Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:14 pm BST

PDB ID	:	2F3M
Title	:	Structure of human GLUTATHIONE S-TRANSFERASE M1A-1A complexed with 1-(S-(GLUTATHIONYL)-2,4,6-TRINITROCYCLOHEXADIENATE ANION
Authors	:	Patskovsky, Y.; Patskovska, L.; Almo, S.C.; Listowsky, I.
Deposited on	:	2005-11-21
Resolution	:	2.70 Å(reported)

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

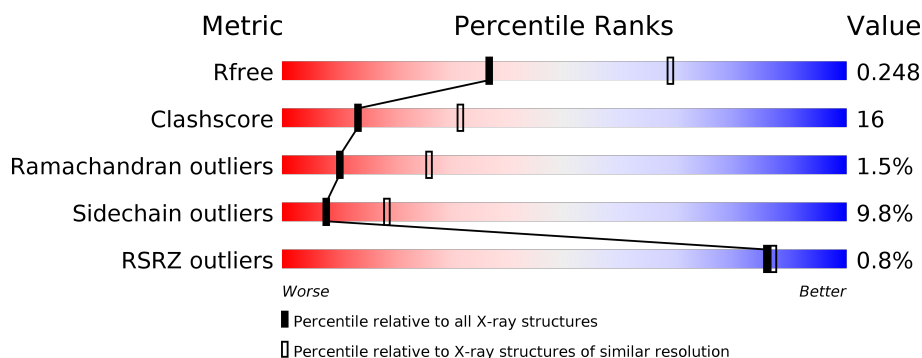|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	Percentile Ranks	Value
Rfree		0.248
Clashscore		16
Ramachandran outliers		1.5%
Sidechain outliers		9.8%
RSRZ outliers		0.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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.

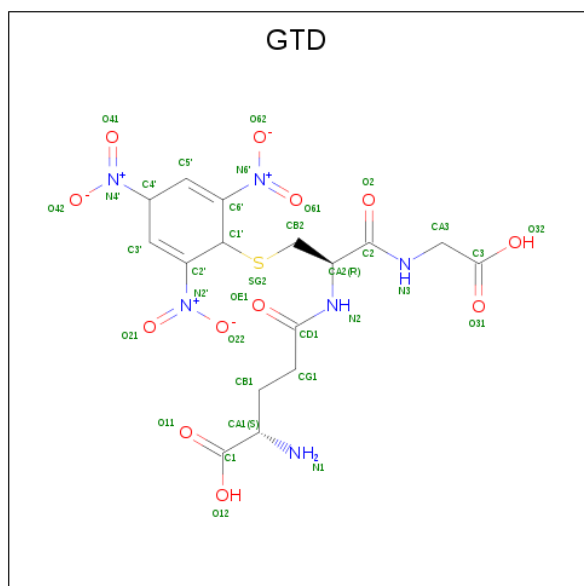| Mol	Chain	Length	Quality of chain
1	A	218	68% 24% 8%
1	B	218	70% 25% 5%
1	C	218	73% 21% 6%
1	D	218	69% 25% 6% ·
1	E	218	65% 28% 6% ·
1	F	218	68% 26% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11167 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 Glutathione S-transferase Mu 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	2	0
			1822	1186	296	327	13			
1	B	218	Total	C	N	O	S	0	1	0
			1817	1183	296	325	13			
1	C	217	Total	C	N	O	S	0	1	0
			1809	1178	295	324	12			
1	D	218	Total	C	N	O	S	0	2	0
			1822	1187	296	325	14			
1	E	218	Total	C	N	O	S	0	1	0
			1817	1183	296	325	13			
1	F	218	Total	C	N	O	S	0	1	0
			1817	1183	296	325	13			

- Molecule 2 is 1-(S-GLUTATHIONYL)-2,4,6-TRINITROCYCLOHEXA-2,5-DIENE (three-letter code: GTD) (formula: $C_{16}H_{20}N_6O_{12}S$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 35	C 16	N 6	O 12	S 1	0	0
2	B	1	Total 35	C 16	N 6	O 12	S 1	0	0
2	C	1	Total 35	C 16	N 6	O 12	S 1	0	0
2	D	1	Total 35	C 16	N 6	O 12	S 1	0	0
2	E	1	Total 35	C 16	N 6	O 12	S 1	0	0
2	F	1	Total 35	C 16	N 6	O 12	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total 13	O 13	0	0
3	B	8	Total 8	O 8	0	0
3	C	8	Total 8	O 8	0	0
3	D	10	Total 10	O 10	0	0
3	E	6	Total 6	O 6	0	0
3	F	8	Total 8	O 8	0	0

3 Residue-property plots ⓘ

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.
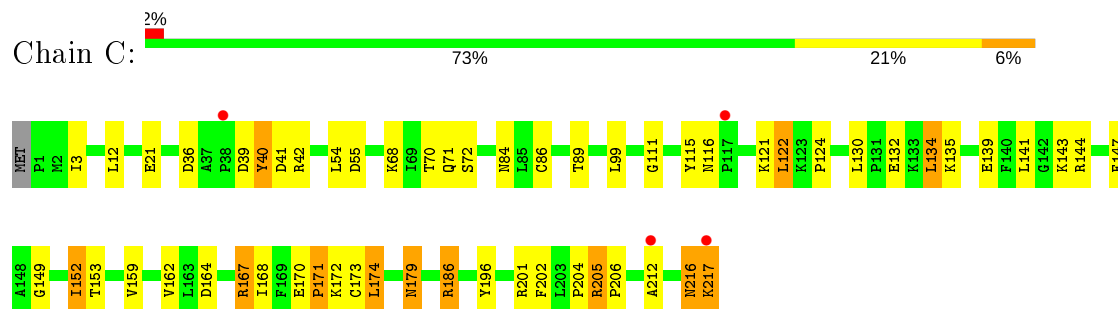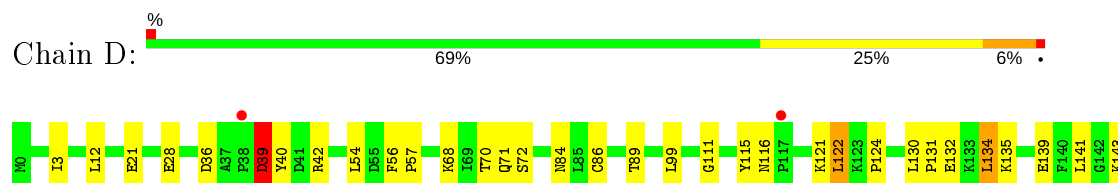
- Molecule 1: Glutathione S-transferase Mu 1
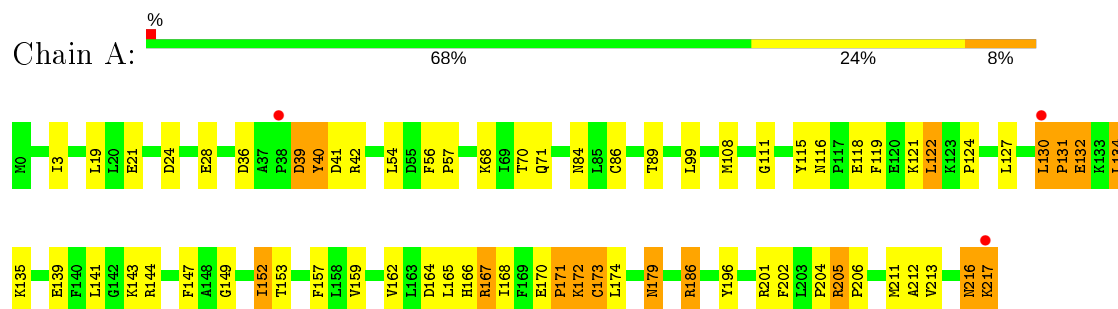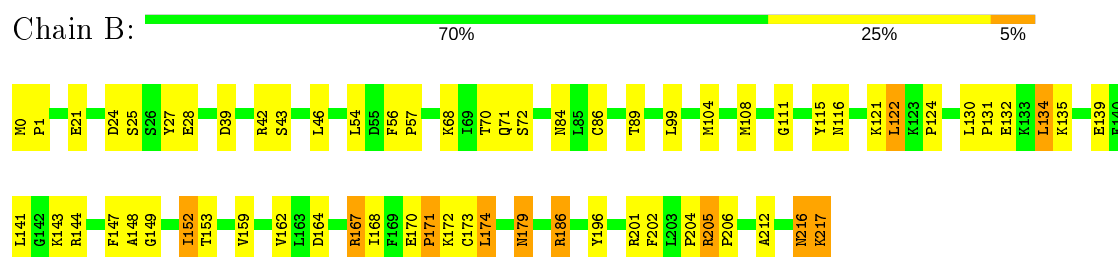
- Molecule 1: Glutathione S-transferase Mu 1

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R144 F147 A148 G149 I152 T153 V159 Y160 D161 V162 L163 D164 L165 H166 R167 I168 F169 E170 P171 K172 C173 L174 D175 A176 F177 P178 N179 L180 K181 R186 Y196 R201 F202 L203 P204 R205 P206 A212 N216 K217

• Molecule 1: Glutathione S-transferase Mu 1

Chain E:

65% 28% 6%

M0 I3 I4 G5 Y6 W7 D8 I9 L19 L20 E21 D24 E28 K31 D36 D39 Y40 D41 R42 W45 L54 L59 K68 I69 T70 Q71 N84 L85 C86 T89 L99 M108 G111 Y115 N116 P117 E118 F119 E120 K121 L122 K123 P124

L130 P131 E132 K133 L134 K135 E139 F140 L141 G142 K143 R144 F147 A148 G149 I152 T153 F157 L158 V159 V162 L165 H166 R167 I168 F169 E170 P171 K172 C173 L174 D175 A176 F177 P178 N179 I184 S185 R186 Y196 R201 F202 L203 P204 R205 P206 S209 K210 M211

A212 V213 N216 K217

• Molecule 1: Glutathione S-transferase Mu 1

Chain F:

68% 26% 5%

M0 P1 M2 I3 D8 E21 D24 E28 T33 D39 R42 S43 L46 L54 D55 F56 P57 N58 K68 I69 T70 Q71 N84 L85 C86 T89 L99 M104 M108 G111 Y115 N116 K121 L122 K123 P124 L130 P131 E132 K133 L134

K135 E139 K143 R144 F147 A148 G149 I152 T153 V159 V162 L163 D164 L165 H166 R167 I168 F169 E170 P171 K172 C173 L174 D175 N179 L180 F183 R186 Y196 R201 F202 L203 P204 R205 P206 A212 N216 K217
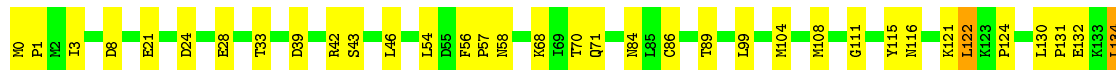
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.97Å　　93.10Å　　93.00Å 120.53°　106.19°　89.97°	Depositor
Resolution (Å)	20.00　–　2.70 19.77　–　2.67	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-2.70) 96.0 (19.77-2.67)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.04	Depositor
$<I/\sigma(I)>$ [1]	1.36 (at 2.67Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.233　,　0.264 0.235　,　0.248	Depositor DCC
R_{free} test set	1143 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 14.3	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-h-l 0.021 for -h,k,-k-l 0.021 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11167	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTD

