



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:57 pm BST

PDB ID : 3N5K
Title : Structure Of The (Sr)Ca²⁺-ATPase E2-AlF₄- Form
Authors : Bublitz, M.; Olesen, C.; Poulsen, H.; Morth, J.P.; Moller, J.V.; Nissen, P.
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

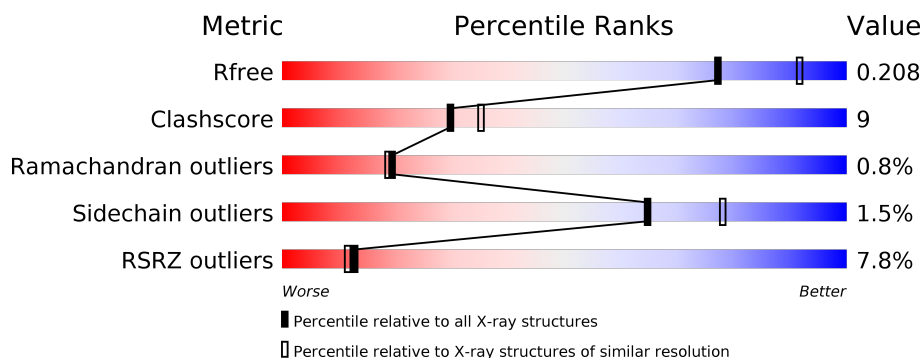
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	994	<div> <div>11%</div> <div> <div></div> <div>82%</div> <div>18%</div> </div> <div></div> </div>
1	B	994	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>17%</div> </div> <div></div> </div>

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.

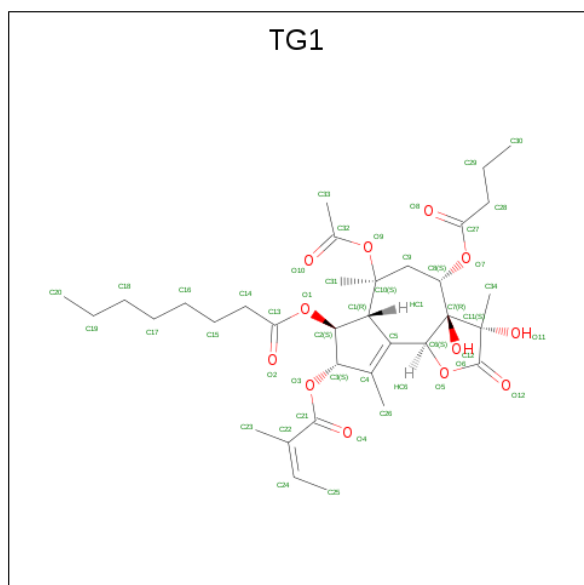
- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

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 (three-letter code: TG1) (formula: C₃₄H₅₀O₁₂).

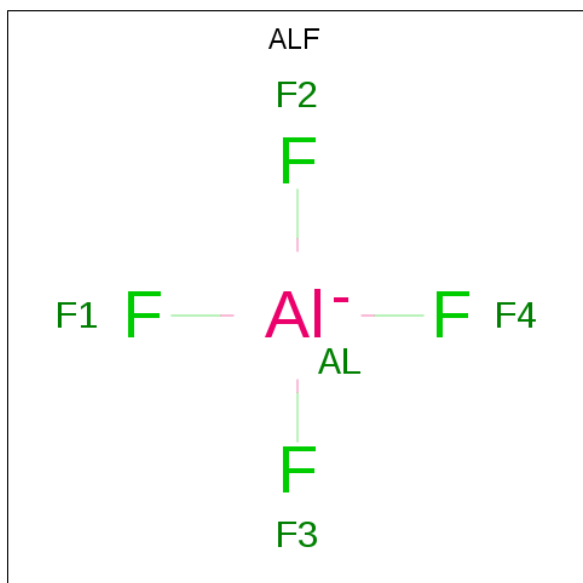


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			46	34	12		
2	B	1	Total	C	O	0	0
			46	34	12		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is TETRAFLUOROALUMINATE ION (three-letter code: 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 (three-letter code: K) (formula: K).

