Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:42 PM BST

PDB ID	:	3W5A
Title	:	Crystal structure of the calcium pump and sarcolipin from rabbit fast twitch skeletal muscle in the E1.Mg2+ state
Authors	:	Toyoshima, C.; Iwasawa, S.; Ogawa, H.; Hirata, A.; Tsueda, J.; Inesi, G.
Deposited on	:	2013-01-27
Resolution	:	3.01 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:

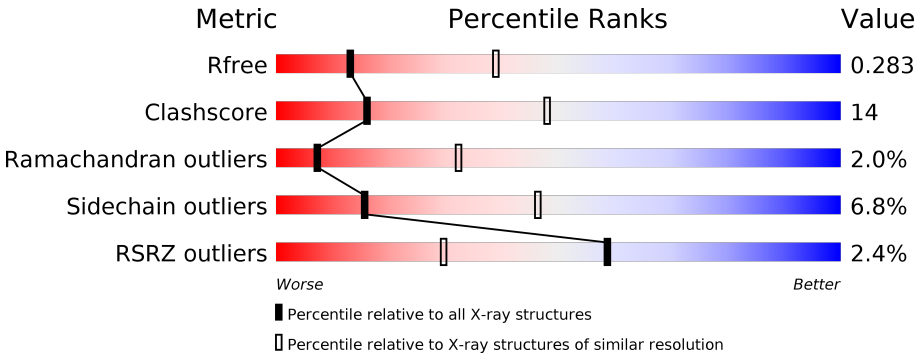
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 <=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% 64% 33% ·
1	B	995	2% 64% 33% ·
2	C	31	35% 55% 42% ·

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15802 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 SERCA1a.

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

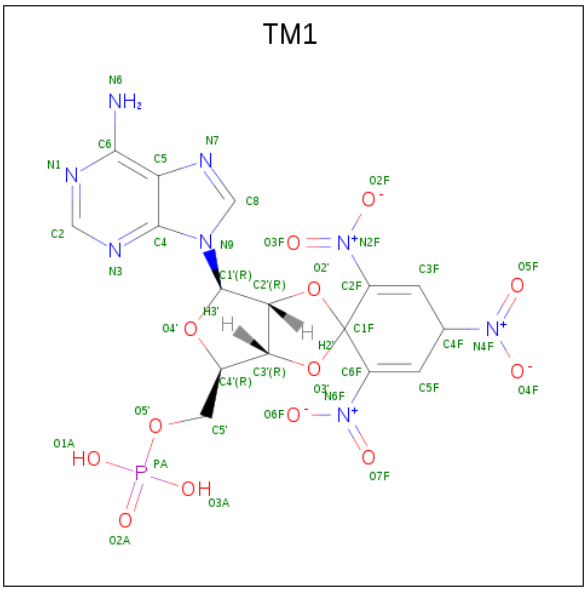
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	ACETYLATION	UNP B6CAM1
B	0	ACE	-	ACETYLATION	UNP B6CAM1

- Molecule 2 is a protein called Sarcolipin.

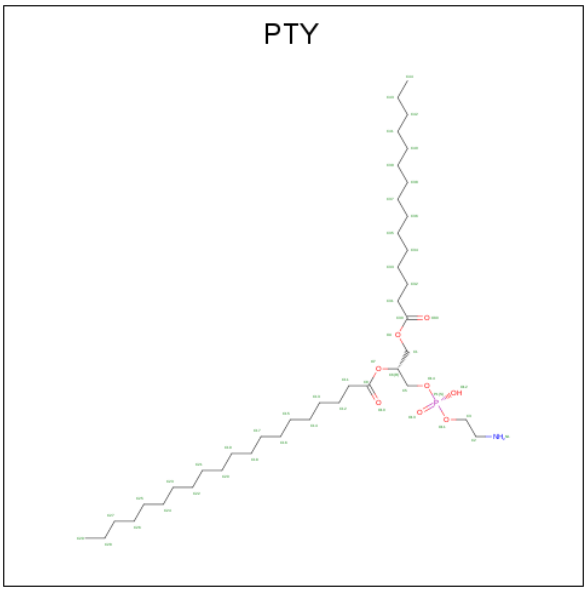
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	31	Total	C	N	O	S	0	0	0
			265	175	43	45	2			

- Molecule 3 is 2',3'-O-[(1r)-2,4,6-trinitrocyclohexa-2,5-diene-1,1-diyl]adenosine 5'-(dihydrogen phosphate) (three-letter code: TM1) (formula: $C_{16}H_{15}N_8O_{13}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			38	16	8	13	1		
3	B	1	Total	C	N	O	P	0	0
			38	16	8	13	1		

- Molecule 4 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 19 9 1 8 1	0	0
4	B	1	Total C N O P 19 9 1 8 1	0	0
4	B	1	Total C N O P 19 9 1 8 1	0	0
4	B	1	Total C N O P 19 9 1 8 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Mg 2 2	0	0
5	A	2	Total Mg 2 2	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Na 1 1	0	0
6	A	1	Total Na 1 1	0	0

- Molecule 7 is water.

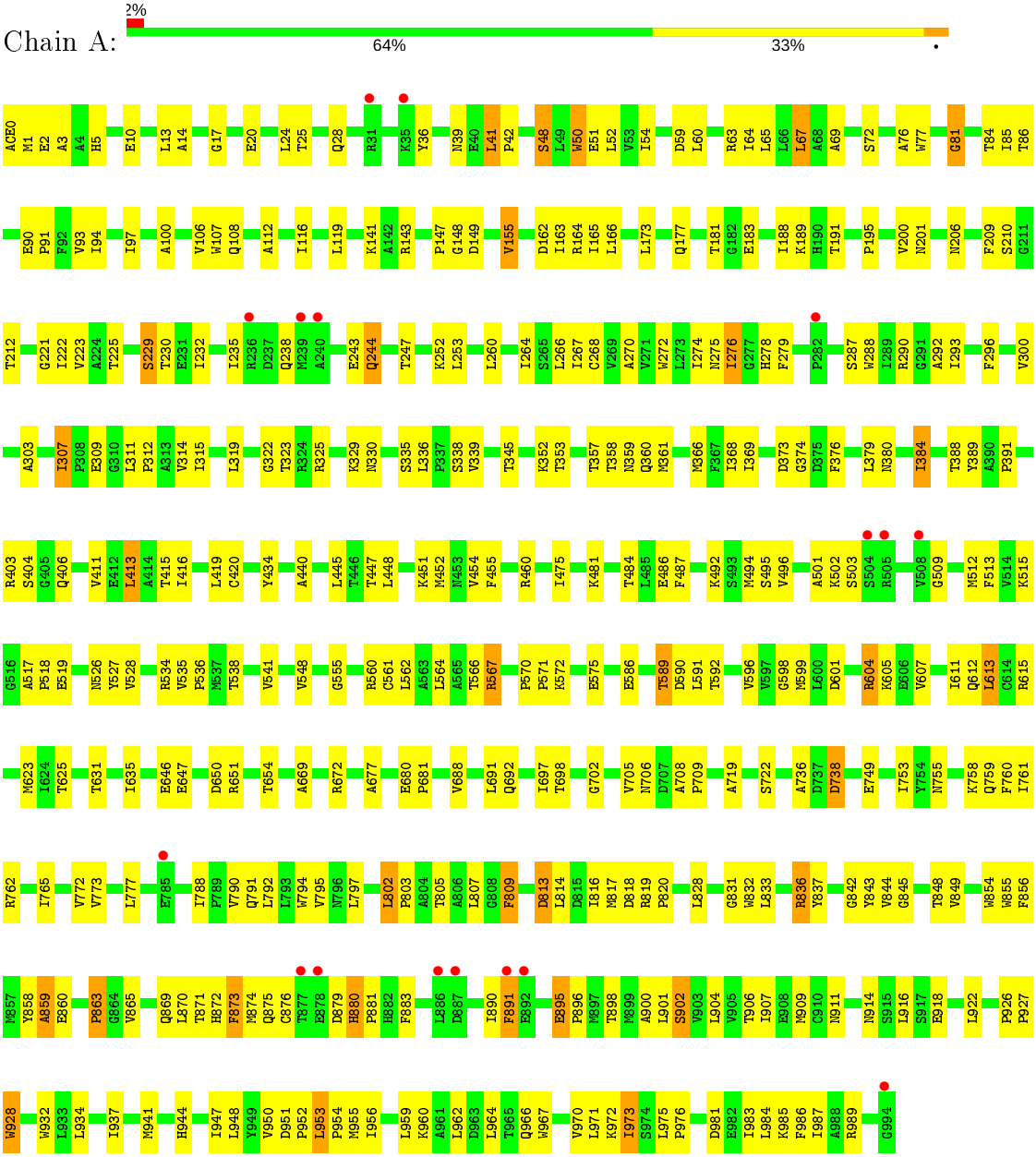
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	6	Total O 6 6	0	0
7	B	6	Total O 6 6	0	0

3 Residue-property plots (i)

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.

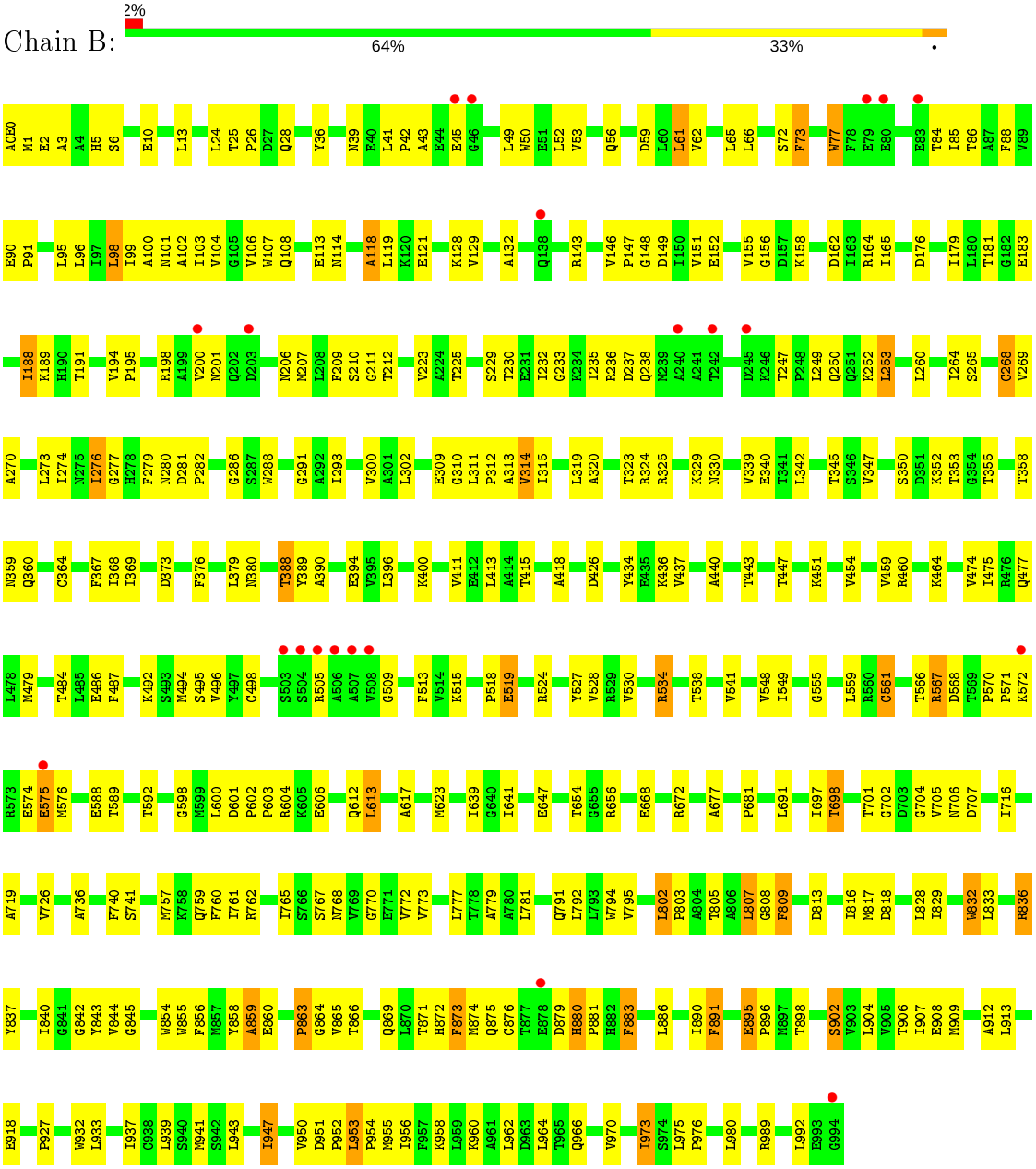
- Molecule 1: SERCA1a

Chain A:



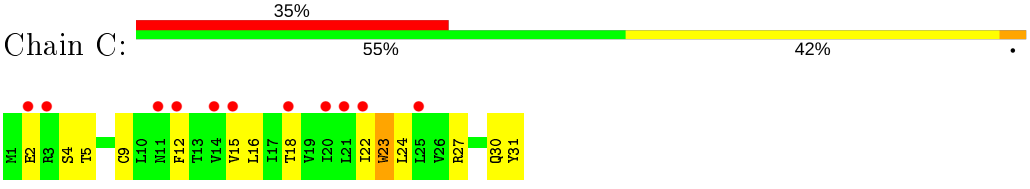
- Molecule 1: SERCA1a

Chain B:



- Molecule 2: Sarcolipin

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	352.88Å 55.73Å 187.95Å 90.00° 119.02° 90.00°	Depositor
Resolution (Å)	15.00 – 3.01 44.24 – 3.01	Depositor EDS
% Data completeness (in resolution range)	95.1 (15.00-3.01) 95.2 (44.24-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 3.01Å)	Xtriage
Refinement program	CNS, REFMAC 5.6.0117	Depositor
R, R_{free}	0.248 , 0.283 0.245 , 0.283	Depositor DCC
R_{free} test set	3113 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 23.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	15802	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TM1, MG, PTY, ACE, NA

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	0.47	10/7813 (0.1%)	0.59	1/10594 (0.0%)
1	B	0.47	6/7813 (0.1%)	0.58	0/10594
2	C	0.60	1/269 (0.4%)	0.76	0/364
All	All	0.47	17/15895 (0.1%)	0.59	1/21552 (0.0%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	794	TRP	CD2-CE2	5.45	1.47	1.41
1	B	794	TRP	CD2-CE2	5.30	1.47	1.41
1	A	832	TRP	CD2-CE2	5.25	1.47	1.41
1	A	77	TRP	CD2-CE2	5.22	1.47	1.41
1	A	928	TRP	CD2-CE2	5.20	1.47	1.41
1	B	288	TRP	CD2-CE2	5.20	1.47	1.41
1	B	50	TRP	CD2-CE2	5.17	1.47	1.41
1	A	932	TRP	CD2-CE2	5.15	1.47	1.41
1	A	288	TRP	CD2-CE2	5.14	1.47	1.41
1	A	967	TRP	CD2-CE2	5.09	1.47	1.41
1	A	107	TRP	CD2-CE2	5.08	1.47	1.41
1	B	832	TRP	CD2-CE2	5.07	1.47	1.41
1	A	50	TRP	CD2-CE2	5.07	1.47	1.41
1	A	272	TRP	CD2-CE2	5.07	1.47	1.41
1	B	854	TRP	CD2-CE2	5.06	1.47	1.41
1	B	77	TRP	CD2-CE2	5.05	1.47	1.41
2	C	23	TRP	CD2-CE2	5.02	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	LEU	CA-CB-CG	5.59	128.17	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	7674	0	7765	234	0
1	B	7674	0	7765	222	0
2	C	265	0	284	13	0
3	A	38	0	12	3	0
3	B	38	0	12	2	0
4	A	38	0	22	1	0
4	B	57	0	33	2	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	6	0	0	0	0
7	B	6	0	0	0	0
All	All	15802	0	15893	458	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 14.

