



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:11 PM UTC

PDB ID : 2CBT / pdb_00002cbt
Title : Crystal structure of the neocarzinostatin 4Tes1 mutant bound testosterone hemisuccinate.
Authors : Drevelle, A.; Graille, M.; Heyd, B.; Sorel, I.; Ulryck, N.; Pecorari, F.; Desmadril, M.; Van Tilbeurgh, H.; Minard, P.
Deposited on : 2006-01-06
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

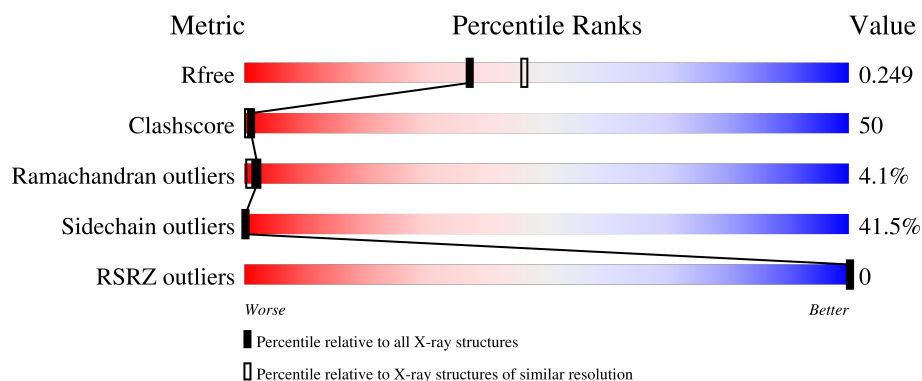
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	112	28% 46% 24% ..
1	B	112	34% 41% 21% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1664 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.

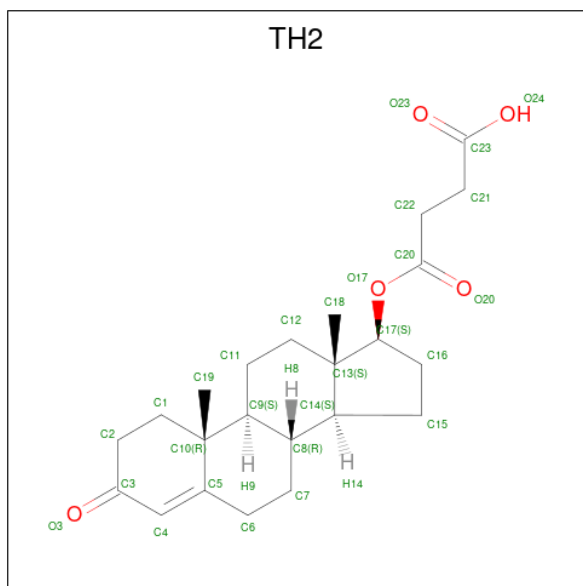
- Molecule 1 is a protein called NEOCARZINOSTATIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			789	489	135	163	2			
1	B	111	Total	C	N	O	S	0	0	0
			789	489	135	163	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1033	TRP	ASP	engineered mutation	UNP P0A3R9
A	1035	ALA	GLY	engineered mutation	UNP P0A3R9
A	1037	SER	CYS	engineered mutation	UNP P0A3R9
A	1045	TYR	LEU	engineered mutation	UNP P0A3R9
A	1047	SER	CYS	engineered mutation	UNP P0A3R9
A	1052	ILE	PHE	engineered mutation	UNP P0A3R9
A	1078	TRP	PHE	engineered mutation	UNP P0A3R9
A	1094	HIS	GLN	engineered mutation	UNP P0A3R9
A	1096	THR	GLY	engineered mutation	UNP P0A3R9
A	1098	ARG	SER	engineered mutation	UNP P0A3R9
A	1101	LEU	ALA	engineered mutation	UNP P0A3R9
A	1102	SER	GLY	engineered mutation	UNP P0A3R9
B	2033	TRP	ASP	engineered mutation	UNP P0A3R9
B	2035	ALA	GLY	engineered mutation	UNP P0A3R9
B	2037	SER	CYS	engineered mutation	UNP P0A3R9
B	2045	TYR	LEU	engineered mutation	UNP P0A3R9
B	2047	SER	CYS	engineered mutation	UNP P0A3R9
B	2052	ILE	PHE	engineered mutation	UNP P0A3R9
B	2078	TRP	PHE	engineered mutation	UNP P0A3R9
B	2094	HIS	GLN	engineered mutation	UNP P0A3R9
B	2096	THR	GLY	engineered mutation	UNP P0A3R9
B	2098	ARG	SER	engineered mutation	UNP P0A3R9
B	2101	LEU	ALA	engineered mutation	UNP P0A3R9
B	2102	SER	GLY	engineered mutation	UNP P0A3R9