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	0.50	0/1877	0.57	1/2529 (0.0%)
1	B	0.50	0/1869	0.56	0/2518
1	C	0.53	0/1861	0.57	1/2507 (0.0%)
1	D	0.54	0/1877	0.58	3/2528 (0.1%)
1	E	0.50	0/1869	0.59	4/2518 (0.2%)
1	F	0.54	1/1869 (0.1%)	0.57	1/2518 (0.0%)
All	All	0.52	1/11222 (0.0%)	0.57	10/15118 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	217	LYS	C-OXT	7.45	1.37	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	8	ASP	CB-CG-OD2	5.27	123.04	118.30
1	E	175	ASP	CB-CG-OD2	5.27	123.04	118.30
1	E	39	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	39	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	36	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	36	ASP	CB-CG-OD2	5.23	123.01	118.30
1	E	36	ASP	CB-CG-OD2	5.23	123.00	118.30
1	D	175	ASP	CB-CG-OD2	5.23	123.00	118.30
1	C	36	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	175	ASP	CB-CG-OD2	5.10	122.89	118.30

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	1822	0	1815	76	0
1	B	1817	0	1811	58	0
1	C	1809	0	1802	45	0
1	D	1822	0	1820	66	0
1	E	1817	0	1811	59	0
1	F	1817	0	1811	51	0
2	A	35	0	18	0	0
2	B	35	0	18	3	0
2	C	35	0	18	2	0
2	D	35	0	18	2	0
2	E	35	0	18	0	0
2	F	35	0	18	0	0
3	A	13	0	0	2	0
3	B	8	0	0	2	0
3	C	8	0	0	1	0
3	D	10	0	0	3	0
3	E	6	0	0	3	0
3	F	8	0	0	2	0
All	All	11167	0	10978	355	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 16.

