



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:25 AM EDT

PDB ID : 3N5K / pdb_00003n5k
Title : Structure Of The (Sr)Ca²⁺-ATPase E2-AlF₄- Form
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Deposited on : 2010-05-25
Resolution : 2.20 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

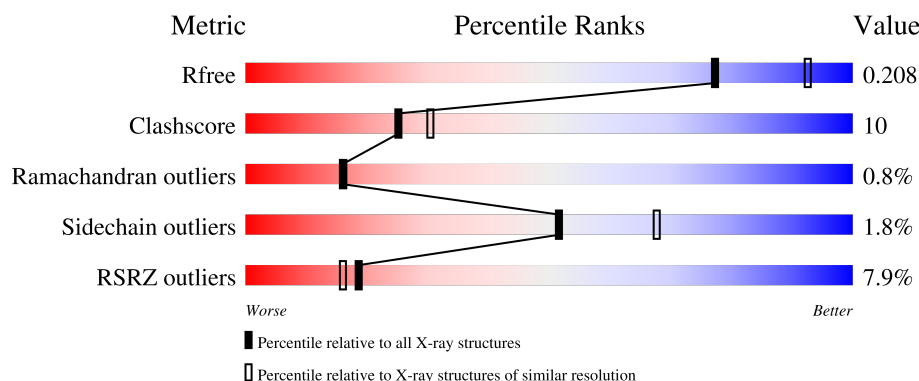
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	994	9% 81% 18% .
1	B	994	7% 81% 18% .

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
4	ALF	B	2002	-	-	X	-
6	ACT	A	3001	-	-	X	-
6	ACT	B	3001	-	-	X	-
6	ACT	B	3002	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16284 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.

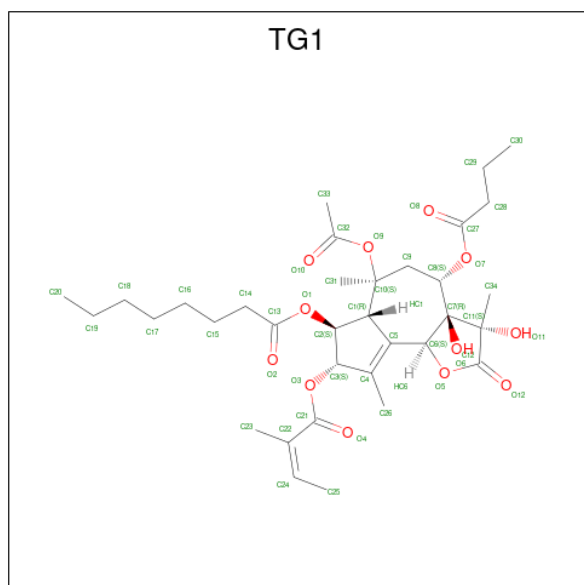
- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	ASP	SEE REMARK 999	UNP P04191
B	994	GLY	ASP	SEE REMARK 999	UNP P04191

- 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).

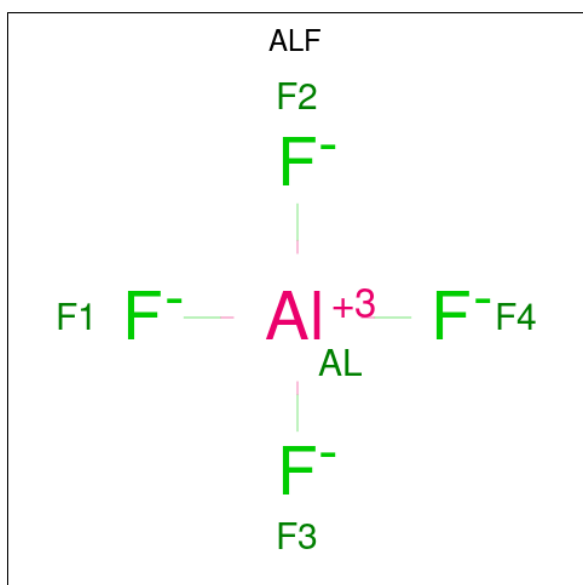


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			46	34	12		
2	B	1	Total	C	O	0	0
			46	34	12		

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

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

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	440	Total O 440 440	0	0
7	B	380	Total O 380 380	0	0

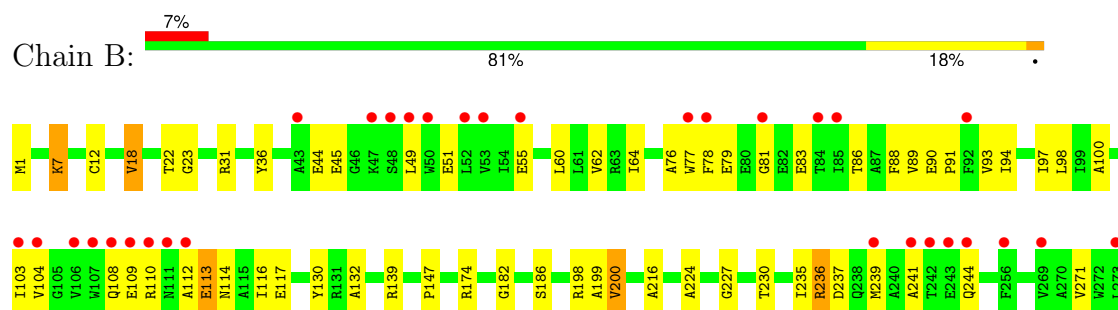
3 Residue-property plots

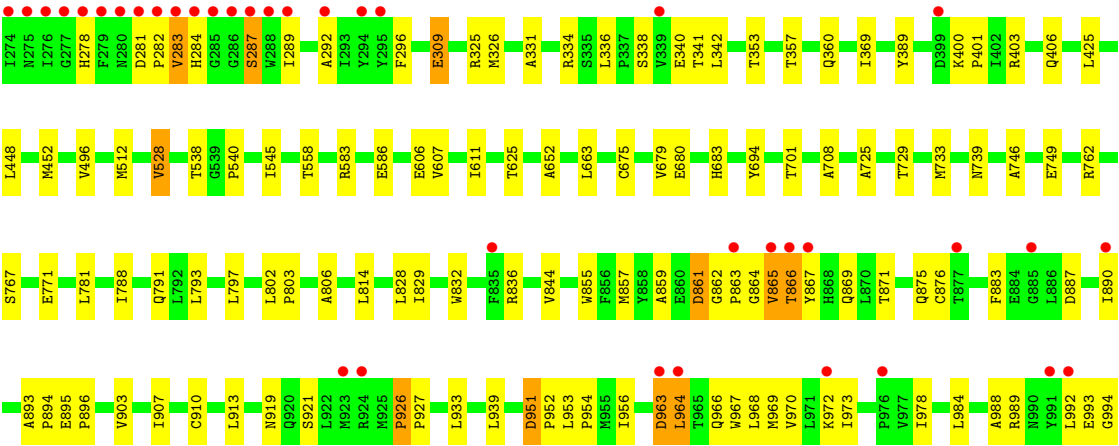
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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/endoplasmic reticulum calcium ATPase 1



- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.93Å 109.42Å 276.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.00 – 2.20 72.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (72.00-2.20) 99.7 (72.00-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.184 , 0.216 0.178 , 0.208	Depositor DCC
R_{free} test set	7823 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.1	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	0.95	EDS
Total number of atoms	16284	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: ALF, K, MG, TG1, ACT

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	0.62	0/7812	0.84	0/10592
1	B	0.60	0/7812	0.85	6/10592 (0.1%)
All	All	0.61	0/15624	0.84	6/21184 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	926	PRO	CA-C-N	6.87	127.16	119.32
1	B	926	PRO	C-N-CA	6.87	127.16	119.32
1	B	861	ASP	N-CA-C	5.89	121.79	113.02
1	B	18	VAL	CB-CA-C	-5.74	102.06	110.62
1	B	7	LYS	CA-CB-CG	5.68	125.45	114.10
1	B	694	TYR	N-CA-C	-5.37	106.60	112.72

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	146	0
1	B	7671	0	7764	148	0
2	A	46	0	50	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	46	0	50	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	8	0	6	3	0
6	B	8	0	6	5	0
7	A	440	0	0	3	0
7	B	380	0	0	0	0
All	All	16284	0	15640	303	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 10.