- Molecule 2 is TESTOSTERONE HEMISUCCINATE (CCD ID: TH2) (formula: $C_{23}H_{32}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			28	23	5		
2	B	1	Total	C	O	0	0
			28	23	5		

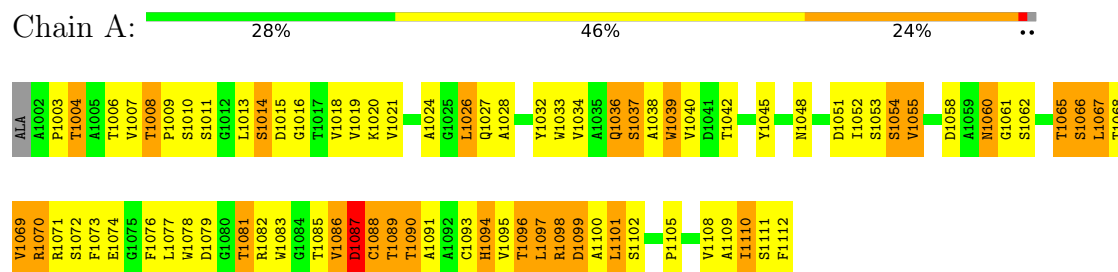
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	14	Total	O	0	0
			14	14		

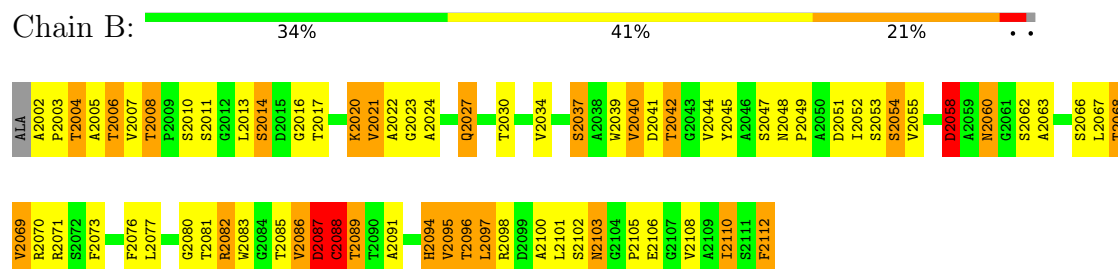
3 Residue-property plots

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

• Molecule 1: NEOCARZINOSTATIN



• Molecule 1: NEOCARZINOSTATIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	52.51Å 52.51Å 128.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.20) 95.5 (20.00-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.20Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.218 , 0.344 0.251 , 0.249	Depositor DCC
R_{free} test set	402 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 81.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.469 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1664	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.24% 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: TH2

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	0.39	0/806	1.27	5/1108 (0.5%)
1	B	0.39	0/806	1.22	3/1108 (0.3%)
All	All	0.39	0/1612	1.24	8/2216 (0.4%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1088	CYS	CA-C-N	5.33	131.73	121.54
1	A	1088	CYS	C-N-CA	5.33	131.73	121.54
1	B	2088	CYS	CA-C-N	5.29	131.64	121.54
1	B	2088	CYS	C-N-CA	5.29	131.64	121.54
1	A	1088	CYS	O-C-N	5.17	127.17	121.85
1	A	1099	ASP	CA-C-N	5.05	127.56	120.28
1	A	1099	ASP	C-N-CA	5.05	127.56	120.28
1	B	2058	ASP	CA-CB-CG	5.02	117.62	112.60

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	789	0	748	93	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	789	0	748	74	0
2	A	28	0	31	3	0
2	B	28	0	31	1	0
3	A	16	0	0	1	0
3	B	14	0	0	1	0
All	All	1664	0	1558	158	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 50.