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

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

- Molecule 6 is ACETATE ION (three-letter code: 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

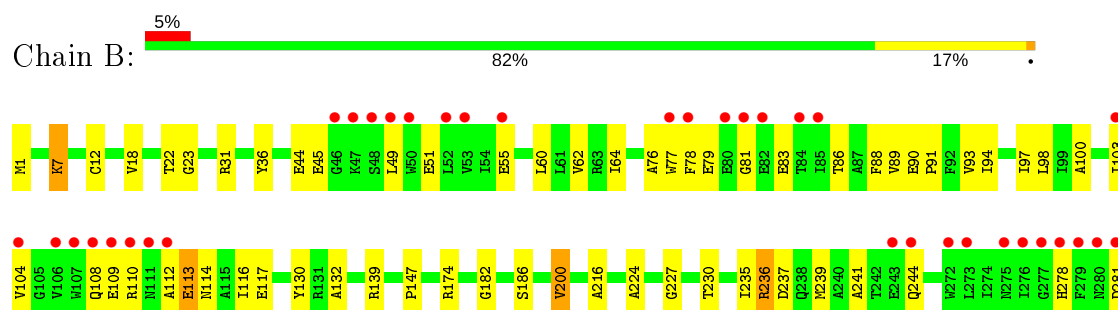
3 Residue-property plots [i](#)

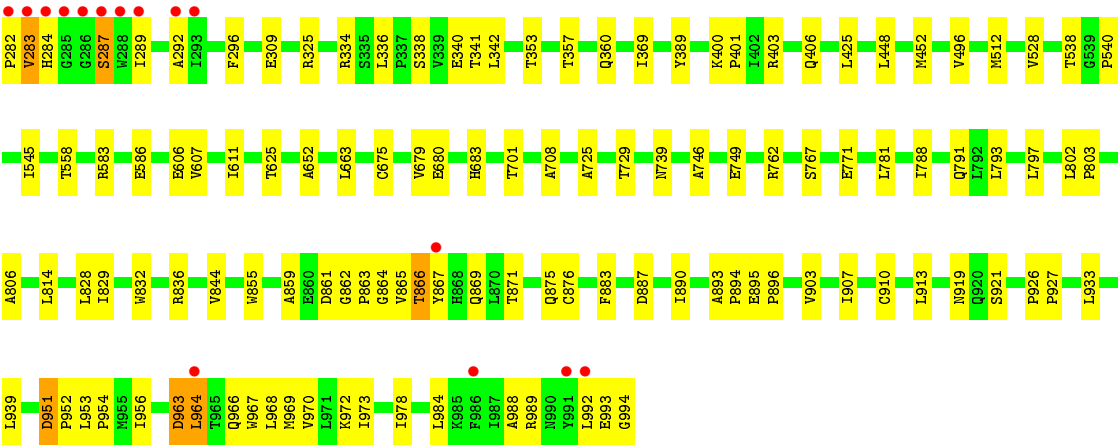
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



- 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 0.177 , 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)	0.29 , 50.0	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	0.96	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, MG, TG1, K, 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	0.51	0/7812	0.58	1/10592 (0.0%)
1	B	0.49	0/7812	0.59	1/10592 (0.0%)
All	All	0.50	0/15624	0.59	2/21184 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	LYS	CA-CB-CG	5.48	125.45	113.40
1	A	425	LEU	CA-CB-CG	5.27	127.42	115.30

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	138	0
1	B	7671	0	7764	146	0
2	A	46	0	50	7	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	293	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 9.

