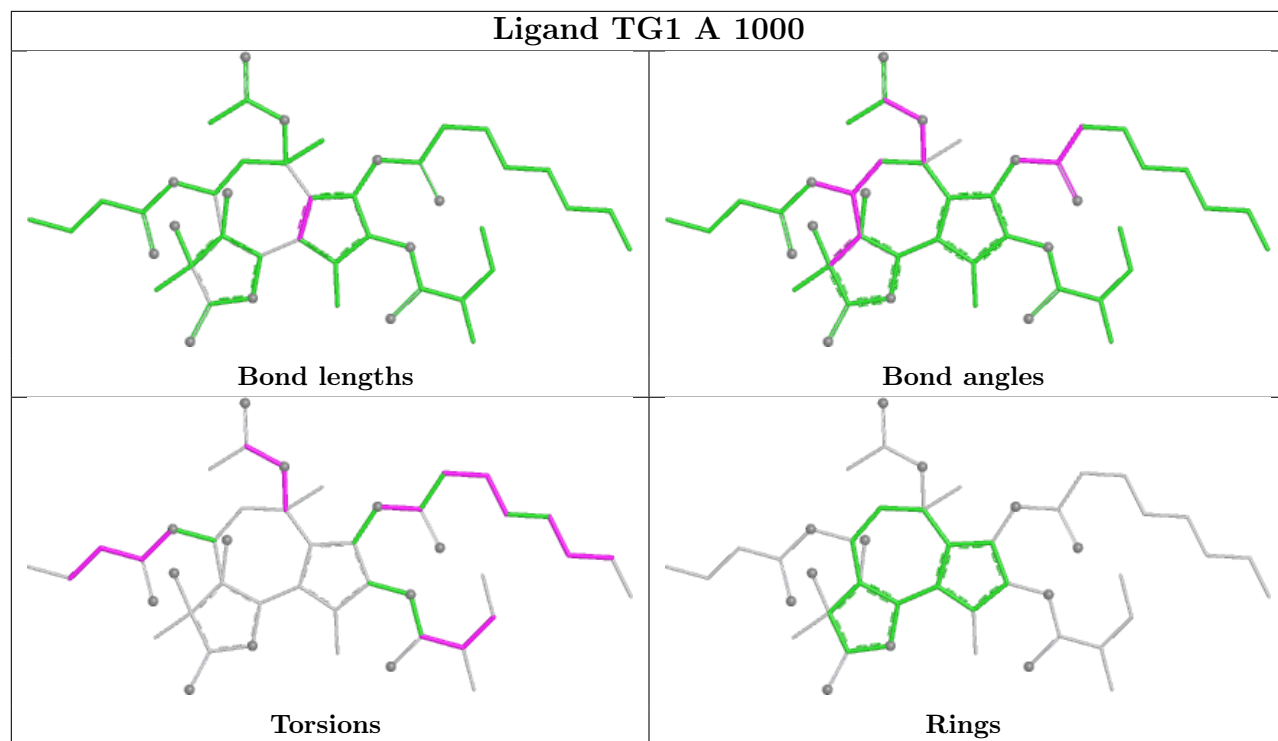
Bond angles

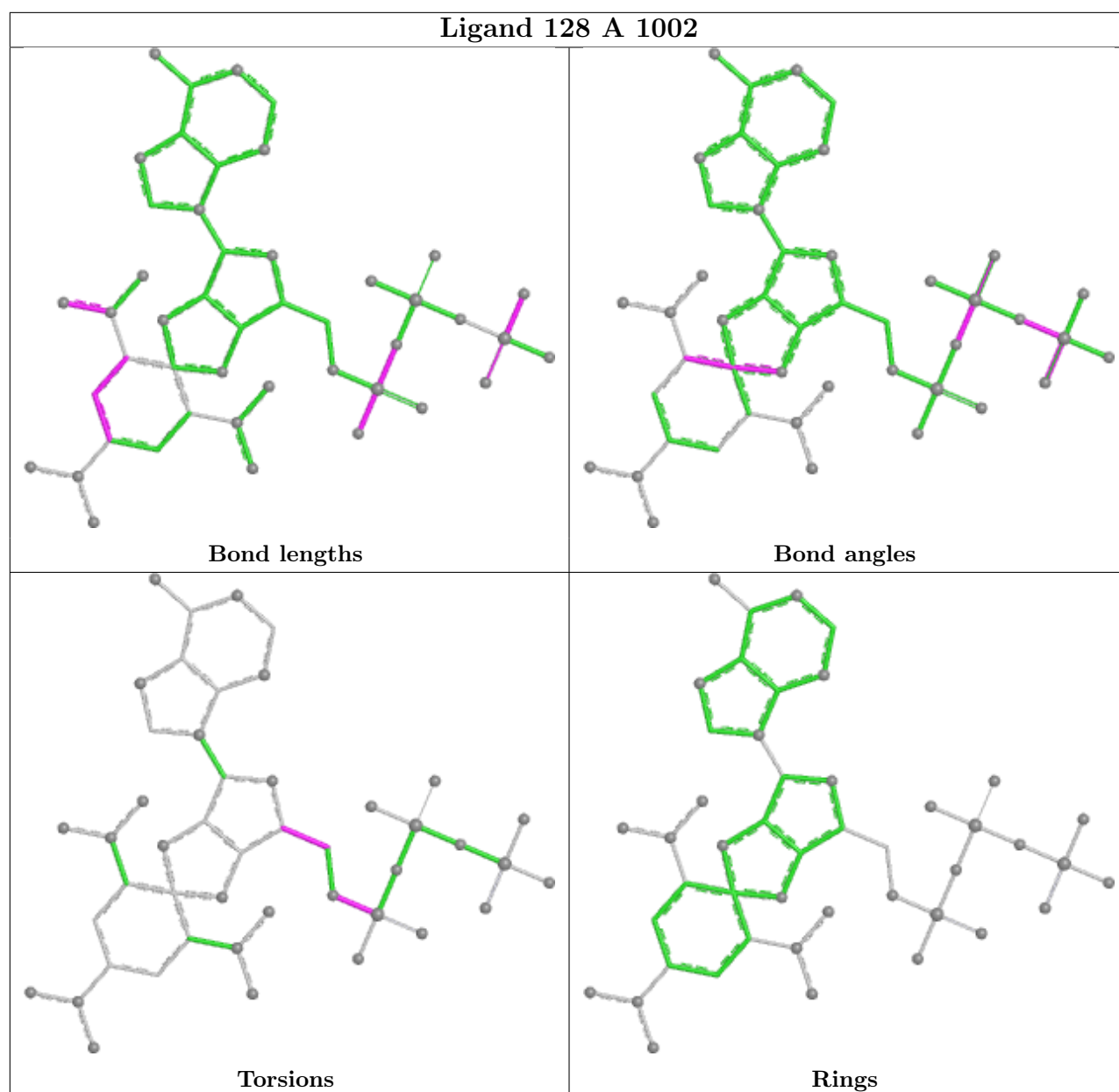


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	994/995 (99%)	0.28	41 (4%)	41 27	51, 110, 250, 425	0
1	B	994/995 (99%)	0.21	29 (2%)	53 35	50, 126, 250, 377	0
All	All	1988/1990 (99%)	0.25	70 (3%)	47 31	50, 119, 250, 425	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	864	GLY	4.6
1	B	787	LEU	4.3
1	B	961	ALA	4.2
1	B	46	GLY	4.0
1	A	853	ALA	4.0
1	A	454	VAL	3.9
1	A	959	LEU	3.9
1	A	786	ALA	3.9
1	A	949	TYR	3.8
1	A	957	PHE	3.7
1	A	787	LEU	3.5
1	B	88	PHE	3.4
1	A	915	SER	3.4
1	A	785	GLU	3.4
1	A	916	LEU	3.2
1	A	508	VAL	3.2
1	A	276	ILE	3.1
1	B	962	LEU	3.1
1	A	289	ILE	3.1
1	B	853	ALA	3.0
1	B	289	ILE	3.0
1	B	740	PHE	3.0
1	A	961	ALA	2.9
1	A	958	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	781	LEU	2.9
1	A	402	ILE	2.8