All (158) 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:1045:TYR:HH	1:A:1094:HIS:CE1	1.45	1.32
1:A:1045:TYR:OH	1:A:1094:HIS:CE1	1.90	1.22
1:A:1045:TYR:OH	1:A:1094:HIS:NE2	1.73	1.17
1:B:2045:TYR:CE1	1:B:2094:HIS:NE2	2.36	0.93
1:B:2008:THR:HG23	1:B:2020:LYS:HB3	1.50	0.92
1:A:1045:TYR:CZ	1:A:1094:HIS:NE2	2.35	0.86
1:A:1045:TYR:CE1	1:A:1094:HIS:NE2	2.46	0.82
1:B:2017:THR:HB	1:B:2069:VAL:HG23	1.62	0.81
1:B:2045:TYR:HE1	1:B:2094:HIS:NE2	1.81	0.79
1:A:1093:CYS:O	1:A:1110:ILE:HG12	1.83	0.78
1:A:1003:PRO:HA	1:A:1024:ALA:O	1.88	0.74
1:A:1013:LEU:HB2	1:A:1112:PHE:CD2	2.23	0.74
1:B:2004:THR:OG1	1:B:2024:ALA:HB3	1.87	0.73
1:B:2067:LEU:HD12	1:B:2068:THR:H	1.51	0.73
1:A:1076:PHE:HE1	1:B:2054:SER:HB3	1.53	0.73
1:B:2034:VAL:HG12	1:B:2067:LEU:HD22	1.69	0.72
1:A:1094:HIS:HB3	1:A:1109:ALA:HA	1.72	0.69
1:B:2027:GLN:HB3	1:B:2030:THR:OG1	1.93	0.69
1:A:1015:ASP:HA	1:A:1070:ARG:HA	1.74	0.69
1:A:1009:PRO:HD2	1:A:1019:VAL:HG12	1.75	0.69
1:A:1036:GLN:NE2	1:A:1069:VAL:HG12	2.09	0.68
1:A:1016:GLY:HA2	1:A:1070:ARG:NH1	2.09	0.68
1:B:2094:HIS:HA	1:B:2110:ILE:HG23	1.76	0.68
1:A:1009:PRO:O	1:A:1013:LEU:HD21	1.94	0.67
1:A:1077:LEU:HG	1:A:1081:THR:HB	1.77	0.67
1:A:1026:LEU:HG	1:A:1061:GLY:O	1.95	0.67
1:A:1054:SER:HB3	1:B:2076:PHE:HE1	1.58	0.67
1:B:2094:HIS:HB2	1:B:2108:VAL:O	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1045:TYR:HE1	1:A:1094:HIS:HE2	1.39	0.66
1:A:1067:LEU:HD12	1:A:1068:THR:H	1.59	0.66
1:A:1018:VAL:HG13	1:A:1067:LEU:O	1.95	0.66
1:A:1101:LEU:HA	2:A:1120:TH2:O24	1.96	0.66
1:B:2014:SER:HA	1:B:2071:ARG:NH1	2.12	0.64
1:B:2067:LEU:HD12	1:B:2068:THR:N	2.12	0.64
1:B:2007:VAL:HG22	1:B:2021:VAL:HG13	1.80	0.63
1:B:2017:THR:HB	1:B:2069:VAL:CG2	2.28	0.63
1:A:1034:VAL:HG22	1:A:1097:LEU:CD1	2.29	0.62
1:A:1078:TRP:HH2	1:A:1098:ARG:HD3	1.63	0.62
1:A:1055:VAL:HG23	1:A:1065:THR:HB	1.82	0.61
1:B:2006:THR:HG23	1:B:2022:ALA:HB3	1.83	0.60
1:A:1008:THR:HG23	1:A:1020:LYS:HB3	1.83	0.60
1:B:2016:GLY:HA2	1:B:2070:ARG:NH1	2.17	0.60
1:B:2020:LYS:HE2	1:B:2020:LYS:O	2.01	0.59
1:B:2034:VAL:HB	1:B:2053:SER:HB3	1.83	0.59
1:B:2045:TYR:OH	1:B:2094:HIS:NE2	2.35	0.59
1:A:1008:THR:CG2	1:A:1020:LYS:HE2	2.33	0.59
1:A:1013:LEU:HB2	1:A:1112:PHE:CE2	2.38	0.59
1:A:1026:LEU:O	1:A:1061:GLY:HA3	2.03	0.59
1:A:1110:ILE:HG13	1:A:1112:PHE:CE1	2.39	0.57
1:B:2016:GLY:HA2	1:B:2070:ARG:HH11	1.69	0.57
1:A:1004:THR:HG23	1:A:1024:ALA:HB3	1.87	0.57
1:B:2034:VAL:HG22	1:B:2097:LEU:CD1	2.35	0.57
1:A:1040:VAL:HB	1:A:1083:TRP:CZ2	2.40	0.56