All (355) 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:D:173:CYS:SG	1:D:174:LEU:CD1	2.30	1.19
1:D:173:CYS:SG	1:D:174:LEU:HD13	1.83	1.17
1:F:186:ARG:HG3	1:F:186:ARG:HH11	1.07	1.10
1:E:186:ARG:HG3	1:E:186:ARG:HH11	1.03	1.09
1:A:186:ARG:HG3	1:A:186:ARG:HH11	1.07	1.07
1:C:186:ARG:HH11	1:C:186:ARG:HG3	1.13	1.07
1:B:186:ARG:HG3	1:B:186:ARG:HH11	1.14	1.06
1:E:211:MET:HE1	3:E:5223:HOH:O	1.58	1.03
1:A:173:CYS:O	1:A:174:LEU:HD12	1.58	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108[B]:MET:HE1	2:B:2218:GTD:O41	1.57	1.01
1:D:186:ARG:HG3	1:D:186:ARG:HH11	1.27	0.97
1:A:170:GLU:O	1:A:173:CYS:HB3	1.66	0.95
1:A:211:MET:HE1	3:A:1221:HOH:O	1.67	0.92
1:E:170:GLU:O	1:E:173:CYS:HB3	1.70	0.91
1:E:186:ARG:HG3	1:E:186:ARG:NH1	1.81	0.90
1:A:130:LEU:HB3	1:A:131:PRO:HD3	1.55	0.88
1:A:186:ARG:HG3	1:A:186:ARG:NH1	1.84	0.88
1:E:186:ARG:CG	1:E:186:ARG:HH11	1.89	0.85
1:A:170:GLU:HB3	1:A:173:CYS:HB3	1.61	0.83
1:A:127:LEU:HD23	1:A:130:LEU:HD23	1.60	0.82
1:E:162:VAL:HG23	3:E:5222:HOH:O	1.77	0.82
1:A:186:ARG:HH11	1:A:186:ARG:CG	1.93	0.82
1:F:186:ARG:HG3	1:F:186:ARG:NH1	1.85	0.81
1:B:170:GLU:HG3	1:B:173:CYS:HB3	1.60	0.81
1:A:170:GLU:CB	1:A:173:CYS:HB3	2.11	0.81
1:A:173:CYS:O	1:A:174:LEU:CD1	2.30	0.80
1:C:186:ARG:HG3	1:C:186:ARG:NH1	1.90	0.80
1:A:127:LEU:CD2	1:A:130:LEU:HD23	2.12	0.79
1:A:170:GLU:O	1:A:173:CYS:CB	2.30	0.79
1:F:204:PRO:C	1:F:205:ARG:HG2	2.04	0.78
1:F:179:ASN:ND2	1:F:180:LEU:H	1.83	0.77
1:B:186:ARG:HG3	1:B:186:ARG:NH1	1.91	0.76
1:A:170:GLU:HG3	1:A:173:CYS:HB3	1.66	0.75
1:A:212:ALA:HB3	1:A:216:ASN:HB3	1.69	0.74
1:A:216:ASN:H	1:A:216:ASN:HD22	1.34	0.74
1:B:216:ASN:H	1:B:216:ASN:HD22	1.33	0.73
1:C:170:GLU:HG3	1:C:170:GLU:O	1.87	0.73
1:E:216:ASN:HD22	1:E:216:ASN:H	1.35	0.72
1:C:212:ALA:HB3	1:C:216:ASN:HB3	1.71	0.72
1:F:216:ASN:H	1:F:216:ASN:HD22	1.35	0.72
1:A:127:LEU:HD23	1:A:130:LEU:CD2	2.20	0.71
1:E:212:ALA:HB3	1:E:216:ASN:HB3	1.72	0.71
1:B:0:MET:HA	1:B:0:MET:HE2	1.73	0.71
1:A:170:GLU:CG	1:A:173:CYS:HB3	2.21	0.70
1:F:179:ASN:HD22	1:F:180:LEU:H	1.40	0.70
1:D:212:ALA:HB3	1:D:216:ASN:HB3	1.73	0.70
1:B:170:GLU:CG	1:B:173:CYS:HB3	2.22	0.69
1:A:39:ASP:O	1:A:40:TYR:C	2.30	0.69
1:A:170:GLU:HB3	1:A:173:CYS:CB	2.21	0.69
1:D:217:LYS:HA	1:D:217:LYS:HZ2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:ASN:ND2	1:F:180:LEU:N	2.42	0.68
1:D:173:CYS:SG	1:D:174:LEU:HD12	2.31	0.68
1:A:127:LEU:HA	1:A:130:LEU:HB2	1.74	0.68
1:B:212:ALA:HB3	1:B:216:ASN:HB3	1.76	0.67
1:C:186:ARG:HH11	1:C:186:ARG:CG	1.97	0.67
1:C:216:ASN:H	1:C:216:ASN:HD22	1.41	0.67
1:F:212:ALA:HB3	1:F:216:ASN:HB3	1.76	0.67
1:A:173:CYS:SG	1:A:174:LEU:HD13	2.35	0.67
1:D:216:ASN:H	1:D:216:ASN:HD22	1.42	0.66
1:E:144:ARG:HD3	1:E:149:GLY:HA2	1.77	0.66
1:A:130:LEU:O	1:A:130:LEU:HD12	1.96	0.66
1:F:186:ARG:HH11	1:F:186:ARG:CG	1.92	0.66
1:E:39:ASP:O	1:E:40:TYR:C	2.33	0.66
1:C:217:LYS:HA	1:C:217:LYS:HZ2	1.61	0.66
1:D:172:LYS:O	1:D:174:LEU:N	2.28	0.66
1:D:202:PHE:CE2	1:D:204:PRO:HG3	2.32	0.65
1:B:0:MET:HE1	1:B:1:PRO:HD2	1.78	0.65
1:E:186:ARG:CG	1:E:186:ARG:NH1	2.53	0.65
1:A:144:ARG:HD3	1:A:149:GLY:HA2	1.79	0.65
1:F:172:LYS:O	1:F:174:LEU:N	2.29	0.65
1:D:186:ARG:HG3	1:D:186:ARG:NH1	2.03	0.65
1:B:148:ALA:HB3	3:B:2225:HOH:O	1.97	0.64
1:D:99:LEU:HD11	1:D:147:PHE:HB3	1.79	0.64
1:F:186:ARG:NH1	1:F:186:ARG:CG	2.57	0.64
1:C:39:ASP:O	1:C:40:TYR:C	2.36	0.64
1:A:39:ASP:O	1:A:41:ASP:N	2.31	0.63
1:C:144:ARG:HD3	1:C:149:GLY:HA2	1.79	0.63
1:E:21:GLU:HG3	1:E:196:TYR:CD1	2.34	0.63
1:A:21:GLU:HG3	1:A:196:TYR:CD1	2.34	0.63
1:C:72:SER:H	2:C:3218:GTD:C1	2.11	0.63
1:D:144:ARG:HD3	1:D:149:GLY:HA2	1.80	0.63
1:A:186:ARG:NH1	1:A:186:ARG:CG	2.56	0.63
1:E:116:ASN:ND2	1:E:122:LEU:HD21	2.14	0.63
1:A:170:GLU:O	1:A:173:CYS:N	2.30	0.62
1:B:217:LYS:HZ2	1:B:217:LYS:HA	1.64	0.62
1:C:202:PHE:CE2	1:C:204:PRO:HG3	2.34	0.62
1:A:171:PRO:C	1:A:173:CYS:H	2.03	0.62
1:A:131:PRO:O	1:A:134:LEU:N	2.32	0.62
1:B:144:ARG:HD3	1:B:149:GLY:HA2	1.80	0.62
1:B:186:ARG:CG	1:B:186:ARG:HH11	1.99	0.62
1:D:167:ARG:HD3	3:D:4226:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:LEU:HD12	2:D:4218:GTD:SG2	2.40	0.62
1:D:21:GLU:HG3	1:D:196:TYR:CD1	2.34	0.61
1:F:144:ARG:HD3	1:F:149:GLY:HA2	1.81	0.61
1:A:70:THR:O	1:A:71:GLN:HB2	2.00	0.61
1:C:21:GLU:HG3	1:C:196:TYR:CD1	2.34	0.61
1:C:99:LEU:HD11	1:C:147:PHE:HB3	1.83	0.60
1:A:99:LEU:HD11	1:A:147:PHE:HB3	1.83	0.60
1:F:130:LEU:HG	1:F:134:LEU:CD2	2.30	0.60
1:B:186:ARG:CG	1:B:186:ARG:NH1	2.62	0.60
1:E:205:ARG:HA	1:E:206:PRO:C	2.22	0.60
1:A:131:PRO:O	1:A:132:GLU:C	2.38	0.60
1:A:130:LEU:O	1:A:134:LEU:HD22	2.01	0.60
1:B:0:MET:CE	1:B:1:PRO:HD2	2.32	0.60
1:E:70:THR:O	1:E:71:GLN:HB2	2.02	0.59
1:B:130:LEU:HG	1:B:134:LEU:CD2	2.31	0.59
1:B:108[B]:MET:CE	2:B:2218:GTD:O41	2.42	0.59
1:B:170:GLU:HG3	1:B:170:GLU:O	2.02	0.59
1:F:70:THR:O	1:F:71:GLN:HB2	2.02	0.59
1:D:135:LYS:HE3	1:D:139:GLU:OE1	2.01	0.59
1:E:99:LEU:HD11	1:E:147:PHE:HB3	1.85	0.59
1:A:116:ASN:ND2	1:A:122:LEU:HD21	2.18	0.59
1:E:8:ASP:OD1	1:E:31:LYS:HE3	2.02	0.59
1:B:170:GLU:O	1:B:173:CYS:HB3	2.03	0.59
1:D:170:GLU:O	1:D:170:GLU:HG3	2.03	0.58
1:E:202:PHE:CE2	1:E:204:PRO:HG3	2.38	0.58
1:C:186:ARG:CG	1:C:186:ARG:NH1	2.59	0.58
1:D:164:ASP:HA	1:D:167:ARG:HD2	1.86	0.58
1:B:99:LEU:HD11	1:B:147:PHE:HB3	1.85	0.58
1:F:99:LEU:HD11	1:F:147:PHE:HB3	1.85	0.58
1:E:39:ASP:O	1:E:41:ASP:N	2.37	0.58
1:E:170:GLU:O	1:E:173:CYS:CB	2.50	0.58
1:A:205:ARG:HA	1:A:206:PRO:C	2.24	0.57
1:D:116:ASN:ND2	1:D:122:LEU:HD21	2.19	0.57
1:F:21:GLU:HG3	1:F:196:TYR:CD1	2.39	0.57
1:A:132:GLU:OE2	1:A:132:GLU:HA	2.03	0.57
1:C:116:ASN:ND2	1:C:122:LEU:HD21	2.19	0.57
1:D:186:ARG:CG	1:D:186:ARG:HH11	2.08	0.57
1:F:206:PRO:HG3	1:F:217:LYS:OXT	2.04	0.57
1:F:202:PHE:CE2	1:F:204:PRO:HG3	2.39	0.57
1:A:166:HIS:O	1:A:170:GLU:N	2.26	0.56
1:B:202:PHE:CE2	1:B:204:PRO:HG3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASN:N	1:A:179:ASN:HD22	2.03	0.56
1:A:202:PHE:CE2	1:A:204:PRO:HG3	2.41	0.56
1:B:70:THR:O	1:B:71:GLN:HB2	2.05	0.56
1:C:130:LEU:HG	1:C:134:LEU:CD2	2.36	0.56
1:D:130:LEU:HG	1:D:134:LEU:CD2	2.36	0.56
1:D:148:ALA:HB3	3:D:4222:HOH:O	2.04	0.56
1:A:130:LEU:HD12	1:A:130:LEU:C	2.26	0.56
1:B:21:GLU:HG3	1:B:196:TYR:CD1	2.42	0.55
1:C:135:LYS:HE3	1:C:139:GLU:OE1	2.06	0.55
1:C:173:CYS:SG	1:C:174:LEU:HD13	2.47	0.55
1:B:0:MET:HA	1:B:0:MET:CE	2.35	0.55
1:B:135:LYS:HE3	1:B:139:GLU:OE1	2.07	0.54
1:D:172:LYS:O	1:D:175:ASP:N	2.34	0.54
1:A:170:GLU:HG3	1:A:173:CYS:CB	2.35	0.54
1:E:176:ALA:O	1:E:177:PHE:CD1	2.61	0.54
1:E:173:CYS:SG	1:E:174:LEU:HG	2.48	0.54
1:E:217:LYS:HZ2	1:E:217:LYS:HA	1.72	0.54
1:B:217:LYS:HE3	1:B:217:LYS:OXT	2.07	0.53
1:C:201:ARG:HG3	1:C:201:ARG:HH11	1.71	0.53
1:B:173:CYS:SG	1:B:174:LEU:HD13	2.48	0.53
1:F:205:ARG:HA	1:F:206:PRO:C	2.28	0.53
1:C:70:THR:O	1:C:71:GLN:HB2	2.08	0.53
1:E:130:LEU:HG	1:E:134:LEU:CD2	2.39	0.53
1:E:165:LEU:O	1:E:168:ILE:HB	2.08	0.53
1:D:116:ASN:ND2	1:D:122:LEU:CD2	2.72	0.53
1:A:135:LYS:HE3	1:A:139:GLU:OE1	2.08	0.53
1:C:179:ASN:HD22	1:C:179:ASN:N	2.06	0.53
1:D:3:ILE:HD12	1:D:28:GLU:OE2	2.08	0.53
1:E:179:ASN:HD22	1:E:179:ASN:N	2.07	0.53
1:A:130:LEU:HB3	1:A:131:PRO:CD	2.35	0.52
1:C:116:ASN:ND2	1:C:122:LEU:CD2	2.72	0.52
1:D:175:ASP:C	1:D:177:PHE:H	2.13	0.52
1:D:170:GLU:O	1:D:171:PRO:C	2.46	0.52
1:D:179:ASN:N	1:D:179:ASN:HD22	2.06	0.52
1:C:170:GLU:CG	1:C:170:GLU:O	2.54	0.52
1:D:173:CYS:SG	1:D:174:LEU:HD11	2.42	0.52
1:B:205:ARG:HA	1:B:206:PRO:C	2.30	0.52
1:E:116:ASN:ND2	1:E:122:LEU:CD2	2.72	0.52
1:F:116:ASN:ND2	1:F:122:LEU:HD21	2.24	0.52
1:F:170:GLU:O	1:F:170:GLU:HG3	2.09	0.51
1:E:147:PHE:CZ	1:E:159:VAL:HG11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:GLU:O	1:B:171:PRO:C	2.49	0.51
1:D:174:LEU:N	1:D:174:LEU:CD1	2.73	0.51
1:A:171:PRO:O	1:A:173:CYS:N	2.42	0.51
1:C:12:LEU:HD12	2:C:3218:GTD:SG2	2.50	0.51
1:F:164:ASP:OD1	1:F:167:ARG:HD3	2.11	0.51
1:A:216:ASN:HD22	1:A:216:ASN:N	2.06	0.51
1:F:179:ASN:N	1:F:179:ASN:HD22	2.07	0.51
1:A:147:PHE:CE1	1:A:159:VAL:HG11	2.46	0.51
