Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:52 am BST

PDB ID	:	5OGK
Title	:	Crystal structure of a nucleotide sugar transporter with bound nucleotide sugar.
Authors	:	Newstead, S.; Parker, J.L.
Deposited on	:	2017-07-13
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

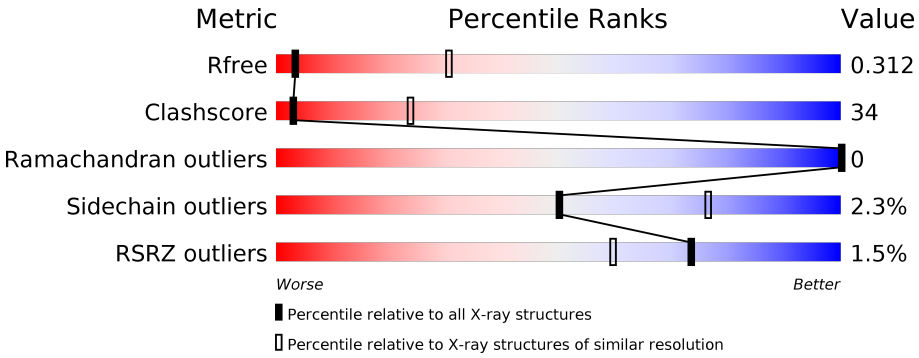
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	337	2% 42% 43% • 13%
1	B	337	% 39% 47% • 12%
1	C	337	% 34% 52% • 13%
1	D	337	2% 41% 45% • 13%
1	E	337	2% 42% 45% • 12%
1	F	337	41% 45% • 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	337	40% 45% 12%
1	H	337	% 42% 44% 13%

2 Entry composition (i)

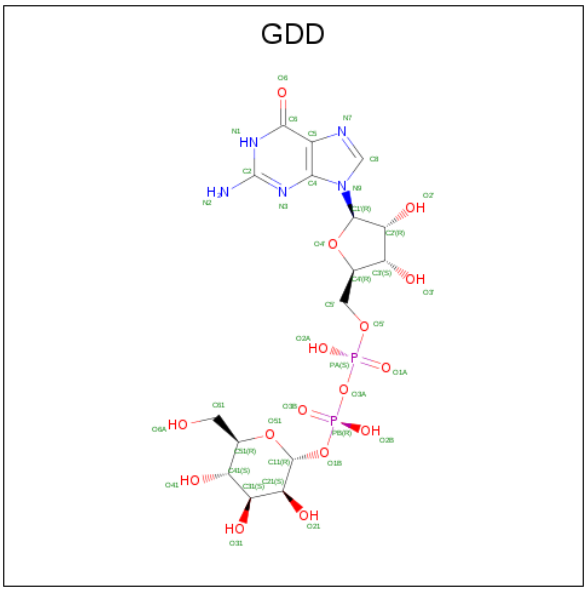
There are 3 unique types of molecules in this entry. The entry contains 19204 atoms, of which 395 are hydrogens and 0 are deuteriums.

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 GDP-mannose transporter 1.

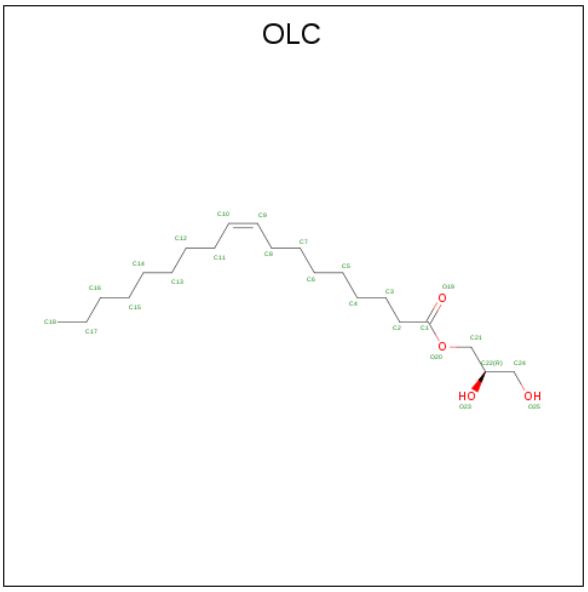
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2291	1516	355	403	17			
1	B	297	Total	C	N	O	S	0	0	0
			2325	1539	360	409	17			
1	C	294	Total	C	N	O	S	0	0	0
			2307	1528	357	405	17			
1	D	294	Total	C	N	O	S	0	0	0
			2307	1528	357	405	17			
1	E	298	Total	C	N	O	S	0	0	0
			2330	1542	361	410	17			
1	F	294	Total	C	N	O	S	0	0	0
			2307	1528	357	405	17			
1	G	296	Total	C	N	O	S	0	0	0
			2318	1534	359	408	17			
1	H	294	Total	C	N	O	S	0	0	0
			2307	1528	357	405	17			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE-ALPHA-D-MANNOSE (three-letter code: GDD) (formula: $C_{16}H_{25}N_5O_{16}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			64	16	25	5	16	2		
2	D	1	Total	C	H	N	O	P	0	0
			64	16	25	5	16	2		
2	E	1	Total	C	H	N	O	P	0	0
			64	16	25	5	16	2		