1:B:2077:LEU:HD12	1:B:2081:THR:HB	1.88	0.56
1:A:1014:SER:HA	1:A:1071:ARG:NH1	2.21	0.56
1:A:1094:HIS:HB2	1:A:1108:VAL:O	2.06	0.56
1:A:1007:VAL:HG22	1:A:1021:VAL:HG22	1.87	0.55
1:B:2037:SER:OG	1:B:2096:THR:OG1	2.22	0.55
1:A:1054:SER:HB3	1:B:2076:PHE:CE1	2.41	0.55
1:A:1088:CYS:O	1:A:1089:THR:HG23	2.07	0.55
1:B:2005:ALA:HB2	1:B:2105:PRO:HG2	1.89	0.55
1:B:2045:TYR:HH	1:B:2094:HIS:CE1	2.24	0.55
1:A:1026:LEU:HB3	1:A:1032:TYR:CE1	2.41	0.54
1:A:1004:THR:CG2	1:A:1024:ALA:HB3	2.39	0.53
1:B:2087:ASP:OD1	1:B:2091:ALA:HB3	2.09	0.53
1:A:1072:SER:OG	1:A:1088:CYS:HA	2.08	0.53
1:A:1033:TRP:O	1:A:1097:LEU:HA	2.08	0.53
1:A:1045:TYR:OH	1:A:1094:HIS:HE1	1.79	0.53
2:B:2120:TH2:O20	2:B:2120:TH2:H183	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:PRO:HG2	1:A:1013:LEU:CD2	2.39	0.52
1:A:1076:PHE:CE1	1:B:2054:SER:HB3	2.39	0.52
1:B:2040:VAL:HG11	1:B:2083:TRP:NE1	2.25	0.52
1:B:2034:VAL:CG1	1:B:2067:LEU:HD22	2.38	0.52
1:A:1073:PHE:CZ	1:A:1086:VAL:HG11	2.45	0.52
1:A:1094:HIS:HA	1:A:1110:ILE:HD13	1.92	0.51
1:A:1100:ALA:O	2:A:1120:TH2:C21	2.58	0.51
1:A:1055:VAL:CG2	1:A:1065:THR:HB	2.40	0.51
1:A:1068:THR:HG22	1:A:1068:THR:O	2.10	0.51
1:B:2048:ASN:HB2	1:B:2073:PHE:CD1	2.46	0.51
1:A:1086:VAL:O	1:A:1086:VAL:HG12	2.10	0.50
1:A:1034:VAL:HG22	1:A:1097:LEU:HD11	1.92	0.50
1:B:2017:THR:O	1:B:2069:VAL:HG22	2.12	0.50
1:A:1034:VAL:HG12	1:A:1034:VAL:O	2.11	0.50
1:B:2045:TYR:OH	1:B:2094:HIS:CE1	2.65	0.50
1:B:2101:LEU:O	1:B:2103:ASN:OD1	2.30	0.50
1:A:1037:SER:O	1:A:1093:CYS:HA	2.11	0.50
1:B:2068:THR:O	1:B:2068:THR:HG22	2.12	0.50
1:A:1086:VAL:O	1:A:1087:ASP:O	2.29	0.50
1:A:1108:VAL:O	1:A:1108:VAL:HG12	2.11	0.50
1:A:1008:THR:HG21	1:A:1020:LYS:HE2	1.92	0.49
1:A:1078:TRP:CH2	1:A:1098:ARG:HD3	2.45	0.49
1:A:1037:SER:OG	1:A:1096:THR:OG1	2.30	0.49
1:A:1082:ARG:NH2	1:B:2054:SER:O	2.46	0.49
1:B:2007:VAL:HG21	1:B:2095:VAL:CG2	2.42	0.48
1:A:1079:ASP:HA	1:B:2100:ALA:HB2	1.96	0.48
1:B:2034:VAL:HG22	1:B:2097:LEU:HD11	1.96	0.48
1:A:1100:ALA:O	2:A:1120:TH2:H211	2.13	0.47
1:B:2112:PHE:CD1	1:B:2112:PHE:N	2.82	0.47
1:A:1014:SER:HA	1:A:1071:ARG:CZ	2.43	0.47
1:B:2013:LEU:O	1:B:2112:PHE:HA	2.15	0.47
1:A:1037:SER:HB2	1:A:1045:TYR:CD1	2.50	0.47
1:A:1097:LEU:O	1:A:1105:PRO:HD2	2.14	0.47
1:B:2088:CYS:O	1:B:2089:THR:HG23	2.14	0.47
1:A:1099:ASP:OD2	1:A:1101:LEU:HD12	2.14	0.47
1:A:1016:GLY:HA2	1:A:1070:ARG:HH11	1.79	0.46
1:A:1074:GLU:HG3	3:A:2007:HOH:O	2.15	0.46
1:B:2048:ASN:ND2	1:B:2051:ASP:OD2	2.49	0.46
1:A:1087:ASP:OD1	1:A:1091:ALA:N	2.48	0.46