All (303) 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:1:MET:H2	1:B:7:LYS:NZ	1.59	0.99
2:A:1000:TG1:H232	2:A:1000:TG1:H161	1.40	0.98
1:B:1:MET:H2	1:B:7:LYS:HZ1	0.99	0.98
1:B:239:MET:HE2	1:B:708:ALA:CB	1.93	0.96
1:B:1:MET:HG3	1:B:224:ALA:O	1.65	0.94
1:A:242:THR:HA	1:A:243:GLU:CB	1.98	0.94
1:B:239:MET:HE2	1:B:708:ALA:HB3	1.59	0.84
1:A:909:MET:HE3	1:A:937:ILE:HG23	1.61	0.82
1:B:239:MET:HE2	1:B:708:ALA:HB1	1.62	0.81
1:B:762:ARG:HG2	1:B:829:ILE:HD11	1.64	0.80
1:B:1:MET:N	1:B:7:LYS:NZ	2.30	0.80
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.66	0.77
1:A:671:ARG:HD2	1:A:694:TYR:CE2	2.20	0.77
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.67	0.76
1:A:242:THR:HA	1:A:243:GLU:HB3	1.68	0.76
1:B:969:MET:HE3	1:B:973:ILE:HD11	1.66	0.76
1:B:216:ALA:HB1	6:B:3001:ACT:H2	1.68	0.76
1:A:242:THR:HA	1:A:243:GLU:HB2	1.66	0.75
1:A:862:GLY:H	1:A:863:PRO:HD3	1.51	0.75
1:B:861:ASP:N	1:B:862:GLY:HA3	2.02	0.74
1:A:774:CYS:O	1:A:778:THR:HG22	1.86	0.74
1:B:235:ILE:CG2	1:B:239:MET:HE3	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:TRP:CE3	1:A:896:PRO:HG3	2.25	0.71
1:B:90:GLU:HB3	1:B:91:PRO:HD3	1.73	0.71
1:A:267:ILE:HD11	2:A:1000:TG1:H182	1.72	0.70
1:B:338:SER:HA	1:B:341:THR:CG2	2.21	0.70
1:A:31:ARG:HH21	1:A:34:GLU:HG3	1.57	0.70
1:A:247:THR:HG23	1:A:250:GLN:H	1.56	0.69
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.27	0.69
1:B:7:LYS:HD2	1:B:12:CYS:SG	2.32	0.69
1:A:31:ARG:NH2	1:A:34:GLU:HG3	2.09	0.68
1:A:114:ASN:HB3	1:A:117:GLU:HG2	1.73	0.68
1:B:239:MET:CE	1:B:708:ALA:HB3	2.23	0.67
1:B:338:SER:HA	1:B:341:THR:HG22	1.77	0.67
1:B:230:THR:OG1	6:B:3002:ACT:H2	1.94	0.67
1:B:762:ARG:HG2	1:B:829:ILE:CD1	2.24	0.67
1:B:89:VAL:O	1:B:93:VAL:HG23	1.95	0.67
1:A:814:LEU:HD12	1:A:814:LEU:H	1.59	0.66
1:B:963:ASP:HB3	1:B:966:GLN:H	1.62	0.64
1:A:606:GLU:HG3	1:A:739:ASN:OD1	1.99	0.63
1:B:863:PRO:HB2	1:B:864:GLY:HA2	1.81	0.63
1:B:887:ASP:O	1:B:890:ILE:HG12	2.00	0.62
2:A:1000:TG1:H333	2:A:1000:TG1:HC91	1.82	0.62
1:B:282:PRO:HD2	1:B:284:HIS:CE1	2.33	0.62
1:B:583:ARG:O	1:B:586:GLU:HG2	2.00	0.62
1:A:285:GLY:N	1:A:286:GLY:HA3	2.13	0.62
1:A:242:THR:CA	1:A:243:GLU:CB	2.77	0.62
1:A:866:THR:HB	1:A:869:GLN:HB2	1.82	0.61
1:B:1:MET:N	1:B:7:LYS:HZ1	1.85	0.61
1:A:905:VAL:O	1:A:909:MET:HG2	2.00	0.61
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.82	0.61
1:B:100:ALA:O	1:B:103:ILE:HG12	2.00	0.61
1:B:910:CYS:HB3	1:B:978:ILE:HG13	1.82	0.61
1:A:319:LEU:HB3	1:A:336:LEU:HD22	1.82	0.60
1:B:200:VAL:HG22	1:B:680:GLU:HG3	1.84	0.60
1:B:235:ILE:HG23	1:B:239:MET:HE3	1.84	0.60
1:B:836:ARG:HG2	1:B:984:LEU:HB3	1.82	0.60
1:A:342:LEU:CD2	1:A:733:MET:HE1	2.32	0.59
1:B:867:TYR:CZ	1:B:871:THR:HG21	2.37	0.59
1:A:97:ILE:HD11	1:A:797:LEU:HD22	1.83	0.59
1:B:114:ASN:HD22	1:B:117:GLU:H	1.50	0.59
1:B:876:CYS:HA	1:B:883:PHE:CD2	2.37	0.59
1:B:952:PRO:O	1:B:956:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ALA:O	1:B:79:GLU:HB3	2.03	0.58
1:B:988:ALA:HA	1:B:992:LEU:HB2	1.84	0.58
2:B:1000:TG1:H313	2:B:1000:TG1:C33	2.33	0.58
1:A:309:GLU:HG3	1:A:793:LEU:HD23	1.85	0.58
1:A:864:GLY:O	1:A:866:THR:HG23	2.04	0.58
1:A:342:LEU:HD22	1:A:733:MET:HE1	1.86	0.58
1:B:865:VAL:HG12	1:B:869:GLN:HB2	1.86	0.58
1:B:855:TRP:CE3	1:B:896:PRO:HG3	2.40	0.57
1:A:242:THR:CA	1:A:243:GLU:HB2	2.33	0.57
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.87	0.57
1:B:353:THR:HA	1:B:357:THR:OG1	2.05	0.57
1:A:247:THR:CG2	1:A:250:GLN:H	2.17	0.57
1:B:866:THR:HG23	1:B:869:GLN:H	1.70	0.57
1:B:51:GLU:O	1:B:55:GLU:HG3	2.05	0.56
1:A:278:HIS:O	1:A:282:PRO:HB3	2.05	0.56
1:A:893:ALA:O	1:A:896:PRO:HD2	2.05	0.56
1:A:863:PRO:CB	1:A:864:GLY:HA2	2.34	0.56
1:A:120:LYS:HG2	1:A:123:GLU:OE2	2.06	0.56
1:B:863:PRO:HB2	1:B:864:GLY:CA	2.36	0.56
1:A:679:VAL:HB	1:A:683:HIS:HB2	1.86	0.56
1:A:863:PRO:HB2	1:A:864:GLY:HA2	1.88	0.55
1:B:844:VAL:HG22	1:B:907:ILE:HG21	1.88	0.55
1:B:216:ALA:CB	6:B:3001:ACT:H2	2.36	0.55
1:B:963:ASP:H	1:B:966:GLN:HB2	1.70	0.55
2:A:1000:TG1:H161	2:A:1000:TG1:C23	2.27	0.55
1:B:227:GLY:O	6:B:3002:ACT:H3	2.07	0.55
1:A:120:LYS:HA	1:A:123:GLU:OE2	2.07	0.55
1:B:893:ALA:O	1:B:896:PRO:HD2	2.07	0.55
1:A:247:THR:OG1	1:A:248:PRO:HD2	2.07	0.54
1:A:829:ILE:HD13	2:A:1000:TG1:H333	1.89	0.54
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.88	0.54
1:A:880:HIS:HD2	1:A:888:CYS:SG	2.30	0.54
1:A:107:TRP:HA	1:A:110:ARG:HD3	1.89	0.54
1:B:963:ASP:HB2	1:B:966:GLN:CG	2.38	0.54
1:A:952:PRO:HB2	1:A:955:MET:HE2	1.89	0.54
1:B:287:SER:C	1:B:289:ILE:H	2.16	0.54
1:B:857:MET:HE2	1:B:867:TYR:HA	1.89	0.54
