



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:19 PM EDT

PDB ID : 3AR8 / pdb_00003ar8
Title : Calcium pump crystal structure with bound AlF₄, TNP-AMP and TG
Authors : Toyoshima, C.; Yonekura, S.; Tsueda, J.; Iwasawa, S.
Deposited on : 2010-11-24
Resolution : 2.60 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

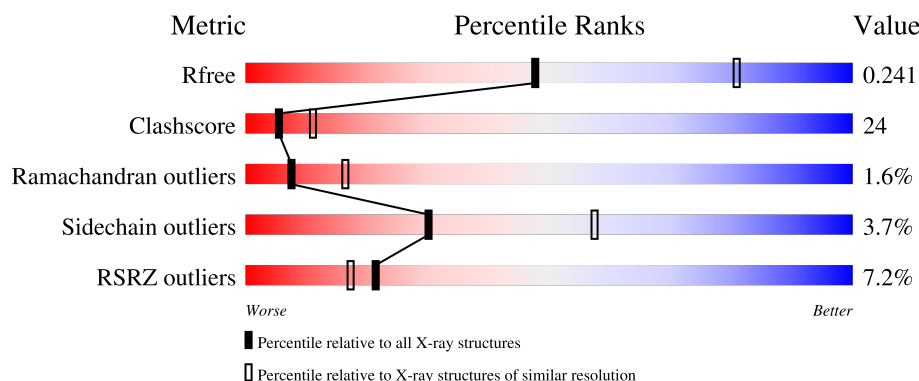
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7871 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
1	A	995	Total	C	N	O	S	1	0	0
			7674	4878	1287	1452	57			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1A	ACE	-	acetylation	UNP P04191
A	994	GLY	ASP	SEE REMARK 999	UNP P04191

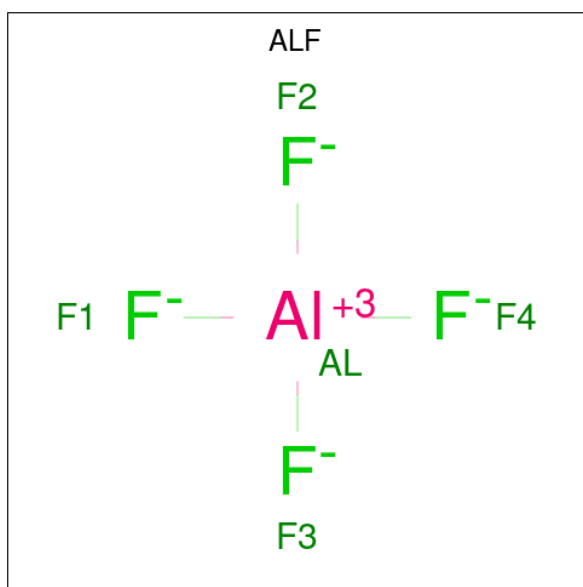
- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

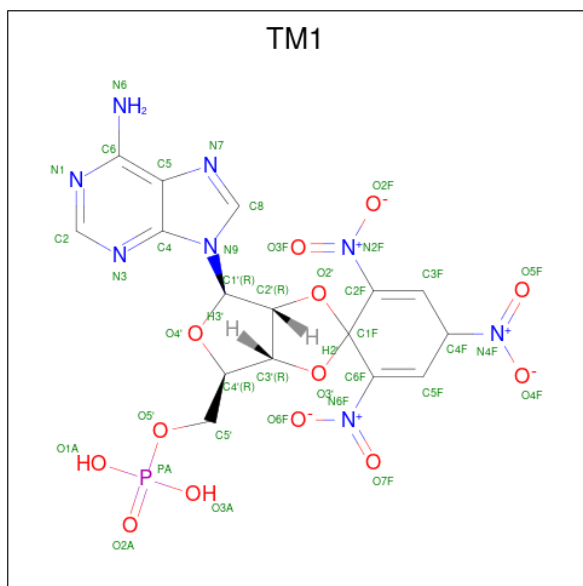
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).

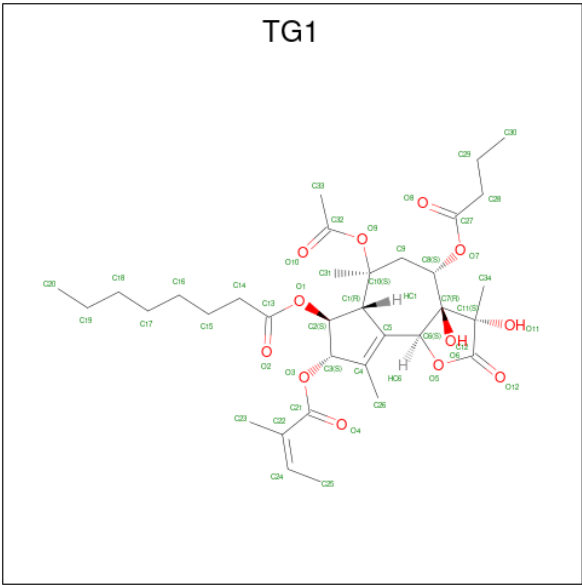


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Al	F	0	0
			5	1	4		

- Molecule 5 is 2',3'-O-[(1r)-2,4,6-trinitrocyclohexa-2,5-diene-1,1-diyl]adenosine 5'-(dihydrogen phosphate) (CCD ID: TM1) (formula: C₁₆H₁₅N₈O₁₃P).



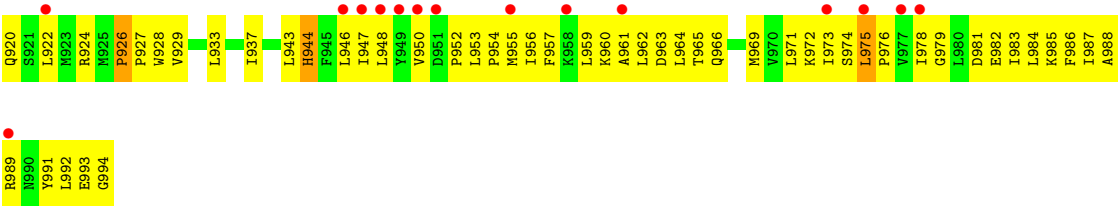
DRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (CCD ID: TG1) (formula: C₃₄H₅₀O₁₂).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	106	Total	O	0	0
			106	106		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	176.86Å 69.87Å 141.81Å 90.00° 106.71° 90.00°	Depositor
Resolution (Å)	14.99 – 2.60 14.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (14.99-2.60) 99.3 (14.99-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.253 0.214 , 0.241	Depositor DCC
R_{free} test set	2531 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7871	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: TG1, TM1, ACE, MG, NA, ALF

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	0.43	0/7813	0.93	23/10594 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	PRO	N-CA-C	8.47	119.65	110.58
1	A	601	ASP	CA-C-N	7.97	125.40	119.66
1	A	601	ASP	C-N-CA	7.97	125.40	119.66
1	A	732	GLU	N-CA-C	-6.88	105.01	113.41
1	A	605	LYS	N-CA-C	6.12	117.95	111.28
1	A	944	HIS	N-CA-C	-5.90	105.92	113.23
1	A	351	ASP	N-CA-C	-5.85	102.81	110.53
1	A	444	ALA	N-CA-C	-5.83	105.01	111.36
1	A	628	ASN	N-CA-C	5.78	118.65	110.50
1	A	194	VAL	CA-C-N	5.77	127.06	119.84
1	A	194	VAL	C-N-CA	5.77	127.06	119.84
1	A	470	ALA	N-CA-C	5.70	117.97	111.02
1	A	350	SER	N-CA-C	5.63	118.64	109.24
1	A	654	THR	N-CA-C	-5.57	101.79	110.42
1	A	163	ILE	N-CA-C	5.50	116.51	108.53
1	A	516	GLY	N-CA-C	5.40	117.87	110.69
1	A	556	ARG	N-CA-C	-5.37	106.69	113.18
1	A	99	ILE	N-CA-C	-5.37	108.61	113.71
1	A	514	VAL	N-CA-C	5.35	116.29	108.53
1	A	164	ARG	N-CA-C	-5.24	100.76	109.46
1	A	159	VAL	CA-C-N	5.16	124.66	119.19
1	A	159	VAL	C-N-CA	5.16	124.66	119.19
1	A	110	ARG	N-CA-C	-5.00	107.15	113.20

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	7674	0	7765	371	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	5	0	0	1	0
5	A	38	0	12	0	0
6	A	46	0	50	3	0
7	A	106	0	0	4	0
All	All	7871	0	7827	371	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 24.