1:A:1054:SER:O	1:B:2082:ARG:NH2	2.49	0.46
1:B:2007:VAL:HG21	1:B:2095:VAL:HG21	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2023:GLY:O	1:B:2024:ALA:HB2	2.16	0.46
1:A:1013:LEU:O	1:A:1071:ARG:NH1	2.49	0.46
1:B:2058:ASP:OD1	1:B:2060:ASN:N	2.50	0.45
1:B:2103:ASN:OD1	1:B:2103:ASN:N	2.50	0.45
1:B:2071:ARG:HE	1:B:2112:PHE:HB3	1.82	0.45
1:A:1052:ILE:HG21	1:B:2049:PRO:HB2	1.98	0.45
1:B:2041:ASP:OD2	1:B:2042:THR:N	2.49	0.45
1:A:1038:ALA:O	1:A:1040:VAL:N	2.50	0.45
1:A:1054:SER:OG	1:B:2080:GLY:O	2.28	0.45
1:A:1028:ALA:HA	1:A:1058:ASP:O	2.17	0.44
1:A:1090:THR:OG1	1:A:1091:ALA:N	2.47	0.44
1:B:2003:PRO:HA	1:B:2024:ALA:O	2.17	0.44
1:A:1058:ASP:OD1	1:A:1060:ASN:ND2	2.50	0.44
1:A:1065:THR:HG23	1:A:1066:SER:N	2.33	0.44
1:B:2047:SER:O	1:B:2049:PRO:HD3	2.18	0.44
1:B:2067:LEU:HD23	1:B:2095:VAL:CG1	2.47	0.44
1:B:2087:ASP:OD1	1:B:2091:ALA:N	2.50	0.44
1:A:1079:ASP:OD1	1:A:1081:THR:OG1	2.30	0.44
1:B:2088:CYS:O	1:B:2089:THR:OG1	2.30	0.44
1:A:1098:ARG:HE	1:A:1098:ARG:HB3	1.54	0.44
1:B:2045:TYR:CZ	1:B:2094:HIS:NE2	2.63	0.44
1:A:1024:ALA:O	1:A:1026:LEU:HD23	2.18	0.43
1:A:1053:SER:OG	1:A:1054:SER:N	2.50	0.43
1:A:1013:LEU:HD12	1:A:1112:PHE:CE2	2.53	0.43
1:A:1048:ASN:ND2	1:A:1051:ASP:OD2	2.52	0.43
1:A:1099:ASP:CG	1:A:1101:LEU:HD12	2.44	0.43
1:B:2002:ALA:HB1	1:B:2003:PRO:HD2	2.00	0.43
1:B:2008:THR:HG23	1:B:2020:LYS:CB	2.35	0.43
1:A:1015:ASP:OD1	1:A:1070:ARG:HB3	2.19	0.43
1:A:1033:TRP:N	1:A:1098:ARG:O	2.52	0.43
1:B:2101:LEU:HB2	1:B:2103:ASN:OD1	2.18	0.43
1:A:1033:TRP:CH2	1:B:2080:GLY:HA2	2.55	0.42
1:A:1067:LEU:HD12	1:A:1068:THR:N	2.33	0.42
1:B:2020:LYS:HB3	1:B:2020:LYS:HE2	1.51	0.42
1:B:2077:LEU:HD12	1:B:2081:THR:CB	2.49	0.42
1:A:1099:ASP:OD1	1:A:1101:LEU:HD12	2.20	0.42
1:B:2007:VAL:HG12	1:B:2008:THR:N	2.34	0.42
1:B:2049:PRO:HG3	1:B:2076:PHE:CD2	2.55	0.41
1:B:2071:ARG:HE	1:B:2112:PHE:CB	2.33	0.41
1:B:2020:LYS:HE2	1:B:2020:LYS:C	2.45	0.41
1:A:1096:THR:HG22	1:A:1098:ARG:HD2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2041:ASP:HB3	1:B:2044:VAL:HB	2.02	0.41
1:B:2108:VAL:HG22	3:B:5014:HOH:O	2.20	0.41
1:A:1014:SER:HB3	1:A:1071:ARG:HH22	1.85	0.41
1:B:2086:VAL:O	1:B:2087:ASP:O	2.39	0.41
1:A:1007:VAL:HG21	1:A:1095:VAL:HB	2.03	0.41
1:B:2004:THR:N	1:B:2024:ALA:O	2.50	0.41
1:A:1087:ASP:OD1	1:A:1091:ALA:O	2.40	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	109/112 (97%)	89 (82%)	16 (15%)	4 (4%)	2	1
1	B	109/112 (97%)	88 (81%)	16 (15%)	5 (5%)	2	1
All	All	218/224 (97%)	177 (81%)	32 (15%)	9 (4%)	2	1