2:B:1000:TG1:HC91	2:B:1000:TG1:H333	1.89	0.53
1:B:832:TRP:CD1	1:B:988:ALA:HB2	2.44	0.53
1:A:270:ALA:O	1:A:274:ILE:HG12	2.09	0.53
1:A:855:TRP:HA	1:A:859:ALA:CB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:HB2	1:B:139:ARG:NH1	2.23	0.52
1:A:80:GLU:HG3	1:A:81:GLY:H	1.75	0.52
1:B:325:ARG:NH1	1:B:749:GLU:OE2	2.38	0.52
1:A:862:GLY:N	1:A:863:PRO:HD3	2.23	0.52
1:B:887:ASP:HB3	1:B:890:ILE:HD11	1.91	0.52
1:B:953:LEU:HB2	1:B:954:PRO:HD3	1.90	0.52
1:A:947:ILE:HG22	1:A:959:LEU:HD12	1.91	0.52
1:A:984:LEU:HA	1:A:987:ILE:HD11	1.92	0.52
1:B:97:ILE:HG13	1:B:797:LEU:HD21	1.91	0.52
1:A:326:MET:SD	1:A:749:GLU:HG2	2.50	0.52
1:A:863:PRO:CD	1:A:864:GLY:HA2	2.40	0.51
1:A:949:TYR:CZ	1:A:961:ALA:HB1	2.45	0.51
1:B:88:PHE:C	1:B:91:PRO:HD2	2.34	0.51
1:B:309:GLU:HG3	1:B:793:LEU:CD2	2.40	0.51
1:A:267:ILE:O	1:A:271:VAL:HG23	2.09	0.51
1:A:832:TRP:HZ2	1:A:987:ILE:HD11	1.75	0.51
1:A:894:PRO:HD2	1:A:895:GLU:OE1	2.10	0.51
1:B:836:ARG:HA	1:B:984:LEU:HD13	1.93	0.51
1:A:864:GLY:O	1:A:865:VAL:C	2.54	0.51
1:A:909:MET:CE	1:A:937:ILE:HA	2.41	0.51
1:A:918:GLU:HG2	1:A:919:ASN:OD1	2.11	0.51
1:A:953:LEU:HB2	1:A:954:PRO:HD3	1.92	0.51
1:B:802:LEU:HB2	1:B:803:PRO:HD3	1.93	0.51
1:A:79:GLU:HG2	1:A:80:GLU:N	2.25	0.50
1:A:79:GLU:HG2	1:A:80:GLU:H	1.77	0.50
1:A:277:GLY:C	1:A:279:PHE:H	2.18	0.50
1:B:109:GLU:O	1:B:109:GLU:HG2	2.11	0.50
1:B:369:ILE:HG13	1:B:528:VAL:HG13	1.93	0.50
1:B:969:MET:O	1:B:973:ILE:HG13	2.12	0.50
1:A:93:VAL:O	1:A:97:ILE:HG12	2.11	0.50
1:B:863:PRO:HB2	1:B:865:VAL:N	2.27	0.50
1:B:867:TYR:CE2	1:B:871:THR:HG21	2.47	0.50
1:B:77:TRP:HD1	1:B:78:PHE:CE1	2.30	0.49
1:B:200:VAL:HG22	1:B:680:GLU:CG	2.41	0.49
1:B:292:ALA:O	1:B:296:PHE:HD1	1.95	0.49
1:B:863:PRO:CB	1:B:864:GLY:HA2	2.42	0.49
1:A:172:THR:OG1	6:A:3001:ACT:H1	2.13	0.49
1:A:100:ALA:O	1:A:103:ILE:HG12	2.13	0.49
1:B:227:GLY:O	6:B:3002:ACT:CH3	2.61	0.49
1:A:305:ALA:HB2	1:A:792:LEU:HD13	1.95	0.49
1:A:866:THR:O	1:A:867:TYR:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:LEU:O	1:B:452:MET:HG3	2.13	0.49
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.96	0.48
1:A:811:PRO:HG2	1:A:929:VAL:HG13	1.94	0.48
1:B:963:ASP:CB	1:B:966:GLN:H	2.26	0.48
1:A:185:VAL:HG13	1:A:185:VAL:O	2.12	0.48
1:A:489:ARG:HD3	7:A:1316:HOH:O	2.13	0.48
1:A:639:ILE:HD11	1:A:641:ILE:HD12	1.95	0.48
1:B:88:PHE:O	1:B:91:PRO:HD2	2.14	0.48
1:A:31:ARG:O	1:A:34:GLU:HG2	2.13	0.48
1:B:992:LEU:O	1:B:994:GLY:HA3	2.13	0.48
1:A:969:MET:HE3	1:A:973:ILE:HD11	1.95	0.48
6:A:3002:ACT:H1	7:A:1082:HOH:O	2.14	0.48
1:B:919:ASN:O	1:B:989:ARG:HD3	2.14	0.48
1:A:256:PHE:CZ	1:A:765:ILE:HD13	2.49	0.48
1:A:795:VAL:HA	1:A:799:THR:HB	1.96	0.48
2:A:1000:TG1:H162	2:A:1000:TG1:H191	1.52	0.48
1:B:113:GLU:HG2	1:B:729:THR:HG22	1.94	0.48
1:A:402:ILE:C	1:A:402:ILE:HD12	2.39	0.48
1:A:950:VAL:O	1:A:953:LEU:HB2	2.14	0.47
1:B:44:GLU:HG3	1:B:45:GLU:N	2.29	0.47
1:B:114:ASN:HD21	1:B:116:ILE:HB	1.79	0.47
1:A:800:ASP:C	1:A:803:PRO:HD2	2.38	0.47
1:B:90:GLU:O	1:B:94:ILE:HG13	2.14	0.47
1:A:44:GLU:HB3	1:A:114:ASN:HD21	1.78	0.47
1:A:857:MET:HA	1:A:865:VAL:HA	1.96	0.47
1:B:369:ILE:HD11	1:B:545:ILE:HD11	1.96	0.47
1:A:276:ILE:O	1:A:279:PHE:HB3	2.14	0.47
1:B:859:ALA:O	1:B:862:GLY:HA3	2.15	0.47
1:A:256:PHE:CE1	1:A:765:ILE:HD13	2.49	0.47
1:B:60:LEU:O	1:B:64:ILE:HG12	2.14	0.47
1:A:373:ASP:O	1:A:375:ASP:N	2.47	0.47
1:B:236:ARG:HG3	1:B:237:ASP:N	2.28	0.47
1:B:802:LEU:HD13	1:B:939:LEU:HD23	1.97	0.47
1:A:44:GLU:HB2	1:A:116:ILE:HD12	1.95	0.47
1:A:962:LEU:HB3	1:A:966:GLN:HB2	1.96	0.47
1:B:725:ALA:O	1:B:729:THR:HG23	2.15	0.47
1:B:62:VAL:HG13	1:B:98:LEU:HD22	1.96	0.47
1:A:309:GLU:HG3	1:A:793:LEU:CD2	2.45	0.47
1:A:495:SER:HB3	1:A:514:VAL:HG22	1.96	0.46
1:A:577:VAL:HG11	7:A:1375:HOH:O	2.14	0.46
1:B:910:CYS:O	1:B:913:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:PRO:N	1:A:864:GLY:HA2	2.30	0.46
1:A:898:THR:HG23	1:A:948:LEU:HD21	1.97	0.46
1:A:909:MET:HE1	1:A:940:SER:HB2	1.97	0.46
1:B:342:LEU:HD23	1:B:746:ALA:HB1	1.98	0.46
1:A:876:CYS:HA	1:A:883:PHE:CD2	2.50	0.46
1:A:910:CYS:HB3	1:A:978:ILE:HG13	1.98	0.46
1:A:909:MET:CE	1:A:940:SER:HB2	2.46	0.46
1:B:963:ASP:HB2	1:B:966:GLN:HG3	1.98	0.46
1:B:403:ARG:HB2	1:B:406:GLN:HG2	1.97	0.46
1:B:876:CYS:HA	1:B:883:PHE:CE2	2.51	0.46
1:A:353:THR:HA	1:A:357:THR:OG1	2.16	0.46
1:A:863:PRO:N	1:A:864:GLY:CA	2.79	0.46
1:B:865:VAL:HG12	1:B:866:THR:H	1.80	0.45
2:B:1000:TG1:H313	2:B:1000:TG1:H333	1.98	0.45
1:A:115:ALA:HB1	1:A:239:MET:CE	2.46	0.45
1:B:951:ASP:CG	1:B:952:PRO:HA	2.41	0.45
1:A:650:ASP:O	1:A:672:ARG:HD2	2.17	0.45