All (458) 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:909:MET:CE	1:A:937:ILE:HA	1.97	0.94
1:B:773:VAL:HG23	1:B:845:GLY:HA3	1.49	0.93
1:A:561:CYS:HB3	1:A:598:GLY:HA2	1.51	0.90
1:B:373:ASP:HB3	1:B:376:PHE:HD2	1.38	0.88
1:B:561:CYS:HB3	1:B:598:GLY:HA2	1.56	0.85
1:A:303:ALA:O	1:A:307:ILE:HG22	1.76	0.84
1:B:358:THR:HB	1:B:360:GLN:HG2	1.58	0.84
1:B:62:VAL:HG13	1:B:98:LEU:HD11	1.59	0.82
1:A:984:LEU:HA	1:A:987:ILE:HD12	1.62	0.81
1:B:0:ACE:H3	1:B:36:TYR:CE1	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:THR:HG22	1:A:496:VAL:HG12	1.64	0.79
1:A:572:LYS:HB2	1:A:575:GLU:HG2	1.63	0.79
1:B:909:MET:CE	1:B:937:ILE:HA	2.11	0.79
1:A:898:THR:O	1:A:902:SER:HB2	1.82	0.79
1:A:358:THR:HB	1:A:360:GLN:HG2	1.65	0.79
1:B:72:SER:HB3	1:B:293:ILE:HG21	1.65	0.79
1:B:41:LEU:HG	1:B:42:PRO:HD2	1.63	0.78
1:B:52:LEU:HD23	1:B:106:VAL:HG23	1.66	0.78
1:A:345:THR:HA	1:A:697:ILE:HG22	1.67	0.77
1:A:67:LEU:HD21	2:C:24:LEU:HD11	1.66	0.76
1:B:103:ILE:O	1:B:106:VAL:HG12	1.84	0.76
1:B:162:ASP:OD1	1:B:209:PHE:HA	1.85	0.76
1:B:1:MET:HG2	1:B:2:GLU:H	1.52	0.75
1:A:515:LYS:HE3	3:A:1001:TM1:O5F	1.87	0.75
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.69	0.74
1:A:909:MET:HE2	1:A:937:ILE:HA	1.70	0.74
1:B:249:LEU:HD12	1:B:340:GLU:HG3	1.70	0.73
1:A:311:LEU:O	1:A:314:VAL:HG12	1.88	0.72
1:B:809:PHE:HE1	2:C:4:SER:HB2	1.54	0.72
1:B:209:PHE:O	1:B:212:THR:HG22	1.88	0.72
1:B:373:ASP:HB3	1:B:376:PHE:CD2	2.24	0.71
1:B:148:GLY:H	1:B:223:VAL:HB	1.54	0.71
1:A:762:ARG:HG3	1:A:837:TYR:HE1	1.53	0.71
1:A:287:SER:HB2	1:A:290:ARG:HB3	1.73	0.70
1:B:527:TYR:HB3	1:B:534:ARG:HG3	1.71	0.70
1:B:761:ILE:HG23	1:B:765:ILE:HD13	1.73	0.70
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.74	0.69
1:B:487:PHE:HE2	1:B:492:LYS:HA	1.57	0.69
1:A:909:MET:HE3	1:A:937:ILE:HA	1.74	0.69
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.24	0.68
1:A:773:VAL:HG23	1:A:845:GLY:HA3	1.74	0.67
1:B:119:LEU:HD11	1:B:323:THR:HG23	1.77	0.67
1:B:681:PRO:HB3	1:B:706:ASN:HD22	1.59	0.67
1:B:369:ILE:HG13	1:B:528:VAL:CG1	2.26	0.66
1:B:484:THR:HG22	1:B:496:VAL:HG12	1.75	0.66
1:B:840:ILE:HD13	1:B:980:LEU:HD23	1.78	0.66
1:B:302:LEU:HD21	1:B:772:VAL:HG13	1.76	0.66
1:A:69:ALA:O	1:A:91:PRO:HG3	1.96	0.66
1:B:72:SER:HB3	1:B:293:ILE:CG2	2.25	0.66
1:A:181:THR:HG23	1:A:183:GLU:H	1.59	0.66
1:A:264:ILE:O	1:A:268:CYS:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ILE:HD12	1:B:772:VAL:HG21	1.77	0.65
1:A:373:ASP:HB3	1:A:376:PHE:HD2	1.61	0.65
1:B:808:GLY:C	1:B:809:PHE:HD2	1.99	0.65
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.77	0.65
1:A:869:GLN:NE2	1:A:872:HIS:ND1	2.45	0.65
1:B:950:VAL:O	1:B:954:PRO:HD2	1.97	0.65
1:A:112:ALA:O	1:A:116:ILE:HG12	1.97	0.65
1:B:909:MET:HE2	1:B:937:ILE:HA	1.78	0.65
1:B:513:PHE:HD1	1:B:566:THR:HG22	1.62	0.64
1:A:379:LEU:HD12	1:A:548:VAL:HG21	1.78	0.64
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.80	0.64
1:B:379:LEU:HD12	1:B:548:VAL:HG21	1.78	0.64
1:B:515:LYS:HE3	3:B:1001:TM1:O5F	1.97	0.63
1:B:898:THR:O	1:B:902:SER:HB2	1.98	0.63
1:B:345:THR:HA	1:B:697:ILE:HG22	1.80	0.62
1:A:761:ILE:HG23	1:A:765:ILE:HD13	1.81	0.62
1:A:947:ILE:HA	1:A:953:LEU:HD23	1.80	0.62
1:B:25:THR:HG22	1:B:28:GLN:OE1	1.99	0.62
1:A:567:ARG:CD	1:A:570:PRO:HA	2.29	0.62
1:A:260:LEU:O	1:A:264:ILE:HG12	1.98	0.62
1:B:181:THR:HG23	1:B:183:GLU:H	1.64	0.62
1:B:528:VAL:HG21	1:B:541:VAL:HG11	1.81	0.62
1:B:487:PHE:CE2	1:B:492:LYS:HA	2.35	0.61
1:A:52:LEU:HD23	1:A:106:VAL:HG23	1.83	0.61
1:A:1:MET:HG2	1:A:2:GLU:H	1.66	0.61
1:B:280:ASN:O	1:B:286:GLY:HA2	2.01	0.61
1:B:781:LEU:O	1:B:871:THR:HG23	2.00	0.61
1:B:770:GLY:HA3	1:B:844:VAL:CG2	2.31	0.61
1:A:162:ASP:OD1	1:A:209:PHE:HA	2.00	0.61
1:B:879:ASP:C	1:B:881:PRO:HD2	2.21	0.60
1:B:56:GLN:HG2	1:B:102:ALA:CB	2.32	0.60
1:A:773:VAL:HG21	1:A:842:GLY:HA2	1.82	0.60
1:B:947:ILE:HA	1:B:953:LEU:HD23	1.82	0.60
1:B:56:GLN:HG2	1:B:102:ALA:HB1	1.84	0.60
1:B:210:SER:HB3	1:B:230:THR:HG21	1.84	0.60
1:B:572:LYS:HB2	1:B:575:GLU:HG2	1.84	0.60
1:A:353:THR:HG22	1:A:359:ASN:HD22	1.65	0.60
1:A:72:SER:HB3	1:A:293:ILE:HG21	1.83	0.60
1:A:252:LYS:HE2	1:A:828:LEU:H	1.68	0.59
1:A:148:GLY:H	1:A:223:VAL:HB	1.68	0.59
1:A:5:HIS:HA	1:A:206:ASN:HD21	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ILE:HG13	1:A:528:VAL:HG12	1.83	0.59
1:A:100:ALA:HB3	1:A:797:LEU:HD11	1.85	0.59
1:A:526:ASN:ND2	1:A:590:ASP:HA	2.17	0.59
1:B:165:ILE:HG22	1:B:191:THR:HG22	1.84	0.59
1:B:1:MET:HG2	1:B:2:GLU:N	2.18	0.58
1:B:762:ARG:HH21	1:B:918:GLU:HA	1.68	0.58
1:A:527:TYR:HB2	1:A:592:THR:HG23	1.85	0.58
1:A:681:PRO:HB3	1:A:706:ASN:HD22	1.68	0.58
1:A:25:THR:HG22	1:A:28:GLN:OE1	2.03	0.58
1:A:879:ASP:C	1:A:881:PRO:HD2	2.23	0.58
1:A:702:GLY:O	1:A:719:ALA:HA	2.04	0.58
1:A:276:ILE:HG22	1:A:279:PHE:CE2	2.38	0.58
1:B:876:CYS:O	1:B:880:HIS:HB3	2.04	0.58
1:B:567:ARG:HD3	1:B:570:PRO:HA	1.85	0.58
1:B:809:PHE:CE1	2:C:4:SER:HB2	2.39	0.57
1:B:84:THR:O	1:B:86:THR:N	2.37	0.57
1:B:809:PHE:N	1:B:809:PHE:CD2	2.73	0.56
1:A:345:THR:HA	1:A:697:ILE:CG2	2.35	0.56
1:A:253:LEU:HD21	1:A:311:LEU:HD22	1.88	0.56
1:A:41:LEU:HG	1:A:42:PRO:HD2	1.87	0.56
1:A:773:VAL:O	1:A:777:LEU:HB2	2.05	0.56
1:A:876:CYS:O	1:A:880:HIS:HB3	2.06	0.56
1:B:513:PHE:CD1	1:B:566:THR:HG22	2.41	0.56
1:A:276:ILE:H	1:A:276:ILE:HD13	1.70	0.56
1:A:369:ILE:HD13	1:A:379:LEU:HD23	1.88	0.56
1:A:264:ILE:HD12	1:A:772:VAL:HG21	1.86	0.56
1:B:200:VAL:HG12	1:B:201:ASN:H	1.70	0.56
1:B:347:VAL:HB	1:B:698:THR:HG23	1.88	0.56
1:A:319:LEU:HD22	1:A:339:VAL:CG2	2.35	0.56
1:A:777:LEU:HD23	1:A:849:VAL:HG21	1.88	0.55
1:B:809:PHE:N	1:B:809:PHE:HD2	2.03	0.55
1:B:869:GLN:NE2	1:B:872:HIS:ND1	2.55	0.55
1:B:639:ILE:HD11	1:B:641:ILE:HD12	1.88	0.55
1:A:210:SER:HB3	1:A:230:THR:HG21	1.88	0.55
1:B:90:GLU:HB3	1:B:91:PRO:HD3	1.88	0.55
1:A:373:ASP:HB3	1:A:376:PHE:CD2	2.41	0.55
1:A:856:PHE:CD1	1:A:870:LEU:HD11	2.42	0.55
1:B:179:ILE:HG21	1:B:211:GLY:O	2.06	0.55
1:A:319:LEU:HD22	1:A:339:VAL:HG21	1.89	0.55
1:A:447:THR:HG22	1:A:451:LYS:HE3	1.89	0.55
1:A:970:VAL:O	1:A:973:ILE:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LEU:HD22	1:B:149:ASP:HB3	1.88	0.55
1:A:572:LYS:HB2	1:A:575:GLU:CG	2.34	0.54
1:B:773:VAL:HG21	1:B:842:GLY:HA2	1.89	0.54
1:A:403:ARG:HH21	1:A:406:GLN:NE2	2.04	0.54
1:A:948:LEU:CD2	1:A:959:LEU:HB3	2.37	0.54
1:B:24:LEU:HD13	1:B:149:ASP:HA	1.89	0.54
1:B:330:ASN:HB3	1:B:736:ALA:HB3	1.89	0.54
1:A:492:LYS:HE3	3:A:1001:TM1:H2	1.89	0.54
1:A:494:MET:HG2	3:A:1001:TM1:O4F	2.08	0.54
1:A:361:MET:SD	1:A:601:ASP:HB3	2.48	0.54
1:B:863:PRO:HB2	1:B:890:ILE:HD11	1.89	0.54
1:B:912:ALA:HB1	1:B:933:LEU:HD11	1.90	0.53
1:A:39:ASN:O	1:A:143:ARG:HA	2.08	0.53
1:A:873:PHE:CE1	1:A:891:PHE:HB3	2.44	0.53
1:B:61:LEU:HD23	1:B:300:VAL:HG13	1.90	0.53
1:B:773:VAL:O	1:B:777:LEU:HB2	2.09	0.53
1:A:1:MET:HG2	1:A:2:GLU:N	2.22	0.53
1:B:264:ILE:O	1:B:268:CYS:HB2	2.08	0.53
1:B:379:LEU:CD1	1:B:548:VAL:HG21	2.37	0.53
1:A:934:LEU:HA	1:A:937:ILE:HD12	1.91	0.53
1:B:249:LEU:HD12	1:B:340:GLU:CG	2.37	0.53
1:A:76:ALA:O	1:A:81:GLY:HA2	2.08	0.53
1:B:353:THR:CG2	1:B:359:ASN:HD22	2.21	0.53
1:B:389:TYR:OH	1:B:440:ALA:HB1	2.09	0.53
1:B:527:TYR:O	1:B:592:THR:HA	2.09	0.53
1:A:950:VAL:O	1:A:954:PRO:HD2	2.08	0.53
1:B:770:GLY:HA3	1:B:844:VAL:HG22	1.91	0.53
1:A:487:PHE:HE2	1:A:492:LYS:HA	1.74	0.52
1:A:527:TYR:HB3	1:A:534:ARG:HG3	1.91	0.52
1:A:948:LEU:HD21	1:A:959:LEU:HB3	1.91	0.52
1:B:250:GLN:CG	1:B:315:ILE:HD12	2.39	0.52
1:A:225:THR:HB	1:A:229:SER:HB2	1.90	0.52
1:A:235:ILE:O	1:A:238:GLN:HB3	2.08	0.52
1:B:276:ILE:HD13	1:B:277:GLY:H	1.74	0.52
1:B:364:CYS:SG	1:B:600:LEU:HB3	2.49	0.52
1:A:368:ILE:HG13	1:A:380:ASN:HB2	1.92	0.52
1:B:762:ARG:HG3	1:B:837:TYR:HE1	1.73	0.52
1:B:952:PRO:HG2	2:C:23:TRP:CD1	2.45	0.52
1:A:322:GLY:HA3	1:A:753:ILE:CD1	2.39	0.52
1:B:230:THR:HG21	1:B:232:ILE:HG22	1.91	0.52
1:B:767:SER:HB2	1:B:908:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:855:TRP:CZ2	1:B:863:PRO:HD2	2.45	0.52
1:B:880:HIS:N	1:B:881:PRO:HD2	2.24	0.52
1:A:379:LEU:CD1	1:A:548:VAL:HG21	2.39	0.51
1:A:487:PHE:CE2	1:A:492:LYS:HA	2.45	0.51
1:B:970:VAL:O	1:B:973:ILE:HG22	2.09	0.51
1:A:788:ILE:HG12	1:A:791:GLN:CD	2.30	0.51
1:A:916:LEU:HD11	1:A:927:PRO:HA	1.93	0.51
1:B:898:THR:HG21	1:B:960:LYS:O	2.09	0.51
1:A:981:ASP:OD1	1:A:985:LYS:HE3	2.11	0.51
1:B:832:TRP:N	4:B:1002:PTY:HC51	2.26	0.51
1:B:49:LEU:O	1:B:53:VAL:HG23	2.11	0.51
1:B:843:TYR:OH	1:B:976:PRO:HG2	2.10	0.51
1:B:883:PHE:HD1	1:B:886:LEU:H	1.57	0.51
1:A:48:SER:HB3	1:A:51:GLU:OE1	2.10	0.51
1:A:84:THR:O	1:A:86:THR:N	2.44	0.51
1:B:200:VAL:HG12	1:B:201:ASN:N	2.26	0.50
1:B:147:PRO:HA	1:B:223:VAL:CG1	2.42	0.50
1:B:369:ILE:HD13	1:B:379:LEU:HD23	1.92	0.50
1:B:352:LYS:HG3	1:B:623:MET:SD	2.50	0.50
1:A:59:ASP:O	1:A:63:ARG:HG3	2.12	0.50
1:B:279:PHE:HA	1:B:291:GLY:HA3	1.94	0.50
1:A:335:SER:O	1:A:338:SER:HB2	2.12	0.50
1:A:336:LEU:O	1:A:339:VAL:HG22	2.10	0.50
1:A:513:PHE:HD1	1:A:566:THR:HG22	1.75	0.50
1:B:353:THR:HG22	1:B:359:ASN:HD22	1.76	0.50
1:B:768:ASN:O	1:B:772:VAL:HG23	2.11	0.50
1:A:253:LEU:HD21	1:A:311:LEU:HB3	1.93	0.50
1:B:474:VAL:HA	1:B:477:GLN:HG2	1.93	0.50
1:B:6:SER:HA	1:B:194:VAL:O	2.12	0.50
1:B:415:THR:HA	1:B:475:ILE:HD13	1.93	0.50
1:B:527:TYR:HB2	1:B:592:THR:HG23	1.93	0.50
1:B:155:VAL:HG12	1:B:705:VAL:HG21	1.92	0.50
1:A:880:HIS:N	1:A:881:PRO:HD2	2.27	0.50
1:B:350:SER:HA	1:B:701:THR:OG1	2.12	0.50
1:B:230:THR:HB	1:B:233:GLY:H	1.76	0.49
1:B:311:LEU:N	1:B:312:PRO:HD2	2.26	0.49
2:C:12:PHE:O	2:C:16:LEU:HB2	2.12	0.49
1:A:369:ILE:HD13	1:A:379:LEU:CD2	2.42	0.49
1:A:952:PRO:O	1:A:956:ILE:HG12	2.11	0.49
1:B:230:THR:CG2	1:B:232:ILE:HG22	2.42	0.49
1:B:880:HIS:HB2	1:B:883:PHE:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LYS:HB2	1:B:152:GLU:O	2.12	0.49
1:B:574:GLU:C	1:B:576:MET:H	2.15	0.49
1:B:913:LEU:HD22	1:B:927:PRO:HB3	1.94	0.49
1:A:173:LEU:HD23	1:A:189:LYS:HB2	1.95	0.49
1:B:880:HIS:N	1:B:881:PRO:CD	2.76	0.49
1:A:814:LEU:C	1:A:816:ILE:H	2.14	0.49
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.95	0.49
1:B:250:GLN:HG3	1:B:315:ILE:HD12	1.94	0.49
1:A:495:SER:HA	1:A:513:PHE:O	2.12	0.49
1:B:518:PRO:HB3	1:B:549:ILE:HD13	1.95	0.49
1:A:833:LEU:O	1:A:836:ARG:HB3	2.13	0.49
1:A:762:ARG:CG	1:A:837:TYR:HE1	2.20	0.48
1:A:762:ARG:NH2	1:A:918:GLU:HA	2.28	0.48
1:B:320:ALA:O	1:B:323:THR:HB	2.14	0.48
1:B:654:THR:HA	1:B:677:ALA:O	2.13	0.48
1:A:855:TRP:CD1	1:A:896:PRO:HG3	2.48	0.48