All (371) 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:836:ARG:HG3	1:A:984:LEU:HD13	1.45	0.98
1:A:235:ILE:HG22	1:A:239:MET:HE2	1.46	0.97
1:A:421:ASN:ND2	1:A:423:SER:H	1.66	0.93
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.50	0.92
1:A:484:THR:HB	1:A:496:VAL:HG12	1.52	0.92
1:A:988:ALA:HA	1:A:992:LEU:HD12	1.56	0.88
1:A:762:ARG:HG2	1:A:829:ILE:HD11	1.56	0.86
1:A:41:LEU:HG	1:A:236:ARG:HG3	1.59	0.85
1:A:90:GLU:HB2	1:A:790:VAL:HG22	1.62	0.82
1:A:737:ASP:OD2	1:A:739:ASN:HB2	1.79	0.81
1:A:833:LEU:HD13	1:A:836:ARG:HH21	1.45	0.81
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.63	0.79
1:A:342:LEU:HA	1:A:716:ILE:HD13	1.65	0.79
1:A:30:LYS:O	1:A:34:GLU:HG3	1.82	0.78
1:A:49:LEU:HD13	1:A:110:ARG:HD2	1.63	0.78
1:A:247:THR:HG22	1:A:250:GLN:H	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:THR:HG21	1:A:956:ILE:HA	1.66	0.77
1:A:20:GLU:HA	1:A:150:ILE:CD1	2.14	0.77
1:A:311:LEU:HD11	1:A:761:ILE:HD13	1.68	0.74
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.70	0.73
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.91	0.71
1:A:97:ILE:HA	1:A:100:ALA:HB3	1.72	0.71
1:A:421:ASN:HD22	1:A:422:ASP:N	1.87	0.71
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.72	0.71
1:A:45:GLU:H	1:A:45:GLU:CD	1.97	0.71
1:A:794:TRP:HH2	1:A:943:LEU:HB3	1.55	0.71
1:A:79:GLU:HG2	1:A:87:ALA:HB2	1.71	0.71
1:A:421:ASN:HD22	1:A:423:SER:H	1.36	0.71
1:A:116:ILE:H	1:A:116:ILE:HD12	1.56	0.69
1:A:853:ALA:HB1	1:A:857:MET:HE2	1.74	0.69
1:A:981:ASP:HA	1:A:984:LEU:HD12	1.74	0.69
1:A:557:ASP:HA	1:A:638:ARG:HH12	1.57	0.69
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.76	0.68
1:A:326:MET:HE1	1:A:339:VAL:HG22	1.75	0.68
1:A:972:LYS:HA	1:A:972:LYS:HE2	1.74	0.68
1:A:49:LEU:HA	1:A:52:LEU:HD12	1.76	0.68
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.76	0.68
1:A:52:LEU:HD13	1:A:110:ARG:HB2	1.76	0.68
1:A:271:VAL:HG12	1:A:275:ASN:ND2	2.09	0.67
1:A:342:LEU:HG	1:A:716:ILE:HG21	1.76	0.67
1:A:917:SER:OG	1:A:920:GLN:HB2	1.94	0.67
1:A:749:GLU:O	1:A:753:ILE:HG12	1.96	0.66
1:A:773:VAL:HB	1:A:845:GLY:HA3	1.78	0.65
1:A:486:GLU:O	1:A:491:ARG:NH2	2.26	0.65
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.32	0.65
1:A:482:GLU:CD	1:A:573:ARG:HH12	2.04	0.64
1:A:895:GLU:H	1:A:896:PRO:HD2	1.62	0.64
1:A:975:LEU:N	1:A:976:PRO:HD2	2.13	0.64
1:A:52:LEU:HA	1:A:55:GLU:CD	2.23	0.64
1:A:777:LEU:HB2	1:A:849:VAL:HG21	1.80	0.63
1:A:765:ILE:O	1:A:769:VAL:HG23	1.97	0.63
1:A:23:GLY:HA3	1:A:130:TYR:O	1.99	0.63
1:A:326:MET:HE1	1:A:339:VAL:CG2	2.28	0.63
1:A:791:GLN:O	1:A:795:VAL:HG23	1.99	0.63
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.80	0.63
1:A:342:LEU:HD12	1:A:733:MET:CE	2.29	0.62
1:A:557:ASP:HA	1:A:638:ARG:HH22	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:LEU:HB3	1:A:698:THR:HG21	1.82	0.62
1:A:174:ARG:HB2	1:A:216:ALA:HB3	1.81	0.62
1:A:114:ASN:HB3	1:A:117:GLU:HG2	1.81	0.62
1:A:791:GLN:NE2	1:A:959:LEU:HD21	2.15	0.62
1:A:85:ILE:HG23	1:A:86:THR:HG23	1.82	0.62
1:A:174:ARG:HG3	1:A:188:ILE:CD1	2.31	0.61
1:A:342:LEU:HD22	1:A:747:VAL:HG22	1.82	0.61
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.30	0.61
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.82	0.61
1:A:644:GLU:CD	1:A:644:GLU:H	2.08	0.61
1:A:342:LEU:HA	1:A:716:ILE:CD1	2.29	0.61
1:A:926:PRO:O	1:A:929:VAL:HG23	2.00	0.61
1:A:297:LYS:HA	1:A:300:VAL:HG22	1.82	0.61
1:A:8:SER:OG	1:A:11:GLU:HG3	2.01	0.61
1:A:116:ILE:HD12	1:A:116:ILE:N	2.16	0.61
1:A:342:LEU:HD12	1:A:733:MET:HE1	1.83	0.60
1:A:353:THR:HA	1:A:357:THR:OG1	2.01	0.60
1:A:271:VAL:HG12	1:A:275:ASN:HD21	1.66	0.60
1:A:557:ASP:HA	1:A:638:ARG:NH1	2.16	0.60
1:A:974:SER:C	1:A:976:PRO:HD2	2.26	0.60
1:A:756:ASN:HB3	1:A:808:GLY:HA2	1.83	0.60
1:A:946:LEU:O	1:A:953:LEU:HD12	2.02	0.59
1:A:986:PHE:HA	1:A:989:ARG:HG2	1.84	0.59
1:A:314:VAL:HG13	1:A:805:THR:OG1	2.02	0.59
1:A:757:MET:HA	1:A:760:PHE:CE2	2.38	0.59
1:A:114:ASN:HD21	1:A:116:ILE:HD13	1.68	0.59
1:A:491:ARG:NH1	1:A:588:GLU:OE1	2.36	0.59
1:A:119:LEU:HD22	1:A:239:MET:CE	2.33	0.58
1:A:788:ILE:CG1	1:A:791:GLN:HG3	2.32	0.58
1:A:893:ALA:O	1:A:896:PRO:HD2	2.03	0.58
1:A:600:LEU:HD13	1:A:600:LEU:O	2.02	0.58