1:B:342:LEU:HD22	1:B:733:MET:HE1	1.98	0.45
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.99	0.45
1:B:862:GLY:H	1:B:863:PRO:HD3	1.82	0.45
1:A:115:ALA:HB1	1:A:239:MET:HE1	1.98	0.45
1:A:62:VAL:HG13	1:A:98:LEU:HD22	1.99	0.44
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.43	0.44
1:A:50:TRP:O	1:A:54:ILE:HG12	2.18	0.44
1:A:377:CYS:HB3	1:A:544:LYS:HG2	2.00	0.44
1:B:104:VAL:O	1:B:108:GLN:HG2	2.17	0.44
1:B:993:GLU:HA	1:B:994:GLY:HA3	1.75	0.44
1:B:857:MET:HE1	1:B:867:TYR:HD1	1.81	0.44
1:A:880:HIS:N	1:A:881:PRO:CD	2.80	0.44
1:B:538:THR:OG1	1:B:540:PRO:HD2	2.18	0.44
1:B:110:ARG:HH22	1:B:112:ALA:HB2	1.83	0.44
1:B:558:THR:O	1:B:558:THR:HG22	2.18	0.44
1:A:784:PRO:O	1:A:785:GLU:C	2.61	0.44
1:B:607:VAL:O	1:B:611:ILE:HG12	2.18	0.44
1:B:22:THR:HG22	1:B:132:ALA:HB2	1.99	0.43
1:B:282:PRO:O	1:B:283:VAL:HB	2.18	0.43
1:B:894:PRO:HD2	1:B:895:GLU:OE1	2.18	0.43
1:B:968:LEU:O	1:B:972:LYS:HG2	2.18	0.43
2:B:1000:TG1:H141	2:B:1000:TG1:H171	1.62	0.43
1:A:893:ALA:HA	1:A:894:PRO:HD3	1.83	0.43
1:B:606:GLU:HG3	1:B:739:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:LEU:N	1:A:976:PRO:CD	2.82	0.43
1:B:283:VAL:CG2	1:B:875:GLN:HE21	2.31	0.43
1:B:893:ALA:HA	1:B:894:PRO:HD3	1.81	0.43
1:A:880:HIS:CD2	1:A:888:CYS:SG	3.11	0.43
1:B:7:LYS:HB2	1:B:12:CYS:SG	2.59	0.43
1:B:23:GLY:HA3	1:B:130:TYR:O	2.18	0.43
1:A:367:PHE:C	1:A:367:PHE:CD2	2.96	0.43
1:B:281:ASP:N	1:B:282:PRO:HD3	2.32	0.43
1:B:967:TRP:O	1:B:970:VAL:HB	2.17	0.43
1:B:336:LEU:HD23	1:B:336:LEU:HA	1.88	0.43
1:B:855:TRP:HA	1:B:859:ALA:CB	2.49	0.43
1:B:903:VAL:O	1:B:907:ILE:HG13	2.18	0.43
1:A:106:VAL:O	1:A:110:ARG:HG3	2.19	0.43
1:A:922:LEU:HA	1:A:925:MET:O	2.19	0.43
1:B:972:LYS:HA	1:B:972:LYS:HD3	1.78	0.43
1:A:305:ALA:HB1	1:A:771:GLU:HB3	1.99	0.42
1:A:883:PHE:HB3	1:A:886:LEU:HD11	2.01	0.42
1:A:895:GLU:N	1:A:896:PRO:CD	2.82	0.42
1:B:652:ALA:HA	1:B:675:CYS:O	2.19	0.42
1:B:855:TRP:HA	1:B:859:ALA:HB2	2.01	0.42
1:A:333:VAL:HG22	1:A:733:MET:HE2	2.01	0.42
1:B:198:ARG:O	1:B:199:ALA:C	2.62	0.42
1:B:964:LEU:H	1:B:964:LEU:HG	1.39	0.42
1:B:182:GLY:HA3	4:B:2002:ALF:F1	2.09	0.42
1:B:836:ARG:HG2	1:B:984:LEU:HD13	2.02	0.42
1:A:33:LEU:HD13	1:A:146:VAL:CG1	2.49	0.42
1:A:85:ILE:HD12	1:A:85:ILE:N	2.33	0.42
1:A:625:THR:HA	4:A:2002:ALF:F4	2.09	0.42
1:B:389:TYR:HB3	1:B:425:LEU:HD21	2.01	0.42
1:A:31:ARG:HA	1:A:34:GLU:HG2	2.00	0.42
1:A:135:LYS:HD2	1:A:135:LYS:HA	1.88	0.42
1:A:769:VAL:O	1:A:773:VAL:HG23	2.20	0.42
1:B:83:GLU:HG2	1:B:86:THR:OG1	2.19	0.42
1:A:654:THR:HA	1:A:677:ALA:O	2.20	0.42
1:A:671:ARG:CD	1:A:694:TYR:CZ	2.99	0.42
1:A:753:ILE:O	1:A:757:MET:HG3	2.20	0.42
1:B:926:PRO:HA	1:B:927:PRO:HD3	1.94	0.42
1:A:80:GLU:HG3	1:A:81:GLY:N	2.34	0.42
1:A:71:ILE:O	1:A:75:LEU:HD13	2.20	0.41
1:A:341:THR:HG22	1:A:716:ILE:HD11	2.01	0.41
1:B:326:MET:HE3	1:B:331:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:ILE:HG12	1:B:791:GLN:OE1	2.20	0.41
1:A:67:LEU:O	1:A:71:ILE:HG13	2.20	0.41
1:B:400:LYS:HA	1:B:401:PRO:HD3	1.92	0.41
1:B:36:TYR:CG	1:B:147:PRO:HG2	2.56	0.41
1:B:679:VAL:HB	1:B:683:HIS:HB2	2.01	0.41
1:A:216:ALA:HB1	6:A:3001:ACT:H2	2.03	0.41
1:A:288:TRP:CD1	1:A:289:ILE:HG13	2.56	0.41
1:A:708:ALA:HB3	1:A:709:PRO:HD3	2.02	0.41
1:A:836:ARG:HG3	1:A:984:LEU:HD13	2.02	0.41
1:A:868:HIS:CE1	1:A:872:HIS:CE1	3.09	0.41
1:B:139:ARG:HB2	1:B:139:ARG:HH11	1.85	0.41
1:B:174:ARG:HB3	1:B:186:SER:HB3	2.02	0.41
1:B:951:ASP:OD1	1:B:952:PRO:HA	2.20	0.41
1:A:898:THR:CG2	1:A:948:LEU:HD21	2.50	0.41
1:B:200:VAL:HG22	1:B:680:GLU:CD	2.45	0.41
1:B:814:LEU:HD12	1:B:814:LEU:N	2.36	0.41
1:A:984:LEU:HA	1:A:987:ILE:CD1	2.50	0.41
1:A:833:LEU:O	1:A:836:ARG:HB3	2.21	0.41
1:B:94:ILE:HG12	1:B:793:LEU:HD11	2.03	0.41
1:B:309:GLU:HG3	1:B:793:LEU:HD23	2.02	0.41
1:B:282:PRO:C	1:B:284:HIS:H	2.29	0.41
1:B:496:VAL:O	1:B:512:MET:HA	2.22	0.41
1:A:956:ILE:HD11	1:A:957:PHE:CE1	2.56	0.40
1:B:767:SER:O	1:B:771:GLU:HG3	2.21	0.40
1:B:625:THR:HA	4:B:2002:ALF:F4	2.11	0.40
1:A:88:PHE:C	1:A:91:PRO:HD2	2.45	0.40
1:A:256:PHE:HB2	2:A:1000:TG1:H291	2.02	0.40
1:A:855:TRP:CZ3	1:A:896:PRO:HG3	2.56	0.40
1:B:278:HIS:O	1:B:278:HIS:CG	2.73	0.40
1:B:788:ILE:HG12	1:B:791:GLN:CD	2.47	0.40
1:B:806:ALA:HB1	1:B:933:LEU:HA	2.02	0.40
1:B:887:ASP:HB3	1:B:890:ILE:CD1	2.52	0.40
1:A:703:ASP:HB2	1:A:723:GLY:HA3	2.04	0.40
1:A:947:ILE:HD13	1:A:957:PHE:CE1	2.56	0.40
1:B:828:LEU:N	1:B:828:LEU:HD12	2.36	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%)	941 (95%)	41 (4%)	10 (1%)	12	11
1	B	992/994 (100%)	951 (96%)	36 (4%)	5 (0%)	24	27
All	All	1984/1988 (100%)	1892 (95%)	77 (4%)	15 (1%)	16	16