1	B	61	LEU	2.8
1	A	563	ALA	2.8
1	B	957	PHE	2.7
1	B	964	LEU	2.7
1	B	431	LYS	2.7
1	B	296	PHE	2.7
1	A	752	ALA	2.7
1	B	546	LEU	2.7
1	B	520	GLY	2.7
1	A	963	ASP	2.5
1	B	779	ALA	2.5
1	B	611	ILE	2.5
1	A	870	LEU	2.5
1	B	43	ALA	2.5
1	B	273	LEU	2.5
1	A	284	HIS	2.5
1	B	276	ILE	2.4
1	A	417	CYS	2.4
1	B	561	CYS	2.4
1	B	968	LEU	2.4
1	A	960	LYS	2.4
1	A	422	ASP	2.4
1	A	564	LEU	2.3
1	A	867	TYR	2.3
1	A	321	LEU	2.3
1	B	849	VAL	2.3
1	A	829	ILE	2.3
1	A	850	GLY	2.3
1	A	211	GLY	2.3
1	A	919	ASN	2.2
1	A	783	LEU	2.2
1	B	668	GLU	2.2
1	A	891	PHE	2.2
1	B	963	ASP	2.1
1	A	77	TRP	2.1
1	A	848	THR	2.1
1	B	401	PRO	2.1
1	A	639	ILE	2.1
1	A	272	TRP	2.1
1	A	509	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	866	THR	2.0
1	B	857	MET	2.0
1	A	754	TYR	2.0
1	B	861	ASP	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](#)