1:A:147:PHE:CZ	1:A:159:VAL:HG11	2.46	0.51
1:A:217:LYS:HZ2	1:A:217:LYS:HA	1.75	0.51
1:D:70:THR:O	1:D:71:GLN:HB2	2.11	0.51
1:D:186:ARG:CG	1:D:186:ARG:NH1	2.69	0.50
1:E:135:LYS:HE3	1:E:139:GLU:OE1	2.11	0.50
1:E:111:GLY:O	1:E:115:TYR:HD2	1.94	0.50
1:A:164:ASP:HA	1:A:167:ARG:HD2	1.92	0.50
1:F:148:ALA:HB3	3:F:6225:HOH:O	2.10	0.50
1:B:216:ASN:HD22	1:B:216:ASN:N	2.07	0.49
1:C:205:ARG:HA	1:C:206:PRO:C	2.32	0.49
1:B:179:ASN:HD22	1:B:179:ASN:N	2.10	0.49
1:B:116:ASN:ND2	1:B:122:LEU:HD21	2.27	0.49
1:D:132:GLU:HA	1:D:132:GLU:OE2	2.12	0.49
1:B:164:ASP:OD1	1:B:167:ARG:HD3	2.12	0.49
1:B:1:PRO:CG	1:B:28:GLU:OE2	2.60	0.49
1:D:99:LEU:CD1	1:D:147:PHE:HB3	2.41	0.49
1:A:167:ARG:HG2	1:A:168:ILE:N	2.28	0.49
1:D:205:ARG:HA	1:D:206:PRO:C	2.32	0.49
1:F:147:PHE:CZ	1:F:159:VAL:HG11	2.47	0.49
1:A:164:ASP:OD1	1:A:167:ARG:HD3	2.12	0.49
1:B:164:ASP:HA	1:B:167:ARG:HD2	1.94	0.49
1:A:116:ASN:ND2	1:A:122:LEU:CD2	2.76	0.48
1:A:170:GLU:O	1:A:171:PRO:C	2.51	0.48
1:D:172:LYS:O	1:D:173:CYS:C	2.51	0.48
1:F:135:LYS:HE3	1:F:139:GLU:OE1	2.14	0.48
1:F:58:ASN:HB3	3:F:6220:HOH:O	2.13	0.48
1:F:99:LEU:CD1	1:F:147:PHE:HB3	2.44	0.48
1:C:121:LYS:O	1:C:124:PRO:HD2	2.14	0.48
1:F:116:ASN:ND2	1:F:122:LEU:CD2	2.76	0.48
1:C:111:GLY:O	1:C:115:TYR:HD2	1.97	0.48
1:E:170:GLU:O	1:E:170:GLU:HG3	2.13	0.48
1:A:111:GLY:O	1:A:115:TYR:HD2	1.97	0.48
1:E:147:PHE:CE1	1:E:159:VAL:HG11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:GLY:O	1:D:115:TYR:HD2	1.96	0.48
1:C:132:GLU:HA	1:C:132:GLU:OE2	2.14	0.47
1:C:99:LEU:CD1	1:C:147:PHE:HB3	2.43	0.47
1:B:201:ARG:HG3	1:B:201:ARG:HH11	1.80	0.47
1:C:164:ASP:HA	1:C:167:ARG:HD2	1.95	0.47
1:B:132:GLU:OE2	1:B:132:GLU:HA	2.14	0.47
1:D:72:SER:H	2:D:4218:GTD:C1	2.28	0.47
1:E:7:TRP:O	1:E:9:ILE:N	2.36	0.47
1:A:99:LEU:CD1	1:A:147:PHE:HB3	2.44	0.47
1:A:216:ASN:ND2	1:A:216:ASN:H	2.09	0.47
1:C:167:ARG:O	1:C:171:PRO:HA	2.15	0.47
1:D:135:LYS:HA	1:D:177:PHE:CE1	2.50	0.47
1:E:132:GLU:OE2	1:E:132:GLU:HA	2.14	0.47
1:A:21:GLU:HG3	1:A:196:TYR:CG	2.50	0.47
1:E:21:GLU:HG3	1:E:196:TYR:CG	2.50	0.47
1:B:99:LEU:CD1	1:B:147:PHE:HB3	2.46	0.46
1:B:54:LEU:HD23	1:B:68:LYS:HB3	1.97	0.46
1:D:167:ARG:HG2	1:D:168:ILE:N	2.30	0.46
1:E:54:LEU:HD23	1:E:68:LYS:HB3	1.96	0.46
1:A:171:PRO:C	1:A:173:CYS:N	2.68	0.46
1:A:211:MET:CE	3:A:1221:HOH:O	2.41	0.46
1:B:116:ASN:ND2	1:B:122:LEU:CD2	2.77	0.46
1:C:39:ASP:O	1:C:41:ASP:N	2.47	0.46
1:F:121:LYS:O	1:F:124:PRO:HD2	2.15	0.46
1:D:201:ARG:HH11	1:D:201:ARG:HG3	1.79	0.46
1:B:56:PHE:O	1:B:57:PRO:C	2.54	0.46
1:D:130:LEU:N	1:D:131:PRO:CD	2.78	0.46
1:D:202:PHE:CD2	1:D:204:PRO:HG3	2.50	0.46
1:F:216:ASN:N	1:F:216:ASN:HD22	2.08	0.46
1:C:202:PHE:CD2	1:C:204:PRO:HG3	2.50	0.46
1:D:54:LEU:HD23	1:D:68:LYS:HB3	1.97	0.46
1:F:164:ASP:HA	1:F:167:ARG:HD2	1.97	0.46
1:A:19:LEU:HA	1:A:157:PHE:CE2	2.51	0.46
1:F:147:PHE:CE1	1:F:159:VAL:HG11	2.51	0.45
1:B:27:TYR:C	1:B:27:TYR:CD2	2.89	0.45
1:E:121:LYS:O	1:E:124:PRO:HD2	2.17	0.45
1:E:99:LEU:CD1	1:E:147:PHE:HB3	2.46	0.45
1:A:3:ILE:HD13	1:A:3:ILE:N	2.31	0.45
1:D:147:PHE:CE1	1:D:159:VAL:HG11	2.52	0.45
1:D:39:ASP:O	1:D:40:TYR:C	2.55	0.45
1:B:130:LEU:N	1:B:131:PRO:CD	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:TRP:C	1:E:9:ILE:H	2.18	0.45
1:B:43:SER:HA	1:B:46:LEU:HB2	1.99	0.45
1:E:166:HIS:O	1:E:170:GLU:N	2.30	0.45
1:F:130:LEU:N	1:F:131:PRO:CD	2.78	0.45
1:A:201:ARG:HG3	1:A:201:ARG:HH11	1.81	0.45
1:D:170:GLU:HG3	1:D:173:CYS:HB3	1.98	0.45
1:B:111:GLY:O	1:B:115:TYR:HD2	1.98	0.45
1:B:202:PHE:CD2	1:B:204:PRO:HG3	2.52	0.45
1:D:121:LYS:O	1:D:124:PRO:HD2	2.17	0.45
1:D:147:PHE:CZ	1:D:159:VAL:HG11	2.51	0.45
1:E:176:ALA:C	1:E:177:PHE:CG	2.90	0.45
1:F:56:PHE:O	1:F:57:PRO:C	2.55	0.45
1:B:121:LYS:O	1:B:124:PRO:HD2	2.17	0.45
1:F:54:LEU:HD23	1:F:68:LYS:HB3	1.99	0.45
1:A:54:LEU:HD23	1:A:68:LYS:HB3	1.98	0.44
1:D:3:ILE:N	1:D:3:ILE:HD13	2.32	0.44
1:E:19:LEU:HA	1:E:157:PHE:CE2	2.52	0.44
1:C:170:GLU:HG3	1:C:173:CYS:HB3	2.00	0.44
1:E:216:ASN:H	1:E:216:ASN:ND2	2.11	0.44
1:E:39:ASP:OD1	1:E:39:ASP:N	2.50	0.44
1:F:201:ARG:HG3	1:F:201:ARG:HH11	1.83	0.44
1:D:172:LYS:C	1:D:174:LEU:N	2.71	0.44
1:B:1:PRO:HG3	1:B:28:GLU:OE2	2.17	0.44
1:B:104:MET:CE	1:B:108[B]:MET:HG2	2.47	0.44
1:C:147:PHE:CE1	1:C:159:VAL:HG11	2.53	0.44
1:D:161:ASP:O	1:D:165:LEU:HG	2.17	0.44
1:B:72:SER:H	2:B:2218:GTD:C1	2.29	0.44
1:C:54:LEU:HD23	1:C:68:LYS:HB3	1.99	0.44
1:E:201:ARG:HG3	1:E:201:ARG:HH11	1.83	0.44
1:F:132:GLU:OE2	1:F:132:GLU:HA	2.17	0.44
1:A:152:ILE:HG13	1:A:153:THR:N	2.33	0.44
1:C:167:ARG:HG2	1:C:168:ILE:N	2.32	0.44
1:F:152:ILE:HG13	1:F:153:THR:N	2.32	0.44
1:C:164:ASP:OD1	1:C:167:ARG:HD3	2.17	0.43
1:D:174:LEU:N	1:D:174:LEU:HD12	2.32	0.43
1:A:39:ASP:OD1	1:A:39:ASP:N	2.51	0.43
1:C:147:PHE:CZ	1:C:159:VAL:HG11	2.53	0.43
1:D:21:GLU:HG3	1:D:196:TYR:CG	2.54	0.43
1:E:45:TRP:CZ3	1:E:59:LEU:HD21	2.53	0.43
1:F:43:SER:HA	1:F:46:LEU:HB2	2.00	0.43
1:A:127:LEU:HD22	1:A:130:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:ASP:OD1	1:E:31:LYS:CE	2.65	0.43
1:A:119:PHE:HB3	1:A:213:VAL:HG11	2.01	0.43
1:F:0:MET:SD	1:F:1:PRO:HD2	2.59	0.43
1:F:202:PHE:CD2	1:F:204:PRO:HG3	2.54	0.43
1:A:141:LEU:HB2	1:A:147:PHE:CE2	2.54	0.43
1:C:216:ASN:N	1:C:216:ASN:HD22	2.13	0.43
1:D:216:ASN:HD22	1:D:216:ASN:N	2.13	0.43
1:D:175:ASP:C	1:D:177:PHE:N	2.72	0.43
1:E:152:ILE:HG13	1:E:153:THR:N	2.34	0.43
1:B:152:ILE:HG13	1:B:153:THR:N	2.33	0.43
1:D:165:LEU:HA	1:D:165:LEU:HD23	1.78	0.43
1:A:173:CYS:O	1:A:173:CYS:SG	2.77	0.42
1:D:177:PHE:O	1:D:181:LYS:HG3	2.19	0.42
1:E:118:GLU:O	1:E:119:PHE:C	2.56	0.42
1:C:3:ILE:HD13	1:C:3:ILE:N	2.34	0.42
1:C:21:GLU:HG3	1:C:196:TYR:CG	2.55	0.42
1:E:202:PHE:CD2	1:E:204:PRO:HG3	2.55	0.42
1:E:211:MET:CE	3:E:5223:HOH:O	2.37	0.42
1:A:118:GLU:O	1:A:119:PHE:C	2.56	0.42
1:A:121:LYS:O	1:A:124:PRO:HD2	2.20	0.42
1:B:147:PHE:CZ	1:B:159:VAL:HG11	2.54	0.42
1:F:104:MET:CE	1:F:108[B]:MET:HG2	2.50	0.42
1:F:167:ARG:O	1:F:171:PRO:HA	2.20	0.42
1:D:167:ARG:O	1:D:171:PRO:HA	2.20	0.42
1:E:216:ASN:HD22	1:E:216:ASN:N	2.09	0.42
1:F:165:LEU:HD23	1:F:165:LEU:HA	1.88	0.42
1:B:147:PHE:CE1	1:B:159:VAL:HG11	2.55	0.42
1:D:148:ALA:CB	3:D:4222:HOH:O	2.65	0.42
1:E:119:PHE:HB3	1:E:213:VAL:HG11	2.02	0.42
1:F:111:GLY:O	1:F:115:TYR:HD2	2.01	0.42
1:B:167:ARG:HG2	1:B:168:ILE:N	2.35	0.41
1:E:167:ARG:NH1	1:E:184:ILE:HG21	2.35	0.41
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.90	0.41
1:F:167:ARG:HG2	1:F:168:ILE:N	2.35	0.41
1:A:118:GLU:HB3	1:A:122:LEU:HD22	2.02	0.41
1:F:180:LEU:O	1:F:183:PHE:HB3	2.21	0.41
1:B:148:ALA:CB	3:B:2225:HOH:O	2.60	0.41
1:E:141:LEU:HB2	1:E:147:PHE:CE2	2.56	0.41
1:E:170:GLU:HG3	1:E:173:CYS:HB3	2.03	0.41
1:E:5:GLY:O	1:E:6:TYR:HB2	2.21	0.41
1:B:216:ASN:ND2	1:B:216:ASN:H	2.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LEU:HB2	1:C:147:PHE:CE2	2.56	0.41
1:A:56:PHE:O	1:A:57:PRO:C	2.59	0.41
1:C:152:ILE:HG13	1:C:153:THR:N	2.35	0.41
1:E:176:ALA:O	1:E:177:PHE:CG	2.74	0.41
1:A:202:PHE:CD2	1:A:204:PRO:HG3	2.56	0.41
1:D:56:PHE:O	1:D:57:PRO:C	2.59	0.40
1:B:141:LEU:HB2	1:B:147:PHE:CE2	2.56	0.40
1:D:166:HIS:O	1:D:169:PHE:N	2.54	0.40
1:E:3:ILE:HD13	1:E:3:ILE:N	2.36	0.40
1:D:141:LEU:HB2	1:D:147:PHE:CE2	2.57	0.40
1:F:8:ASP:OD2	1:F:33:THR:HG23	2.22	0.40
1:B:104:MET:CE	1:B:108[B]:MET:CE	2.99	0.40
1:C:55:ASP:HB2	3:C:3225:HOH:O	2.20	0.40
1:D:130:LEU:HB3	1:D:131:PRO:HD3	2.03	0.40
1:F:3:ILE:HD13	1:F:3:ILE:N	2.36	0.40
1:D:152:ILE:HG13	1:D:153:THR:N	2.36	0.40
1:D:170:GLU:O	1:D:170:GLU:CG	2.69	0.40
1:F:173:CYS:SG	1:F:174:LEU:HD13	2.62	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	218/218 (100%)	202 (93%)	11 (5%)	5 (2%)	6	16
1	B	217/218 (100%)	207 (95%)	9 (4%)	1 (0%)	29	54
1	C	216/218 (99%)	205 (95%)	9 (4%)	2 (1%)	17	40
1	D	218/218 (100%)	202 (93%)	12 (6%)	4 (2%)	8	21
1	E	217/218 (100%)	202 (93%)	11 (5%)	4 (2%)	8	21
1	F	217/218 (100%)	204 (94%)	10 (5%)	3 (1%)	11	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1303/1308 (100%)	1222 (94%)	62 (5%)	19 (2%)	10 26