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	GLU
1	A	889	GLU
1	B	283	VAL
1	A	374	GLY
1	A	865	VAL
1	A	992	LEU
1	B	241	ALA
1	A	283	VAL
1	A	785	GLU
1	A	47	LYS
1	A	877	THR
1	B	244	GLN
1	B	287	SER
1	A	867	TYR
1	B	81	GLY

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%)	830 (99%)	10 (1%)	63	78
1	B	840/840 (100%)	819 (98%)	21 (2%)	42	56
All	All	1680/1680 (100%)	1649 (98%)	31 (2%)	51	68

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

Mol	Chain	Res	Type
1	A	220	LEU
1	A	255	GLU
1	A	309	GLU
1	A	323	THR
1	A	577	VAL
1	A	814	LEU
1	A	929	VAL
1	A	975	LEU
1	A	982	GLU
1	A	987	ILE
1	B	18	VAL
1	B	31	ARG
1	B	49	LEU
1	B	113	GLU
1	B	200	VAL
1	B	236	ARG
1	B	271	VAL
1	B	309	GLU
1	B	334	ARG
1	B	340	GLU
1	B	360	GLN
1	B	528	VAL
1	B	663	LEU
1	B	701	THR
1	B	781	LEU
1	B	865	VAL
1	B	866	THR
1	B	921	SER
1	B	951	ASP
1	B	963	ASP
1	B	964	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	259	GLN
1	A	868	HIS
1	A	880	HIS
1	A	911	ASN
1	A	920	GLN
1	B	38	HIS
1	B	114	ASN
1	B	278	HIS
1	B	284	HIS
1	B	359	ASN
1	B	406	GLN
1	B	456	ASN
1	B	692	GLN
1	B	875	GLN
1	B	920	GLN
1	B	990	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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
4	ALF	A	2002	7,1	4,4,4	1.30	0	-		
4	ALF	B	2002	7,1	4,4,4	1.37	0	-		
2	TG1	B	1000	-	44,48,48	2.12	10 (22%)	47,72,72	3.59	14 (29%)
6	ACT	A	3001	-	3,3,3	0.84	0	3,3,3	0.62	0
6	ACT	B	3001	-	3,3,3	0.94	0	3,3,3	0.70	0
2	TG1	A	1000	-	44,48,48	2.12	10 (22%)	47,72,72	3.71	14 (29%)
6	ACT	A	3002	-	3,3,3	0.71	0	3,3,3	1.90	1 (33%)
6	ACT	B	3002	-	3,3,3	0.81	0	3,3,3	0.81	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
2	TG1	A	1000	-	-	17/33/99/99	0/3/3/3
2	TG1	B	1000	-	-	17/33/99/99	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	TG1	O12-C12	8.20	1.38	1.20
2	A	1000	TG1	O12-C12	7.85	1.38	1.20
2	B	1000	TG1	C4-C5	4.93	1.55	1.33
2	A	1000	TG1	C4-C5	4.88	1.54	1.33
2	A	1000	TG1	C3-C4	3.97	1.55	1.50
2	A	1000	TG1	O5-C12	3.92	1.41	1.35
2	B	1000	TG1	C24-C22	3.80	1.54	1.31
2	B	1000	TG1	O5-C12	3.79	1.41	1.35
2	A	1000	TG1	C24-C22	3.74	1.53	1.31
2	B	1000	TG1	C3-C4	3.70	1.55	1.50
2	A	1000	TG1	O9-C10	-3.17	1.43	1.48
2	A	1000	TG1	O7-C8	-3.15	1.41	1.46
2	B	1000	TG1	O9-C10	-3.15	1.43	1.48
2	B	1000	TG1	O7-C8	-3.07	1.41	1.46
2	A	1000	TG1	C11-C7	2.48	1.58	1.55
2	B	1000	TG1	O3-C21	2.26	1.39	1.34
2	A	1000	TG1	O3-C21	2.08	1.39	1.34
2	B	1000	TG1	C11-C7	2.07	1.58	1.55
2	B	1000	TG1	O6-C7	-2.06	1.39	1.43