1:B:418:ALA:HB3	1:B:475:ILE:HG21	1.94	0.48
1:A:50:TRP:O	1:A:54:ILE:HG12	2.13	0.48
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.94	0.48
1:B:104:VAL:O	1:B:108:GLN:HG2	2.13	0.48
1:B:873:PHE:CE1	1:B:891:PHE:HB3	2.49	0.48
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.96	0.48
1:A:797:LEU:O	1:A:797:LEU:HD23	2.14	0.48
1:A:844:VAL:HB	1:A:907:ILE:HG21	1.95	0.48
1:B:534:ARG:NH2	1:B:568:ASP:HB2	2.28	0.48
1:B:950:VAL:HG12	1:B:952:PRO:HD2	1.95	0.48
1:A:831:GLY:H	4:A:1002:PTY:HC32	1.79	0.48
1:A:904:LEU:O	1:A:907:ILE:HG22	2.14	0.48
1:B:426:ASP:HB2	1:B:437:VAL:HG21	1.95	0.48
1:A:253:LEU:HD13	1:A:315:ILE:HD11	1.96	0.48
1:A:535:VAL:HB	1:A:536:PRO:HD2	1.96	0.48
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.79	0.48
1:A:119:LEU:HD21	1:A:323:THR:HG22	1.96	0.48
1:B:342:LEU:HD12	1:B:716:ILE:HG12	1.94	0.48
1:A:762:ARG:HG3	1:A:837:TYR:CE1	2.43	0.48
1:A:762:ARG:CG	1:A:837:TYR:CE1	2.97	0.48
1:A:843:TYR:HE2	1:A:907:ILE:HD11	1.78	0.48
1:B:856:PHE:CZ	1:B:896:PRO:HG2	2.49	0.48
1:A:352:LYS:HD2	1:A:635:ILE:HD13	1.96	0.47
1:A:975:LEU:N	1:A:976:PRO:HD2	2.29	0.47
1:B:252:LYS:HE2	1:B:828:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:PHE:HE2	1:A:475:ILE:HG12	1.79	0.47
1:B:791:GLN:O	1:B:795:VAL:HG23	2.14	0.47
1:B:939:LEU:O	1:B:943:LEU:HD13	2.15	0.47
1:A:366:MET:HG2	1:A:384:ILE:HD11	1.95	0.47
1:B:943:LEU:HD21	2:C:15:VAL:CG2	2.43	0.47
1:A:253:LEU:CD2	1:A:311:LEU:HB3	2.44	0.47
1:A:809:PHE:N	1:A:809:PHE:CD2	2.81	0.47
1:A:962:LEU:HB2	1:A:966:GLN:OE1	2.15	0.47
1:B:567:ARG:CD	1:B:570:PRO:HA	2.43	0.47
1:B:329:LYS:O	1:B:330:ASN:HB2	2.14	0.47
1:B:235:ILE:O	1:B:238:GLN:HB3	2.15	0.47
1:B:324:ARG:HG2	1:B:325:ARG:N	2.30	0.47
1:A:108:GLN:NE2	1:A:805:THR:HG22	2.29	0.47
1:A:502:LYS:O	1:A:502:LYS:HG3	2.15	0.47
1:A:880:HIS:N	1:A:881:PRO:CD	2.78	0.47
1:B:108:GLN:HE22	1:B:805:THR:HG22	1.79	0.47
1:A:177:GLN:O	1:A:181:THR:HG22	2.15	0.47
1:A:270:ALA:O	1:A:274:ILE:HG12	2.14	0.47
1:A:819:ARG:HB3	1:A:820:PRO:HD2	1.97	0.47
1:B:773:VAL:CG2	1:B:845:GLY:HA3	2.34	0.47
1:A:60:LEU:O	1:A:64:ILE:HG12	2.15	0.46
1:A:646:GLU:OE1	1:A:651:ARG:NH1	2.48	0.46
1:B:265:SER:O	1:B:269:VAL:HG23	2.15	0.46
1:A:586:GLU:O	1:A:589:THR:OG1	2.33	0.46
1:B:315:ILE:HG12	1:B:757:MET:SD	2.56	0.46
1:A:164:ARG:CZ	1:A:206:ASN:HD22	2.28	0.46
1:A:200:VAL:HG12	1:A:201:ASN:H	1.80	0.46
1:A:403:ARG:HH21	1:A:406:GLN:HE21	1.63	0.46
1:A:528:VAL:HG21	1:A:541:VAL:HG11	1.98	0.46
1:B:311:LEU:O	1:B:314:VAL:HG12	2.16	0.46
1:A:10:GLU:HA	1:A:13:LEU:HD12	1.97	0.46
1:A:65:LEU:CD2	1:A:94:ILE:HG21	2.46	0.46
1:B:989:ARG:NH2	4:B:1003:PTY:HC52	2.31	0.46
1:A:613:LEU:HD22	1:A:817:MET:CE	2.47	0.45
1:A:869:GLN:C	1:A:871:THR:N	2.68	0.45
1:B:426:ASP:HB2	1:B:437:VAL:CG2	2.47	0.45
1:A:863:PRO:HB2	1:A:890:ILE:HD11	1.98	0.45
1:B:319:LEU:HD22	1:B:339:VAL:HG21	1.98	0.45
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.98	0.45
1:A:419:LEU:O	1:A:481:LYS:HE2	2.16	0.45
1:A:330:ASN:HB3	1:A:736:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ILE:CG2	1:B:530:VAL:HG22	2.47	0.45
1:B:807:LEU:HD13	1:B:933:LEU:HD13	1.99	0.45
1:B:617:ALA:HB2	1:B:817:MET:HE3	1.98	0.45
1:A:292:ALA:O	1:A:296:PHE:HB2	2.16	0.45
1:B:273:LEU:O	1:B:276:ILE:HG23	2.16	0.45
1:B:668:GLU:HG3	1:B:672:ARG:NH2	2.31	0.45
1:B:156:GLY:HA2	1:B:726:VAL:HG23	1.99	0.45
1:B:355:THR:HG22	1:B:740:PHE:HB2	1.98	0.45
1:B:975:LEU:N	1:B:976:PRO:HD2	2.30	0.45
1:A:25:THR:HG23	1:A:28:GLN:H	1.82	0.45
1:A:416:ILE:O	1:A:420:CYS:HB2	2.16	0.45
1:A:604:ARG:HB2	1:A:607:VAL:CG2	2.46	0.45
1:B:164:ARG:HG2	1:B:207:MET:SD	2.57	0.45
1:B:369:ILE:HG21	1:B:530:VAL:HG22	1.99	0.45
1:B:904:LEU:O	1:B:907:ILE:HG22	2.17	0.45
1:B:260:LEU:O	1:B:264:ILE:HG12	2.16	0.45
1:A:200:VAL:HG12	1:A:201:ASN:N	2.31	0.45
1:A:654:THR:HA	1:A:677:ALA:O	2.17	0.45
1:B:939:LEU:HD13	2:C:12:PHE:HB2	1.99	0.44
1:A:166:LEU:HG	1:A:221:GLY:HA2	1.98	0.44
1:A:448:LEU:O	1:A:452:MET:HG3	2.16	0.44
1:A:567:ARG:CZ	1:A:571:PRO:HD3	2.48	0.44
1:B:319:LEU:HD22	1:B:339:VAL:CG2	2.47	0.44
2:C:27:ARG:HA	2:C:30:GLN:HB2	1.99	0.44
1:A:325:ARG:NE	1:A:749:GLU:OE2	2.51	0.44
1:A:631:THR:O	1:A:635:ILE:HG13	2.17	0.44
1:A:755:ASN:O	1:A:758:LYS:HB2	2.17	0.44
1:B:118:ALA:O	1:B:121:GLU:HB3	2.16	0.44
1:B:66:LEU:HD21	1:B:95:LEU:HD12	1.99	0.44
1:A:165:ILE:HG22	1:A:191:THR:HG22	1.98	0.44
1:A:858:TYR:O	1:A:860:GLU:HG3	2.17	0.44
1:A:950:VAL:HB	1:A:953:LEU:HD22	2.00	0.44
1:B:495:SER:HA	1:B:513:PHE:O	2.16	0.44
1:B:909:MET:HE3	1:B:937:ILE:HG12	1.98	0.44
1:B:932:TRP:CZ3	2:C:5:THR:HA	2.53	0.44
1:A:163:ILE:CD1	1:A:223:VAL:HG22	2.48	0.44
1:B:176:ASP:O	1:B:212:THR:OG1	2.32	0.44
1:A:266:LEU:C	1:A:268:CYS:H	2.20	0.44
1:A:357:THR:C	1:A:604:ARG:HD2	2.38	0.44
1:A:848:THR:HG22	1:A:900:ALA:HB1	1.99	0.44
1:A:562:LEU:N	1:A:562:LEU:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:PHE:O	1:A:212:THR:HG22	2.17	0.44
1:B:394:GLU:HG3	1:B:396:LEU:HD21	1.98	0.44
1:B:802:LEU:HB2	1:B:803:PRO:HD3	1.99	0.44
1:B:855:TRP:O	1:B:859:ALA:HB2	2.18	0.44
1:B:65:LEU:HD13	1:B:300:VAL:HB	1.99	0.44
1:B:829:ILE:HD13	1:B:837:TYR:HE2	1.83	0.44
1:A:856:PHE:CZ	1:A:896:PRO:HG2	2.53	0.43
1:A:986:PHE:HA	1:A:989:ARG:HH21	1.83	0.43
1:B:494:MET:HG2	3:B:1001:TM1:O4F	2.18	0.43
1:A:72:SER:HB3	1:A:293:ILE:CG2	2.47	0.43
1:A:90:GLU:O	1:A:94:ILE:HG12	2.18	0.43
1:A:155:VAL:HG12	1:A:705:VAL:HG21	1.99	0.43
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.17	0.43
1:B:524:ARG:HD2	1:B:588:GLU:O	2.17	0.43
1:A:311:LEU:N	1:A:312:PRO:HD2	2.32	0.43
1:A:926:PRO:HB3	1:A:928:TRP:CZ2	2.53	0.43
1:B:411:VAL:HG22	1:B:454:VAL:HB	2.00	0.43
1:B:956:ILE:HD11	2:C:22:ILE:CG2	2.48	0.43
1:A:276:ILE:C	1:A:278:HIS:H	2.22	0.43
1:B:188:ILE:H	1:B:188:ILE:HG13	1.61	0.43
1:B:704:GLY:O	1:B:707:ASP:HB2	2.18	0.43
1:A:65:LEU:HB2	1:A:300:VAL:CG1	2.48	0.43
1:A:611:ILE:O	1:A:615:ARG:HG3	2.19	0.43
1:A:650:ASP:OD1	1:A:650:ASP:N	2.51	0.43
1:A:560:ARG:O	1:A:599:MET:HG2	2.18	0.43
1:A:795:VAL:HG11	1:A:904:LEU:CD2	2.49	0.43
1:A:613:LEU:HD22	1:A:817:MET:HE3	2.00	0.43
1:B:479:MET:HB3	1:B:498:CYS:HB3	2.00	0.43
1:A:360:GLN:HA	1:A:360:GLN:NE2	2.34	0.43
1:A:802:LEU:HB2	1:A:803:PRO:HD3	2.01	0.43
1:B:559:LEU:CD2	1:B:600:LEU:HB2	2.49	0.43
1:B:702:GLY:O	1:B:719:ALA:HA	2.19	0.43
1:A:898:THR:HG22	1:A:962:LEU:HD22	2.00	0.43
1:B:274:ILE:HD11	1:B:779:ALA:HB1	2.01	0.43
1:B:100:ALA:HB2	2:C:18:THR:HG21	2.01	0.42
1:B:225:THR:HB	1:B:229:SER:HB2	2.00	0.42
1:B:252:LYS:HE2	1:B:828:LEU:H	1.84	0.42
1:A:244:GLN:HE21	1:A:244:GLN:HB3	1.57	0.42
1:B:601:ASP:HA	1:B:602:PRO:HD2	1.93	0.42
1:B:770:GLY:HA2	1:B:773:VAL:HG22	2.01	0.42
1:B:863:PRO:CB	1:B:890:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:PRO:HD2	1:A:434:TYR:CE1	2.54	0.42
1:A:517:ALA:HA	1:A:518:PRO:HD3	1.87	0.42
1:A:512:MET:HB2	1:A:567:ARG:HB3	2.01	0.42
1:A:65:LEU:HB2	1:A:300:VAL:HG12	2.02	0.42
1:B:762:ARG:CZ	1:B:836:ARG:HH12	2.32	0.42
1:A:983:ILE:O	1:A:987:ILE:HG13	2.20	0.42
1:B:129:VAL:HG12	1:B:151:VAL:HG22	2.00	0.42
1:B:39:ASN:O	1:B:143:ARG:HA	2.18	0.42
1:B:388:THR:C	1:B:390:ALA:H	2.22	0.42
1:B:567:ARG:CZ	1:B:571:PRO:HD3	2.49	0.42
1:B:932:TRP:HZ3	2:C:5:THR:HA	1.84	0.42
1:A:93:VAL:O	1:A:97:ILE:HG12	2.20	0.42
1:B:518:PRO:O	1:B:519:GLU:C	2.58	0.42
1:B:253:LEU:HD11	1:B:761:ILE:HD11	2.01	0.42
1:A:561:CYS:HB3	1:A:598:GLY:CA	2.37	0.42
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.99	0.42
1:A:854:TRP:O	1:A:859:ALA:HA	2.20	0.42
1:B:958:LYS:HG3	1:B:958:LYS:O	2.19	0.42
1:A:0:ACE:H3	1:A:36:TYR:CE1	2.54	0.42
1:B:10:GLU:HA	1:B:13:LEU:HD12	2.02	0.42
1:B:253:LEU:HD12	1:B:315:ILE:HD11	2.02	0.42
1:A:141:LYS:H	1:A:141:LYS:HG2	1.68	0.42
1:A:415:THR:HA	1:A:475:ILE:HD13	2.01	0.42
1:A:971:LEU:C	1:A:973:ILE:H	2.24	0.42
1:B:436:LYS:HB3	1:B:443:THR:HG21	2.02	0.42
1:A:411:VAL:HA	1:A:454:VAL:HG11	2.01	0.41
1:B:230:THR:HG22	1:B:232:ILE:H	1.84	0.41
1:B:613:LEU:HD22	1:B:817:MET:CE	2.50	0.41
1:B:858:TYR:O	1:B:860:GLU:HG3	2.20	0.41
1:A:329:LYS:O	1:A:330:ASN:HB2	2.20	0.41
1:A:762:ARG:HA	1:A:837:TYR:CE1	2.54	0.41
1:B:99:ILE:O	1:B:103:ILE:HG12	2.20	0.41
1:B:73:PHE:CE1	1:B:88:PHE:HD1	2.38	0.41
1:B:962:LEU:HB2	1:B:966:GLN:OE1	2.20	0.41
1:A:916:LEU:CD1	1:A:927:PRO:HA	2.49	0.41
1:A:898:THR:HG21	1:A:960:LYS:O	2.20	0.41
1:A:816:ILE:HG23	1:A:817:MET:N	2.35	0.41
1:B:367:PHE:CD2	1:B:379:LEU:HD22	2.55	0.41
1:A:688:VAL:O	1:A:692:GLN:HG3	2.21	0.41
1:B:606:GLU:HB2	1:B:741:SER:OG	2.21	0.41
1:B:950:VAL:HB	1:B:953:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:HG22	1:A:232:ILE:H	1.85	0.41
1:A:287:SER:HB2	1:A:290:ARG:CB	2.48	0.41
1:A:567:ARG:HG3	1:A:591:LEU:HD23	2.03	0.41
1:A:14:ALA:O	1:A:17:GLY:N	2.54	0.41
1:A:669:ALA:HA	1:A:672:ARG:NH1	2.35	0.41
1:A:875:GLN:HE21	1:A:875:GLN:HB2	1.66	0.41
1:A:901:LEU:HD22	1:A:944:HIS:CE1	2.56	0.41
1:B:281:ASP:CG	1:B:282:PRO:HD2	2.41	0.41
1:B:368:ILE:HG13	1:B:380:ASN:HB2	2.01	0.41
1:A:481:LYS:HD3	1:A:484:THR:CG2	2.51	0.41
1:A:329:LYS:NZ	1:A:749:GLU:OE1	2.53	0.41
1:B:447:THR:HG22	1:B:451:LYS:HE3	2.03	0.41
1:B:943:LEU:HD21	2:C:15:VAL:HG21	2.02	0.41
1:A:389:TYR:OH	1:A:440:ALA:HB1	2.20	0.41
1:B:56:GLN:HG2	1:B:102:ALA:HB2	2.03	0.41
1:B:5:HIS:HA	1:B:206:ASN:HD21	1.86	0.41
1:B:106:VAL:CG1	1:B:107:TRP:N	2.84	0.41
1:B:602:PRO:HA	1:B:603:PRO:HD3	1.87	0.41
1:A:366:MET:HA	1:A:596:VAL:O	2.21	0.41
1:A:623:MET:HE3	1:A:625:THR:HG21	2.03	0.41
1:B:108:GLN:HE22	1:B:805:THR:CG2	2.33	0.41
1:A:13:LEU:HD21	1:A:20:GLU:HB3	2.02	0.40
1:A:322:GLY:HA3	1:A:753:ILE:HD11	2.03	0.40
1:B:833:LEU:O	1:B:836:ARG:HB3	2.20	0.40
1:A:148:GLY:O	1:A:222:ILE:HG13	2.22	0.40
1:A:36:TYR:CD2	1:A:147:PRO:HG2	2.56	0.40
1:B:270:ALA:O	1:B:274:ILE:HG23	2.21	0.40
1:B:310:GLY:O	1:B:313:ALA:HB3	2.21	0.40
1:B:434:TYR:OH	1:B:464:LYS:HG3	2.22	0.40
1:A:604:ARG:HH11	1:A:604:ARG:CG	2.34	0.40
1:A:65:LEU:HD21	1:A:94:ILE:HG21	2.02	0.40
1:B:165:ILE:CD1	1:B:189:LYS:HB3	2.52	0.40
1:A:177:GLN:C	1:A:181:THR:HG22	2.41	0.40
1:A:605:LYS:HG2	1:A:605:LYS:H	1.57	0.40
1:A:97:ILE:HG23	1:A:797:LEU:HD12	2.02	0.40
1:B:26:PRO:HD3	1:B:132:ALA:HB3	2.04	0.40
1:A:119:LEU:HD11	1:A:323:THR:HG21	2.02	0.40
1:A:722:SER:OG	1:A:738:ASP:OD2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	993/995 (100%)	865 (87%)	109 (11%)	19 (2%)	8	34
1	B	993/995 (100%)	861 (87%)	112 (11%)	20 (2%)	7	32
2	C	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	3	19
All	All	2015/2021 (100%)	1752 (87%)	223 (11%)	40 (2%)	7	32