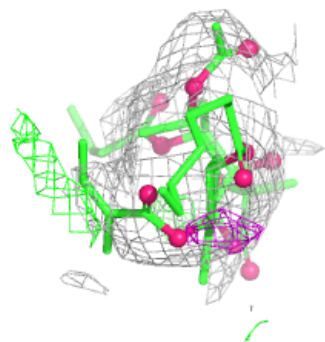
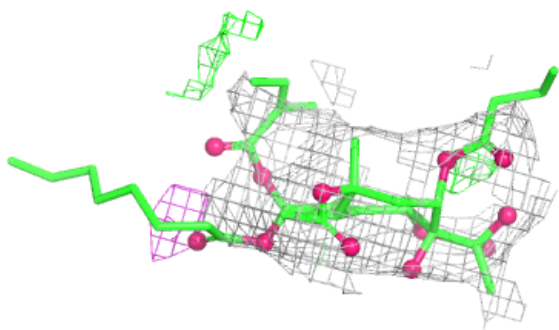
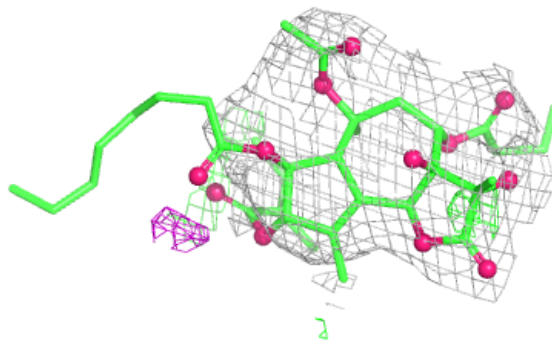
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TG1	B	1000	46/46	0.80	0.16	157,200,218,226	0
5	MG	A	1004	1/1	0.80	0.14	142,142,142,142	0
4	128	B	1002	46/46	0.85	0.18	153,187,205,208	0
5	MG	B	1004	1/1	0.86	0.17	195,195,195,195	0
4	128	A	1002	46/46	0.90	0.13	107,144,157,169	0
2	TG1	A	1000	46/46	0.92	0.14	122,165,182,193	0
7	CL	B	1009	1/1	0.93	0.13	74,74,74,74	0
6	K	B	1008	1/1	0.97	0.05	106,106,106,106	0
7	CL	A	1009	1/1	0.97	0.12	74,74,74,74	0
6	K	A	1008	1/1	0.97	0.05	94,94,94,94	0
5	MG	A	1003	1/1	0.99	0.15	92,92,92,92	0
3	VN4	A	1001	4/4	0.99	0.14	85,95,118,119	0
5	MG	B	1003	1/1	0.99	0.03	102,102,102,102	0
3	VN4	B	1001	4/4	0.99	0.09	88,92,121,134	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.