2	A	1000	TG1	C2-C3	2.05	1.56	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	TG1	O12-C12-C11	-17.42	110.66	128.28
2	B	1000	TG1	O12-C12-C11	-16.15	111.95	128.28
2	B	1000	TG1	O5-C12-O12	-12.15	105.88	121.60
2	A	1000	TG1	O5-C12-O12	-12.14	105.89	121.60
2	B	1000	TG1	C10-O9-C32	6.29	136.10	121.36
2	A	1000	TG1	C10-O9-C32	6.00	135.42	121.36
2	A	1000	TG1	O5-C6-C5	-4.75	104.13	111.17
2	B	1000	TG1	O3-C21-O4	-4.26	115.46	123.40
2	A	1000	TG1	C23-C22-C24	-4.24	106.86	123.12
2	A	1000	TG1	C10-C1-C5	4.03	120.54	115.07
2	B	1000	TG1	O5-C6-C5	-3.97	105.29	111.17
2	A	1000	TG1	O3-C21-O4	-3.95	116.03	123.40
2	B	1000	TG1	C23-C22-C24	-3.91	108.11	123.12
2	B	1000	TG1	C26-C4-C3	-3.87	114.79	121.24
2	B	1000	TG1	O1-C2-C3	-3.82	102.97	110.18
2	A	1000	TG1	O1-C2-C3	-3.40	103.75	110.18
2	B	1000	TG1	C10-C1-C5	3.36	119.64	115.07
2	A	1000	TG1	C23-C22-C21	-3.11	108.12	116.12
2	B	1000	TG1	C23-C22-C21	-2.73	109.11	116.12
2	A	1000	TG1	C26-C4-C3	-2.69	116.75	121.24
2	B	1000	TG1	C26-C4-C5	-2.62	123.51	130.03
2	A	1000	TG1	C26-C4-C5	-2.61	123.54	130.03
6	A	3002	ACT	OXT-C-CH3	2.58	125.89	115.05
2	B	1000	TG1	O7-C8-C9	2.47	111.05	106.63
2	A	1000	TG1	O7-C8-C9	2.45	111.01	106.63
2	B	1000	TG1	O1-C13-O2	-2.38	118.14	123.70
2	A	1000	TG1	O9-C32-C33	-2.27	106.82	110.67
2	A	1000	TG1	O9-C32-O10	-2.20	119.78	123.61
2	B	1000	TG1	O9-C32-O10	-2.05	120.04	123.61

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	TG1	C9-C10-O9-C32
2	A	1000	TG1	C1-C10-O9-C32
2	A	1000	TG1	C31-C10-O9-C32
2	A	1000	TG1	C14-C13-O1-C2
2	A	1000	TG1	C22-C21-O3-C3
2	A	1000	TG1	O3-C21-C22-C24
2	A	1000	TG1	O10-C32-O9-C10

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Mol	Chain	Res	Type	Atoms
2	A	1000	TG1	C33-C32-O9-C10
2	B	1000	TG1	C9-C10-O9-C32
2	B	1000	TG1	C1-C10-O9-C32
2	B	1000	TG1	O3-C21-C22-C24
2	B	1000	TG1	C21-C22-C24-C25
2	B	1000	TG1	O10-C32-O9-C10
2	B	1000	TG1	C33-C32-O9-C10
2	A	1000	TG1	O2-C13-O1-C2
2	A	1000	TG1	O4-C21-O3-C3
2	B	1000	TG1	O4-C21-O3-C3
2	B	1000	TG1	C22-C21-O3-C3
2	A	1000	TG1	C16-C17-C18-C19
2	B	1000	TG1	C14-C15-C16-C17
2	A	1000	TG1	C21-C22-C24-C25
2	B	1000	TG1	C13-C14-C15-C16
2	B	1000	TG1	C16-C17-C18-C19
2	A	1000	TG1	O4-C21-C22-C24
2	B	1000	TG1	C15-C16-C17-C18
2	B	1000	TG1	O2-C13-O1-C2
2	A	1000	TG1	C15-C16-C17-C18
2	B	1000	TG1	O4-C21-C22-C24
2	A	1000	TG1	C14-C15-C16-C17
2	B	1000	TG1	C17-C18-C19-C20
2	A	1000	TG1	C13-C14-C15-C16
2	A	1000	TG1	C17-C18-C19-C20
2	B	1000	TG1	C31-C10-O9-C32
2	B	1000	TG1	O4-C21-C22-C23

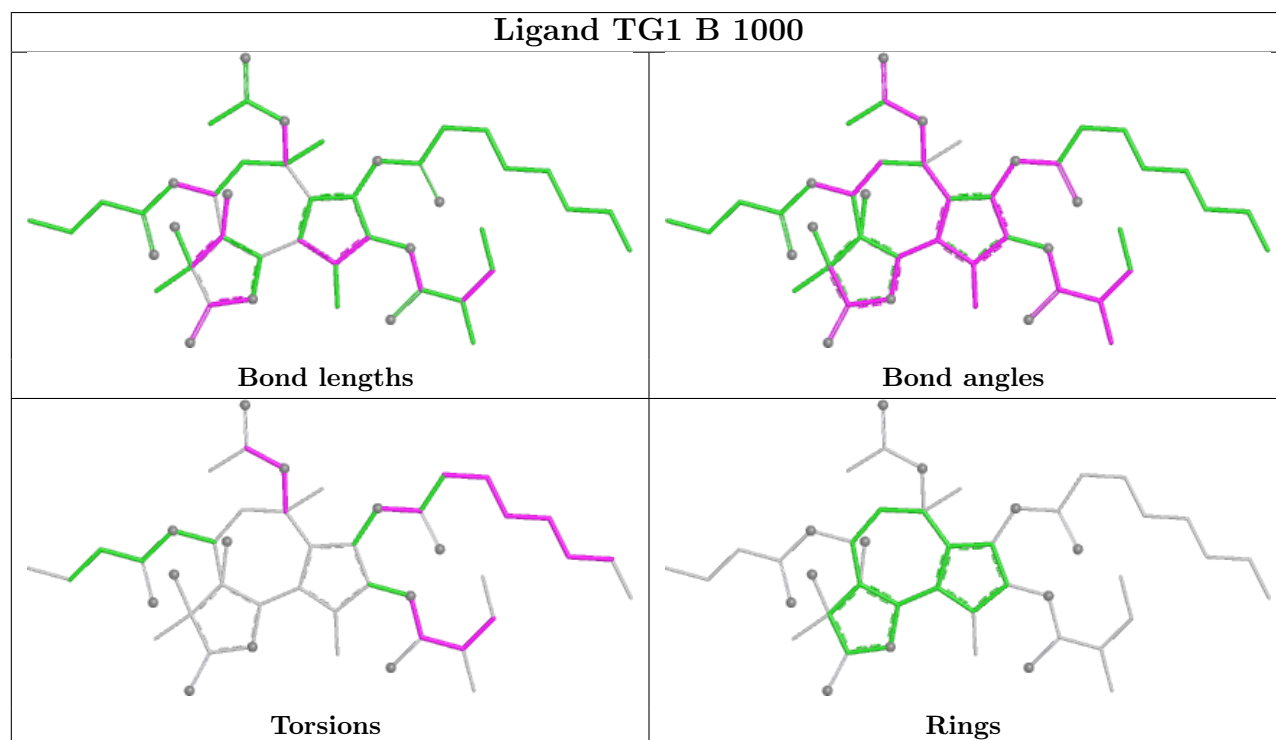
There are no ring outliers.