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	ILE
1	A	519	GLU
1	A	863	PRO
1	B	85	ILE
1	B	309	GLU
1	B	863	PRO
1	A	81	GLY
1	A	195	PRO
1	A	267	ILE
1	B	195	PRO
1	B	519	GLU
2	C	2	GLU
1	A	374	GLY
1	A	501	ALA
1	A	503	SER
1	A	813	ASP
1	B	43	ALA
1	A	3	ALA
1	A	972	LYS
1	B	45	GLU
1	B	575	GLU
1	A	509	GLY
1	A	859	ALA
1	A	895	GLU

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Mol	Chain	Res	Type
1	B	118	ALA
1	B	509	GLY
1	A	865	VAL
1	A	880	HIS
1	B	3	ALA
1	B	859	ALA
1	B	880	HIS
1	B	802	LEU
1	B	555	GLY
1	B	864	GLY
1	B	895	GLU
1	A	802	LEU
1	B	459	VAL
1	A	555	GLY
1	B	865	VAL
1	B	816	ILE

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%)	788 (94%)	52 (6%)	18 50
1	B	840/840 (100%)	777 (92%)	63 (8%)	13 42
2	C	31/31 (100%)	29 (94%)	2 (6%)	17 48
All	All	1711/1711 (100%)	1594 (93%)	117 (7%)	16 46

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	48	SER
1	A	67	LEU
1	A	155	VAL
1	A	188	ILE
1	A	229	SER

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Mol	Chain	Res	Type
1	A	243	GLU
1	A	244	GLN
1	A	247	THR
1	A	275	ASN
1	A	276	ILE
1	A	307	ILE
1	A	309	GLU
1	A	384	ILE
1	A	388	THR
1	A	404	SER
1	A	445	LEU
1	A	460	ARG
1	A	486	GLU
1	A	538	THR
1	A	567	ARG
1	A	589	THR
1	A	604	ARG
1	A	612	GLN
1	A	613	LEU
1	A	647	GLU
1	A	691	LEU
1	A	698	THR
1	A	738	ASP
1	A	759	GLN
1	A	760	PHE
1	A	790	VAL
1	A	792	LEU
1	A	807	LEU
1	A	809	PHE
1	A	813	ASP
1	A	818	ASP
1	A	836	ARG
1	A	873	PHE
1	A	874	MET
1	A	883	PHE
1	A	891	PHE
1	A	895	GLU
1	A	902	SER
1	A	906	THR
1	A	922	LEU
1	A	941	MET
1	A	951	ASP

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Mol	Chain	Res	Type
1	A	953	LEU
1	A	955	MET
1	A	964	LEU
1	A	973	ILE
1	B	59	ASP
1	B	61	LEU
1	B	73	PHE
1	B	77	TRP
1	B	96	LEU
1	B	98	LEU
1	B	101	ASN
1	B	113	GLU
1	B	114	ASN
1	B	146	VAL
1	B	158	LYS
1	B	188	ILE
1	B	198	ARG
1	B	236	ARG
1	B	237	ASP
1	B	247	THR
1	B	253	LEU
1	B	268	CYS
1	B	276	ILE
1	B	314	VAL
1	B	388	THR
1	B	400	LYS
1	B	413	LEU
1	B	460	ARG
1	B	486	GLU
1	B	505	ARG
1	B	534	ARG
1	B	538	THR
1	B	561	CYS
1	B	567	ARG
1	B	589	THR
1	B	604	ARG
1	B	612	GLN
1	B	613	LEU
1	B	647	GLU
1	B	656	ARG
1	B	691	LEU
1	B	698	THR

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Mol	Chain	Res	Type
1	B	759	GLN
1	B	760	PHE
1	B	792	LEU
1	B	807	LEU
1	B	809	PHE
1	B	813	ASP
1	B	818	ASP
1	B	836	ARG
1	B	866	THR
1	B	873	PHE
1	B	874	MET
1	B	875	GLN
1	B	883	PHE
1	B	891	PHE
1	B	895	GLU
1	B	902	SER
1	B	906	THR
1	B	941	MET
1	B	947	ILE
1	B	951	ASP
1	B	953	LEU
1	B	955	MET
1	B	964	LEU
1	B	973	ILE
1	B	992	LEU
2	C	9	CYS
2	C	31	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	206	ASN
1	A	244	GLN
1	A	280	ASN
1	A	330	ASN
1	A	359	ASN
1	A	360	GLN
1	A	406	GLN
1	A	461	ASN
1	A	510	ASN
1	A	526	ASN