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	TYR
1	C	171	PRO
1	D	171	PRO
1	D	173	CYS
1	E	40	TYR
1	F	173	CYS
1	A	132	GLU
1	A	172	LYS
1	C	40	TYR
1	E	8	ASP
1	A	131	PRO
1	A	171	PRO
1	D	172	LYS
1	F	171	PRO
1	F	175	ASP
1	E	171	PRO
1	E	172	LYS
1	B	171	PRO
1	D	178	PRO

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	199/197 (101%)	176 (88%)	23 (12%)	5 12
1	B	198/197 (100%)	178 (90%)	20 (10%)	7 17
1	C	197/197 (100%)	180 (91%)	17 (9%)	10 24
1	D	199/197 (101%)	182 (92%)	17 (8%)	10 24
1	E	198/197 (100%)	175 (88%)	23 (12%)	5 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	198/197 (100%)	180 (91%)	18 (9%)	9	21
All	All	1189/1182 (101%)	1071 (90%)	118 (10%)	8	18

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	28	GLU
1	A	39	ASP
1	A	42	ARG
1	A	84	ASN
1	A	86	CYS
1	A	89	THR
1	A	108[A]	MET
1	A	108[B]	MET
1	A	122	LEU
1	A	130	LEU
1	A	134	LEU
1	A	143	LYS
1	A	152	ILE
1	A	162	VAL
1	A	167	ARG
1	A	172	LYS
1	A	173	CYS
1	A	179	ASN
1	A	186	ARG
1	A	205	ARG
1	A	216	ASN
1	A	217	LYS
1	B	24	ASP
1	B	25	SER
1	B	39	ASP
1	B	42	ARG
1	B	84	ASN
1	B	86	CYS
1	B	89	THR
1	B	122	LEU
1	B	134	LEU
1	B	143	LYS
1	B	152	ILE
1	B	162	VAL
1	B	167	ARG

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Mol	Chain	Res	Type
1	B	172	LYS
1	B	174	LEU
1	B	179	ASN
1	B	186	ARG
1	B	205	ARG
1	B	216	ASN
1	B	217	LYS
1	C	42	ARG
1	C	84	ASN
1	C	86	CYS
1	C	89	THR
1	C	122	LEU
1	C	134	LEU
1	C	143	LYS
1	C	152	ILE
1	C	162	VAL
1	C	167	ARG
1	C	172	LYS
1	C	174	LEU
1	C	179	ASN
1	C	186	ARG
1	C	205	ARG
1	C	216	ASN
1	C	217	LYS
1	D	39	ASP
1	D	42	ARG
1	D	84	ASN
1	D	86	CYS
1	D	89	THR
1	D	122	LEU
1	D	134	LEU
1	D	143	LYS
1	D	152	ILE
1	D	162	VAL
1	D	167	ARG
1	D	172	LYS
1	D	179	ASN
1	D	186	ARG
1	D	205	ARG
1	D	216	ASN
1	D	217	LYS
1	E	24	ASP

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Mol	Chain	Res	Type
1	E	28	GLU
1	E	39	ASP
1	E	42	ARG
1	E	84	ASN
1	E	86	CYS
1	E	89	THR
1	E	108[A]	MET
1	E	108[B]	MET
1	E	122	LEU
1	E	134	LEU
1	E	143	LYS
1	E	152	ILE
1	E	162	VAL
1	E	167	ARG
1	E	172	LYS
1	E	174	LEU
1	E	179	ASN
1	E	186	ARG
1	E	205	ARG
1	E	209	SER
1	E	216	ASN
1	E	217	LYS
1	F	24	ASP
1	F	28	GLU
1	F	39	ASP
1	F	42	ARG
1	F	84	ASN
1	F	86	CYS
1	F	89	THR
1	F	122	LEU
1	F	134	LEU
1	F	143	LYS
1	F	152	ILE
1	F	162	VAL
1	F	167	ARG
1	F	179	ASN
1	F	186	ARG
1	F	205	ARG
1	F	216	ASN
1	F	217	LYS

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

Mol	Chain	Res	Type
1	A	67	HIS
1	A	179	ASN
1	A	216	ASN
1	B	67	HIS
1	B	179	ASN
1	B	216	ASN
1	C	107	HIS
1	C	179	ASN
1	C	216	ASN
1	D	179	ASN
1	D	216	ASN
1	E	67	HIS
1	E	179	ASN
1	E	216	ASN
1	F	67	HIS
1	F	179	ASN
1	F	216	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	GTD	F	6218	-	20,35,35	1.53	2 (10%)	17,48,48	0.85	1 (5%)
2	GTD	D	4218	-	20,35,35	1.71	2 (10%)	17,48,48	0.91	1 (5%)
2	GTD	E	5218	-	20,35,35	1.93	3 (15%)	17,48,48	0.93	1 (5%)
2	GTD	C	3218	-	20,35,35	1.63	2 (10%)	17,48,48	0.98	1 (5%)
2	GTD	B	2218	-	20,35,35	1.57	2 (10%)	17,48,48	0.76	0
2	GTD	A	1218	-	20,35,35	1.74	3 (15%)	17,48,48	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTD	F	6218	-	-	4/25/55/55	0/1/1/1
2	GTD	D	4218	-	-	4/25/55/55	0/1/1/1
2	GTD	E	5218	-	-	5/25/55/55	0/1/1/1
2	GTD	C	3218	-	-	4/25/55/55	0/1/1/1
2	GTD	B	2218	-	-	6/25/55/55	0/1/1/1
2	GTD	A	1218	-	-	6/25/55/55	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4218	GTD	CB2-SG2	-6.17	1.75	1.82
2	A	1218	GTD	CB2-SG2	-5.90	1.75	1.82
2	C	3218	GTD	CB2-SG2	-5.81	1.75	1.82
2	B	2218	GTD	CB2-SG2	-5.77	1.75	1.82
2	F	6218	GTD	CB2-SG2	-5.58	1.76	1.82
2	E	5218	GTD	CB2-SG2	-5.55	1.76	1.82
2	E	5218	GTD	O21-N2'	-5.15	1.14	1.22
2	C	3218	GTD	C1'-SG2	-3.26	1.76	1.83
2	D	4218	GTD	C1'-SG2	-3.26	1.76	1.83
2	A	1218	GTD	C1'-SG2	-3.25	1.76	1.83
2	B	2218	GTD	C1'-SG2	-2.98	1.76	1.83
2	E	5218	GTD	C1'-SG2	-2.93	1.77	1.83
2	F	6218	GTD	C1'-SG2	-2.86	1.77	1.83
2	A	1218	GTD	O21-N2'	-2.58	1.18	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3218	GTD	CA3-N3-C2	-2.38	118.92	122.34
2	D	4218	GTD	CA3-N3-C2	-2.29	119.04	122.34
2	E	5218	GTD	CB1-CG1-CD1	-2.06	108.43	113.04
2	F	6218	GTD	CB2-CA2-C2	2.06	114.19	109.73

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	6218	GTD	C5'-C6'-N6'-O61
2	D	4218	GTD	C5'-C6'-N6'-O61
2	E	5218	GTD	C1-CA1-CB1-CG1
2	E	5218	GTD	C5'-C6'-N6'-O61
2	C	3218	GTD	C1-CA1-CB1-CG1
2	B	2218	GTD	N1-CA1-CB1-CG1
2	B	2218	GTD	C1-CA1-CB1-CG1
2	B	2218	GTD	C5'-C6'-N6'-O61
2	A	1218	GTD	C1-CA1-CB1-CG1
2	A	1218	GTD	C5'-C6'-N6'-O61
2	B	2218	GTD	CA2-CB2-SG2-C1'
2	E	5218	GTD	N1-CA1-CB1-CG1
2	A	1218	GTD	N1-CA1-CB1-CG1
2	C	3218	GTD	C5'-C6'-N6'-O61
2	D	4218	GTD	C3-CA3-N3-C2
2	C	3218	GTD	C3-CA3-N3-C2
2	D	4218	GTD	CA2-CB2-SG2-C1'
2	F	6218	GTD	C3-CA3-N3-C2
2	E	5218	GTD	C3-CA3-N3-C2
2	A	1218	GTD	C3-CA3-N3-C2
2	F	6218	GTD	C5'-C4'-N4'-O41
2	D	4218	GTD	C3'-C4'-N4'-O41
2	E	5218	GTD	C5'-C4'-N4'-O41
2	B	2218	GTD	C5'-C4'-N4'-O41
2	A	1218	GTD	C5'-C4'-N4'-O41
2	F	6218	GTD	O2-C2-CA2-CB2
2	B	2218	GTD	C3-CA3-N3-C2
2	C	3218	GTD	CA2-CB2-SG2-C1'
2	A	1218	GTD	CA2-CB2-SG2-C1'

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4218	GTD	2	0
2	C	3218	GTD	2	0
2	B	2218	GTD	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 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 GTD F 6218