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1039	TRP
1	A	1087	ASP
1	A	1089	THR
1	A	1090	THR
1	B	2058	ASP
1	B	2087	ASP
1	B	2089	THR
1	B	2063	ALA
1	B	2088	CYS

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	82/82 (100%)	49 (60%)	33 (40%)	0	0
1	B	82/82 (100%)	47 (57%)	35 (43%)	0	0
All	All	164/164 (100%)	96 (58%)	68 (42%)	0	0

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1004	THR
1	A	1006	THR
1	A	1008	THR
1	A	1010	SER
1	A	1011	SER
1	A	1014	SER
1	A	1026	LEU
1	A	1027	GLN
1	A	1036	GLN
1	A	1037	SER
1	A	1039	TRP
1	A	1042	THR
1	A	1054	SER
1	A	1055	VAL
1	A	1060	ASN
1	A	1062	SER
1	A	1065	THR
1	A	1066	SER
1	A	1067	LEU
1	A	1069	VAL
1	A	1070	ARG
1	A	1081	THR
1	A	1085	THR
1	A	1086	VAL
1	A	1087	ASP
1	A	1094	HIS
1	A	1096	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1097	LEU
1	A	1098	ARG
1	A	1101	LEU
1	A	1102	SER
1	A	1110	ILE
1	A	1111	SER
1	B	2004	THR
1	B	2006	THR
1	B	2008	THR
1	B	2010	SER
1	B	2011	SER
1	B	2014	SER
1	B	2020	LYS
1	B	2021	VAL
1	B	2027	GLN
1	B	2037	SER
1	B	2039	TRP
1	B	2040	VAL
1	B	2042	THR
1	B	2052	ILE
1	B	2054	SER
1	B	2055	VAL
1	B	2060	ASN
1	B	2062	SER
1	B	2066	SER
1	B	2068	THR
1	B	2069	VAL
1	B	2082	ARG
1	B	2085	THR
1	B	2086	VAL
1	B	2087	ASP
1	B	2094	HIS
1	B	2095	VAL
1	B	2096	THR
1	B	2097	LEU
1	B	2098	ARG
1	B	2102	SER
1	B	2103	ASN
1	B	2106	GLU
1	B	2110	ILE
1	B	2112	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	1036	GLN
1	A	1060	ASN
1	B	2060	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TH2	B	2120	-	31,31,31	1.74	8 (25%)	48,48,48	2.03	14 (29%)
2	TH2	A	1120	-	31,31,31	1.62	6 (19%)	48,48,48	2.04	10 (20%)

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	TH2	B	2120	-	-	6/9/67/67	0/4/4/4
2	TH2	A	1120	-	-	3/9/67/67	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2120	TH2	O17-C17	-3.64	1.40	1.46
2	B	2120	TH2	C10-C5	3.53	1.59	1.52
2	A	1120	TH2	C10-C5	3.24	1.59	1.52
2	B	2120	TH2	O17-C20	-2.63	1.26	1.34
2	A	1120	TH2	C11-C9	2.61	1.58	1.53
2	B	2120	TH2	C10-C9	2.60	1.60	1.56
2	B	2120	TH2	C8-C9	2.56	1.58	1.53
2	A	1120	TH2	C10-C9	2.56	1.60	1.56
2	B	2120	TH2	C11-C9	2.54	1.57	1.53
2	A	1120	TH2	O17-C17	-2.37	1.42	1.46
2	A	1120	TH2	C8-C9	2.24	1.57	1.53
2	B	2120	TH2	C4-C5	2.17	1.37	1.34
2	A	1120	TH2	O3-C3	-2.11	1.19	1.23
2	B	2120	TH2	C16-C17	2.09	1.57	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1120	TH2	C17-O17-C20	5.43	127.94	118.03
2	A	1120	TH2	O17-C17-C16	4.96	123.26	111.06
2	B	2120	TH2	O17-C17-C16	4.92	123.16	111.06
2	A	1120	TH2	C11-C9-C10	-4.77	107.20	113.08
2	B	2120	TH2	O17-C17-C13	4.75	122.34	111.20
2	A	1120	TH2	O17-C17-C13	4.73	122.28	111.20
2	B	2120	TH2	C17-O17-C20	4.68	126.57	118.03
2	B	2120	TH2	C11-C9-C10	-4.64	107.36	113.08
2	B	2120	TH2	C12-C11-C9	-3.66	106.91	113.14
2	B	2120	TH2	O17-C20-O20	3.54	131.99	123.70
2	A	1120	TH2	C12-C11-C9	-3.53	107.14	113.14
2	A	1120	TH2	O17-C20-O20	3.48	131.83	123.70
2	A	1120	TH2	C16-C17-C13	-3.11	102.05	105.18
2	B	2120	TH2	C9-C10-C5	-2.71	105.68	109.65
2	A	1120	TH2	C9-C10-C5	-2.56	105.91	109.65
2	B	2120	TH2	C16-C17-C13	-2.41	102.75	105.18
2	A	1120	TH2	O20-C20-C22	-2.39	114.43	123.78
2	B	2120	TH2	O20-C20-C22	-2.38	114.47	123.78
2	A	1120	TH2	C15-C16-C17	2.35	108.57	104.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2120	TH2	C18-C13-C14	2.23	115.72	111.68
2	B	2120	TH2	O23-C23-C21	-2.12	116.36	123.09
2	B	2120	TH2	C13-C14-C8	-2.09	111.44	114.41
2	B	2120	TH2	C1-C10-C9	2.09	111.50	108.74
2	B	2120	TH2	C15-C16-C17	2.06	108.11	104.76