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Mol	Chain	Res	Type
1	A	612	GLN
1	A	755	ASN
1	A	869	GLN
1	A	875	GLN
1	A	914	ASN
1	A	919	ASN
1	B	32	HIS
1	B	101	ASN
1	B	108	GLN
1	B	114	ASN
1	B	177	GLN
1	B	244	GLN
1	B	280	ASN
1	B	330	ASN
1	B	359	ASN
1	B	360	GLN
1	B	398	ASN
1	B	406	GLN
1	B	461	ASN
1	B	510	ASN
1	B	526	ASN
1	B	612	GLN
1	B	768	ASN
1	B	869	GLN
1	B	875	GLN
1	B	919	ASN
1	B	990	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	PTY	A	1002	-	18,18,49	1.49	2 (11%)	21,23,54	1.28	1 (4%)
3	TM1	B	1001	-	30,42,42	3.63	13 (43%)	31,66,66	3.23	11 (35%)
3	TM1	A	1001	-	30,42,42	3.55	14 (46%)	31,66,66	3.38	9 (29%)
4	PTY	B	1004	-	18,18,49	1.51	2 (11%)	21,23,54	1.33	1 (4%)
4	PTY	A	1003	-	18,18,49	1.50	2 (11%)	21,23,54	1.33	2 (9%)
4	PTY	B	1003	-	18,18,49	1.55	2 (11%)	21,23,54	1.63	2 (9%)
4	PTY	B	1002	-	18,18,49	1.58	2 (11%)	21,23,54	1.33	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PTY	A	1002	-	-	6/20/20/53	-
3	TM1	B	1001	-	-	4/12/68/68	0/5/5/5
3	TM1	A	1001	-	-	5/12/68/68	0/5/5/5
4	PTY	B	1004	-	-	11/20/20/53	-
4	PTY	A	1003	-	-	9/20/20/53	-
4	PTY	B	1003	-	-	12/20/20/53	-
4	PTY	B	1002	-	-	9/20/20/53	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	TM1	C5F-C6F	12.87	1.52	1.33
3	A	1001	TM1	C5F-C6F	11.76	1.50	1.33
3	A	1001	TM1	O3'-C1F	8.25	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	TM1	O2'-C1F	7.83	1.52	1.41
3	B	1001	TM1	O3'-C1F	6.55	1.50	1.41
3	A	1001	TM1	O2'-C1F	6.12	1.49	1.41
4	B	1002	PTY	O7-C8	5.63	1.47	1.35
4	B	1003	PTY	O7-C8	5.42	1.47	1.35
4	B	1004	PTY	O7-C8	5.25	1.47	1.35
4	A	1002	PTY	O7-C8	5.16	1.46	1.35
4	A	1003	PTY	O7-C8	5.09	1.46	1.35
3	A	1001	TM1	C3F-C2F	4.61	1.40	1.33
3	B	1001	TM1	C3'-C4'	-4.53	1.40	1.52
3	B	1001	TM1	C3F-C2F	4.35	1.39	1.33
3	B	1001	TM1	C4F-C3F	-4.15	1.38	1.50
3	A	1001	TM1	C4F-C3F	-3.92	1.38	1.50
3	B	1001	TM1	C2-N3	3.60	1.37	1.32
3	A	1001	TM1	C5'-C4'	3.59	1.62	1.51
3	A	1001	TM1	C2-N3	3.56	1.37	1.32
3	B	1001	TM1	C4-N3	3.43	1.40	1.35
3	A	1001	TM1	C4-N3	3.04	1.39	1.35
3	A	1001	TM1	C2-N1	2.96	1.39	1.33
3	A	1001	TM1	O7F-N6F	-2.89	1.17	1.22
3	A	1001	TM1	C3'-C4'	-2.86	1.45	1.52
3	A	1001	TM1	C4F-C5F	-2.82	1.42	1.50
3	B	1001	TM1	C2-N1	2.79	1.39	1.33
4	A	1003	PTY	O4-C30	2.75	1.46	1.33
4	B	1003	PTY	O4-C30	2.69	1.46	1.33
4	A	1002	PTY	O4-C30	2.66	1.46	1.33
3	B	1001	TM1	C5'-C4'	2.65	1.59	1.51
4	B	1004	PTY	O4-C30	2.58	1.46	1.33
4	B	1002	PTY	O4-C30	2.57	1.46	1.33
3	B	1001	TM1	C4F-C5F	-2.28	1.43	1.50
3	A	1001	TM1	C5-N7	-2.05	1.32	1.39
3	A	1001	TM1	C3'-C2'	-2.04	1.48	1.53
3	B	1001	TM1	C5-N7	-2.02	1.32	1.39
3	B	1001	TM1	C3'-C2'	-2.00	1.48	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	TM1	O5'-C5'-C4'	11.56	148.76	108.99
3	B	1001	TM1	O5'-C5'-C4'	9.92	143.14	108.99
3	A	1001	TM1	O2'-C2'-C3'	7.10	114.92	103.58
3	A	1001	TM1	O3'-C1F-C6F	-6.55	101.50	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1001	TM1	O3'-C1F-C6F	-6.41	101.70	110.47
3	A	1001	TM1	O2'-C1F-C2F	-6.10	102.13	110.47
3	B	1001	TM1	O2'-C2'-C3'	6.08	113.29	103.58
4	B	1003	PTY	O7-C8-C11	5.75	121.66	111.09
3	B	1001	TM1	PA-O5'-C5'	5.07	132.25	118.30
4	B	1002	PTY	O7-C8-C11	4.86	120.03	111.09
3	A	1001	TM1	N3-C2-N1	-4.79	121.19	128.68
3	B	1001	TM1	N3-C2-N1	-4.76	121.24	128.68
4	B	1004	PTY	O7-C8-C11	4.55	119.46	111.09
3	B	1001	TM1	O2'-C1F-C2F	-4.53	104.27	110.47
4	A	1003	PTY	O7-C8-C11	4.36	119.12	111.09
4	A	1002	PTY	O7-C8-C11	4.33	119.05	111.09
3	B	1001	TM1	O4'-C1'-C2'	-4.27	99.19	106.59
3	B	1001	TM1	C2'-C3'-C4'	4.16	113.59	103.72
3	A	1001	TM1	C2'-C3'-C4'	3.78	112.69	103.72
3	A	1001	TM1	O4'-C1'-C2'	-3.64	100.28	106.59
3	B	1001	TM1	O2'-C2'-C1'	2.96	118.27	109.75
3	B	1001	TM1	O3'-C3'-C2'	2.79	108.04	103.58
4	B	1003	PTY	O7-C8-O10	-2.73	117.54	122.96
3	A	1001	TM1	O3'-C1F-C2F	2.68	114.14	110.47
3	B	1001	TM1	O4'-C4'-C5'	2.43	117.38	109.37
3	A	1001	TM1	O2'-C2'-C1'	2.35	116.52	109.75
4	A	1003	PTY	O7-C8-O10	-2.14	118.70	122.96

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1001	TM1	C5'-O5'-PA-O1A
3	B	1001	TM1	C5'-O5'-PA-O2A
3	B	1001	TM1	C5'-O5'-PA-O3A
3	A	1001	TM1	C5'-O5'-PA-O1A
3	A	1001	TM1	C5'-O5'-PA-O2A
3	A	1001	TM1	C5'-O5'-PA-O3A
4	B	1004	PTY	N1-C2-C3-O11
4	B	1004	PTY	C3-O11-P1-O13
4	A	1003	PTY	N1-C2-C3-O11
4	A	1003	PTY	O10-C8-O7-C6
4	A	1003	PTY	C11-C8-O7-C6
4	B	1003	PTY	N1-C2-C3-O11
4	B	1003	PTY	C11-C8-O7-C6
4	B	1002	PTY	C3-O11-P1-O13

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Mol	Chain	Res	Type	Atoms
4	B	1004	PTY	C11-C8-O7-C6
4	B	1003	PTY	O10-C8-O7-C6
4	B	1004	PTY	O10-C8-O7-C6
4	B	1002	PTY	C11-C8-O7-C6
4	B	1002	PTY	C31-C30-O4-C1
4	A	1003	PTY	C31-C30-O4-C1
4	A	1002	PTY	C31-C30-O4-C1
4	B	1004	PTY	C31-C30-O4-C1
4	B	1002	PTY	O30-C30-O4-C1
4	A	1002	PTY	C11-C8-O7-C6
4	A	1003	PTY	O30-C30-O4-C1
4	A	1002	PTY	O30-C30-O4-C1
4	B	1004	PTY	O30-C30-O4-C1
4	B	1002	PTY	O10-C8-O7-C6
4	B	1004	PTY	C3-O11-P1-O14
4	B	1002	PTY	C3-O11-P1-O14
4	B	1003	PTY	C31-C30-O4-C1
4	A	1002	PTY	O10-C8-O7-C6
4	A	1002	PTY	O4-C1-C6-C5
4	B	1002	PTY	O4-C1-C6-C5
4	B	1004	PTY	O14-C5-C6-C1
4	B	1003	PTY	O30-C30-O4-C1
4	A	1003	PTY	O4-C1-C6-C5
4	B	1004	PTY	O14-C5-C6-O7
4	A	1003	PTY	O14-C5-C6-O7
4	B	1003	PTY	O4-C1-C6-O7
4	A	1003	PTY	O14-C5-C6-C1
4	B	1003	PTY	O4-C1-C6-C5
4	B	1002	PTY	O4-C1-C6-O7
4	B	1003	PTY	C3-O11-P1-O14
4	B	1004	PTY	C3-O11-P1-O12
4	A	1003	PTY	O4-C1-C6-O7
4	B	1003	PTY	C1-C6-O7-C8
4	B	1003	PTY	C5-C6-O7-C8
4	A	1002	PTY	O4-C1-C6-O7
4	B	1003	PTY	C5-O14-P1-O11
4	B	1002	PTY	C5-C6-O7-C8
3	B	1001	TM1	C4'-C5'-O5'-PA
3	A	1001	TM1	C3F-C4F-N4F-O5F
3	A	1001	TM1	C5F-C4F-N4F-O5F
4	B	1004	PTY	C5-O14-P1-O13
4	B	1003	PTY	C5-O14-P1-O13

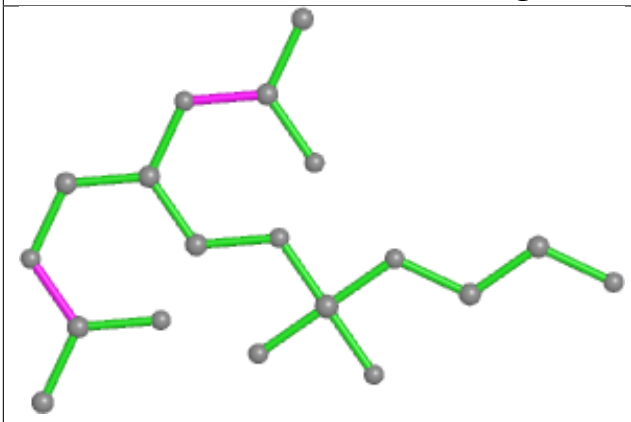
There are no ring outliers.

5 monomers are involved in 8 short contacts:

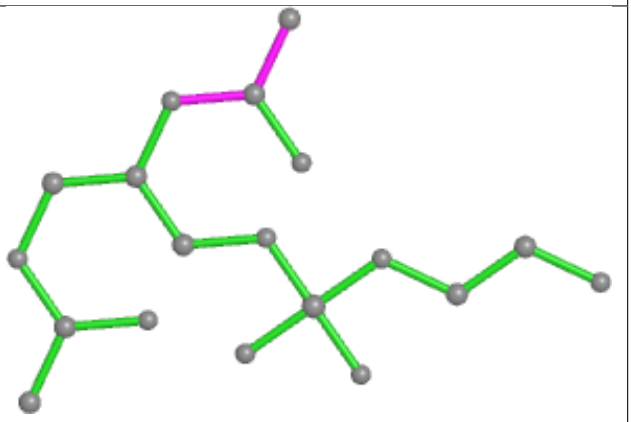
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	PTY	1	0
3	B	1001	TM1	2	0
3	A	1001	TM1	3	0
4	B	1003	PTY	1	0
4	B	1002	PTY	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