1:A:836:ARG:O	1:A:840:ILE:HG12	2.03	0.58
1:A:865:VAL:CG1	1:A:869:GLN:HG3	2.32	0.58
1:A:90:GLU:HB2	1:A:790:VAL:CG2	2.33	0.58
1:A:236:ARG:HD3	1:A:236:ARG:C	2.28	0.58
1:A:310:GLY:O	1:A:314:VAL:HG23	2.02	0.58
1:A:330:ASN:HB3	1:A:737:ASP:HB2	1.85	0.58
1:A:101:ASN:HD21	1:A:313:ALA:HB2	1.68	0.57
1:A:725:ALA:O	1:A:729:THR:HG23	2.03	0.57
1:A:991:TYR:O	1:A:992:LEU:HG	2.03	0.57
1:A:326:MET:CG	1:A:749:GLU:HG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ASN:O	1:A:399:ASP:HB2	2.06	0.56
1:A:100:ALA:O	1:A:103:ILE:HG22	2.05	0.56
1:A:574:GLU:H	1:A:574:GLU:CD	2.14	0.56
1:A:395:VAL:O	1:A:402:ILE:HD13	2.05	0.56
1:A:557:ASP:HA	1:A:638:ARG:NH2	2.20	0.56
1:A:114:ASN:OD1	1:A:117:GLU:HG2	2.06	0.56
1:A:116:ILE:O	1:A:120:LYS:HG3	2.06	0.56
1:A:898:THR:HG21	1:A:960:LYS:O	2.06	0.56
1:A:978:ILE:O	1:A:982:GLU:HB2	2.06	0.56
1:A:508:VAL:HG12	1:A:509:GLY:N	2.21	0.56
1:A:86:THR:HG22	1:A:956:ILE:HG22	1.87	0.56
1:A:549:ILE:CD1	1:A:596:VAL:HG21	2.31	0.56
1:A:557:ASP:CA	1:A:638:ARG:HH22	2.19	0.56
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.86	0.56
1:A:757:MET:O	1:A:761:ILE:HG12	2.06	0.56
1:A:41:LEU:HB2	1:A:123:GLU:OE1	2.07	0.55
1:A:773:VAL:HG11	1:A:842:GLY:HA2	1.88	0.55
1:A:804:ALA:C	1:A:806:ALA:H	2.13	0.55
1:A:962:LEU:HB3	1:A:966:GLN:HB2	1.87	0.55
1:A:783:LEU:HD12	1:A:783:LEU:H	1.71	0.55
1:A:560:ARG:HD3	7:A:9001:HOH:O	2.05	0.55
1:A:79:GLU:HG2	1:A:87:ALA:CB	2.37	0.55
1:A:308:PRO:HA	1:A:768:ASN:HD21	1.70	0.55
1:A:751:ARG:HB3	1:A:816:ILE:HD11	1.88	0.55
1:A:70:CYS:O	1:A:74:VAL:HG23	2.06	0.55
1:A:557:ASP:CB	1:A:638:ARG:HH22	2.19	0.55
1:A:778:THR:HG23	1:A:849:VAL:HG22	1.89	0.55
1:A:855:TRP:CD1	1:A:895:GLU:HB3	2.42	0.54
1:A:403:ARG:HB2	1:A:406:GLN:HG2	1.89	0.54
1:A:874:MET:O	1:A:874:MET:HG2	2.07	0.54
1:A:20:GLU:HA	1:A:150:ILE:HD11	1.89	0.54
1:A:869:GLN:HA	1:A:872:HIS:ND1	2.22	0.54
1:A:421:ASN:HD22	1:A:421:ASN:C	2.15	0.54
1:A:527:TYR:CG	1:A:534:ARG:HD3	2.42	0.54
1:A:485:LEU:HD22	1:A:584:PHE:CE2	2.42	0.54
1:A:819:ARG:CG	1:A:820:PRO:HD2	2.38	0.54
1:A:838:MET:HE3	1:A:838:MET:HA	1.89	0.54
1:A:52:LEU:HB3	1:A:106:VAL:HG13	1.90	0.54
1:A:963:ASP:H	1:A:966:GLN:HE21	1.54	0.54
1:A:66:LEU:HA	1:A:98:LEU:HD11	1.90	0.53
1:A:644:GLU:CD	1:A:644:GLU:N	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLU:OE1	1:A:529:ARG:CD	2.56	0.53
1:A:993:GLU:HG2	1:A:994:GLY:N	2.23	0.53
1:A:49:LEU:HB2	1:A:110:ARG:NH1	2.23	0.53
1:A:944:HIS:O	1:A:947:ILE:HG22	2.09	0.53
1:A:247:THR:HG23	1:A:248:PRO:HD2	1.90	0.53
1:A:926:PRO:HB3	1:A:928:TRP:CE2	2.43	0.53
1:A:20:GLU:HA	1:A:150:ILE:HD13	1.90	0.53
1:A:174:ARG:HD3	1:A:216:ALA:HB3	1.90	0.53
1:A:807:LEU:C	1:A:809:PHE:H	2.17	0.53
1:A:905:VAL:O	1:A:909:MET:HG2	2.09	0.53
1:A:572:LYS:HB2	1:A:575:GLU:HG2	1.90	0.52
1:A:646:GLU:OE2	1:A:651:ARG:NH1	2.39	0.52
1:A:805:THR:HG22	1:A:805:THR:O	2.08	0.52
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.91	0.52
1:A:795:VAL:HA	1:A:799:THR:OG1	2.09	0.52
1:A:887:ASP:HB3	1:A:890:ILE:HG13	1.92	0.52
1:A:85:ILE:HD11	1:A:955:MET:SD	2.48	0.52
1:A:781:LEU:HD23	1:A:783:LEU:HD13	1.92	0.52
1:A:844:VAL:CG2	1:A:907:ILE:HG21	2.37	0.52
1:A:80:GLU:O	1:A:84:THR:HB	2.10	0.52
1:A:856:PHE:CE1	1:A:896:PRO:HB3	2.45	0.52
1:A:857:MET:HG2	1:A:865:VAL:O	2.09	0.52
1:A:865:VAL:HG12	1:A:869:GLN:HG3	1.92	0.52
1:A:308:PRO:HG3	1:A:765:ILE:CD1	2.40	0.52
1:A:877:THR:HA	1:A:880:HIS:CE1	2.45	0.52
1:A:770:GLY:HA2	1:A:841:GLY:O	2.10	0.51
1:A:508:VAL:HG12	1:A:509:GLY:H	1.74	0.51
1:A:624:ILE:HG21	1:A:684:LYS:HG2	1.93	0.51
1:A:922:LEU:O	1:A:927:PRO:HD3	2.09	0.51
1:A:146:VAL:O	1:A:149:ASP:HB2	2.10	0.51
1:A:57:PHE:HZ	1:A:99:ILE:HG12	1.75	0.51
1:A:272:TRP:HA	1:A:295:TYR:OH	2.11	0.51
1:A:494:MET:HG2	1:A:495:SER:N	2.26	0.51
1:A:253:LEU:HD23	6:A:1003:TG1:H301	1.93	0.51
1:A:545:ILE:O	1:A:549:ILE:HG12	2.11	0.51
1:A:875:GLN:HG2	1:A:878:GLU:OE2	2.11	0.51
1:A:60:LEU:HD21	1:A:261:SER:HB2	1.93	0.51
1:A:916:LEU:HD21	1:A:933:LEU:HD22	1.93	0.51
1:A:947:ILE:O	1:A:947:ILE:HG12	2.10	0.50
1:A:885:GLY:C	1:A:886:LEU:HD12	2.36	0.50
1:A:114:ASN:CG	1:A:117:GLU:HG2	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:CYS:O	1:A:544:LYS:HG3	2.11	0.50
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.42	0.50