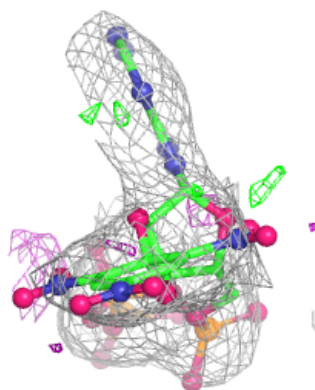
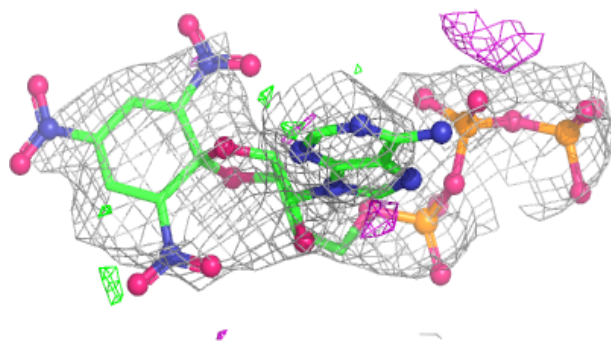
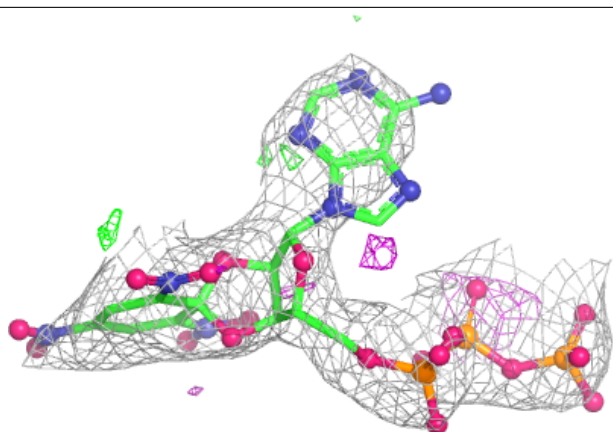
Electron density around TG1 B 1000:

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

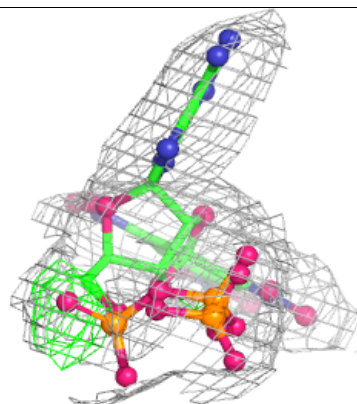
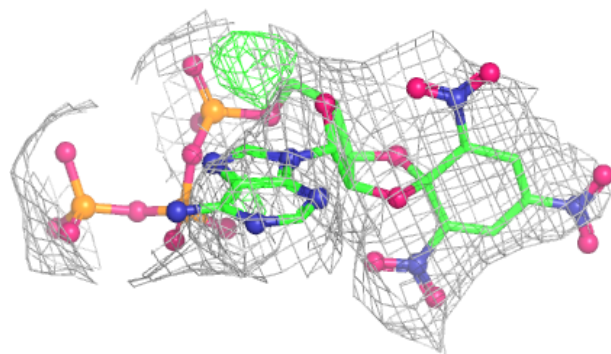
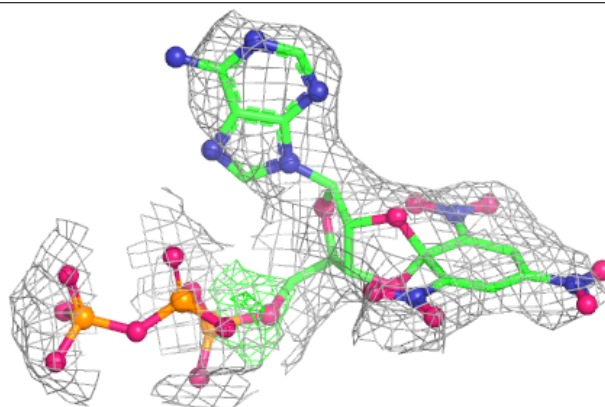