There are no chirality outliers.

All (9) torsion outliers are listed below:

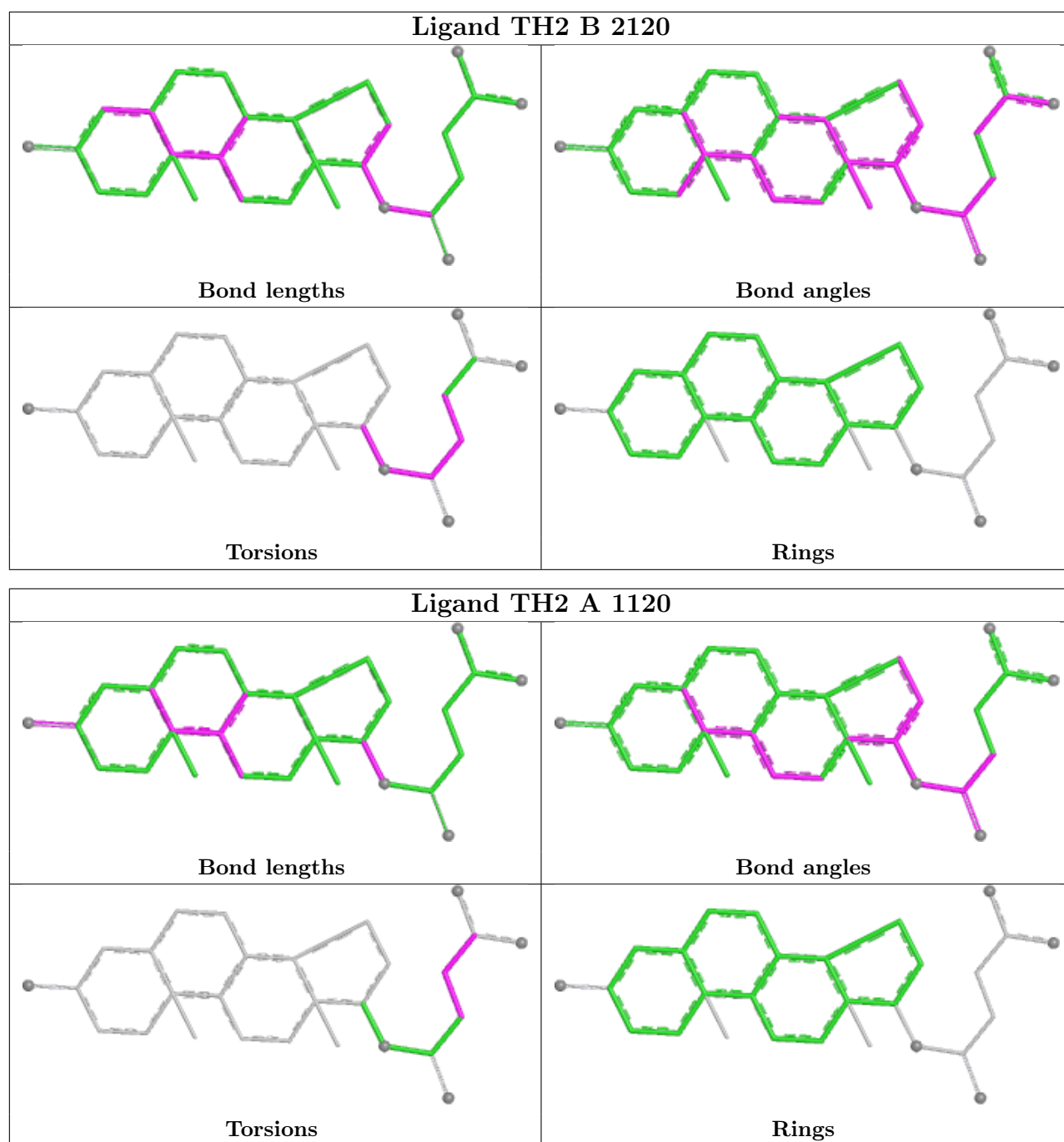
Mol	Chain	Res	Type	Atoms
2	B	2120	TH2	C23-C21-C22-C20
2	A	1120	TH2	C23-C21-C22-C20
2	B	2120	TH2	C22-C20-O17-C17
2	B	2120	TH2	O20-C20-O17-C17
2	B	2120	TH2	C13-C17-O17-C20
2	A	1120	TH2	C22-C21-C23-O24
2	A	1120	TH2	C22-C21-C23-O23
2	B	2120	TH2	O17-C20-C22-C21
2	B	2120	TH2	O20-C20-C22-C21