Bond lengths

Bond angles

Torsions

Rings

Ligand GTD D 4218

Bond lengths

Bond angles

Torsions

Rings

Ligand GTD E 5218

Bond lengths

Bond angles

Torsions

Rings

Ligand GTD C 3218

Bond lengths

Bond angles

Torsions

Rings

Ligand GTD B 2218

Bond lengths

Bond angles

Torsions

Rings

Ligand GTD A 1218

Bond lengths

Bond angles

Torsions

Rings
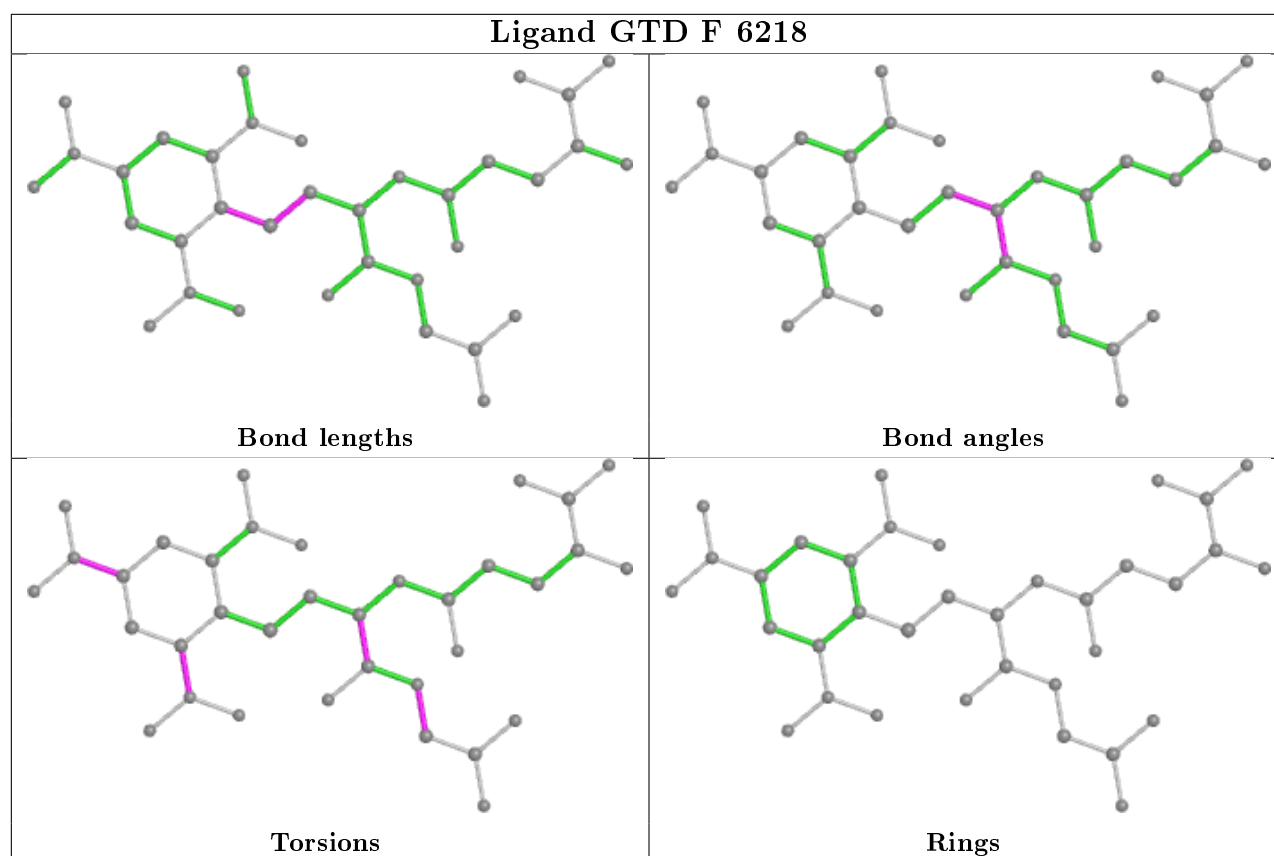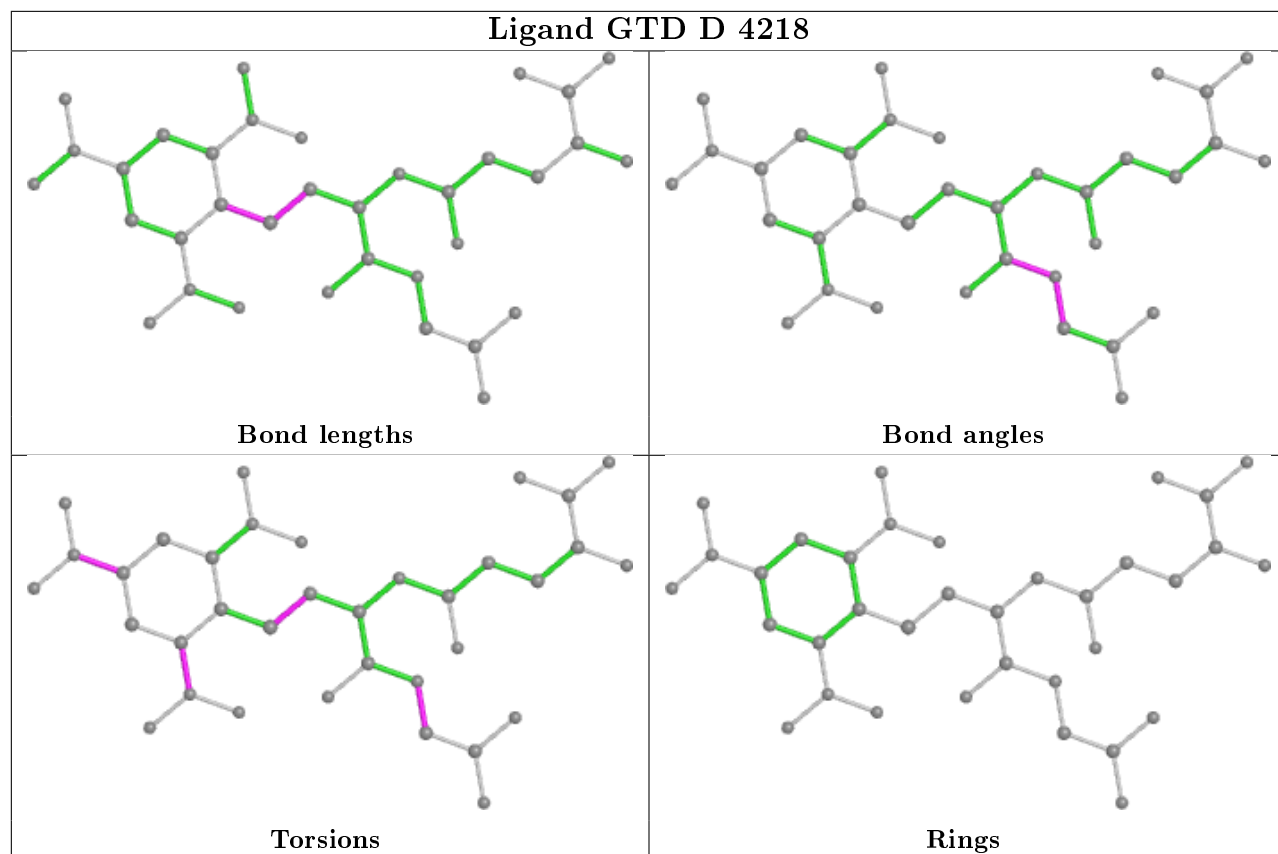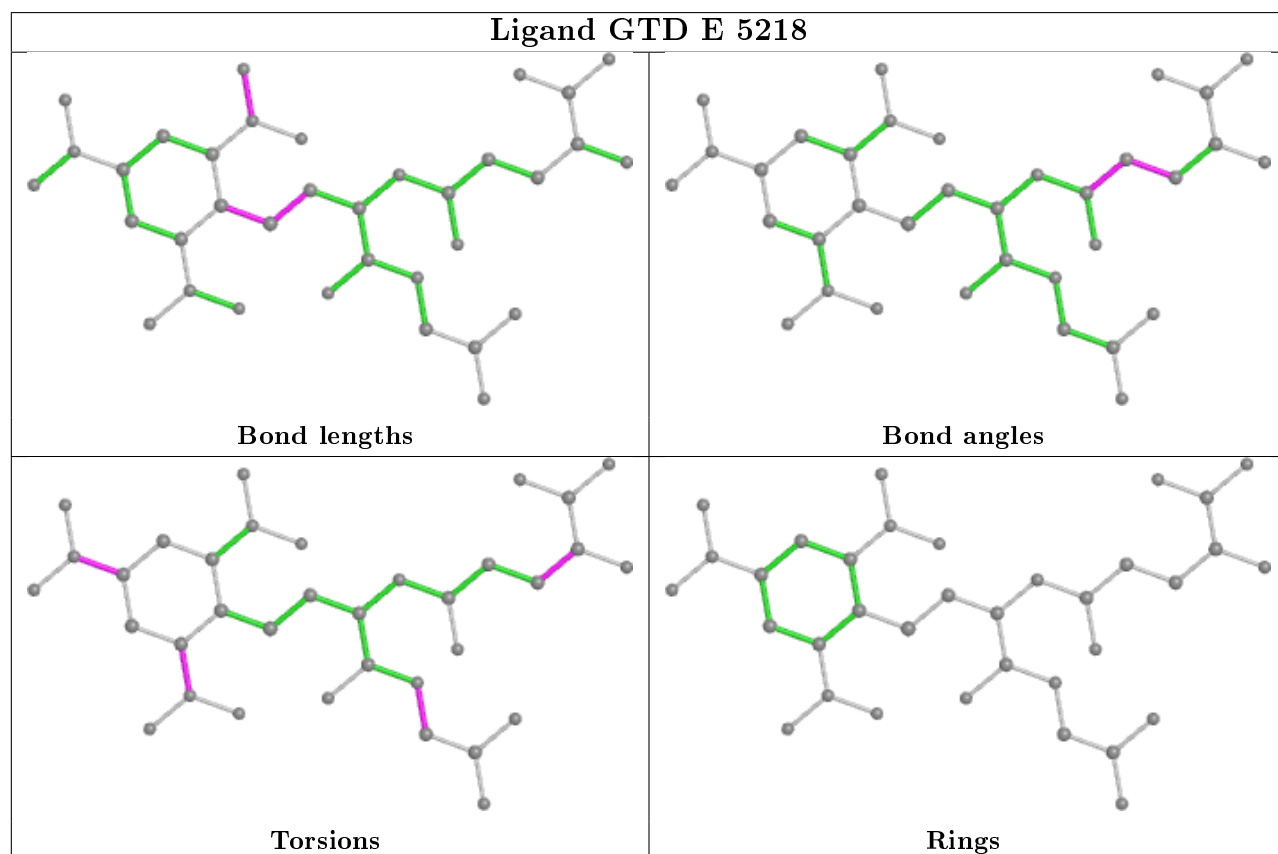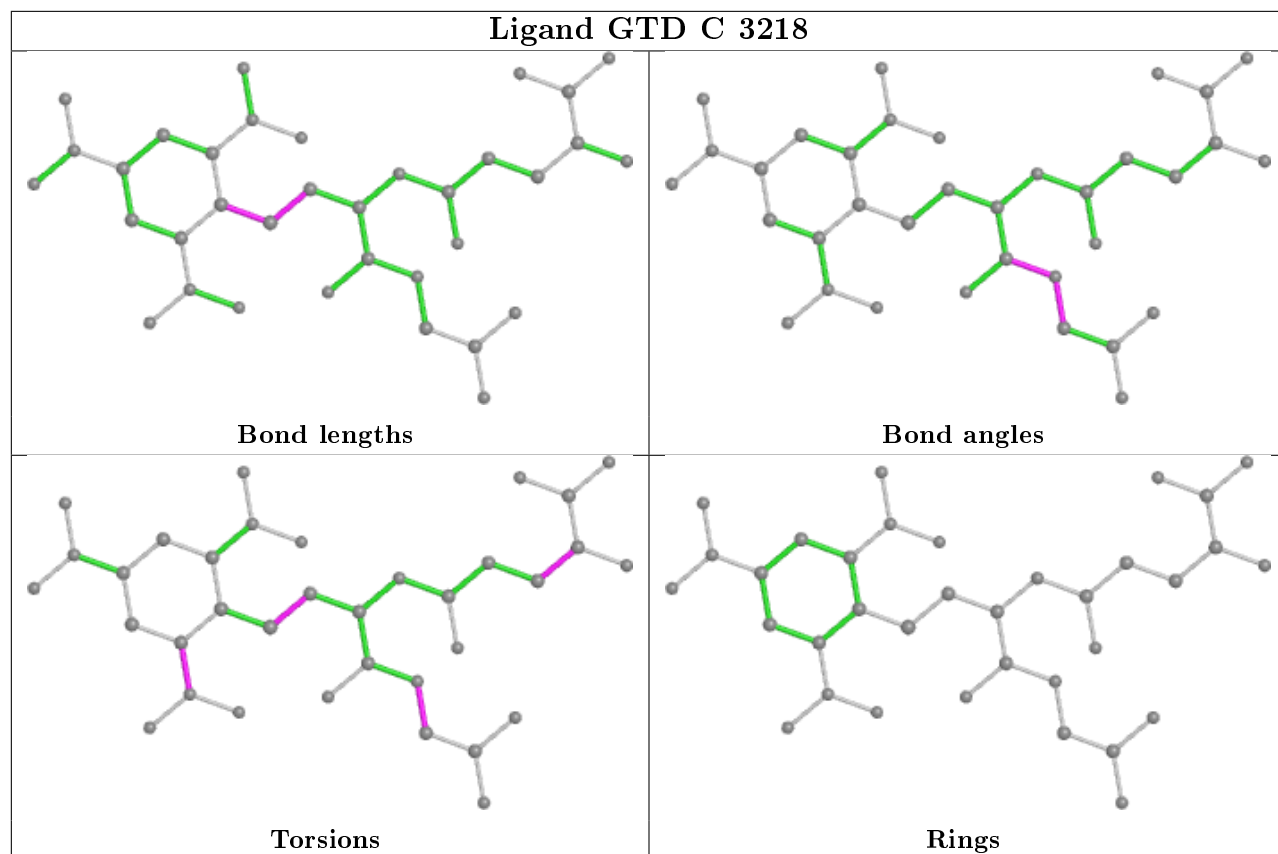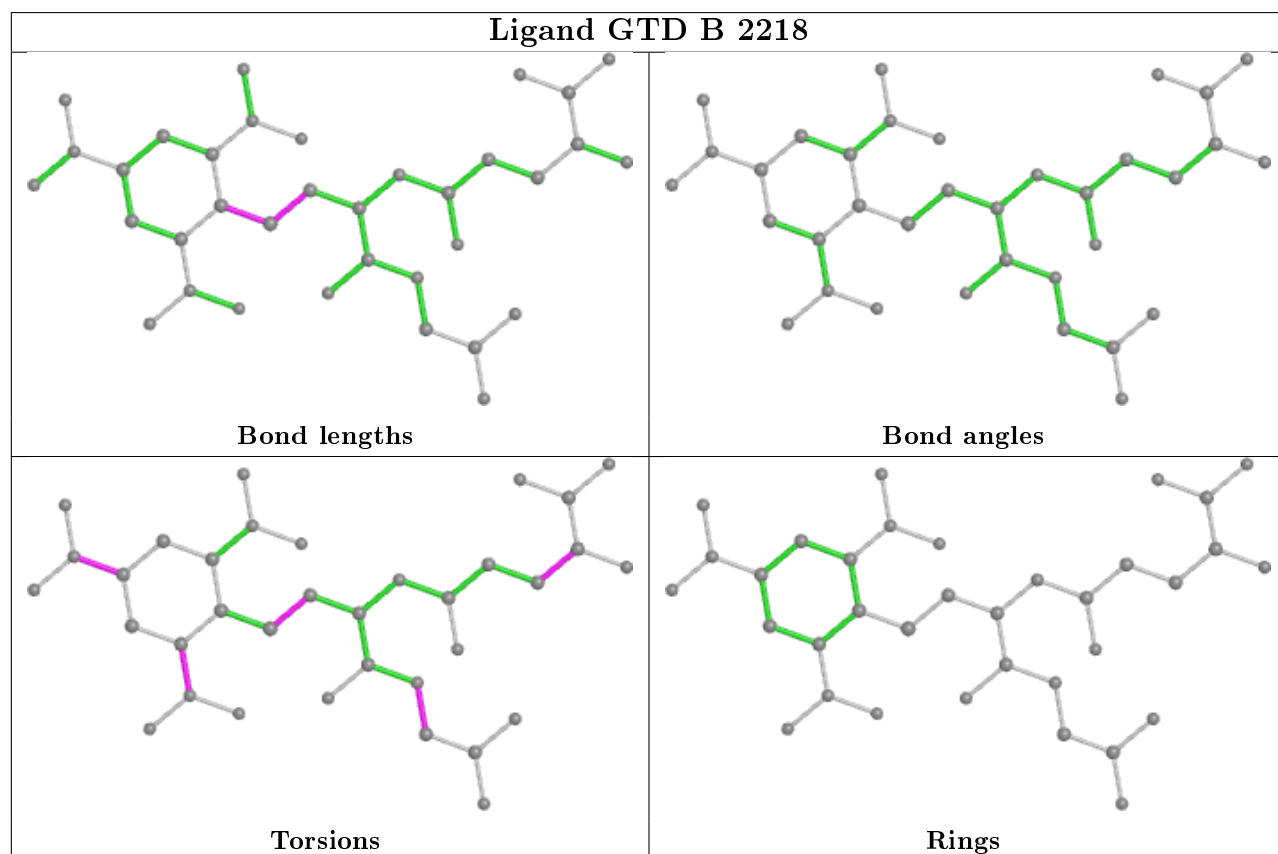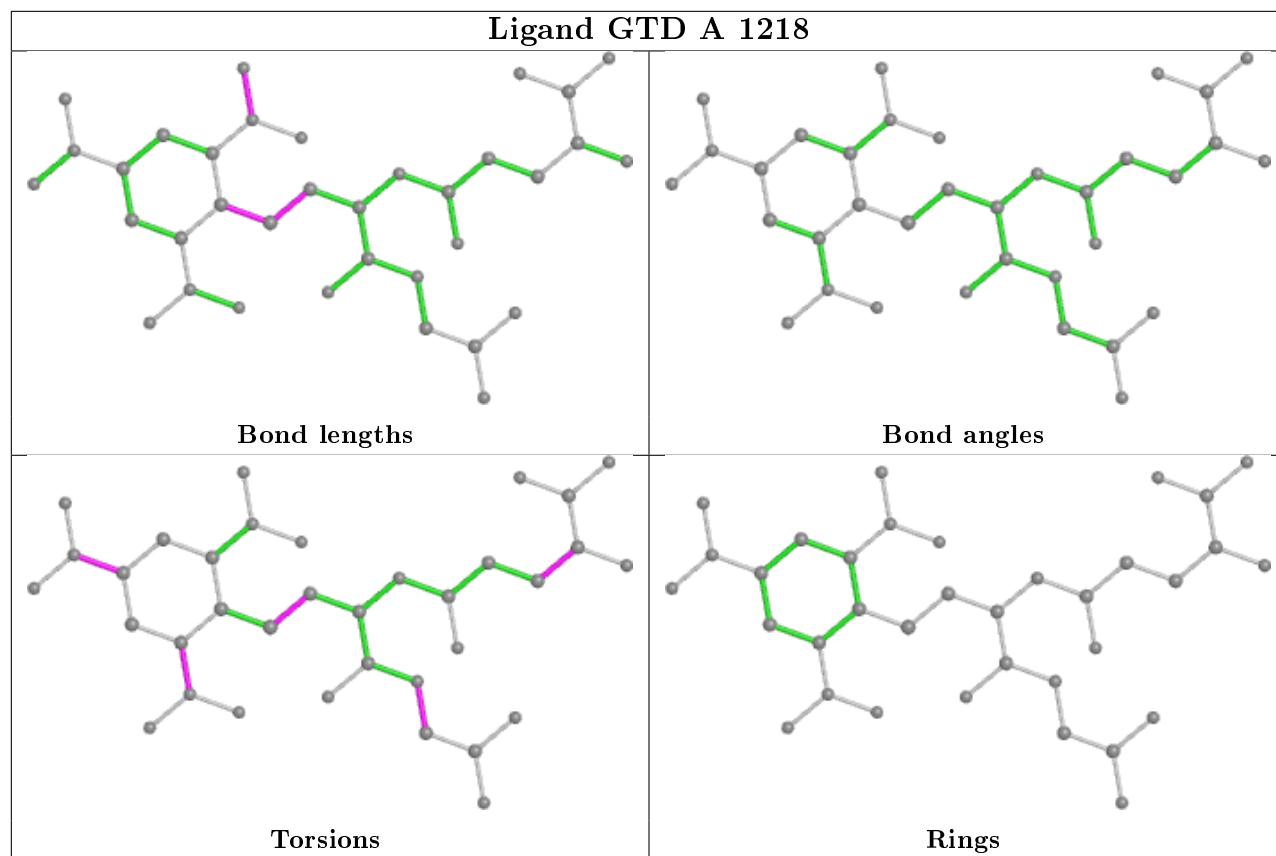
5.7 Other polymers (i)