1:A:796:ASN:O	1:A:797:LEU:HG	2.12	0.50
1:A:697:ILE:HD13	1:A:824:PRO:HG3	1.92	0.50
1:A:907:ILE:O	1:A:910:CYS:HB2	2.11	0.50
1:A:98:LEU:O	1:A:98:LEU:HD23	2.10	0.50
1:A:863:PRO:C	1:A:865:VAL:H	2.19	0.50
1:A:119:LEU:HD22	1:A:239:MET:HE1	1.93	0.50
1:A:247:THR:HB	1:A:250:GLN:HG3	1.94	0.50
1:A:342:LEU:HD12	1:A:733:MET:SD	2.52	0.50
1:A:379:LEU:HD12	1:A:548:VAL:HG21	1.93	0.50
1:A:557:ASP:OD1	1:A:558:THR:N	2.45	0.50
1:A:672:ARG:NH2	7:A:4055:HOH:O	2.41	0.50
1:A:72:SER:O	1:A:76:ALA:HB2	2.12	0.50
1:A:40:GLU:O	1:A:227:GLY:HA2	2.12	0.50
1:A:836:ARG:HD2	1:A:981:ASP:OD1	2.11	0.50
1:A:854:TRP:O	1:A:859:ALA:HB2	2.12	0.49
1:A:962:LEU:HD22	1:A:966:GLN:OE1	2.12	0.49
1:A:92:PHE:O	1:A:96:LEU:HB2	2.11	0.49
1:A:947:ILE:HD11	1:A:957:PHE:CD2	2.47	0.49
1:A:301:ALA:HA	1:A:789:PRO:HB3	1.94	0.49
1:A:924:ARG:O	1:A:926:PRO:HD3	2.13	0.49
1:A:969:MET:HE3	1:A:972:LYS:HB2	1.93	0.49
1:A:203:ASP:OD1	1:A:678:ARG:NH1	2.46	0.49
1:A:979:GLY:O	1:A:983:ILE:HG12	2.13	0.49
1:A:128:LYS:HG2	1:A:139:ARG:HG2	1.95	0.48
1:A:875:GLN:HA	1:A:878:GLU:HG2	1.95	0.48
1:A:600:LEU:HD13	1:A:600:LEU:C	2.38	0.48
1:A:947:ILE:HD11	1:A:957:PHE:CG	2.48	0.48
1:A:347:VAL:HG13	1:A:620:ARG:HG3	1.96	0.48
1:A:520:GLY:O	1:A:524:ARG:HG3	2.14	0.48
1:A:608:MET:HE3	1:A:638:ARG:O	2.14	0.48
1:A:954:PRO:HB2	1:A:959:LEU:O	2.12	0.48
1:A:836:ARG:NH1	1:A:985:LYS:HG2	2.28	0.48
1:A:51:GLU:O	1:A:55:GLU:HG2	2.13	0.48
1:A:114:ASN:CB	1:A:117:GLU:HG2	2.43	0.48
1:A:604:ARG:HB2	1:A:607:VAL:CG2	2.44	0.48
1:A:101:ASN:ND2	1:A:313:ALA:HB2	2.28	0.48
1:A:311:LEU:N	1:A:312:PRO:CD	2.77	0.48
1:A:50:TRP:O	1:A:54:ILE:HG12	2.14	0.47
1:A:485:LEU:HD22	1:A:584:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:VAL:HG21	1:A:541:VAL:HG11	1.96	0.47
1:A:653:TYR:OH	1:A:672:ARG:NH1	2.47	0.47
1:A:963:ASP:C	1:A:965:THR:H	2.22	0.47
1:A:527:TYR:HB3	1:A:534:ARG:CG	2.43	0.47
1:A:950:VAL:O	1:A:954:PRO:HD2	2.14	0.47
1:A:395:VAL:HG12	1:A:402:ILE:HD11	1.95	0.47
1:A:473:SER:O	1:A:477:GLN:HG2	2.13	0.47
1:A:880:HIS:N	1:A:881:PRO:CD	2.78	0.47
1:A:114:ASN:HD22	1:A:115:ALA:N	2.12	0.47
1:A:116:ILE:H	1:A:116:ILE:CD1	2.26	0.47
1:A:363:VAL:HG11	1:A:448:LEU:HD22	1.97	0.47
1:A:769:VAL:HA	6:A:1003:TG1:H231	1.96	0.47
1:A:971:LEU:O	1:A:975:LEU:HB2	2.15	0.47
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.97	0.47
1:A:773:VAL:CB	1:A:845:GLY:HA3	2.44	0.46
1:A:50:TRP:CZ2	1:A:54:ILE:HD11	2.50	0.46
1:A:267:ILE:O	1:A:271:VAL:HG23	2.15	0.46
1:A:293:ILE:CG2	1:A:297:LYS:HE3	2.45	0.46
1:A:527:TYR:HB3	1:A:534:ARG:HG2	1.97	0.46
1:A:795:VAL:O	1:A:799:THR:HB	2.16	0.46
1:A:909:MET:SD	1:A:937:ILE:HG23	2.55	0.46
1:A:917:SER:CB	1:A:920:GLN:HB2	2.46	0.46
1:A:926:PRO:C	1:A:928:TRP:H	2.23	0.46
1:A:20:GLU:HG3	1:A:166:LEU:HD13	1.98	0.46
1:A:247:THR:HG23	1:A:248:PRO:CD	2.45	0.46
1:A:248:PRO:HG2	1:A:340:GLU:OE2	2.16	0.46
1:A:914:ASN:HD22	1:A:922:LEU:HD21	1.81	0.46
1:A:975:LEU:N	1:A:976:PRO:CD	2.78	0.46
1:A:82:GLU:HG3	1:A:83:GLU:N	2.31	0.46
1:A:853:ALA:HB1	1:A:857:MET:CE	2.46	0.46
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.15	0.46
1:A:336:LEU:HB2	1:A:337:PRO:HD3	1.98	0.46
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.46	0.46
1:A:819:ARG:HG3	1:A:820:PRO:HD2	1.97	0.46
1:A:529:ARG:HH22	1:A:568:ASP:CG	2.23	0.46
1:A:295:TYR:O	1:A:298:ILE:HG12	2.15	0.45
1:A:756:ASN:HD22	1:A:808:GLY:C	2.24	0.45
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.51	0.45
1:A:743:ILE:O	1:A:747:VAL:HG23	2.15	0.45
1:A:890:ILE:HG22	1:A:890:ILE:O	2.16	0.45
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:C	1:A:133:ASP:N	2.74	0.45
1:A:670:CYS:HB3	1:A:691:LEU:HD13	1.97	0.45
1:A:791:GLN:HE22	1:A:959:LEU:HD21	1.79	0.45
1:A:975:LEU:HD13	1:A:975:LEU:O	2.16	0.45
1:A:247:THR:HB	1:A:250:GLN:CD	2.42	0.44
1:A:470:ALA:O	1:A:474:VAL:HG23	2.17	0.44
1:A:865:VAL:HG13	1:A:869:GLN:HG3	2.00	0.44
1:A:25:THR:HA	1:A:132:ALA:HB3	1.98	0.44
1:A:759:GLN:OE1	1:A:759:GLN:HA	2.17	0.44
1:A:816:ILE:HG23	1:A:817:MET:HG2	1.99	0.44
1:A:264:ILE:HD11	1:A:306:ALA:HB2	1.98	0.44
1:A:345:THR:HA	1:A:697:ILE:HG22	1.99	0.44
1:A:391:PRO:HB3	1:A:450:GLU:HB3	1.99	0.44
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.82	0.44
1:A:981:ASP:OD2	1:A:985:LYS:HE3	2.18	0.44