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2120	TH2	1	0
2	A	1120	TH2	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	111/112 (99%)	-1.20	0 100 100	8, 32, 49, 59	0
1	B	111/112 (99%)	-1.15	0 100 100	13, 33, 54, 83	0
All	All	222/224 (99%)	-1.18	0 100 100	8, 33, 52, 83	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

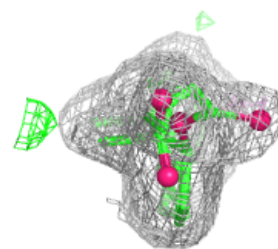
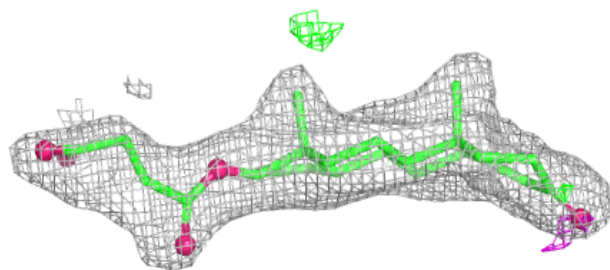
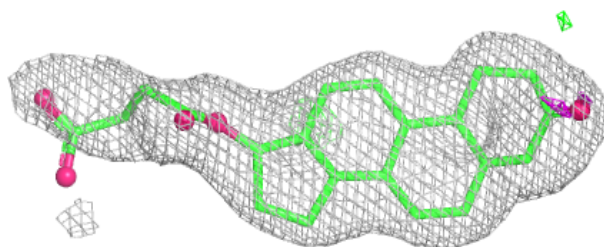
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TH2	A	1120	28/28	0.99	0.04	5,18,43,62	0
2	TH2	B	2120	28/28	0.99	0.03	3,11,27,37	0

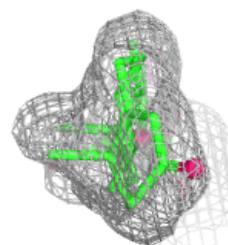
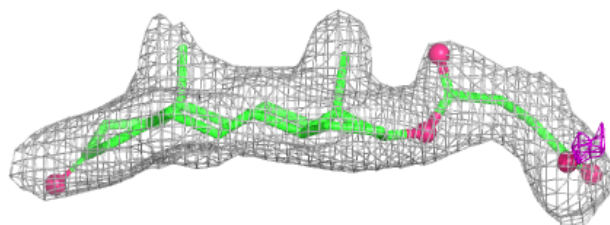
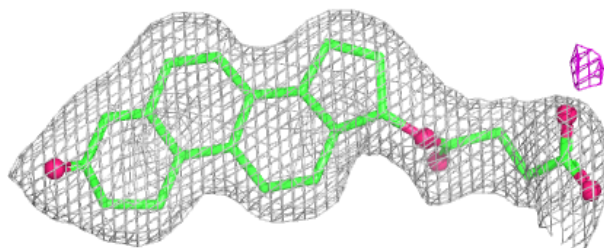
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TH2 A 1120:

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

**Electron density around TH2 B 2120:**

$2mF_o-DF_c$ (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.