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(Å²)	Q<0.9
1	A	218/218 (100%)	-0.51	3 (1%)	75	77	39, 54, 65, 70	0
1	B	218/218 (100%)	-0.54	0	100	100	38, 54, 65, 70	0
1	C	217/218 (99%)	-0.43	4 (1%)	68	70	39, 54, 65, 70	0
1	D	218/218 (100%)	-0.45	3 (1%)	75	77	38, 55, 65, 70	0
1	E	218/218 (100%)	-0.50	0	100	100	39, 54, 65, 70	0
1	F	218/218 (100%)	-0.53	0	100	100	38, 54, 65, 70	0
All	All	1307/1308 (99%)	-0.49	10 (0%)	86	87	38, 55, 65, 70	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	38	PRO	4.1
1	C	38	PRO	3.9
1	D	217	LYS	2.5
1	A	130	LEU	2.4
1	C	217	LYS	2.4
1	C	212	ALA	2.3
1	A	217	LYS	2.2
1	A	38	PRO	2.2
1	C	117	PRO	2.0
1	D	117	PRO	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(Å^2)	Q<0.9
2	GTD	B	2218	35/35	0.89	0.16	51,54,57,57	15
2	GTD	F	6218	35/35	0.90	0.14	51,54,57,57	15
2	GTD	D	4218	35/35	0.91	0.17	51,54,57,57	15
2	GTD	C	3218	35/35	0.92	0.15	51,54,57,57	15
2	GTD	E	5218	35/35	0.92	0.17	51,54,57,57	15
2	GTD	A	1218	35/35	0.92	0.14	51,54,57,57	15