1:A:494:MET:HE2	7:A:4063:HOH:O	2.18	0.44
1:A:761:ILE:O	1:A:765:ILE:HG12	2.17	0.44
1:A:18:VAL:HG22	1:A:19:SER:N	2.32	0.44
1:A:758:LYS:O	1:A:762:ARG:HD2	2.17	0.44
1:A:7:LYS:N	1:A:7:LYS:HD2	2.32	0.44
1:A:899:MET:HE1	1:A:966:GLN:HB3	1.99	0.44
1:A:99:ILE:HA	1:A:102:ALA:HB3	2.00	0.43
1:A:290:ARG:HA	1:A:293:ILE:HD11	2.00	0.43
1:A:452:MET:O	1:A:453:ASN:C	2.61	0.43
1:A:971:LEU:O	1:A:972:LYS:HE2	2.17	0.43
1:A:557:ASP:O	1:A:558:THR:C	2.60	0.43
1:A:666:GLN:O	1:A:669:ALA:HB3	2.18	0.43
1:A:491:ARG:HG3	1:A:585:MET:HB2	1.99	0.43
1:A:656:ARG:CA	1:A:656:ARG:HE	2.30	0.43
1:A:788:ILE:HG12	1:A:791:GLN:HG3	1.99	0.43
1:A:788:ILE:HG13	1:A:791:GLN:HG3	1.98	0.43
1:A:948:LEU:HB3	1:A:961:ALA:HB2	2.00	0.43
1:A:771:GLU:CD	1:A:792:LEU:HD22	2.44	0.43
1:A:773:VAL:HG21	1:A:842:GLY:HA2	2.01	0.43
1:A:259:GLN:O	1:A:263:VAL:HG23	2.19	0.43
1:A:484:THR:HG22	7:A:4106:HOH:O	2.18	0.43
1:A:912:ALA:HB1	1:A:933:LEU:HD11	2.00	0.43
1:A:983:ILE:O	1:A:987:ILE:HG12	2.19	0.43
1:A:544:LYS:HD3	1:A:544:LYS:C	2.44	0.43
1:A:963:ASP:H	1:A:966:GLN:NE2	2.15	0.43
1:A:383:SER:C	1:A:384:ILE:HD13	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:CYS:C	1:A:562:LEU:HD12	2.44	0.43
1:A:834:PHE:O	1:A:838:MET:HB2	2.18	0.43
1:A:256:PHE:HB2	6:A:1003:TG1:H291	2.01	0.43
1:A:662:PRO:HG2	1:A:665:GLU:HG3	2.00	0.43
1:A:161:ALA:HA	1:A:210:SER:HB2	2.01	0.43
1:A:166:LEU:HD11	1:A:222:ILE:HB	2.00	0.43
1:A:397:LYS:O	1:A:398:ASN:HB2	2.19	0.43
1:A:557:ASP:HA	1:A:638:ARG:CZ	2.48	0.43
1:A:329:LYS:O	1:A:330:ASN:HB2	2.19	0.42
1:A:823:SER:HA	1:A:824:PRO:HD3	1.92	0.42
1:A:671:ARG:HD3	1:A:694:TYR:CE2	2.55	0.42
1:A:969:MET:HE3	1:A:969:MET:HA	2.00	0.42
1:A:72:SER:O	1:A:91:PRO:HG3	2.19	0.42
1:A:93:VAL:HA	1:A:96:LEU:HB2	2.00	0.42
1:A:567:ARG:HD2	1:A:570:PRO:CA	2.43	0.42
1:A:49:LEU:O	1:A:53:VAL:HG23	2.20	0.42
1:A:347:VAL:HG22	1:A:620:ARG:HG2	2.01	0.42
1:A:151:VAL:CG1	1:A:152:GLU:N	2.83	0.42
1:A:39:ASN:O	1:A:143:ARG:HA	2.19	0.42
1:A:544:LYS:HD3	1:A:544:LYS:O	2.19	0.42
1:A:898:THR:O	1:A:898:THR:HG22	2.19	0.42
1:A:982:GLU:HA	1:A:982:GLU:OE1	2.20	0.42
1:A:55:GLU:HA	1:A:58:GLU:HG3	2.00	0.42
1:A:82:GLU:CD	1:A:83:GLU:HG3	2.45	0.42
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.54	0.42
1:A:760:PHE:CD1	1:A:760:PHE:C	2.98	0.42
1:A:491:ARG:HH11	1:A:588:GLU:CD	2.27	0.42
1:A:85:ILE:HG12	1:A:955:MET:HE3	2.01	0.42
1:A:408:ASP:OD1	1:A:532:THR:HG23	2.20	0.42
1:A:973:ILE:O	1:A:973:ILE:HG22	2.19	0.42
1:A:52:LEU:O	1:A:56:GLN:HG2	2.20	0.42
1:A:600:LEU:HD22	1:A:601:ASP:C	2.44	0.42
1:A:811:PRO:HA	1:A:812:PRO:HD2	1.96	0.41
1:A:342:LEU:CD2	1:A:747:VAL:HG22	2.47	0.41
1:A:190:HIS:O	1:A:206:ASN:HA	2.20	0.41
1:A:247:THR:HB	1:A:250:GLN:CG	2.50	0.41
1:A:868:HIS:O	1:A:868:HIS:ND1	2.53	0.41
1:A:944:HIS:C	1:A:947:ILE:HG22	2.46	0.41
1:A:256:PHE:CZ	1:A:765:ILE:HD12	2.56	0.41
1:A:708:ALA:HB3	1:A:709:PRO:HD3	2.02	0.41
1:A:739:ASN:OD1	1:A:741:SER:OG	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:LEU:HB2	1:A:954:PRO:CD	2.50	0.41
1:A:80:GLU:H	1:A:80:GLU:CD	2.28	0.41
1:A:326:MET:HE1	1:A:339:VAL:CG1	2.51	0.41
1:A:764:LEU:CD1	1:A:804:ALA:HB2	2.50	0.41
1:A:807:LEU:C	1:A:809:PHE:N	2.76	0.41
1:A:835:PHE:O	1:A:838:MET:HB3	2.20	0.41
1:A:891:PHE:C	1:A:893:ALA:H	2.28	0.41
1:A:270:ALA:O	1:A:274:ILE:HG12	2.20	0.41
1:A:572:LYS:O	1:A:573:ARG:C	2.63	0.41
1:A:804:ALA:C	1:A:806:ALA:N	2.76	0.41
1:A:875:GLN:HG2	1:A:878:GLU:CD	2.46	0.41
1:A:894:PRO:HB2	1:A:960:LYS:N	2.36	0.41
1:A:962:LEU:HA	1:A:966:GLN:NE2	2.35	0.41
1:A:625:THR:HA	4:A:998:ALF:F4	2.11	0.41
1:A:863:PRO:O	1:A:865:VAL:N	2.54	0.41
1:A:308:PRO:HG3	1:A:765:ILE:HD13	2.03	0.41
1:A:488:SER:HB3	1:A:491:ARG:HH21	1.85	0.41
1:A:800:ASP:C	1:A:803:PRO:HD2	2.46	0.41
1:A:50:TRP:CH2	1:A:54:ILE:HD11	2.56	0.40
1:A:67:LEU:O	1:A:71:ILE:HG13	2.21	0.40
1:A:567:ARG:CD	1:A:570:PRO:HA	2.45	0.40
1:A:141:LYS:O	1:A:144:ASP:HB2	2.21	0.40
1:A:482:GLU:CD	1:A:573:ARG:NH1	2.77	0.40
1:A:90:GLU:C	1:A:92:PHE:H	2.29	0.40
1:A:120:LYS:HE2	1:A:120:LYS:HB3	1.88	0.40
1:A:259:GLN:OE1	1:A:259:GLN:HA	2.20	0.40
1:A:575:GLU:HG2	1:A:575:GLU:H	1.66	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	993/995 (100%)	877 (88%)	100 (10%)	16 (2%)	7	16