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



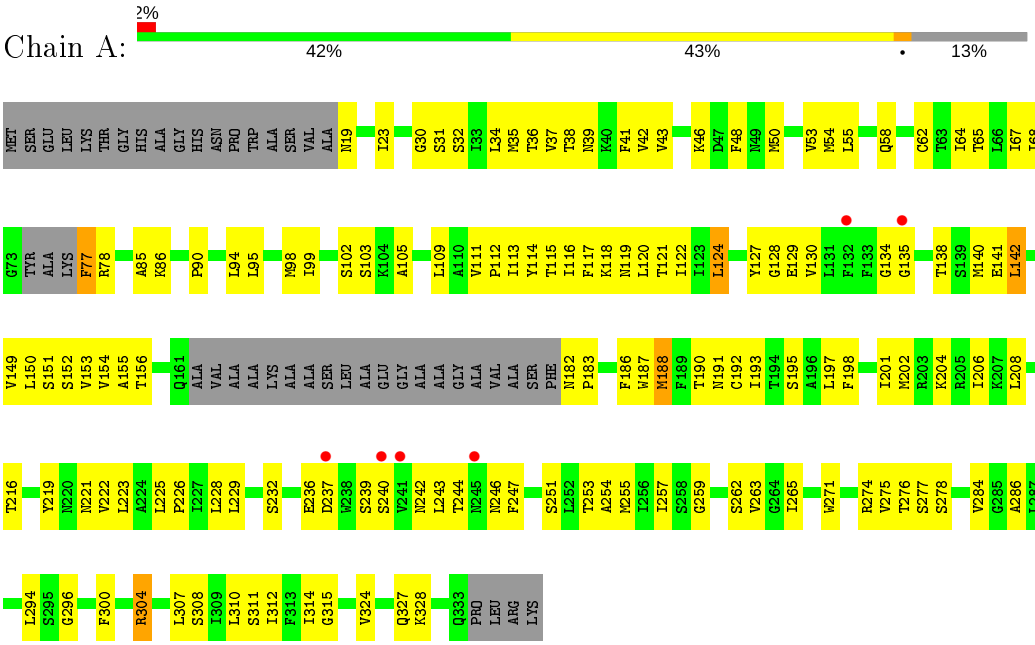
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			65	21	40	4		
3	A	1	Total	C	H	O	0	0
			65	21	40	4		
3	C	1	Total	C	H	O	0	0
			65	21	40	4		
3	C	1	Total	C	H	O	0	0
			65	21	40	4		
3	D	1	Total	C	H	O	0	0
			65	21	40	4		
3	E	1	Total	C	H	O	0	0
			65	21	40	4		
3	G	1	Total	C	H	O	0	0
			65	21	40	4		
3	G	1	Total	C	H	O	0	0
			65	21	40	4		