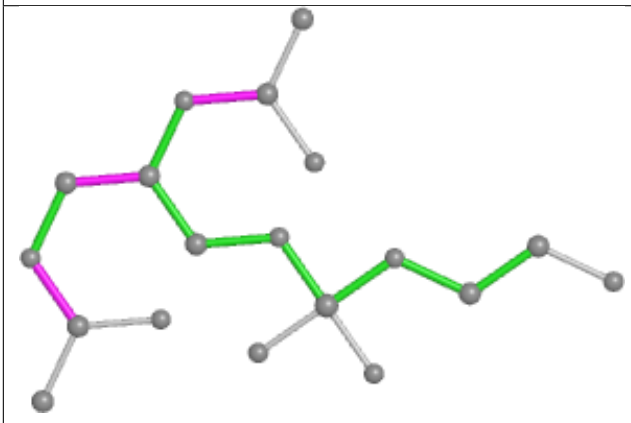
Ligand PTY A 1002



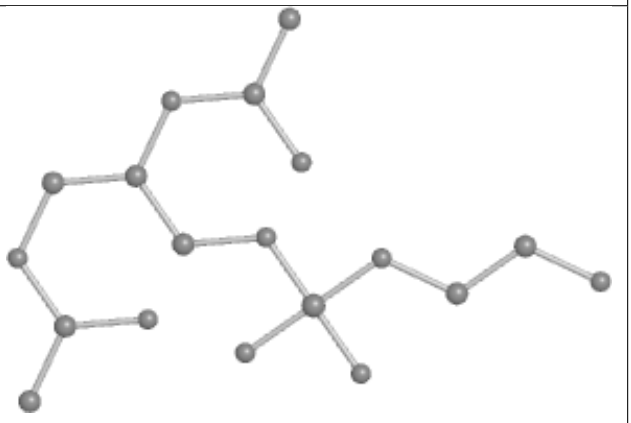
Bond lengths



Bond angles

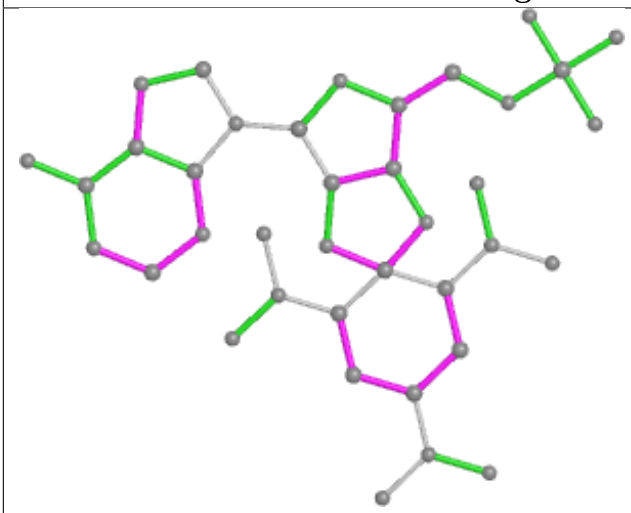


Torsions

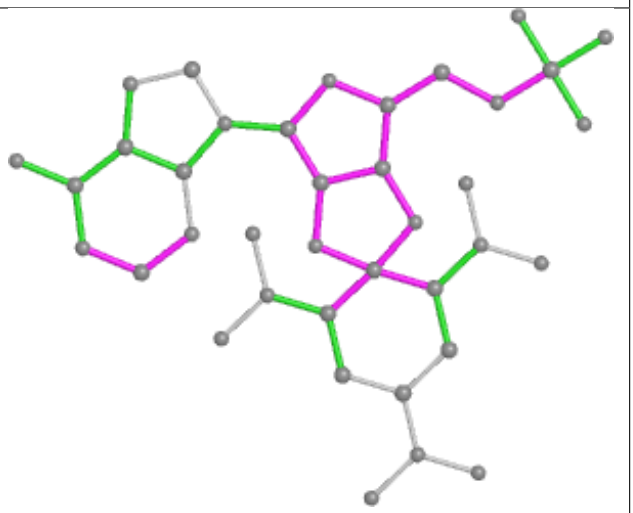


Rings

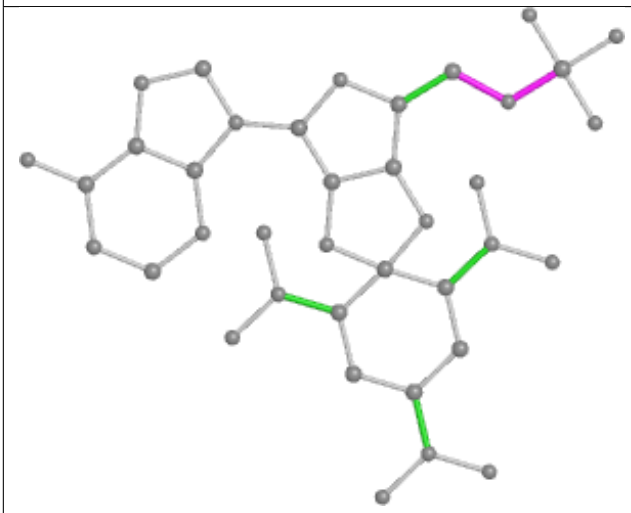
Ligand TM1 B 1001



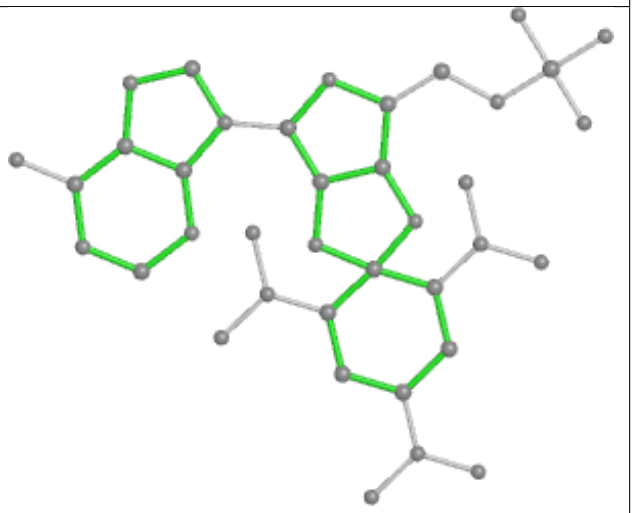
Bond lengths



Bond angles

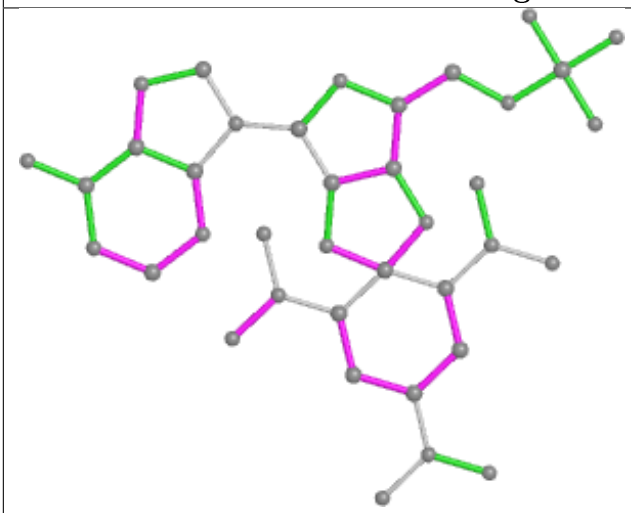


Torsions

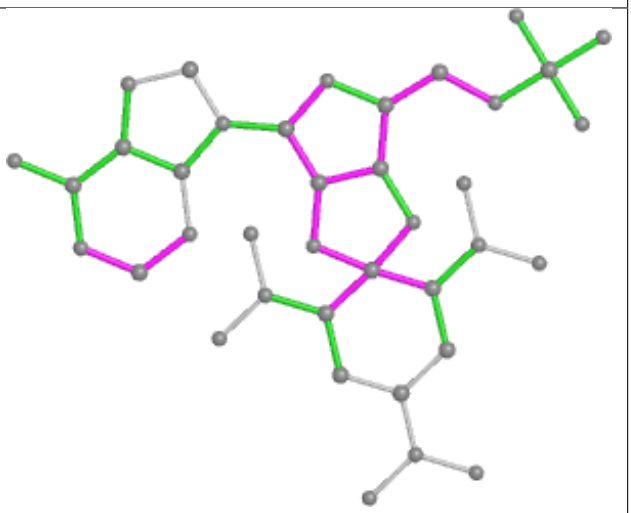


Rings

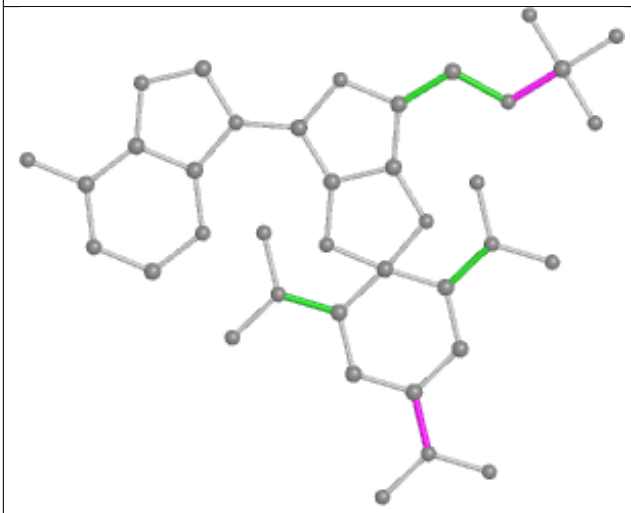
Ligand TM1 A 1001



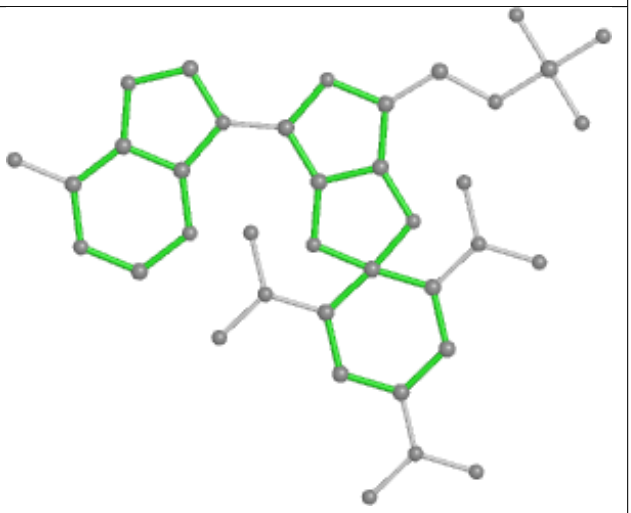
Bond lengths



Bond angles

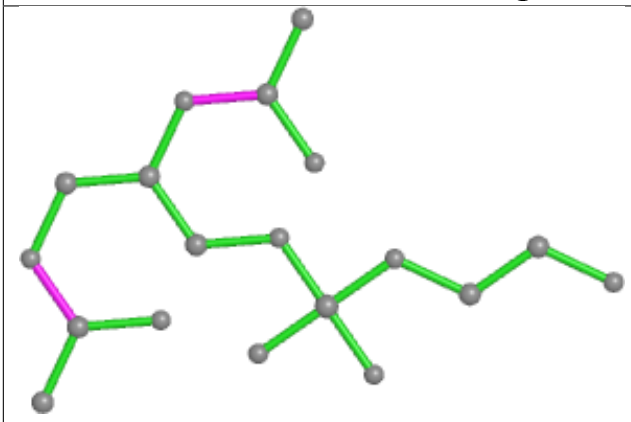


Torsions

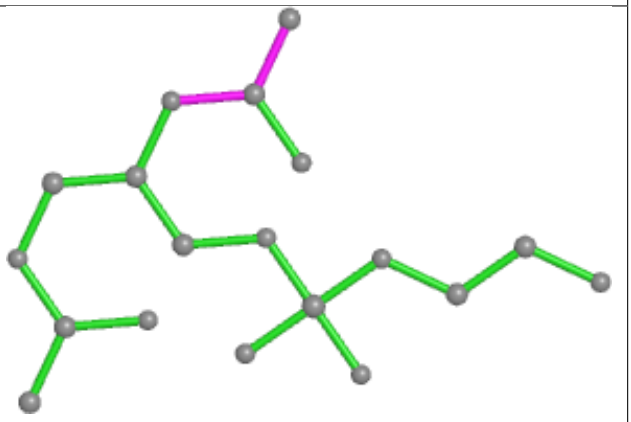


Rings

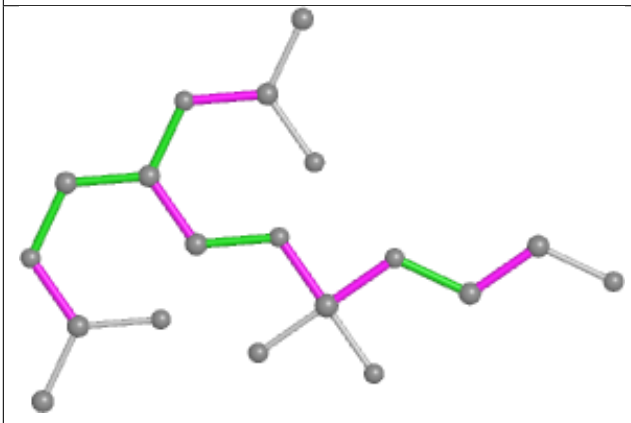
Ligand PTY B 1004



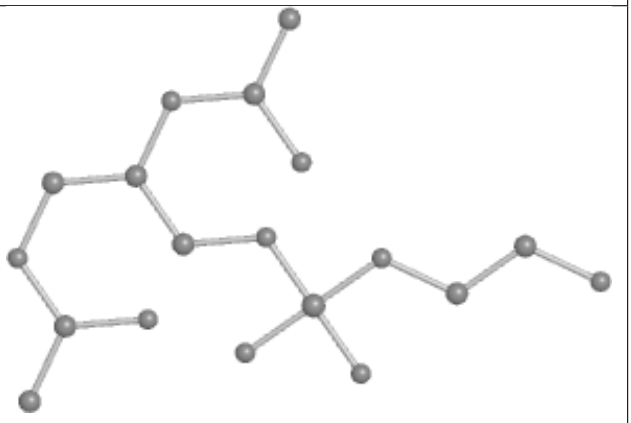
Bond lengths



Bond angles

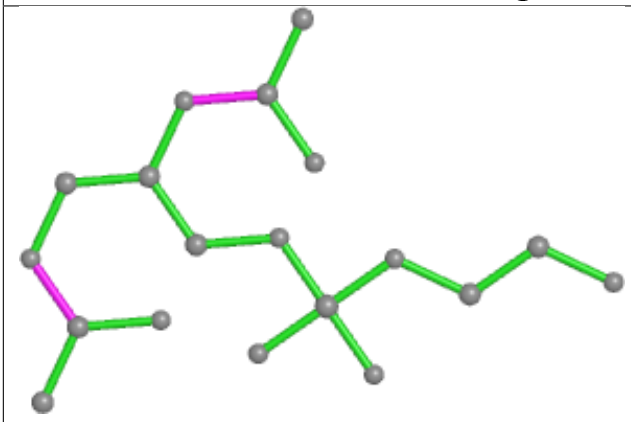


Torsions

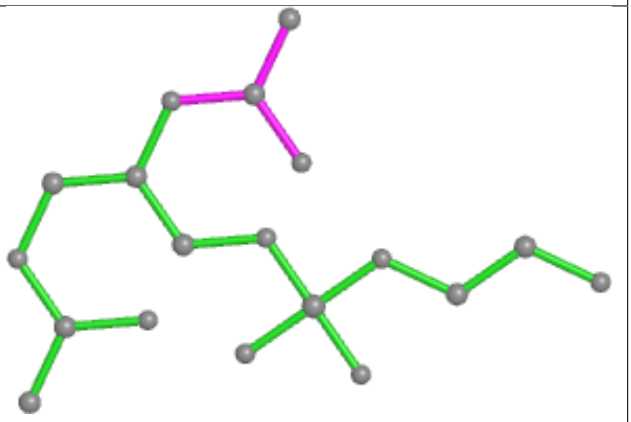


Rings

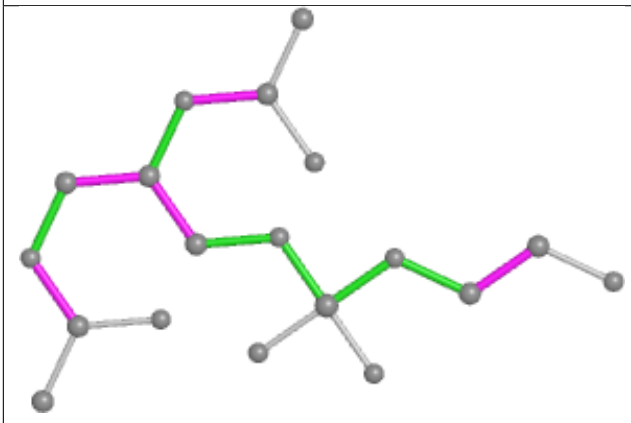
Ligand PTY A 1003



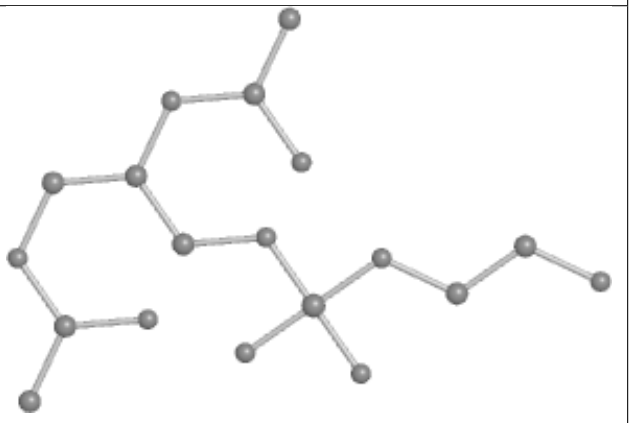
Bond lengths



Bond angles

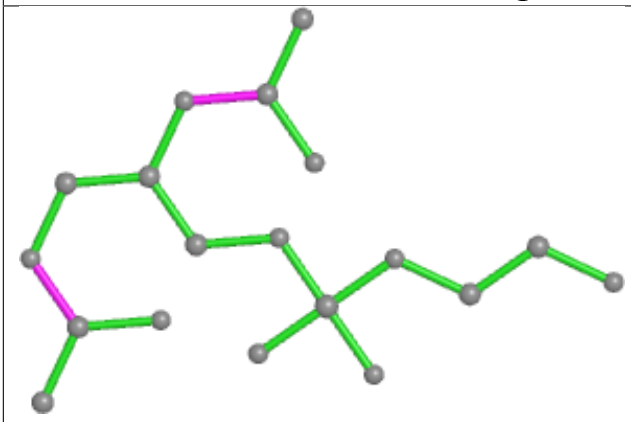


Torsions

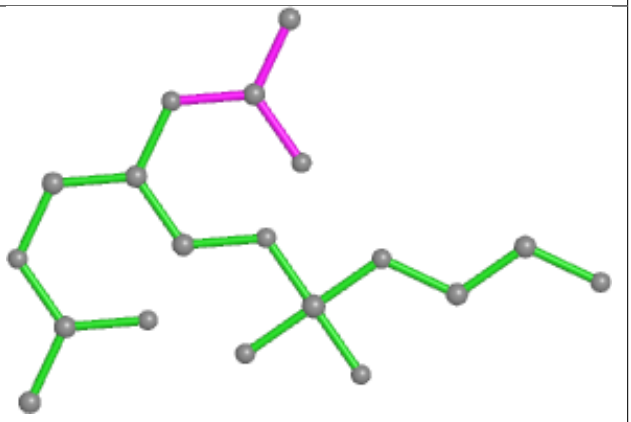


Rings

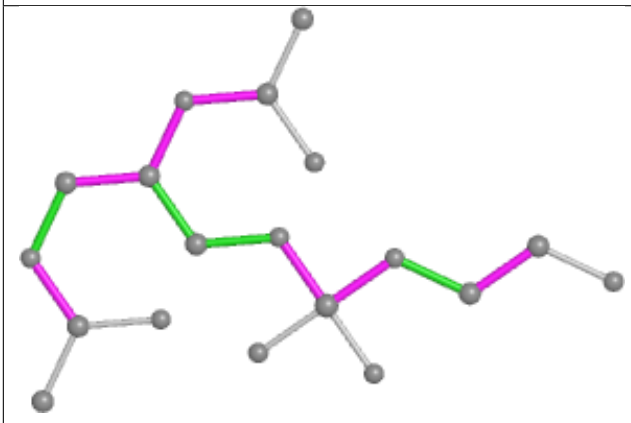
Ligand PTY B 1003



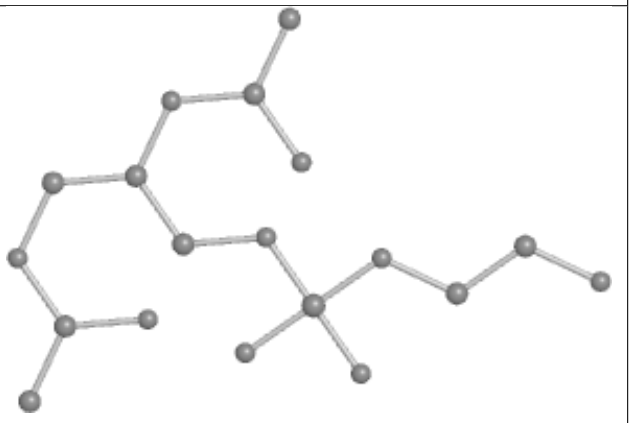
Bond lengths



Bond angles

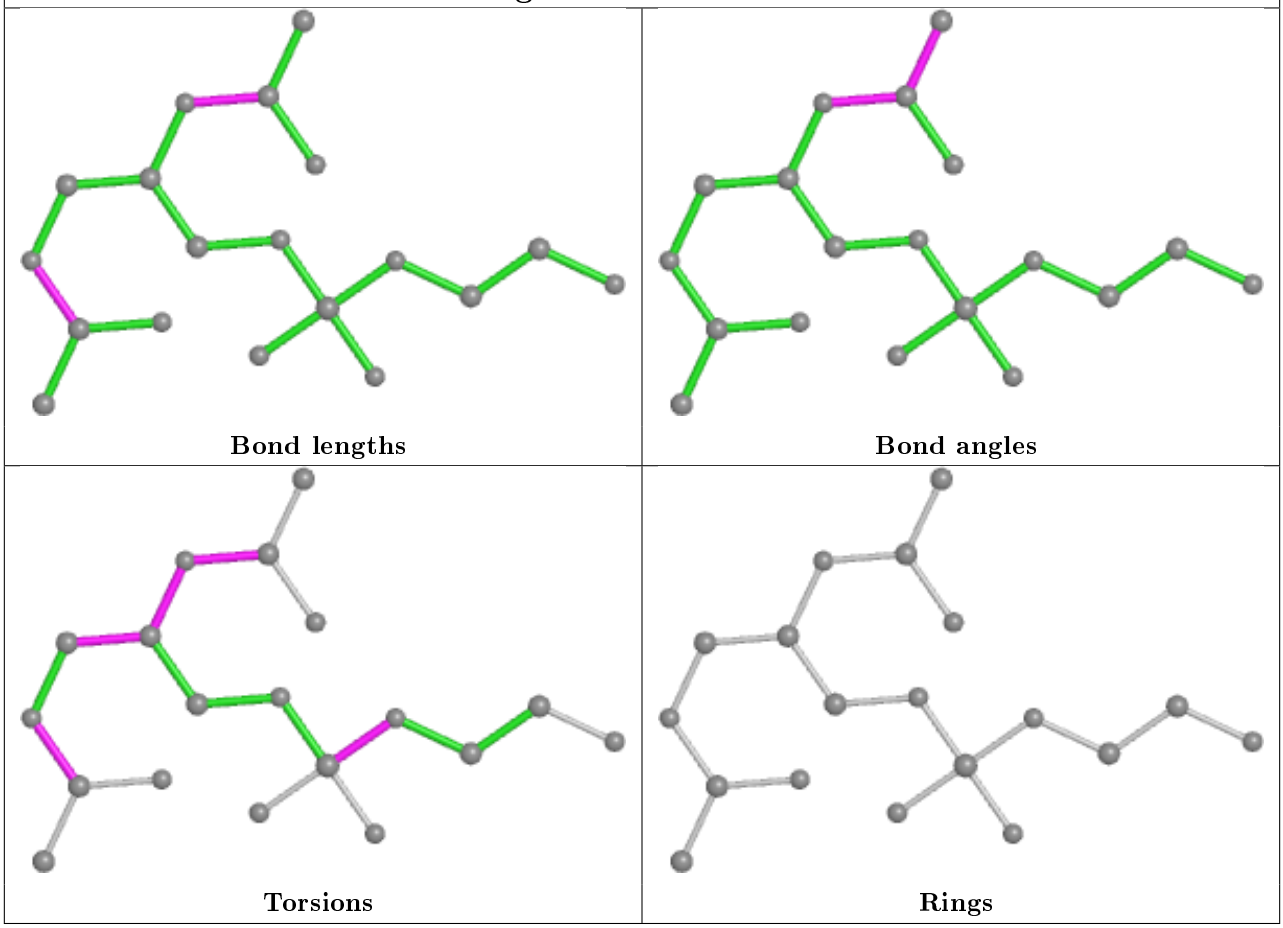


Torsions



Rings

Ligand PTY B 1002



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.29	17 (1%) 70 41	25, 73, 145, 198	0
1	B	994/995 (99%)	-0.26	21 (2%) 63 34	29, 70, 134, 189	0
2	C	31/31 (100%)	1.71	11 (35%) 0 0	118, 137, 159, 164	0
All	All	2019/2021 (99%)	-0.25	49 (2%) 59 30	25, 72, 142, 198	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	878	GLU	7.7
1	B	506	ALA	7.2
1	B	508	VAL	6.7