All (293) 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)
2:A:1000:TG1:H232	2:A:1000:TG1:H161	1.40	0.98
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:A:909:MET:HE3	1:A:937:ILE:HG23	1.57	0.84
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: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:239:MET:HE2	1:B:708:ALA:CB	2.19	0.71
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:239:MET:CE	1:B:708:ALA:HB3	2.23	0.69
1:B:7:LYS:HD2	1:B:12:CYS:SG	2.32	0.69
1:A:114:ASN:HB3	1:A:117:GLU:HG2	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:NH2	1:A:34:GLU:HG3	2.09	0.68
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:B:1:MET:H2	1:B:7:LYS:NZ	1.92	0.66
1:A:814:LEU:H	1:A:814:LEU:HD12	1.59	0.66
1:B:963:ASP:HB3	1:B:966:GLN:H	1.62	0.64
1:B:1:MET:H1	1:B:7:LYS:NZ	1.96	0.63
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:B:1:MET:N	1:B:7:LYS:HZ1	1.98	0.62
1:A:866:THR:HB	1:A:869:GLN:HB2	1.82	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:836:ARG:HG2	1:B:984:LEU:HB3	1.82	0.60
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
2:B:1000:TG1:C33	2:B:1000:TG1:H313	2.33	0.58
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:239:MET:HE3	1:B:708:ALA:HB3	1.86	0.56
1:B:239:MET:CE	1:B:708:ALA:CB	2.80	0.56
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:C23	2:A:1000:TG1:H161	2.27	0.55
1:B:227:GLY:O	6:B:3002:ACT:H3	2.07	0.55
1:B:1:MET:H2	1:B:7:LYS:CE	2.20	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
2:B:1000:TG1:HC91	2:B:1000:TG1:H333	1.89	0.53
1:B:1:MET:H1	1:B:7:LYS:HZ3	1.55	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
1:B:239:MET:HE2	1:B:708:ALA:HB1	1.90	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:MET:H2	1:B:7:LYS:HZ1	1.57	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:918:GLU:HG2	1:A:919:ASN:OD1	2.11	0.51
1:A:909:MET:CE	1:A:937:ILE:HA	2.41	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: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:200:VAL:HG22	1:B:680:GLU:CG	2.41	0.49
1:B:77:TRP:HD1	1:B:78:PHE:CE1	2.30	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:B:287:SER:C	1:B:289:ILE:H	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H191	2:A:1000:TG1:H162	1.52	0.48
1:B:113:GLU:HG2	1:B:729:THR:HG22	1.94	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:B:1:MET:N	1:B:7:LYS:HZ3	2.06	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:B:88:PHE:C	1:B:91:PRO:HD2	2.34	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
1:A:863:PRO:N	1:A:864:GLY:HA2	2.30	0.46
1:A:864:GLY:O	1:A:865:VAL:C	2.54	0.46
1:A:898:THR:HG23	1:A:948:LEU:HD21	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:277:GLY:C	1:A:279:PHE:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1000:TG1:H313	2:B:1000:TG1:H333	1.98	0.45
1:B:865:VAL:HG12	1:B:866:THR:H	1.80	0.45
1:A:115:ALA:HB1	1:A:239:MET:CE	2.46	0.45
1:A:650:ASP:O	1:A:672:ARG:HD2	2.17	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: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:377:CYS:HB3	1:A:544:LYS:HG2	2.00	0.44
1:A:50:TRP:O	1:A:54:ILE:HG12	2.18	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: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:B:235:ILE:CG2	1:B:239:MET:HE1	2.46	0.44
1:B:607:VAL:O	1:B:611:ILE:HG12	2.18	0.44
2:B:1000:TG1:H171	2:B:1000:TG1:H141	1.62	0.43
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
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
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:402:ILE:C	1:A:402:ILE:HD12	2.39	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:235:ILE:CG2	1:B:239:MET:CE	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:ASP:C	1:A:803:PRO:HD2	2.38	0.43
1:A:922:LEU:HA	1:A:925:MET:O	2.19	0.43
1:B:972:LYS:HD3	1:B:972:LYS:HA	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:B:964:LEU:HG	1:B:964:LEU:H	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:625:THR:HA	4:A:2002:ALF:F4	2.09	0.42
1:A:85:ILE:N	1:A:85:ILE:HD12	2.33	0.42
1:B:389:TYR:HB3	1:B:425:LEU:HD21	2.01	0.42
1:A:135:LYS:HD2	1:A:135:LYS:HA	1.88	0.42
1:A:31:ARG:HA	1:A:34:GLU:HG2	2.00	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:341:THR:HG22	1:A:716:ILE:HD11	2.01	0.41
1:A:71:ILE:O	1:A:75:LEU:HD13	2.20	0.41
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:868:HIS:CE1	1:A:872:HIS:CE1	3.09	0.41
1:A:836:ARG:HG3	1:A:984:LEU:HD13	2.02	0.41
1:B:139:ARG:HH11	1:B:139:ARG:HB2	1.85	0.41
1:B:174:ARG:HB3	1:B:186:SER:HB3	2.02	0.41
1:B:1:MET:HE3	1:B:1:MET:HB3	1.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:LEU:N	1:B:814:LEU:HD12	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:A:909:MET:HE1	1:A:937:ILE:HA	2.01	0.41
1:B:309:GLU:HG3	1:B:793:LEU:HD23	2.02	0.41
1:B:94:ILE:HG12	1:B:793:LEU:HD11	2.03	0.41
1:B:239:MET:HE2	1:B:708:ALA:HB3	1.90	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:B:951:ASP:CG	1:B:952:PRO:HA	2.41	0.40
1:A:256:PHE:HB2	2:A:1000:TG1:H291	2.02	0.40
1:A:733:MET:HB2	1:A:733:MET:HE2	1.79	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:887:ASP:HB3	1:B:890:ILE:CD1	2.52	0.40
1:B:806:ALA:HB1	1:B:933:LEU:HA	2.02	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 ⓘ

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	992/994 (100%)	941 (95%)	41 (4%)	10 (1%)	15	14
1	B	992/994 (100%)	951 (96%)	36 (4%)	5 (0%)	29	31
All	All	1984/1988 (100%)	1892 (95%)	77 (4%)	15 (1%)	19	19