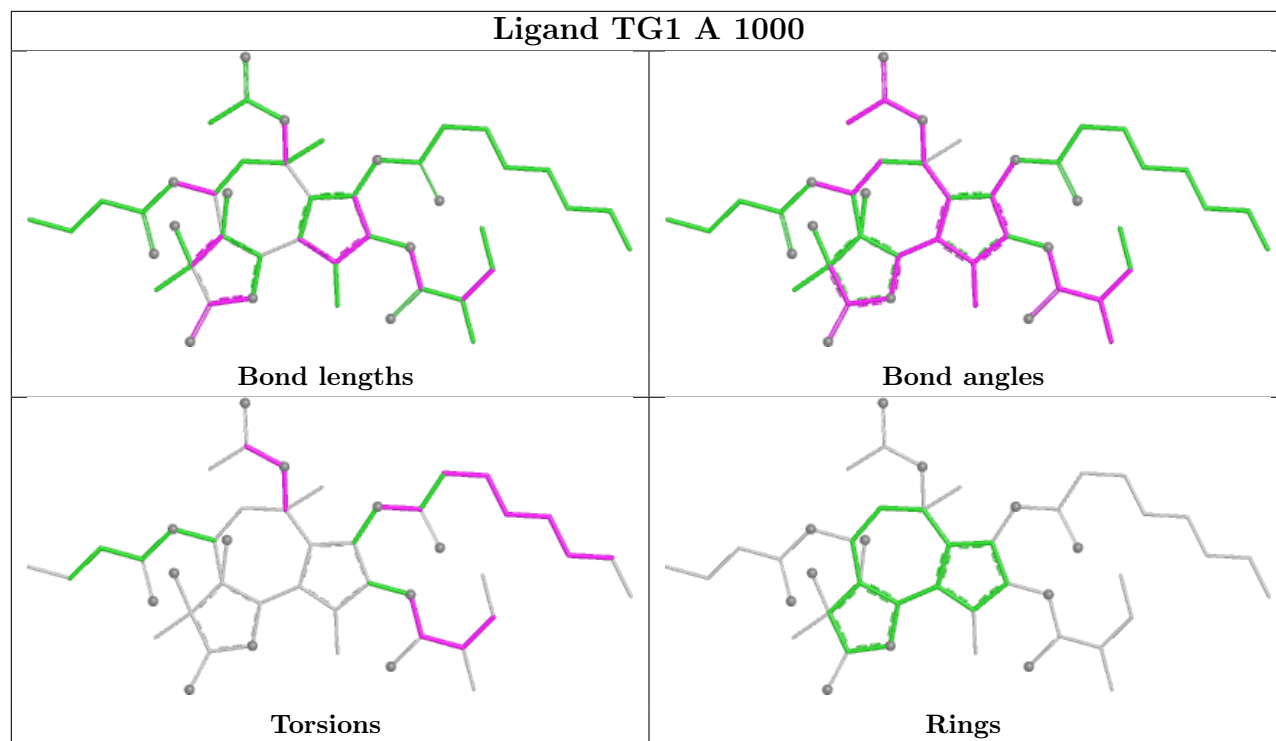
8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2002	ALF	1	0
4	B	2002	ALF	2	0
2	B	1000	TG1	4	0
6	A	3001	ACT	2	0
6	B	3001	ACT	2	0
2	A	1000	TG1	7	0
6	A	3002	ACT	1	0
6	B	3002	ACT	3	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	994/994 (100%)	0.10	89 (8%)	15 12	19, 45, 149, 275	0
1	B	994/994 (100%)	0.09	68 (6%)	23 20	22, 49, 119, 221	0
All	All	1988/1988 (100%)	0.09	157 (7%)	18 16	19, 48, 137, 275	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	964	LEU	7.0
1	A	85	ILE	5.7
1	B	107	TRP	5.7
1	B	49	LEU	5.4
1	B	276	ILE	5.3
1	A	508	VAL	5.3
1	B	85	ILE	5.2
1	A	948	LEU	5.1
1	A	288	TRP	5.0
1	A	279	PHE	4.8
1	B	50	TRP	4.7
1	B	288	TRP	4.7
1	A	78	PHE	4.7
1	B	279	PHE	4.7
1	A	877	THR	4.5
1	B	890	ILE	4.4
1	B	241	ALA	4.4
1	A	890	ILE	4.4
1	B	283	VAL	4.4
1	A	283	VAL	4.3
1	B	108	GLN	4.3
1	A	865	VAL	4.2
1	A	50	TRP	4.1
1	A	947	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	867	TYR	4.1
1	A	885	GLY	4.0
1	B	289	ILE	4.0
1	B	278	HIS	3.9
1	A	881	PRO	3.9
1	A	503	SER	3.9
1	A	949	TYR	3.9
1	B	84	THR	3.8
1	A	107	TRP	3.8
1	A	278	HIS	3.8
1	A	106	VAL	3.8
1	B	77	TRP	3.7
1	A	835	PHE	3.6
1	A	968	LEU	3.6
1	B	112	ALA	3.6
1	B	295	TYR	3.5
1	B	242	THR	3.5
1	A	49	LEU	3.5
1	A	874	MET	3.4
1	A	110	ARG	3.4
1	A	280	ASN	3.4
1	A	957	PHE	3.4
1	A	956	ILE	3.4
1	A	853	ALA	3.4
1	B	92	PHE	3.3
1	B	282	PRO	3.3
1	B	78	PHE	3.3
1	A	507	ALA	3.3
1	B	48	SER	3.3
1	B	106	VAL	3.3
1	B	109	GLU	3.2
1	B	274	ILE	3.2
1	B	924	ARG	3.2
1	A	992	LEU	3.2
1	A	89	VAL	3.2
1	A	506	ALA	3.2
1	A	991	TYR	3.2
1	B	269	VAL	3.1
1	A	374	GLY	3.1
1	B	275	ASN	3.0
1	A	983	ILE	3.0
1	B	52	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	52	LEU	2.9
1	B	273	LEU	2.9
1	B	294	TYR	2.9
1	A	47	LYS	2.9
1	A	972	LYS	2.9
1	A	74	VAL	2.9
1	B	55	GLU	2.9
1	A	788	ILE	2.9
1	B	866	THR	2.9
1	A	81	GLY	2.8
1	B	277	GLY	2.8
1	A	92	PHE	2.8
1	B	972	LYS	2.8
1	A	84	THR	2.8
1	A	289	ILE	2.8
1	A	376	PHE	2.8
1	A	293	ILE	2.7
1	A	104	VAL	2.7
1	B	47	LYS	2.7
1	B	835	PHE	2.7
1	A	48	SER	2.7
1	B	287	SER	2.7
1	A	932	TRP	2.7
1	B	256	PHE	2.6
1	B	104	VAL	2.6
1	A	277	GLY	2.6
1	A	882	HIS	2.6
1	A	891	PHE	2.6
1	A	782	GLY	2.6
1	A	96	LEU	2.6
1	A	284	HIS	2.6
1	A	266	LEU	2.5
1	A	964	LEU	2.5
1	B	863	PRO	2.5
1	A	103	ILE	2.5
1	A	295	TYR	2.5
1	A	814	LEU	2.5
1	A	76	ALA	2.5
1	B	963	ASP	2.5
1	B	867	TYR	2.5
1	A	958	LYS	2.5
1	B	285	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	991	TYR	2.5
1	A	292	ALA	2.5
1	B	292	ALA	2.5
1	B	286	GLY	2.5
1	B	885	GLY	2.5
1	B	339	VAL	2.4
1	A	112	ALA	2.4
1	A	924	ARG	2.4
1	B	110	ARG	2.4
1	A	863	PRO	2.4
1	A	963	ASP	2.3
1	A	109	GLU	2.3
1	A	970	VAL	2.3
1	B	111	ASN	2.3
1	B	81	GLY	2.3
1	A	77	TRP	2.3
1	B	923	MET	2.2
1	A	82	GLU	2.2
1	A	900	ALA	2.2
1	A	86	THR	2.2
1	A	967	TRP	2.2
1	B	244	GLN	2.2
1	A	955	MET	2.2
1	A	854	TRP	2.2
1	B	53	VAL	2.2
1	B	281	ASP	2.2
1	A	961	ALA	2.2
1	B	399	ASP	2.1
1	A	868	HIS	2.1
1	B	103	ILE	2.1
1	A	281	ASP	2.1
1	B	976	PRO	2.1
1	A	46	GLY	2.1
1	B	243	GLU	2.1
1	A	276	ILE	2.1
1	A	294	TYR	2.1
1	B	284	HIS	2.1
1	B	865	VAL	2.1
1	A	873	PHE	2.1
1	A	105	GLY	2.1
1	B	877	THR	2.1
1	A	946	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	43	ALA	2.0
1	B	239	MET	2.0
1	B	280	ASN	2.0
1	A	858	TYR	2.0
1	A	860	GLU	2.0
1	A	965	THR	2.0
1	B	992	LEU	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](#)