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 GTD B 2218:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
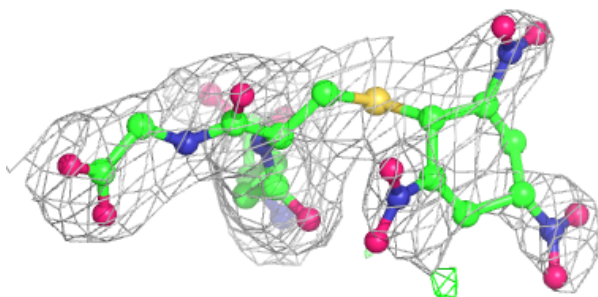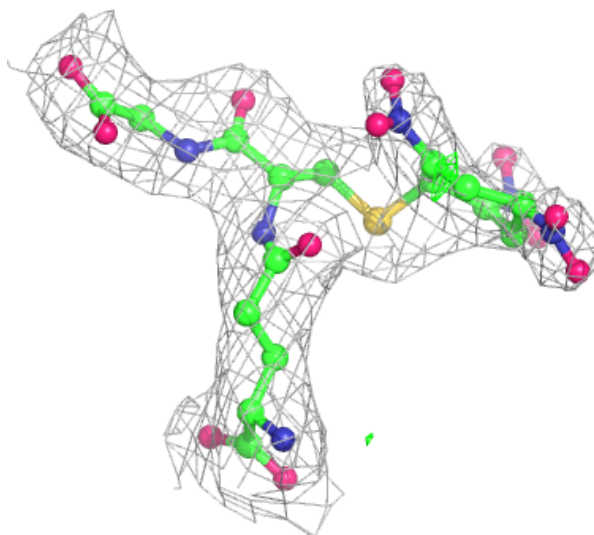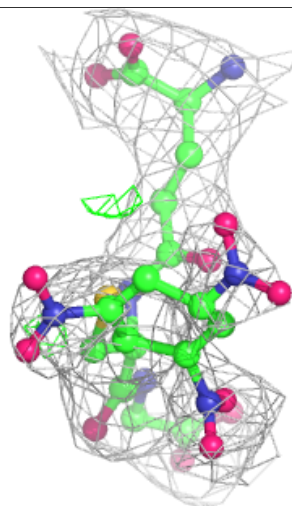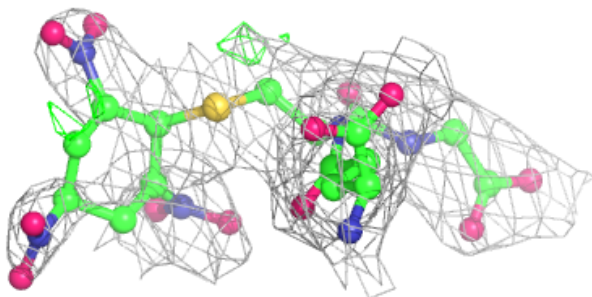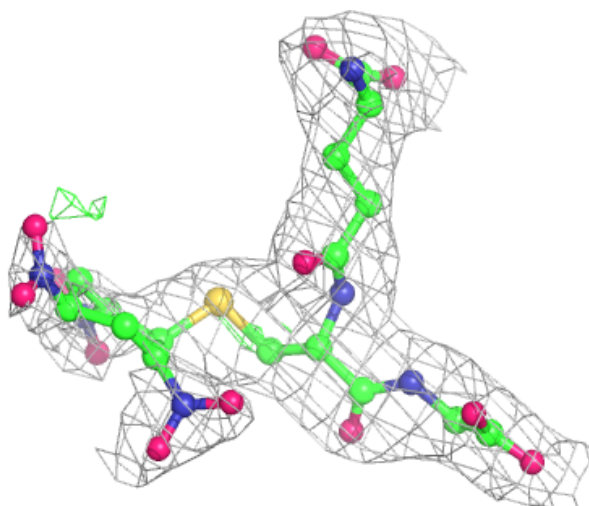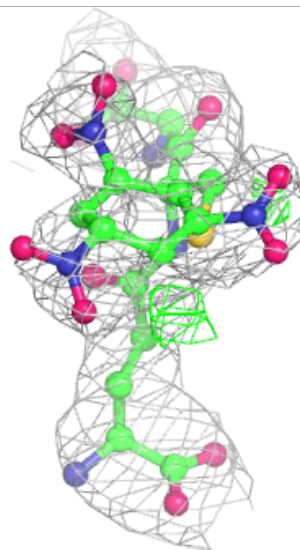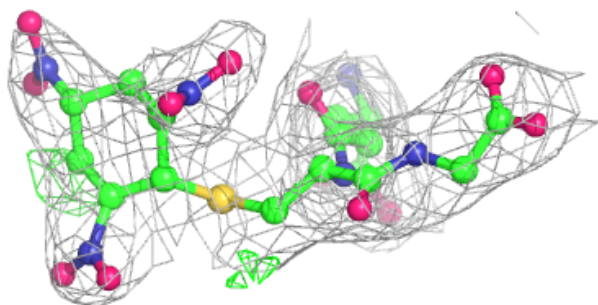and green (positive)
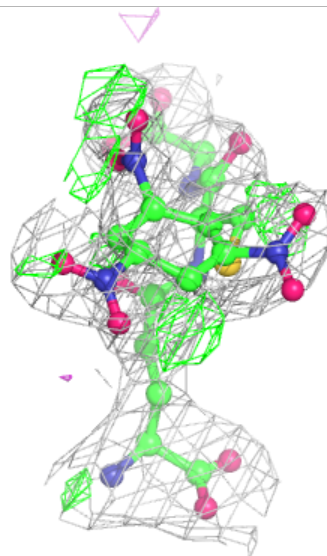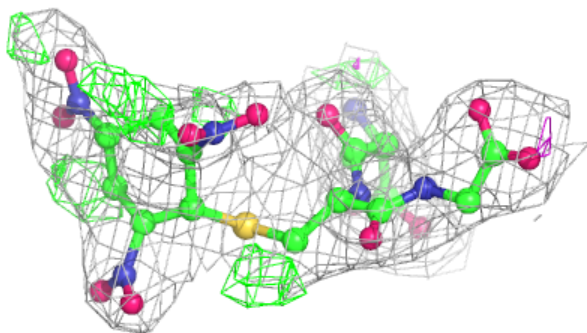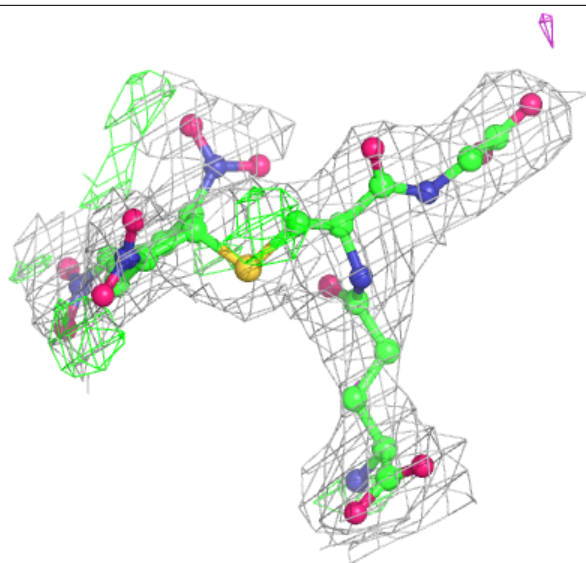
Electron density around GTD F 6218:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
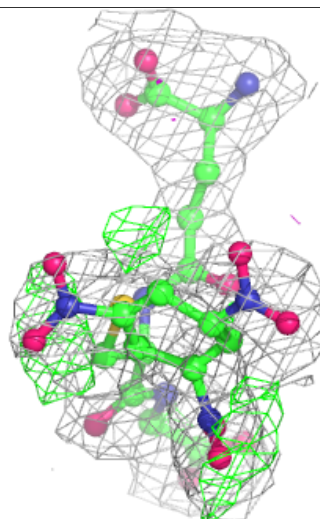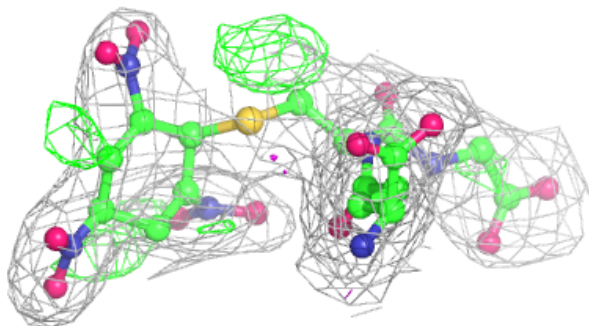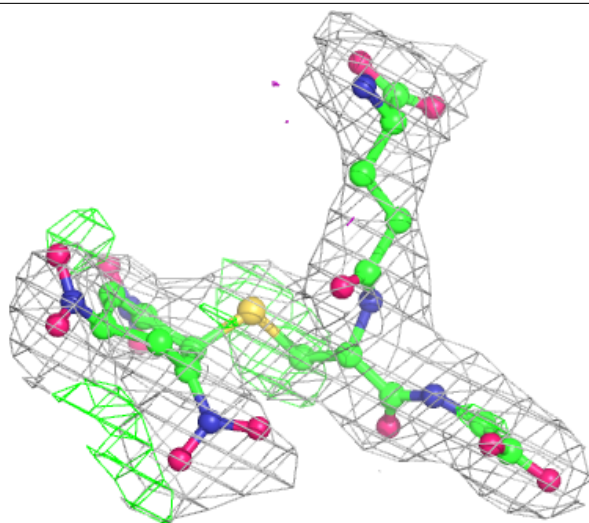
Electron density around GTD D 4218:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
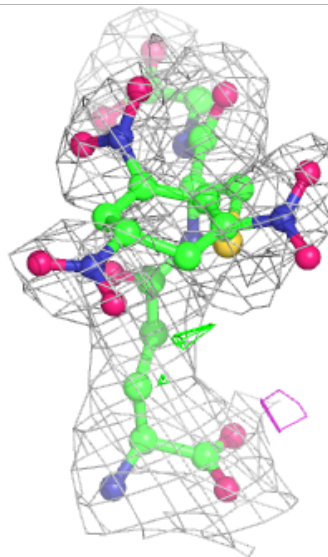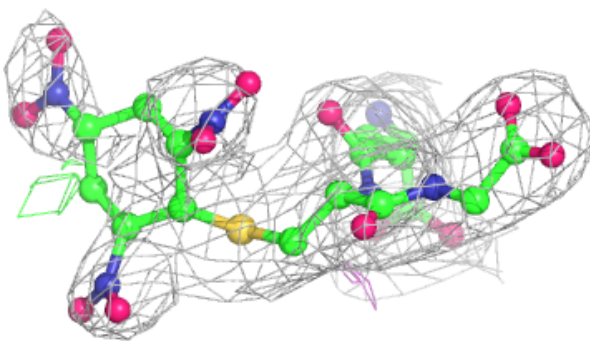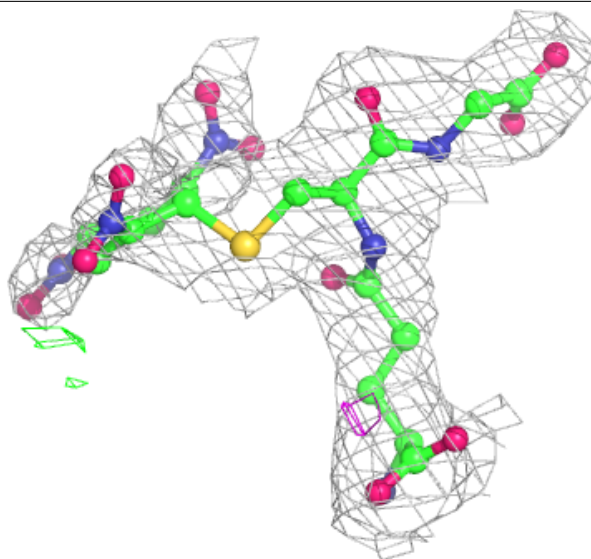
Electron density around GTD C 3218:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
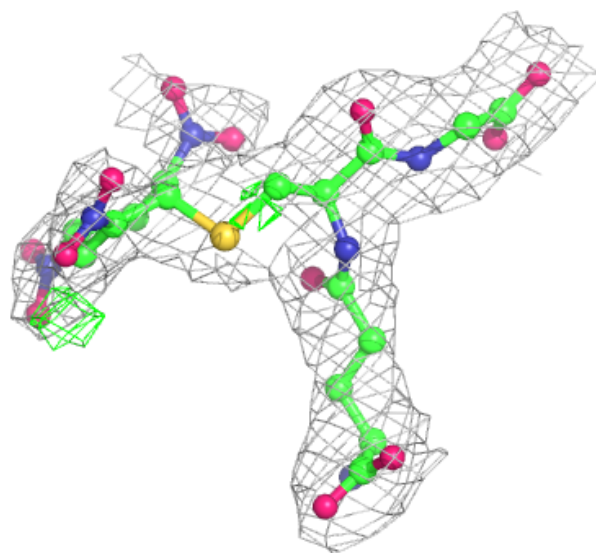$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
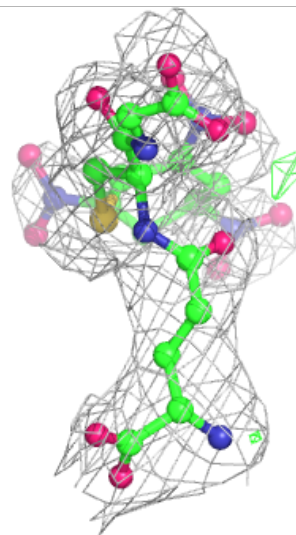
Electron density around GTD E 5218:

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

Electron density around GTD A 1218:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.