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 ⓘ

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%)	831 (99%)	9 (1%)	73	85
1	B	840/840 (100%)	823 (98%)	17 (2%)	55	69
All	All	1680/1680 (100%)	1654 (98%)	26 (2%)	65	78

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	ARG
1	A	255	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

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Mol	Chain	Res	Type
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	334	ARG
1	B	340	GLU
1	B	360	GLN
1	B	663	LEU
1	B	701	THR
1	B	781	LEU
1	B	866	THR
1	B	921	SER
1	B	951	ASP
1	B	963	ASP
1	B	964	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	868	HIS
1	A	880	HIS
1	B	114	ASN
1	B	284	HIS
1	B	875	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
6	ACT	A	3001	-	1,3,3	0.26	0	0,3,3	0.00	-
6	ACT	B	3001	-	1,3,3	0.45	0	0,3,3	0.00	-
4	ALF	B	2002	-	0,4,4	0.00	-	-		
4	ALF	A	2002	-	0,4,4	0.00	-	-		
2	TG1	B	1000	-	43,48,48	4.23	10 (23%)	44,72,72	3.58	12 (27%)
2	TG1	A	1000	-	43,48,48	4.20	9 (20%)	44,72,72	3.71	13 (29%)
6	ACT	B	3002	-	1,3,3	0.20	0	0,3,3	0.00	-
6	ACT	A	3002	-	1,3,3	2.84	1 (100%)	0,3,3	0.00	-

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	B	1000	-	-	16/33/99/99	0/3/3/3
2	TG1	A	1000	-	-	18/33/99/99	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	C4-C5	24.68	1.55	1.34
2	A	1000	TG1	C4-C5	24.40	1.54	1.34
2	B	1000	TG1	O12-C12	7.82	1.38	1.20
2	A	1000	TG1	O12-C12	7.48	1.38	1.20
2	A	1000	TG1	C3-C4	3.87	1.55	1.50
2	A	1000	TG1	O5-C12	3.79	1.41	1.35
2	B	1000	TG1	O5-C12	3.67	1.41	1.35
2	B	1000	TG1	C3-C4	3.61	1.55	1.50
2	B	1000	TG1	C24-C22	3.59	1.54	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	TG1	C24-C22	3.54	1.53	1.31
2	A	1000	TG1	O9-C10	-3.09	1.43	1.48
2	B	1000	TG1	O9-C10	-3.07	1.43	1.48
2	A	1000	TG1	O7-C8	-3.04	1.41	1.46
2	B	1000	TG1	O7-C8	-2.96	1.41	1.46
6	A	3002	ACT	CH3-C	2.84	1.52	1.48
2	A	1000	TG1	C11-C7	2.42	1.58	1.55
2	B	1000	TG1	O3-C21	2.17	1.39	1.34
2	B	1000	TG1	O6-C7	-2.05	1.39	1.43
2	B	1000	TG1	C11-C7	2.02	1.58	1.55
2	A	1000	TG1	C2-C3	2.01	1.56	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	TG1	O12-C12-C11	-17.53	110.66	128.28
2	B	1000	TG1	O12-C12-C11	-16.25	111.95	128.28
2	B	1000	TG1	O5-C12-O12	-11.88	105.88	121.62
2	A	1000	TG1	O5-C12-O12	-11.87	105.89	121.62
2	B	1000	TG1	C10-O9-C32	6.14	136.10	121.53
2	A	1000	TG1	C10-O9-C32	5.85	135.42	121.53
2	A	1000	TG1	C10-C1-C5	4.42	120.54	115.26
2	B	1000	TG1	O3-C21-O4	-4.12	115.46	123.32
2	B	1000	TG1	C26-C4-C3	-4.00	114.79	121.27
2	A	1000	TG1	C23-C22-C24	-3.97	106.86	123.20
2	A	1000	TG1	O3-C21-O4	-3.83	116.03	123.32
2	B	1000	TG1	C23-C22-C24	-3.67	108.11	123.20
2	B	1000	TG1	C10-C1-C5	3.66	119.64	115.26
2	A	1000	TG1	C23-C22-C21	-3.19	108.12	116.09
2	B	1000	TG1	C23-C22-C21	-2.79	109.11	116.09
2	A	1000	TG1	C26-C4-C3	-2.79	116.75	121.27
2	B	1000	TG1	C26-C4-C5	-2.53	123.51	129.82
2	A	1000	TG1	C26-C4-C5	-2.52	123.54	129.82
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	-2.30	118.14	123.70
2	A	1000	TG1	C11-C7-C6	-2.27	98.66	103.03
2	A	1000	TG1	O9-C32-C33	-2.12	106.82	110.68
2	A	1000	TG1	O9-C32-O10	-2.09	119.78	123.61
2	B	1000	TG1	O3-C21-C22	2.00	116.54	111.52