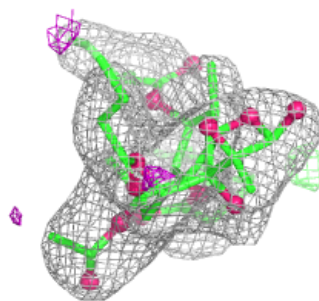
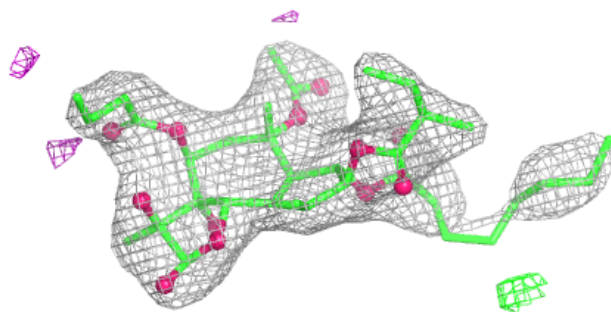
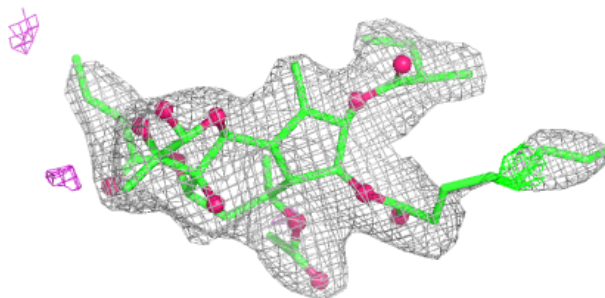
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
6	ACT	A	3002	4/4	0.83	0.18	29,38,42,46	0
2	TG1	B	1000	46/46	0.90	0.14	49,63,87,88	0
6	ACT	B	3002	4/4	0.91	0.14	31,44,45,50	0
2	TG1	A	1000	46/46	0.92	0.13	52,69,119,119	0
6	ACT	A	3001	4/4	0.93	0.18	35,44,45,51	0
6	ACT	B	3001	4/4	0.94	0.12	41,48,49,55	0
5	K	B	2003	1/1	0.98	0.05	40,40,40,40	0
5	K	A	2003	1/1	0.99	0.04	36,36,36,36	0
4	ALF	A	2002	5/5	0.99	0.05	23,23,25,27	0
4	ALF	B	2002	5/5	0.99	0.03	23,23,25,28	0
3	MG	A	2001	1/1	1.00	0.06	26,26,26,26	0
3	MG	B	2001	1/1	1.00	0.05	28,28,28,28	0

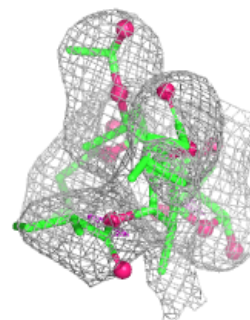
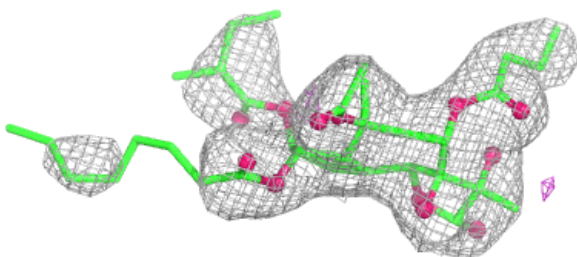
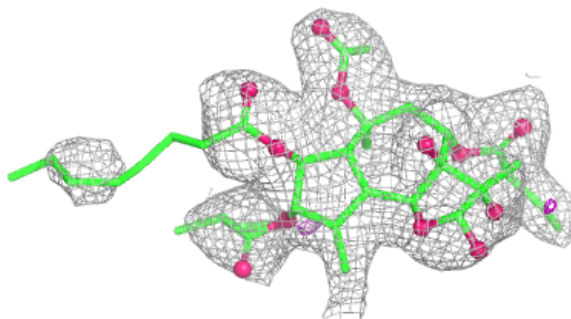
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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 TG1 A 1000:**

$2mF_o-DF_c$ (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.