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	ALA
1	A	857	MET
1	A	964	LEU
1	A	859	ALA
1	A	865	VAL
1	A	918	GLU
1	A	133	ASP
1	A	241	ALA
1	A	243	GLU
1	A	558	THR
1	A	895	GLU
1	A	277	GLY
1	A	797	LEU
1	A	864	GLY
1	A	926	PRO
1	A	885	GLY

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%)	809 (96%)	31 (4%)	30	57

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	82	GLU
1	A	133	ASP
1	A	134	ARG
1	A	149	ASP

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Mol	Chain	Res	Type
1	A	150	ILE
1	A	174	ARG
1	A	238	GLN
1	A	247	THR
1	A	266	LEU
1	A	319	LEU
1	A	342	LEU
1	A	356	LEU
1	A	384	ILE
1	A	402	ILE
1	A	439	GLU
1	A	467	ARG
1	A	484	THR
1	A	491	ARG
1	A	528	VAL
1	A	544	LYS
1	A	567	ARG
1	A	589	THR
1	A	600	LEU
1	A	631	THR
1	A	656	ARG
1	A	691	LEU
1	A	713	LYS
1	A	739	ASN
1	A	911	ASN
1	A	975	LEU

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

Mol	Chain	Res	Type
1	A	56	GLN
1	A	101	ASN
1	A	114	ASN
1	A	177	GLN
1	A	238	GLN
1	A	275	ASN
1	A	359	ASN
1	A	421	ASN
1	A	461	ASN
1	A	510	ASN
1	A	612	GLN
1	A	768	ASN

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Mol	Chain	Res	Type
1	A	880	HIS
1	A	911	ASN
1	A	914	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
5	TM1	A	1002	-	36,42,42	3.58	18 (50%)	43,66,66	3.16	16 (37%)
6	TG1	A	1003	-	44,48,48	1.76	10 (22%)	47,72,72	1.83	11 (23%)
4	ALF	A	998	7,1	4,4,4	1.34	0	-		

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
5	TM1	A	1002	-	-	6/16/68/68	0/5/5/5
6	TG1	A	1003	-	-	9/33/99/99	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002	TM1	C5F-C6F	13.26	1.52	1.33
5	A	1002	TM1	O3'-C1F	6.79	1.51	1.41
5	A	1002	TM1	O2'-C1F	6.69	1.51	1.41
6	A	1003	TG1	O4-C21	5.74	1.33	1.21
5	A	1002	TM1	C1'-N9	5.39	1.61	1.46
5	A	1002	TM1	C4F-C3F	-4.31	1.38	1.50
5	A	1002	TM1	C3F-C2F	4.08	1.39	1.33
5	A	1002	TM1	C5'-C4'	3.85	1.63	1.51
5	A	1002	TM1	C4-N3	3.71	1.41	1.34
5	A	1002	TM1	C5-N7	-3.66	1.32	1.39
6	A	1003	TG1	C3-C4	3.58	1.54	1.50
6	A	1003	TG1	O6-C7	3.20	1.48	1.43
5	A	1002	TM1	C2-N1	3.17	1.39	1.33
5	A	1002	TM1	C3'-C4'	-3.16	1.44	1.52
6	A	1003	TG1	C1-C2	3.15	1.59	1.54
5	A	1002	TM1	O7F-N6F	-3.13	1.17	1.22
6	A	1003	TG1	C11-C7	2.97	1.59	1.55
5	A	1002	TM1	C6-N1	2.88	1.43	1.35
6	A	1003	TG1	C9-C10	2.84	1.59	1.54
6	A	1003	TG1	C1-C5	2.74	1.55	1.51
5	A	1002	TM1	C2-N3	2.51	1.38	1.33
5	A	1002	TM1	C4F-C5F	-2.45	1.43	1.50
6	A	1003	TG1	O3-C3	2.38	1.49	1.44
6	A	1003	TG1	C34-C11	2.34	1.56	1.53
5	A	1002	TM1	O2F-N2F	-2.10	1.21	1.35
6	A	1003	TG1	C9-C8	2.06	1.55	1.52
5	A	1002	TM1	PA-O5'	2.04	1.66	1.60
5	A	1002	TM1	O6F-N6F	-2.03	1.21	1.35

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	TM1	O2'-C1F-C2F	-8.02	99.50	110.47
5	A	1002	TM1	O3'-C1F-C6F	-7.11	100.75	110.47
5	A	1002	TM1	C5-C4-N3	-6.62	117.60	126.72
5	A	1002	TM1	O2'-C2'-C3'	6.34	113.73	103.63
5	A	1002	TM1	N3-C4-N9	5.76	136.96	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1003	TG1	C10-O9-C32	5.59	134.47	121.36
5	A	1002	TM1	C4'-O4'-C1'	5.46	121.53	109.47
5	A	1002	TM1	N3-C2-N1	-4.95	121.09	128.58
5	A	1002	TM1	C2-N3-C4	4.68	123.26	111.83
5	A	1002	TM1	O4'-C1'-C2'	-4.46	98.91	106.59
6	A	1003	TG1	O12-C12-C11	-4.01	124.22	128.28
5	A	1002	TM1	O3'-C1F-C2F	3.82	115.69	110.47
5	A	1002	TM1	C2'-C3'-C4'	3.58	112.07	103.78
5	A	1002	TM1	C1F-O2'-C2'	-3.53	99.80	107.85
6	A	1003	TG1	O3-C21-O4	3.47	129.88	123.40
6	A	1003	TG1	C24-C22-C21	3.46	133.78	120.79
6	A	1003	TG1	C7-C6-C5	3.20	123.82	115.41
6	A	1003	TG1	O1-C2-C3	-2.87	104.75	110.18
6	A	1003	TG1	O5-C12-O12	2.74	125.15	121.60
6	A	1003	TG1	C23-C22-C21	-2.71	109.16	116.12
6	A	1003	TG1	C2-O1-C13	2.66	121.91	117.59
5	A	1002	TM1	O3'-C3'-C2'	2.58	107.74	103.63
5	A	1002	TM1	O5'-C5'-C4'	2.18	116.42	108.99
6	A	1003	TG1	C8-O7-C27	2.12	121.89	118.03
5	A	1002	TM1	N9-C8-N7	-2.11	110.94	113.94
6	A	1003	TG1	O4-C21-C22	-2.08	118.68	125.28
5	A	1002	TM1	C6-C5-C4	2.05	119.98	117.18

There are no chirality outliers.