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	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
2	A	1000	TG1	C33-C32-O9-C10
2	A	1000	TG1	O2-C13-O1-C2
2	B	1000	TG1	O4-C21-O3-C3
2	A	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	B	1000	TG1	C13-C14-C15-C16
2	A	1000	TG1	C21-C22-C24-C25
2	B	1000	TG1	C16-C17-C18-C19
2	B	1000	TG1	C15-C16-C17-C18
2	A	1000	TG1	C15-C16-C17-C18
2	B	1000	TG1	O2-C13-O1-C2
2	B	1000	TG1	O4-C21-C22-C24
2	A	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	O4-C21-C22-C23
2	A	1000	TG1	O7-C27-C28-C29

There are no ring outliers.

8 monomers are involved in 22 short contacts:

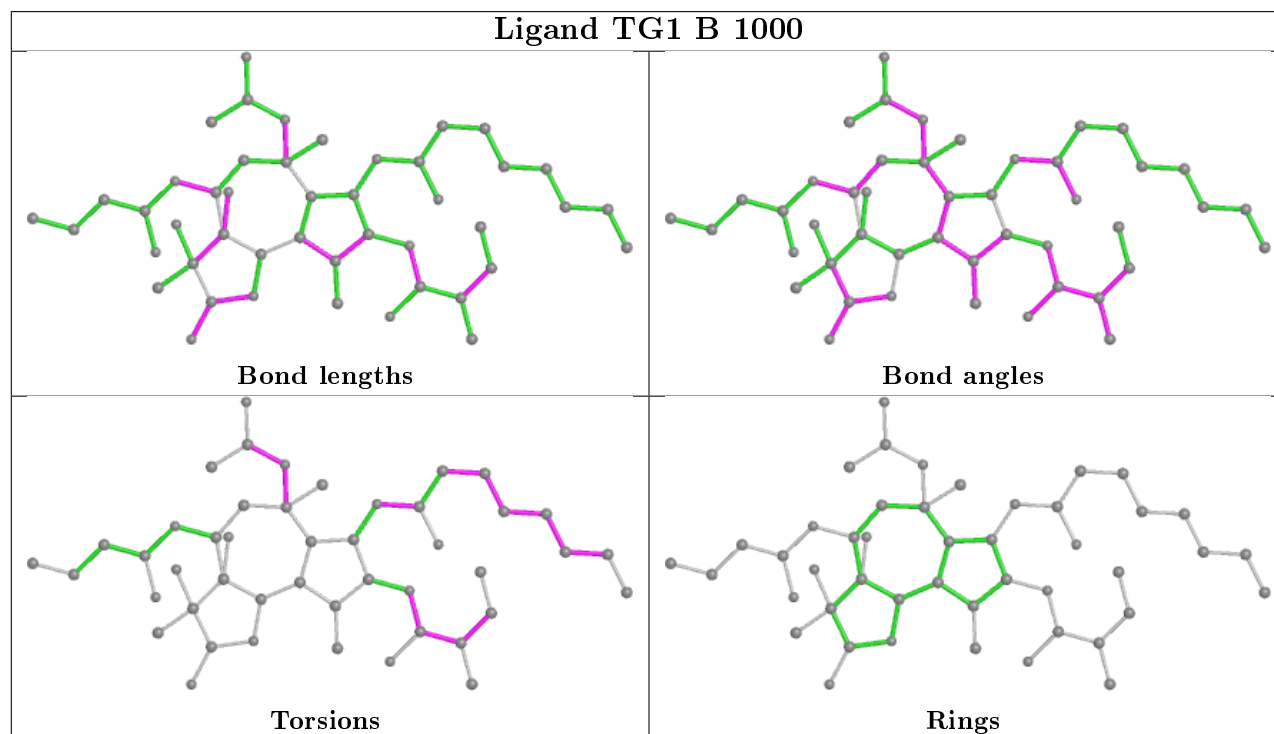
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	3001	ACT	2	0
6	B	3001	ACT	2	0