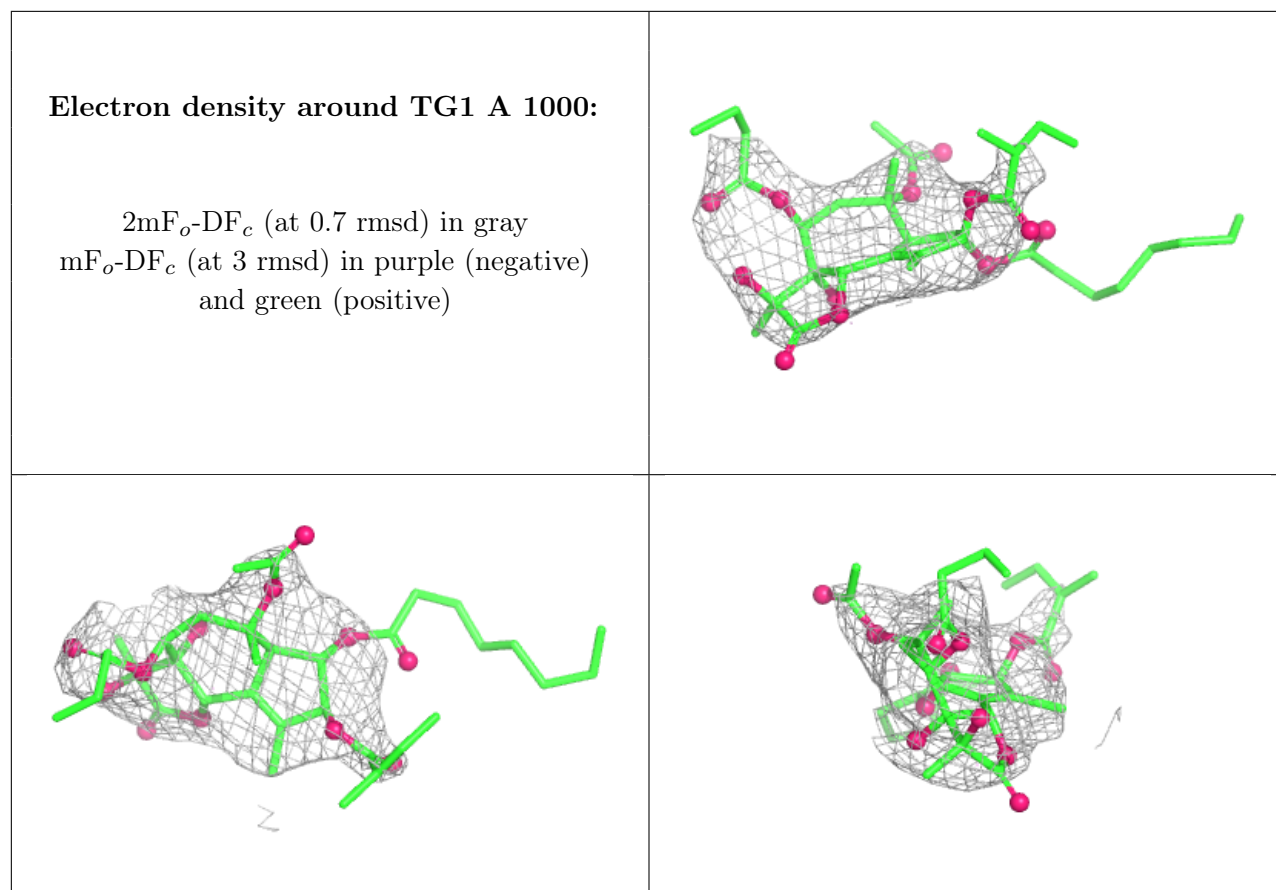
Electron density around 128 B 1002:

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

**Electron density around 128 A 1002:**

$2mF_o-DF_c$ (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.