All (15) torsion outliers are listed below:

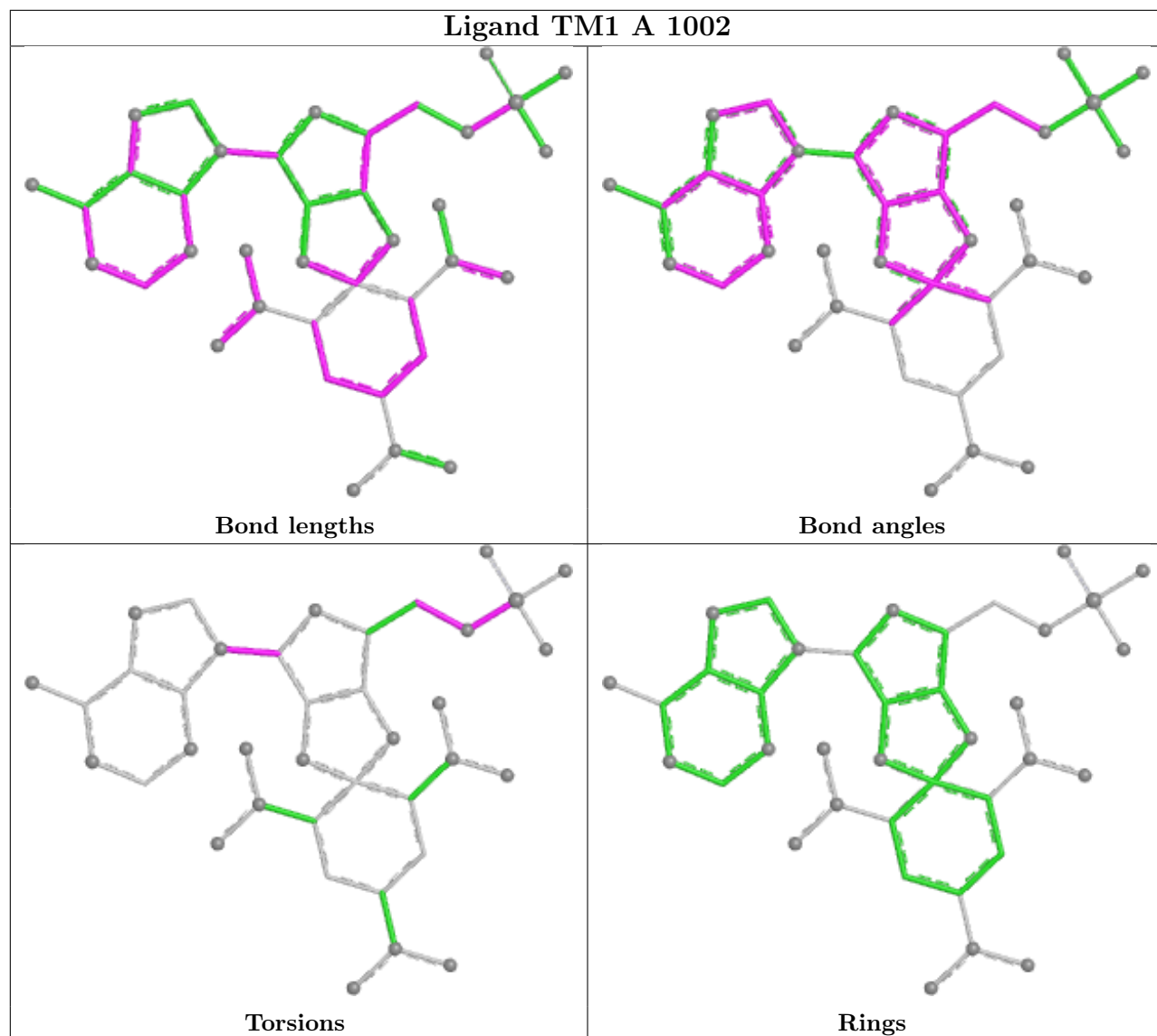
Mol	Chain	Res	Type	Atoms
5	A	1002	TM1	C2'-C1'-N9-C8
5	A	1002	TM1	C5'-O5'-PA-O1A
5	A	1002	TM1	C5'-O5'-PA-O2A
5	A	1002	TM1	C5'-O5'-PA-O3A
5	A	1002	TM1	C4'-C5'-O5'-PA
6	A	1003	TG1	O3-C21-C22-C23
6	A	1003	TG1	O3-C21-C22-C24
5	A	1002	TM1	C2'-C1'-N9-C4
6	A	1003	TG1	O4-C21-C22-C23
6	A	1003	TG1	O4-C21-C22-C24
6	A	1003	TG1	C17-C18-C19-C20
6	A	1003	TG1	C22-C21-O3-C3
6	A	1003	TG1	O1-C13-C14-C15
6	A	1003	TG1	O7-C27-C28-C29
6	A	1003	TG1	O2-C13-C14-C15