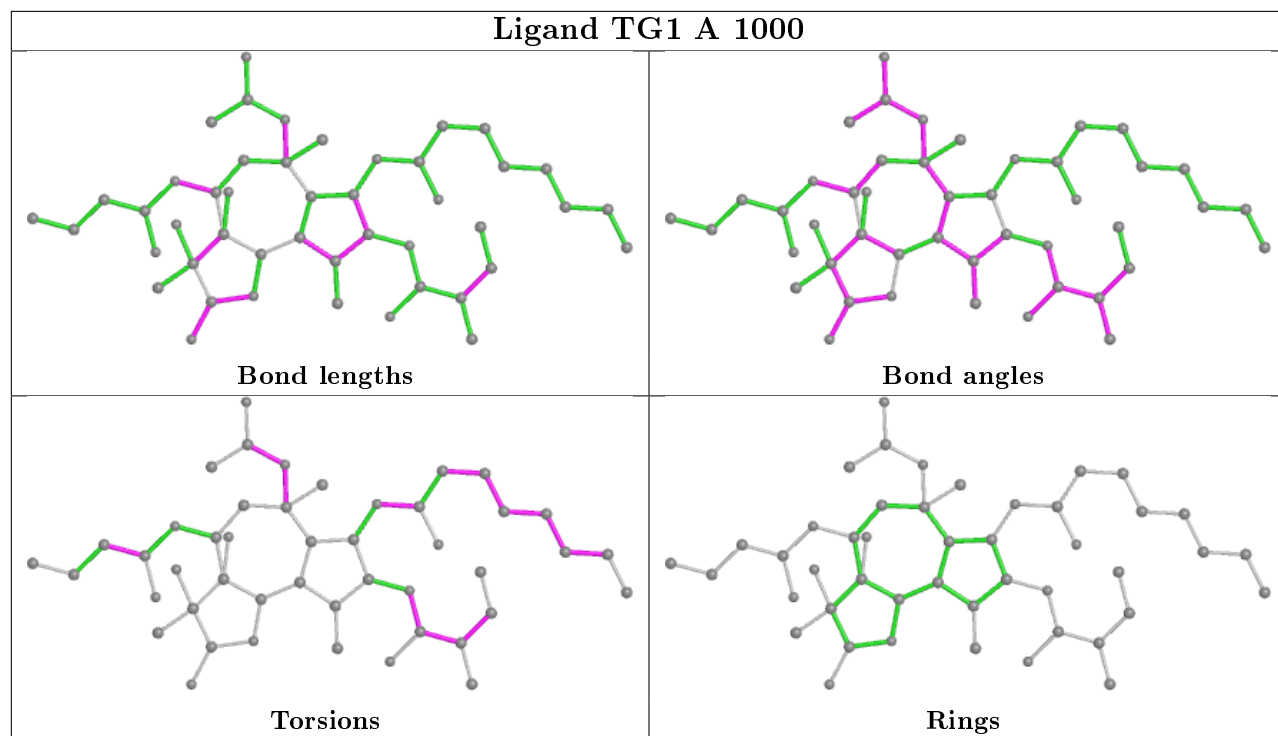
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2002	ALF	2	0
4	A	2002	ALF	1	0
2	B	1000	TG1	4	0
2	A	1000	TG1	7	0
6	B	3002	ACT	3	0
6	A	3002	ACT	1	0