1	A	505	ARG	5.8
1	B	507	ALA	5.6
1	A	994	GLY	5.6
2	C	15	VAL	5.3
1	B	505	ARG	5.3
1	A	877	THR	5.1
1	B	994	GLY	5.1
1	A	240	ALA	4.8
1	B	503	SER	4.7
1	A	239	MET	4.4
2	C	25	LEU	4.3
2	C	11	ASN	4.2
1	B	504	SER	4.1
1	A	236	ARG	4.1
2	C	21	LEU	4.0
2	C	12	PHE	3.9
1	B	878	GLU	3.7
1	A	887	ASP	3.4
2	C	2	GLU	3.4
1	A	886	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	3	ARG	3.0
2	C	22	ILE	3.0
1	A	282	PRO	3.0
2	C	20	ILE	3.0
1	B	240	ALA	2.9
1	B	46	GLY	2.9
1	B	80	GLU	2.8
2	C	14	VAL	2.8
1	A	35	LYS	2.8
1	B	79	GLU	2.6
1	A	31	ARG	2.5
1	B	242	THR	2.5
1	A	892	GLU	2.4
1	A	891	PHE	2.3
1	B	245	ASP	2.3
1	B	83	GLU	2.2
2	C	18	THR	2.2
1	A	785	GLU	2.2
1	B	45	GLU	2.2
1	B	203	ASP	2.1
1	B	200	VAL	2.1
1	B	575	GLU	2.1
1	A	504	SER	2.1
1	B	572	LYS	2.1
1	A	508	VAL	2.0
1	B	138	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

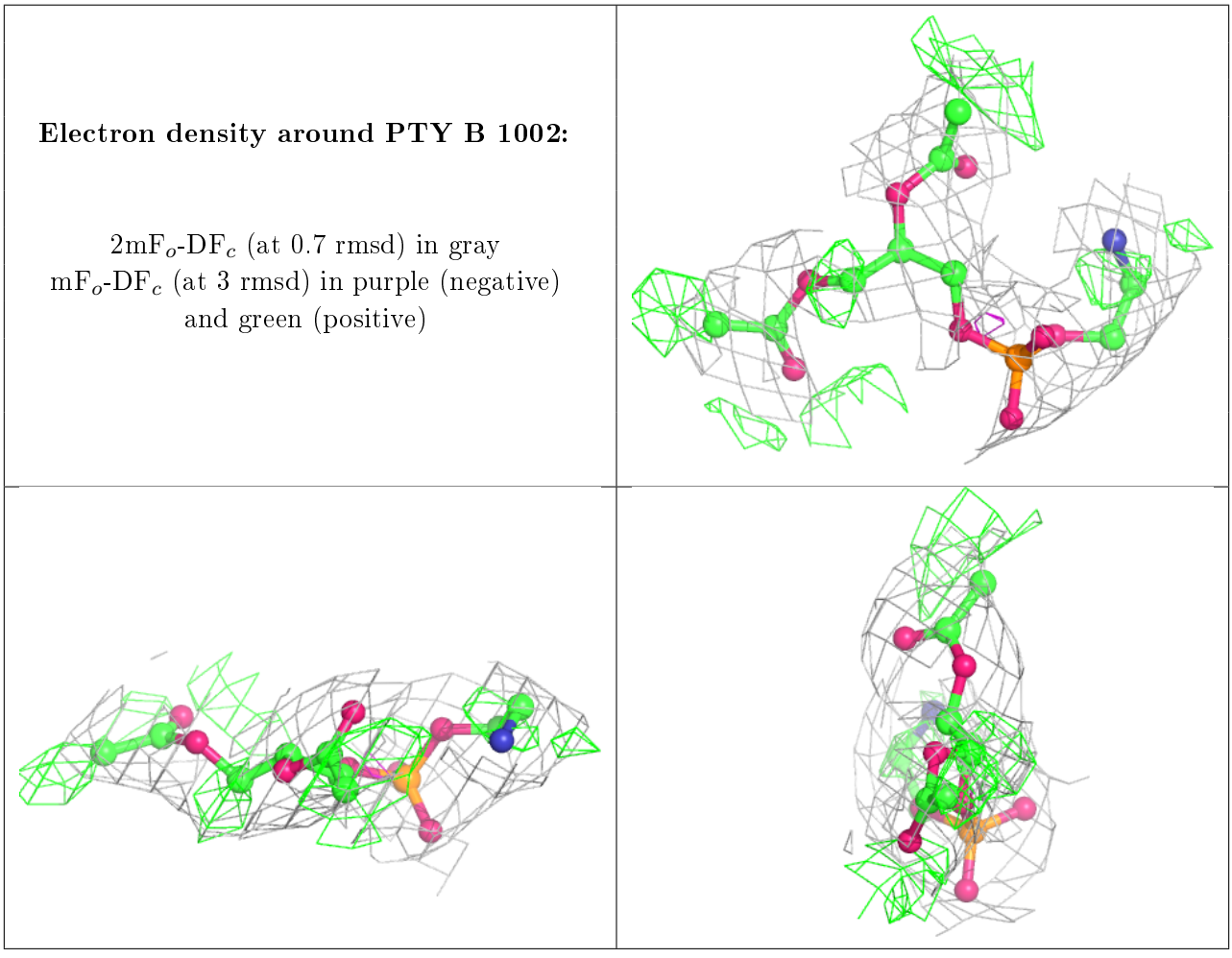
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PTY	B	1002	19/50	0.74	0.20	79,96,134,134	0
4	PTY	A	1002	19/50	0.78	0.19	107,124,149,152	0
4	PTY	B	1004	19/50	0.87	0.26	83,112,120,120	0
4	PTY	A	1003	19/50	0.88	0.21	93,118,130,131	0
3	TM1	B	1001	38/38	0.91	0.25	64,75,100,103	0
3	TM1	A	1001	38/38	0.92	0.23	44,65,92,95	0
5	MG	B	1005	1/1	0.95	0.07	58,58,58,58	0
4	PTY	B	1003	19/50	0.95	0.18	55,76,87,90	0
6	NA	A	1006	1/1	0.97	0.08	37,37,37,37	0
6	NA	B	1007	1/1	0.97	0.21	33,33,33,33	0
5	MG	B	1006	1/1	0.98	0.14	16,16,16,16	0
5	MG	A	1005	1/1	0.99	0.18	19,19,19,19	0
5	MG	A	1004	1/1	0.99	0.07	55,55,55,55	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.

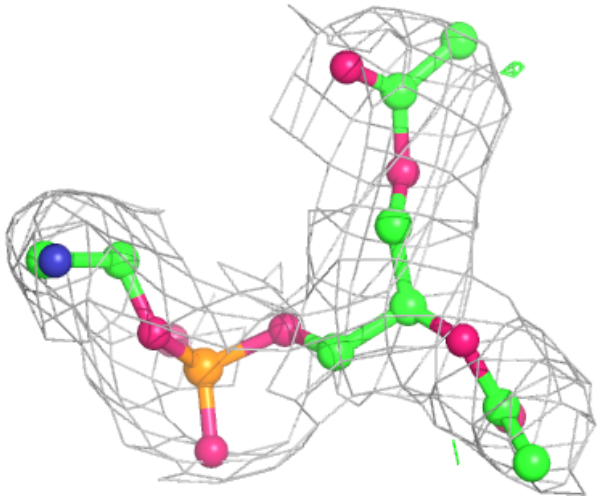
Electron density around PTY B 1002:

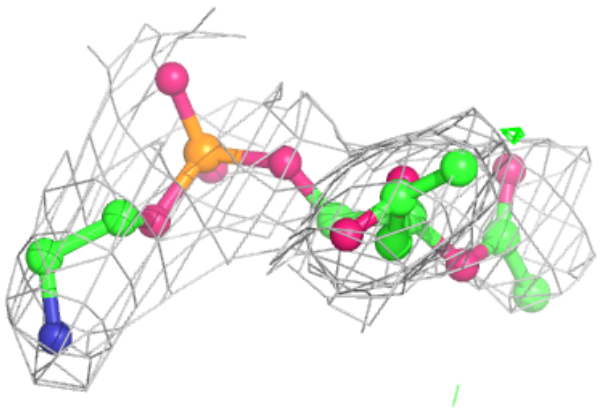
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

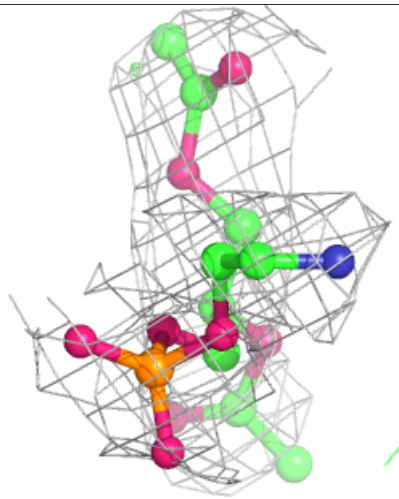


Electron density around PTY A 1002:

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

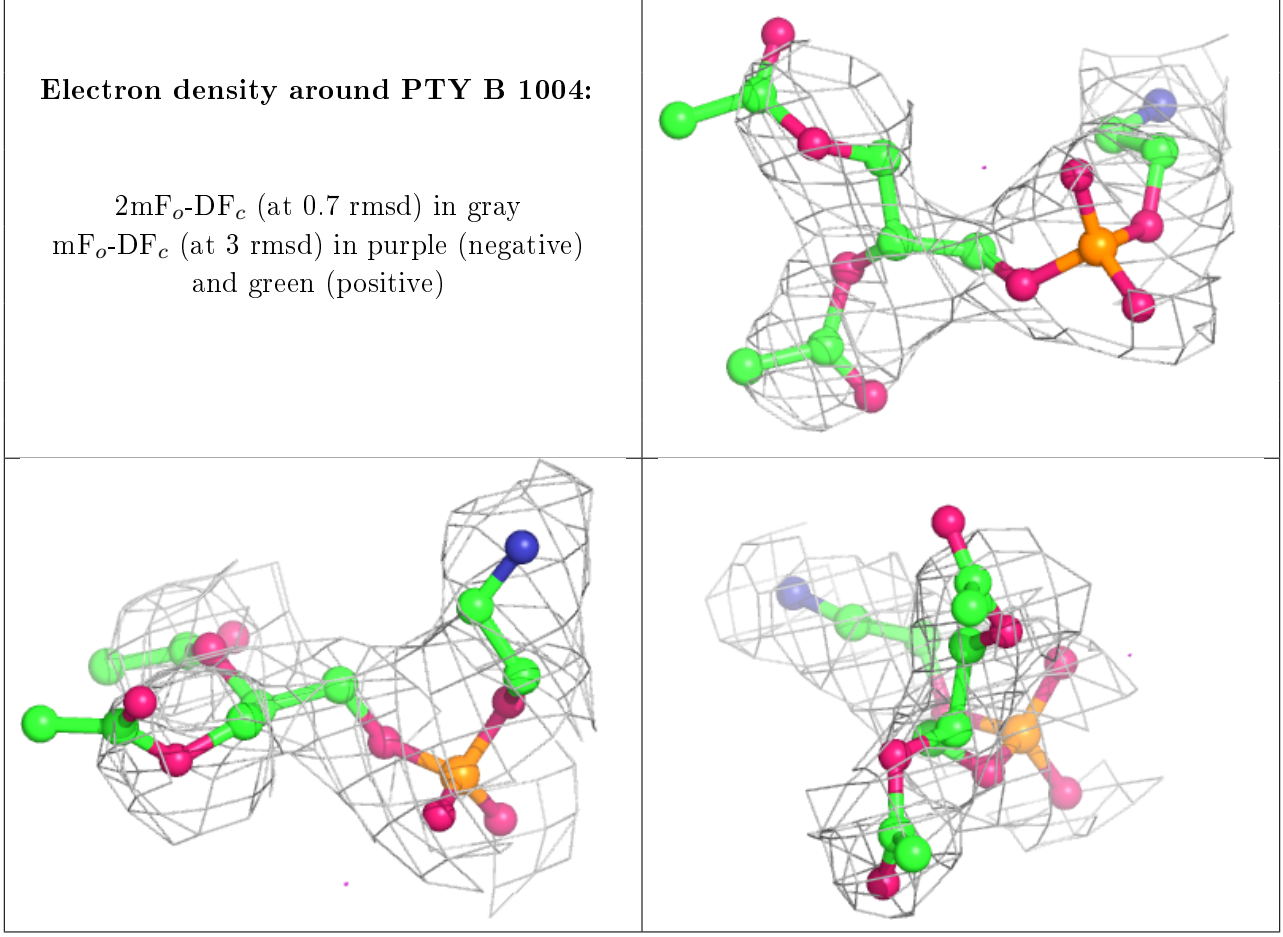






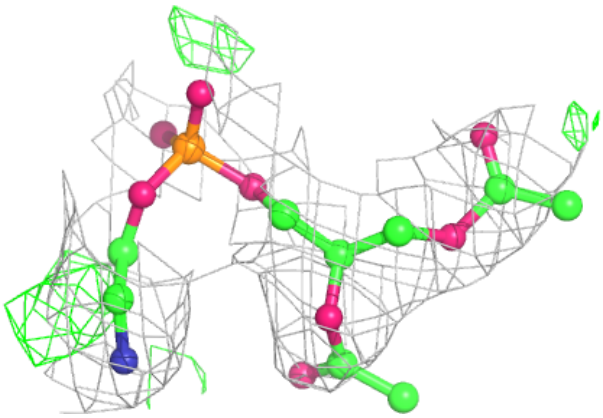
Electron density around PTY B 1004:

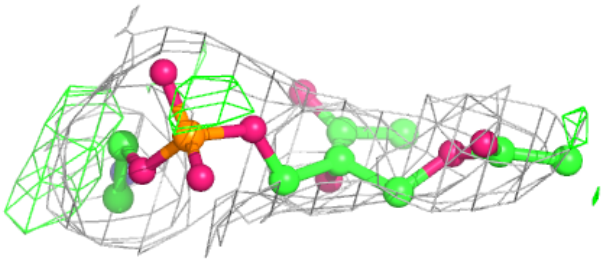
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

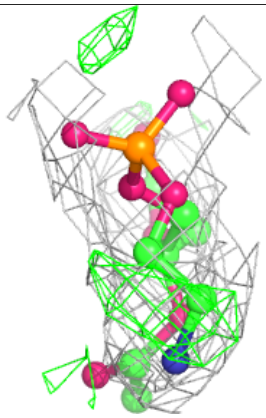


Electron density around PTY A 1003:

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

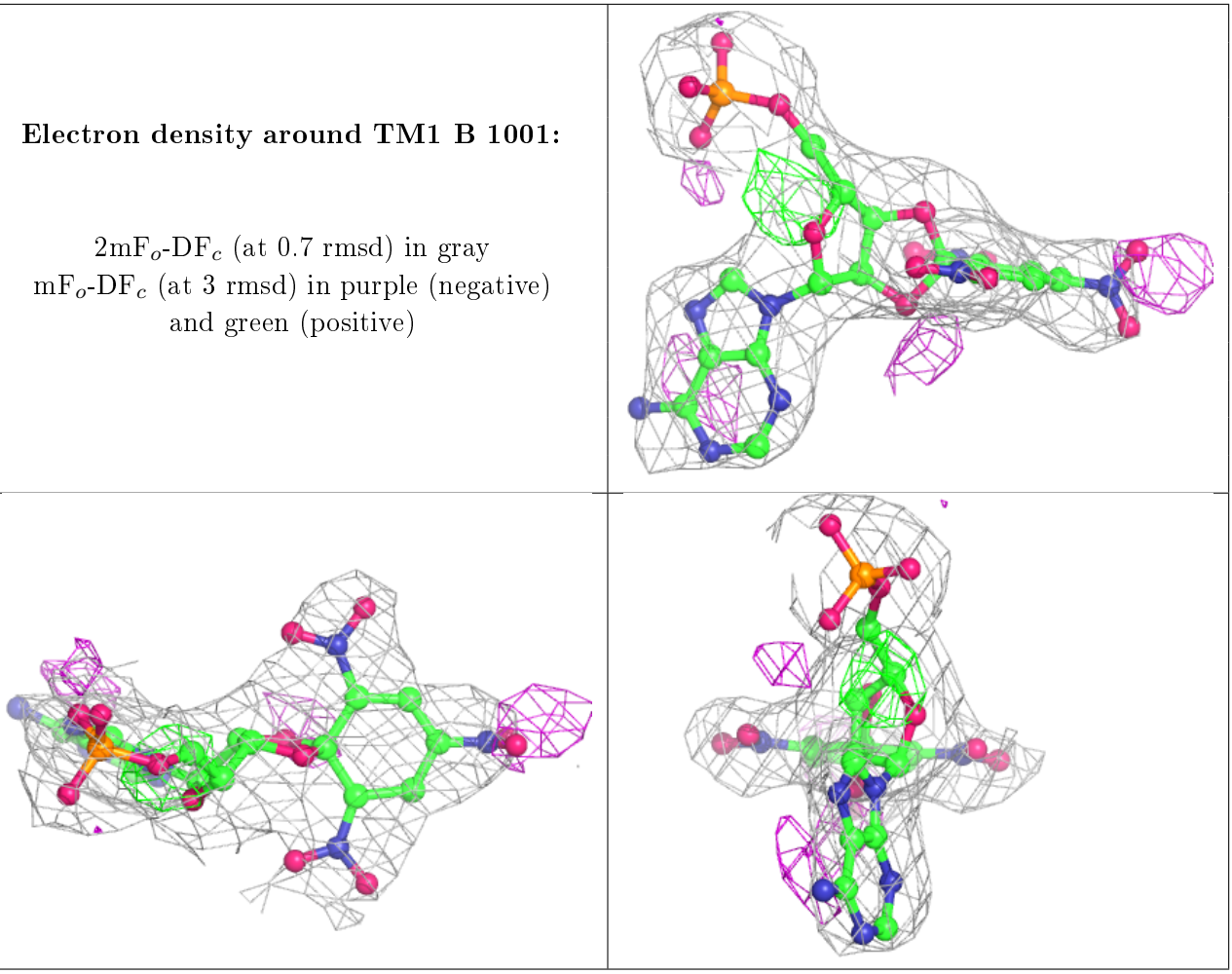






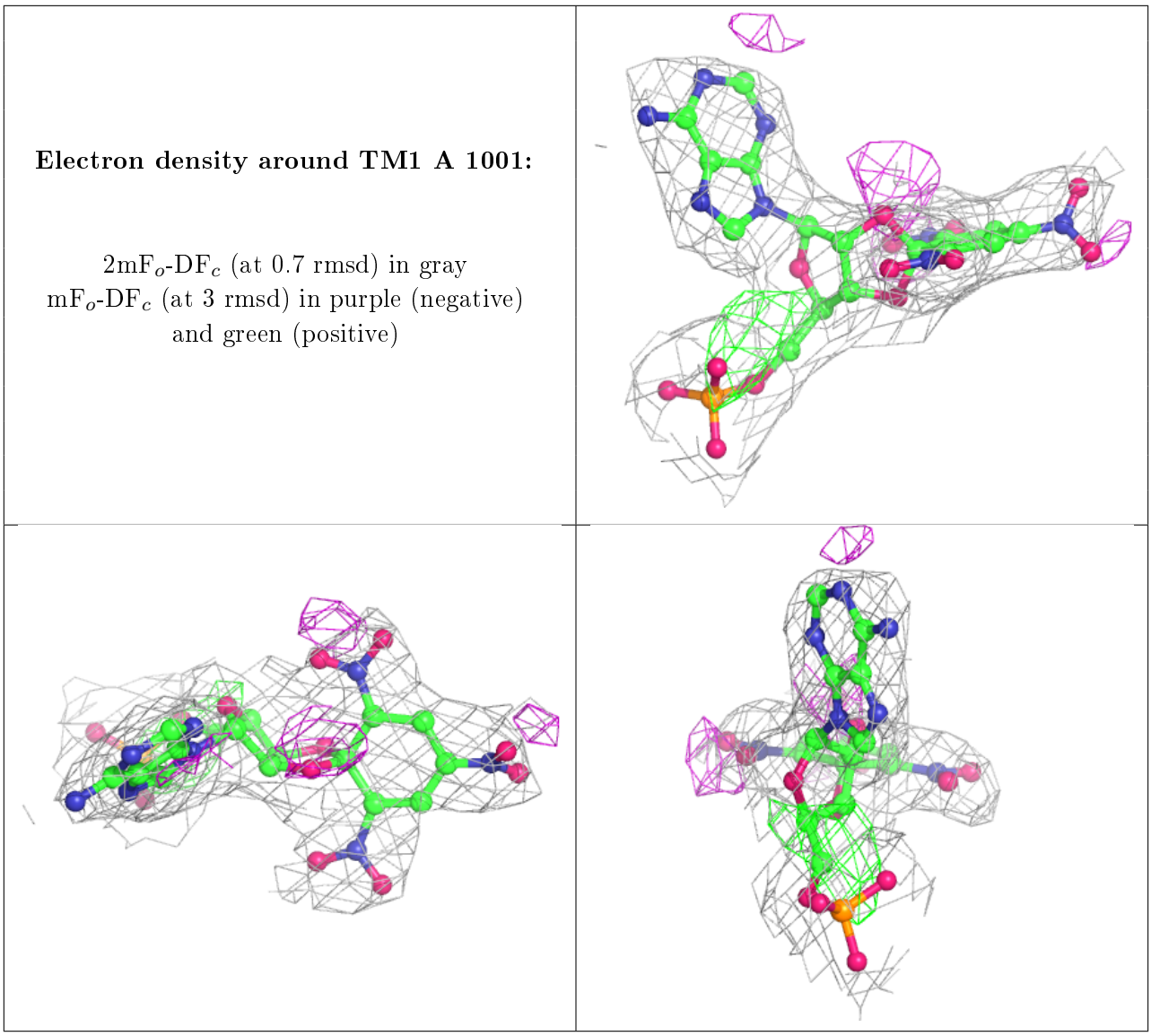
Electron density around TM1 B 1001:

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



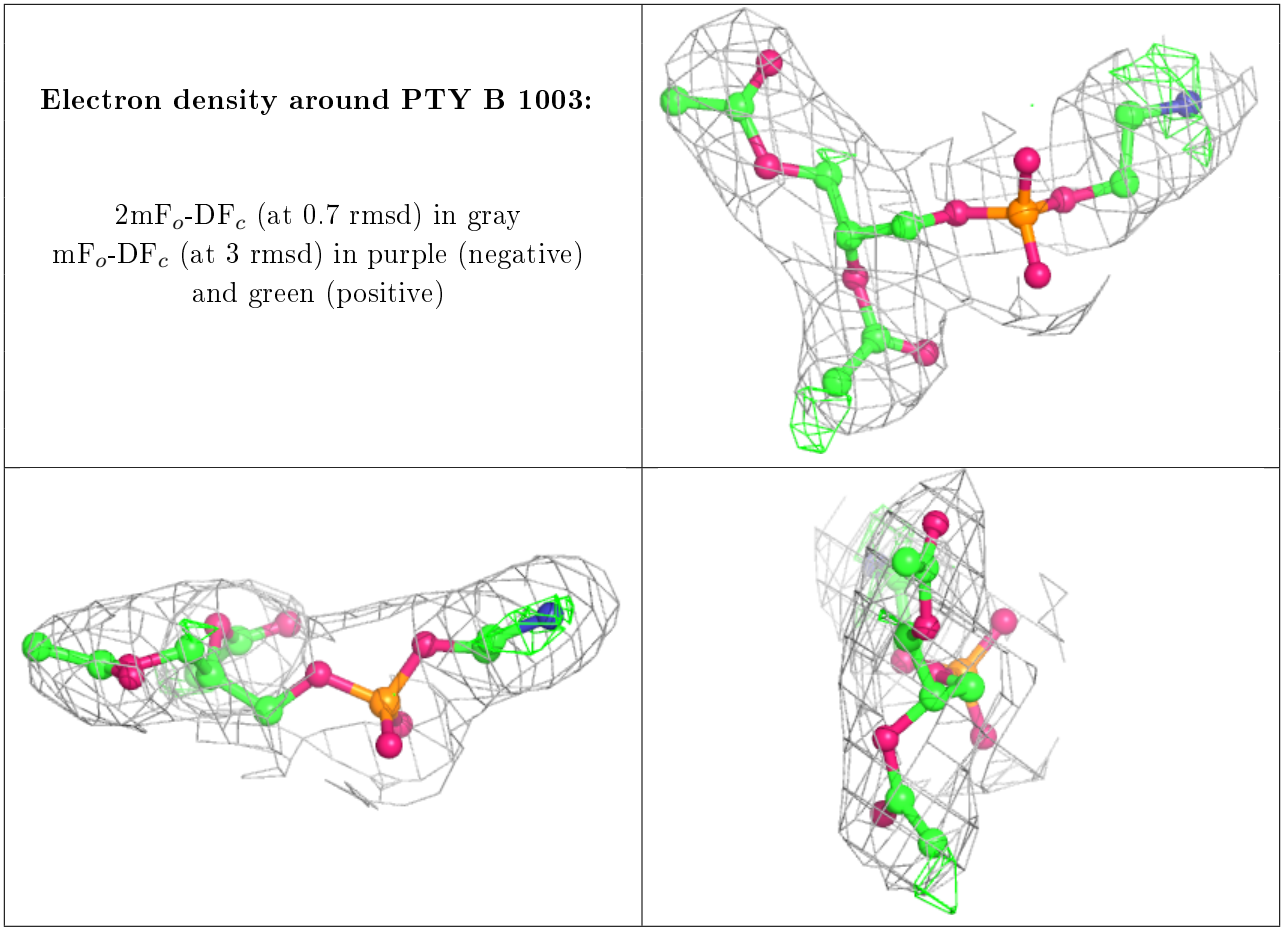
Electron density around TM1 A 1001:

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



Electron density around PTY B 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 (i)

There are no such residues in this entry.