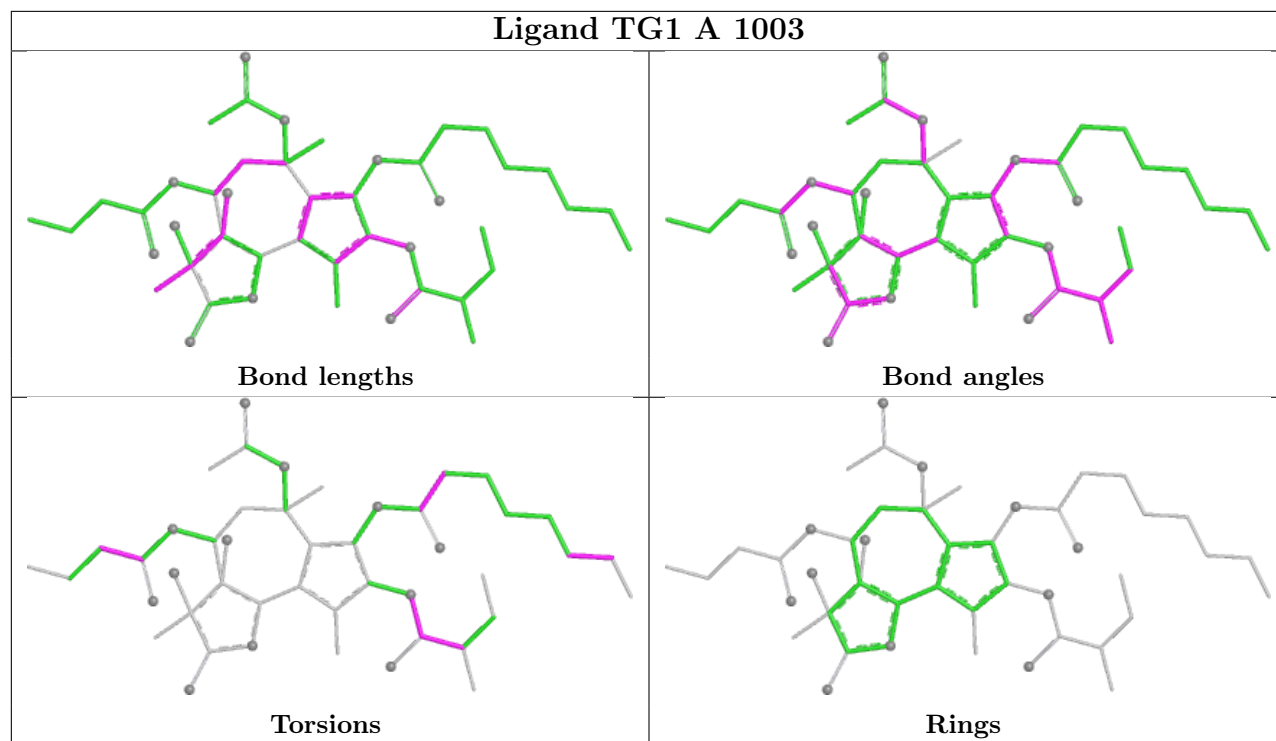
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1003	TG1	3	0
4	A	998	ALF	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	994/995 (99%)	0.27	72 (7%) 21 17	35, 71, 174, 196	1 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	ILE	5.2
1	A	866	THR	4.7
1	A	241	ALA	4.2
1	A	948	LEU	4.0
1	A	85	ILE	3.9
1	A	883	PHE	3.9
1	A	886	LEU	3.6
1	A	870	LEU	3.5
1	A	961	ALA	3.5
1	A	282	PRO	3.4
1	A	877	THR	3.3
1	A	277	GLY	3.2
1	A	276	ILE	3.1
1	A	273	LEU	3.0
1	A	73	PHE	3.0
1	A	106	VAL	3.0
1	A	958	LYS	2.9
1	A	283	VAL	2.9
1	A	867	TYR	2.9
1	A	975	LEU	2.9
1	A	274	ILE	2.8
1	A	75	LEU	2.8
1	A	242	THR	2.8
1	A	74	VAL	2.8
1	A	50	TRP	2.7
1	A	86	THR	2.7
1	A	844	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	890	ILE	2.6
1	A	947	ILE	2.6
1	A	279	PHE	2.6
1	A	858	TYR	2.6
1	A	946	LEU	2.6
1	A	78	PHE	2.5
1	A	859	ALA	2.5
1	A	504	SER	2.5
1	A	884	GLU	2.5
1	A	949	TYR	2.5
1	A	905	VAL	2.5
1	A	916	LEU	2.5
1	A	846	ALA	2.5
1	A	865	VAL	2.4
1	A	880	HIS	2.4
1	A	855	TRP	2.4
1	A	786	ALA	2.4
1	A	87	ALA	2.4
1	A	112	ALA	2.4
1	A	781	LEU	2.3
1	A	76	ALA	2.3
1	A	922	LEU	2.3
1	A	294	TYR	2.3
1	A	881	PRO	2.3
1	A	950	VAL	2.3
1	A	284	HIS	2.3
1	A	857	MET	2.3
1	A	268	CYS	2.2
1	A	868	HIS	2.2
1	A	951	ASP	2.2
1	A	107	TRP	2.2
1	A	989	ARG	2.2
1	A	843	TYR	2.2
1	A	111	ASN	2.1
1	A	763	TYR	2.1
1	A	978	ILE	2.1
1	A	977	VAL	2.1
1	A	955	MET	2.1
1	A	88	PHE	2.1
1	A	871	THR	2.0
1	A	767	SER	2.0
1	A	848	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	764	LEU	2.0
1	A	904	LEU	2.0
1	A	973	ILE	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](#)

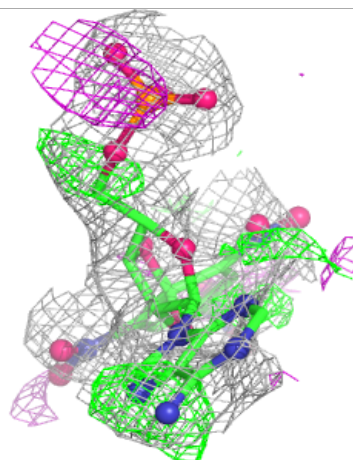
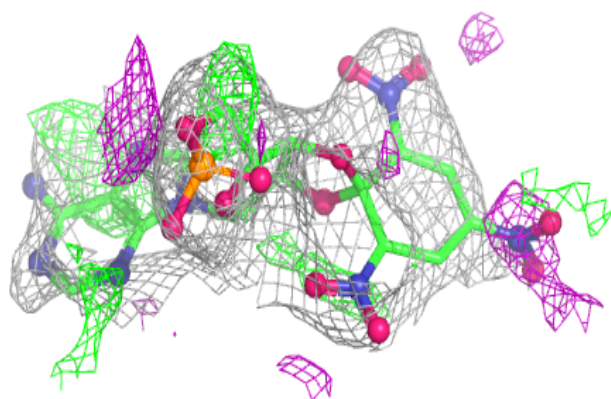
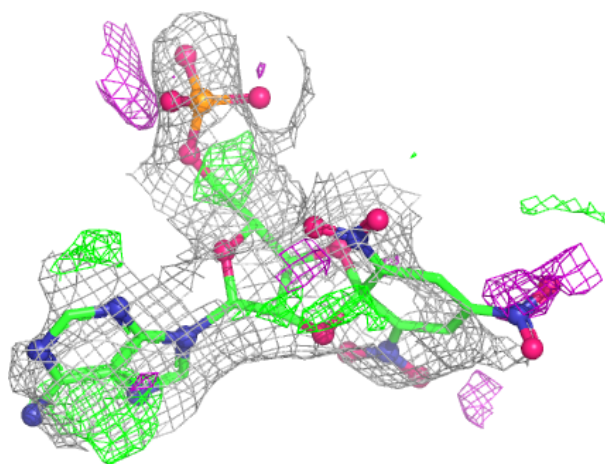
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	TM1	A	1002	38/38	0.73	0.20	146,151,157,159	0
6	TG1	A	1003	46/46	0.84	0.17	143,145,149,150	0
2	NA	A	1000	1/1	0.96	0.10	57,57,57,57	0
4	ALF	A	998	5/5	0.99	0.05	34,34,36,37	0
3	MG	A	995	1/1	1.00	0.01	37,37,37,37	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.

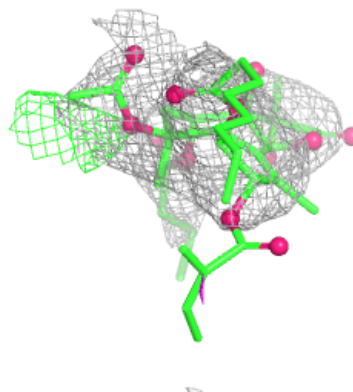
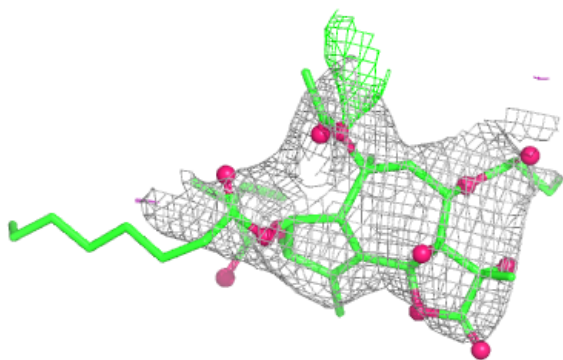
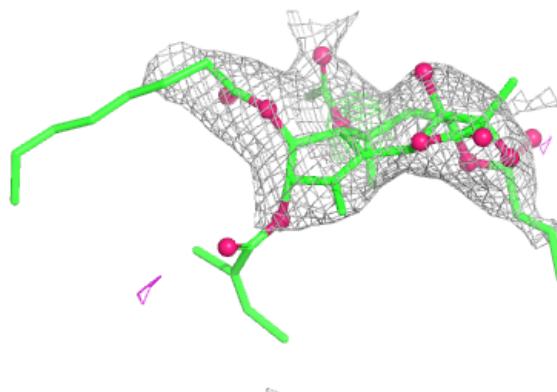
Electron density around TM1 A 1002:

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



Electron density around TG1 A 1003:

$2mF_o-DF_c$ (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.