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	994/994 (100%)	0.39	105 (10%) 6 5	19, 45, 149, 275	0
1	B	994/994 (100%)	0.01	50 (5%) 28 27	22, 49, 119, 221	0
All	All	1988/1988 (100%)	0.20	155 (7%) 13 11	19, 48, 137, 275	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	GLY	13.4
1	A	80	GLU	11.6
1	B	49	LEU	11.3
1	A	84	THR	10.1
1	B	286	GLY	8.8
1	B	80	GLU	8.7
1	A	78	PHE	8.6
1	B	81	GLY	8.6
1	A	81	GLY	8.4
1	B	112	ALA	8.3
1	A	110	ARG	7.4
1	A	77	TRP	7.3
1	B	109	GLU	7.1
1	B	283	VAL	7.1
1	A	85	ILE	6.9
1	A	76	ALA	6.9
1	A	292	ALA	6.8
1	A	891	PHE	6.3
1	A	283	VAL	6.2
1	A	111	ASN	6.2
1	A	888	CYS	6.2
1	A	992	LEU	6.2
1	B	77	TRP	6.1
1	B	280	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	47	LYS	6.0
1	B	108	GLN	5.8
1	B	287	SER	5.8
1	B	285	GLY	5.8
1	B	282	PRO	5.8
1	A	79	GLU	5.6
1	A	82	GLU	5.6
1	A	286	GLY	5.6
1	B	281	ASP	5.5
1	B	78	PHE	5.5
1	B	111	ASN	5.5
1	A	50	TRP	5.4
1	A	949	TYR	5.4
1	B	289	ILE	5.3
1	B	278	HIS	5.2
1	A	883	PHE	5.0
1	A	948	LEU	5.0
1	B	84	THR	4.8
1	B	47	LYS	4.8
1	B	288	TRP	4.8
1	A	994	GLY	4.8
1	A	266	LEU	4.8
1	B	48	SER	4.7
1	B	50	TRP	4.7
1	B	244	GLN	4.6
1	B	276	ILE	4.5
1	A	279	PHE	4.5
1	A	280	ASN	4.5
1	A	781	LEU	4.4
1	A	890	ILE	4.4
1	A	853	ALA	4.4
1	A	106	VAL	4.3
1	A	74	VAL	4.3
1	A	970	VAL	4.3
1	B	273	LEU	4.2
1	B	275	ASN	4.2
1	A	873	PHE	4.1
1	A	281	ASP	4.1
1	A	947	ILE	4.1
1	A	835	PHE	4.1
1	B	279	PHE	4.1
1	B	110	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	52	LEU	4.0
1	B	46	GLY	4.0
1	B	85	ILE	3.9
1	B	107	TRP	3.9
1	A	865	VAL	3.9
1	B	52	LEU	3.9
1	A	295	TYR	3.8
1	A	86	THR	3.8
1	B	243	GLU	3.7
1	A	107	TRP	3.7
1	A	782	GLY	3.7
1	A	104	VAL	3.7
1	B	277	GLY	3.7
1	A	278	HIS	3.6
1	A	46	GLY	3.6
1	A	993	GLU	3.5
1	A	273	LEU	3.4
1	A	243	GLU	3.4
1	A	294	TYR	3.4
1	A	874	MET	3.4
1	B	82	GLU	3.4
1	A	88	PHE	3.4
1	A	856	PHE	3.4
1	A	288	TRP	3.4
1	A	854	TRP	3.3
1	A	289	ILE	3.3
1	A	852	ALA	3.3
1	A	293	ILE	3.3
1	A	291	GLY	3.2
1	A	957	PHE	3.2
1	A	298	ILE	3.2
1	B	106	VAL	3.2
1	A	896	PRO	3.1
1	A	858	TYR	3.1
1	A	108	GLN	3.1
1	A	784	PRO	3.1
1	A	956	ILE	3.1
1	A	83	GLU	3.0
1	A	45	GLU	3.0
1	A	991	TYR	3.0
1	A	886	LEU	3.0
1	A	788	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	109	GLU	3.0
1	A	103	ILE	2.9
1	B	272	TRP	2.9
1	A	287	SER	2.9
1	A	284	HIS	2.9
1	A	282	PRO	2.8
1	A	866	THR	2.8
1	A	958	LYS	2.8
1	A	972	LYS	2.8
1	A	89	VAL	2.8
1	A	900	ALA	2.8
1	A	49	LEU	2.7
1	B	284	HIS	2.7
1	B	867	TYR	2.7
1	A	967	TRP	2.7
1	A	965	THR	2.7
1	B	986	PHE	2.7
1	A	870	LEU	2.7
1	B	293	ILE	2.7
1	A	973	ILE	2.6
1	A	964	LEU	2.6
1	B	292	ALA	2.5
1	A	277	GLY	2.5
1	B	55	GLU	2.5
1	A	893	ALA	2.4
1	A	75	LEU	2.4
1	A	901	LEU	2.4
1	A	955	MET	2.4
1	B	991	TYR	2.4
1	A	112	ALA	2.4
1	B	103	ILE	2.4
1	A	860	GLU	2.3
1	A	272	TRP	2.3
1	A	53	VAL	2.3
1	B	53	VAL	2.3
1	A	968	LEU	2.2
1	A	899	MET	2.2
1	A	863	PRO	2.2
1	A	506	ALA	2.2
1	A	270	ALA	2.2
1	A	780	ALA	2.2
1	B	104	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	785	GLU	2.1
1	A	73	PHE	2.1
1	B	992	LEU	2.1
1	A	87	ALA	2.1
1	B	964	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 carbohydrates in this entry.

6.4 Ligands [i](#)

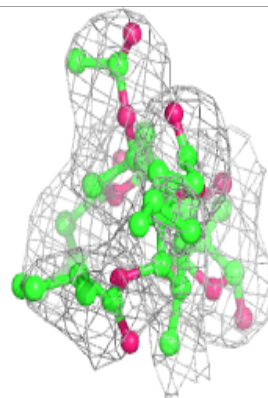
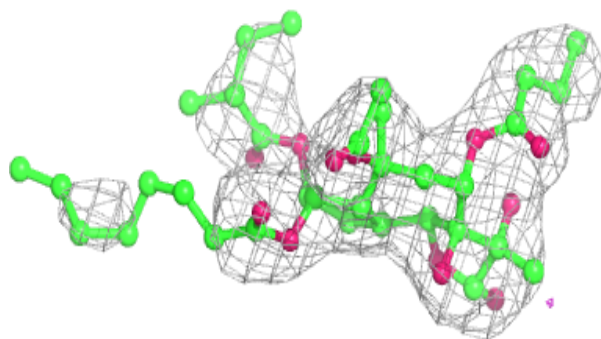
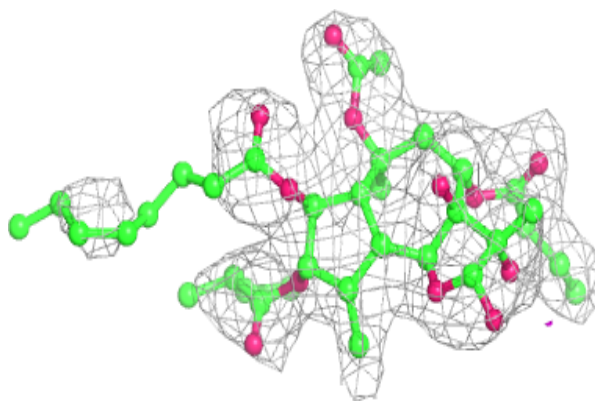
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	ACT	A	3002	4/4	0.89	0.18	29,38,42,46	0
6	ACT	A	3001	4/4	0.90	0.19	35,44,45,51	0
6	ACT	B	3001	4/4	0.92	0.16	41,48,49,55	0
2	TG1	A	1000	46/46	0.93	0.20	52,69,119,119	0
6	ACT	B	3002	4/4	0.93	0.16	31,44,45,50	0
2	TG1	B	1000	46/46	0.94	0.17	49,63,87,88	0
3	MG	A	2001	1/1	0.98	0.16	26,26,26,26	0
5	K	A	2003	1/1	0.98	0.11	36,36,36,36	0
4	ALF	B	2002	5/5	0.99	0.14	23,23,25,28	0
4	ALF	A	2002	5/5	0.99	0.14	23,23,25,27	0
5	K	B	2003	1/1	0.99	0.11	40,40,40,40	0
3	MG	B	2001	1/1	0.99	0.15	28,28,28,28	0

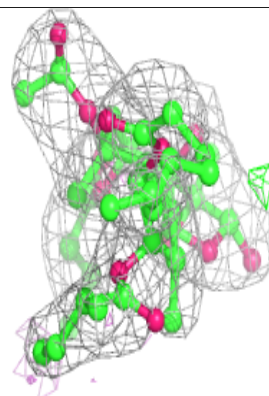
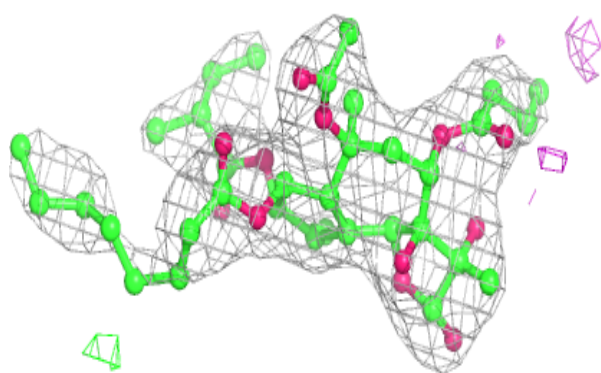
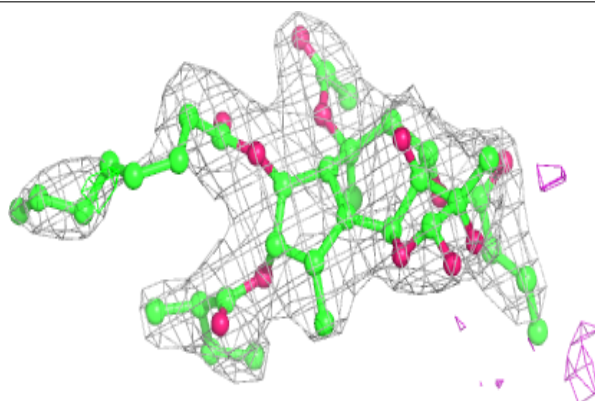
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TG1 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)

**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)



6.5 Other polymers

There are no such residues in this entry.