3 Residue-property plots (i)

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

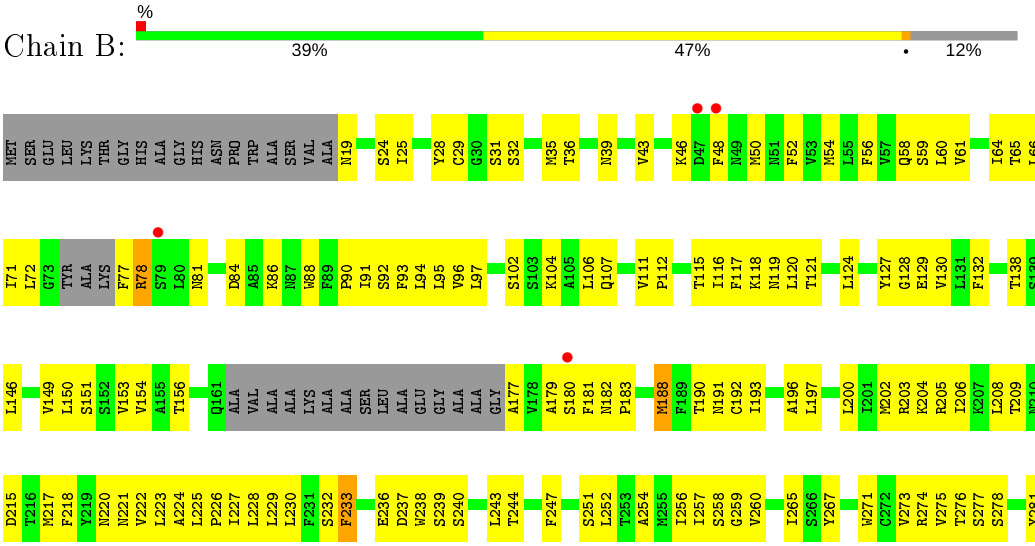
- Molecule 1: GDP-mannose transporter 1

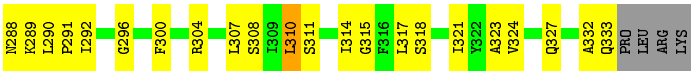
Chain A:



- Molecule 1: GDP-mannose transporter 1

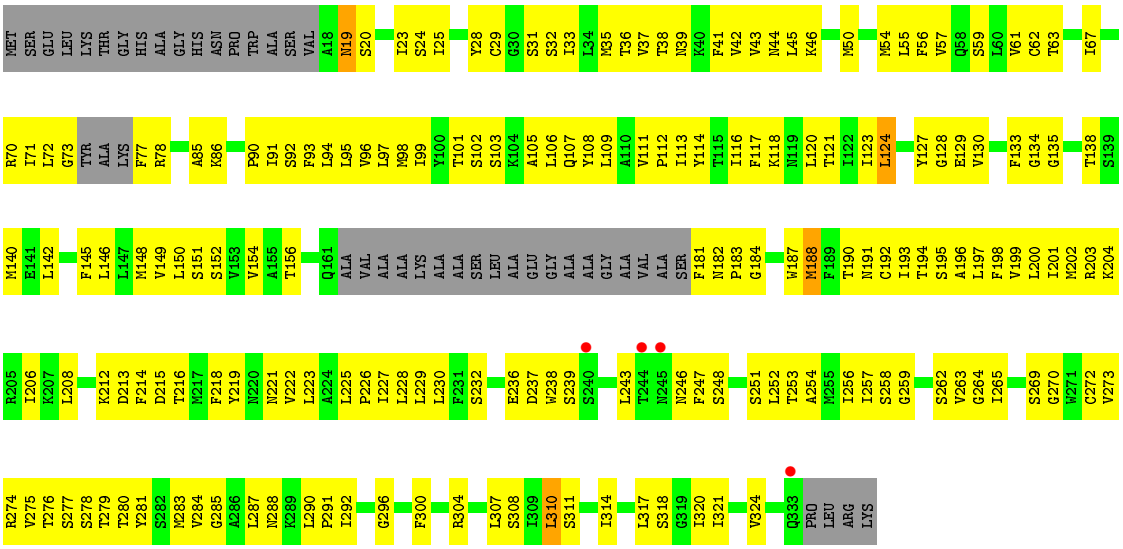
Chain B:





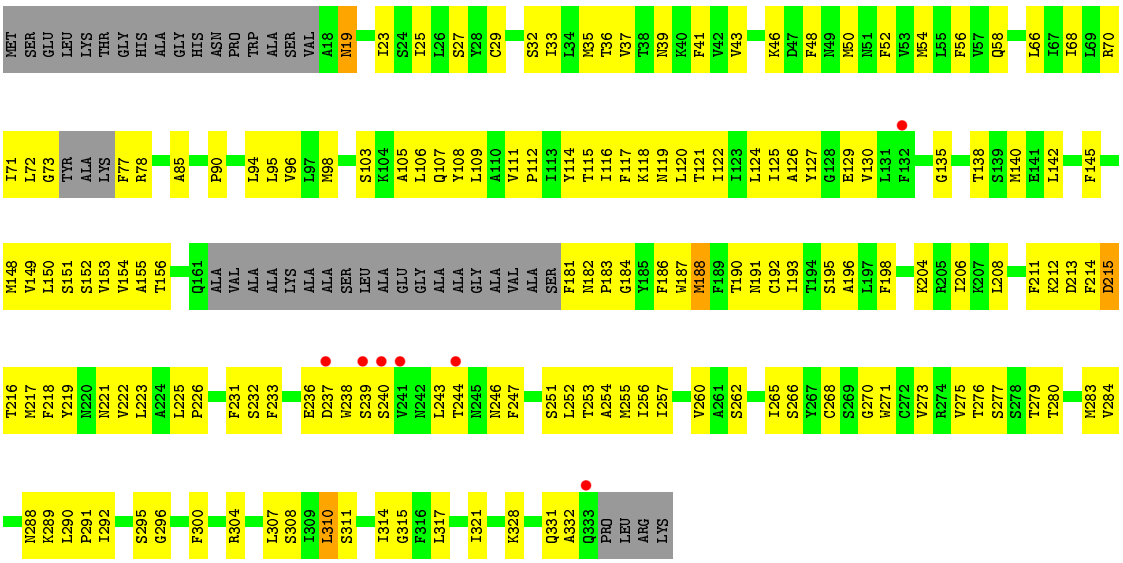
• Molecule 1: GDP-mannose transporter 1

Chain C:



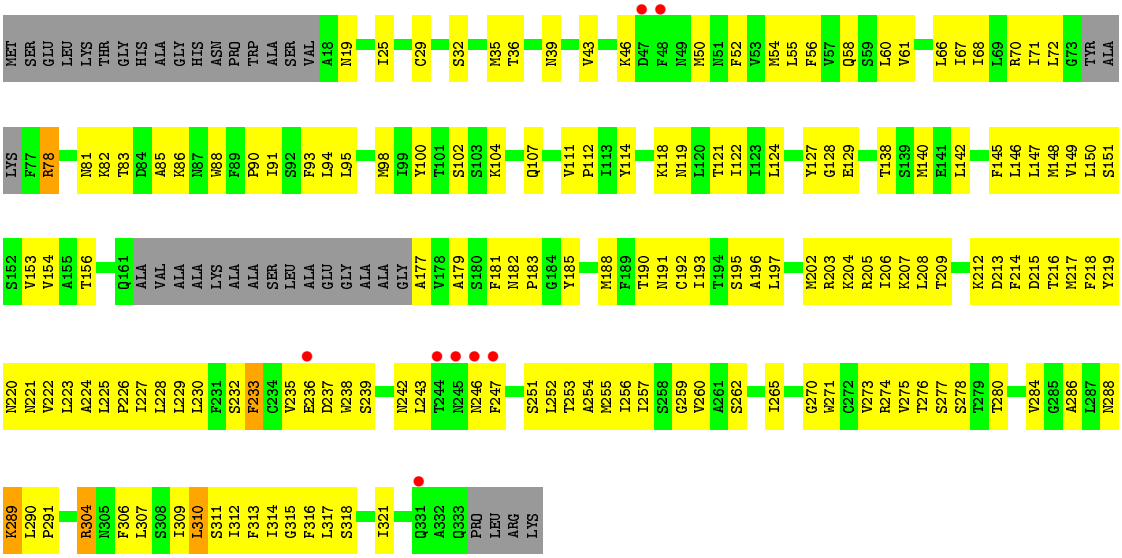
• Molecule 1: GDP-mannose transporter 1

Chain D:



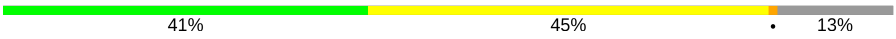
• Molecule 1: GDP-mannose transporter 1

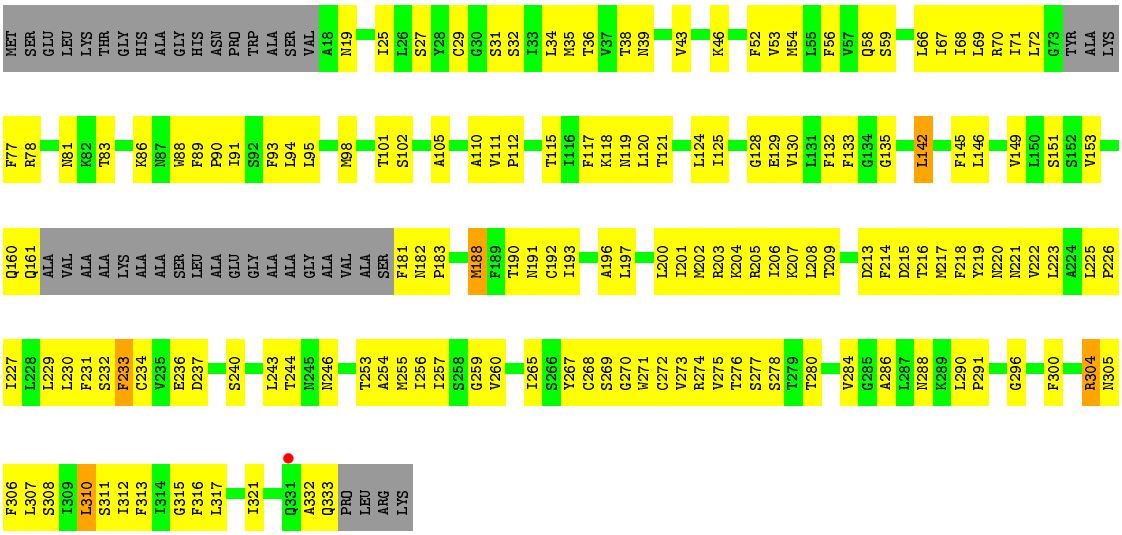
Chain E:



• Molecule 1: GDP-mannose transporter 1

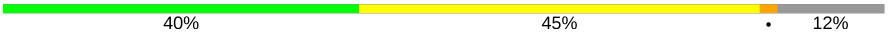
Chain F:

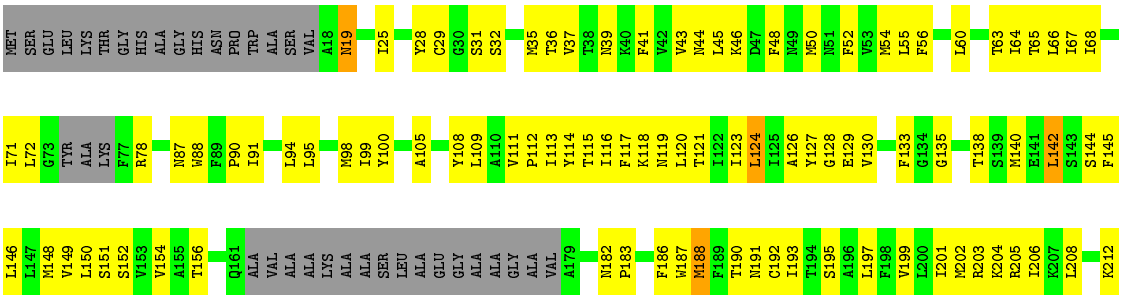


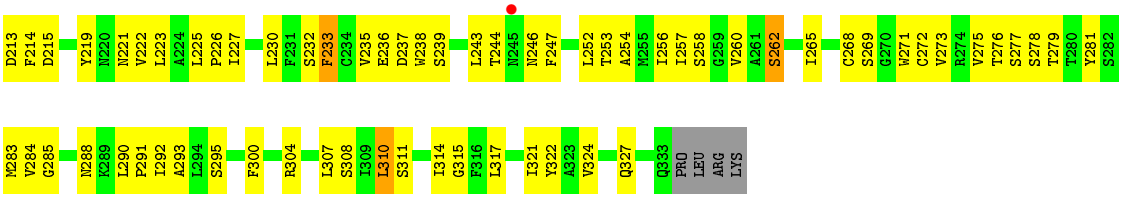


• Molecule 1: GDP-mannose transporter 1

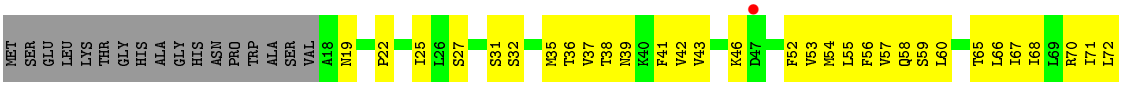
Chain G:

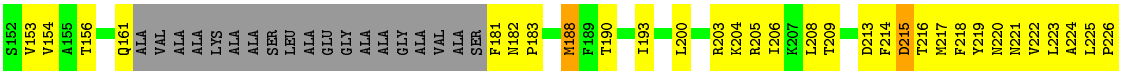


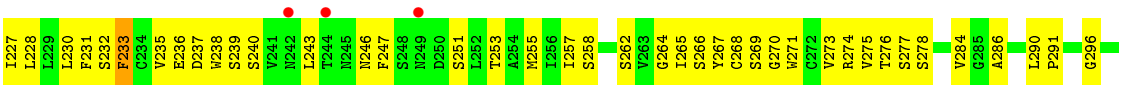


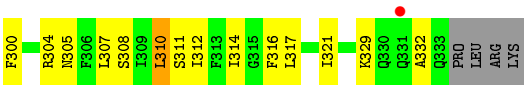


- Molecule 1: GDP-mannose transporter 1









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.32Å 101.69Å 180.19Å 89.86° 90.07° 90.11°	Depositor
Resolution (Å)	44.33 – 3.60 44.33 – 3.60	Depositor EDS
% Data completeness (in resolution range)	96.6 (44.33-3.60) 95.8 (44.33-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.257 , 0.313 0.259 , 0.312	Depositor DCC
R_{free} test set	1950 reflections (5.41%)	wwPDB-VP
Wilson B-factor (Å^2)	92.8	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 17.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.287 for h,-k,-l 0.277 for -h,k,-l 0.277 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19204	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.03% 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: OLC, GDD

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	0.26	0/2340	0.44	0/3174
1	B	0.27	0/2375	0.44	0/3222
1	C	0.27	0/2357	0.44	0/3197
1	D	0.26	0/2357	0.45	0/3197
1	E	0.28	0/2380	0.45	0/3229
1	F	0.26	0/2357	0.45	0/3197
1	G	0.26	0/2368	0.44	0/3212
1	H	0.27	0/2357	0.44	0/3197
All	All	0.27	0/18891	0.44	0/25625

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2291	0	2366	178	0
1	B	2325	0	2399	171	0
1	C	2307	0	2380	189	0
1	D	2307	0	2380	160	0
1	E	2330	0	2404	160	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2307	0	2380	162	0
1	G	2318	0	2390	168	0
1	H	2307	0	2380	132	1
2	A	39	25	23	0	0
2	D	39	25	23	1	0
2	E	39	25	23	4	0
3	A	50	80	80	2	0
3	C	50	80	80	2	0
3	D	25	40	40	2	0
3	E	25	40	40	1	0
3	G	50	80	80	4	0
All	All	18809	395	19468	1305	1

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 34.

All (1305) 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:G:204:LYS:HE3	1:G:208:LEU:HD11	1.29	1.14
1:A:121:THR:HA	1:A:124:LEU:HD21	1.26	1.13
1:C:121:THR:HA	1:C:124:LEU:HD21	1.29	1.12
1:E:204:LYS:HE3	1:E:208:LEU:HD11	1.29	1.12
1:C:43:VAL:HG11	1:C:46:LYS:HD3	1.34	1.09
1:D:204:LYS:HE3	1:D:208:LEU:HD11	1.29	1.08
1:B:227:ILE:HA	1:B:230:LEU:HD12	1.28	1.08
1:F:204:LYS:HE3	1:F:208:LEU:HD11	1.34	1.07
1:C:204:LYS:HE3	1:C:208:LEU:HD11	1.35	1.06
1:G:121:THR:HA	1:G:124:LEU:HD21	1.36	1.05
1:A:48:PHE:HZ	1:A:247:PHE:HB3	1.19	1.03
1:G:43:VAL:HG11	1:G:46:LYS:HD3	1.37	1.02
1:B:67:ILE:HG12	1:B:78:ARG:HH22	1.25	1.01
1:B:247:PHE:HD2	1:B:252:LEU:HD21	1.28	0.99
1:E:227:ILE:HA	1:E:230:LEU:HD12	1.44	0.97
1:F:227:ILE:HA	1:F:230:LEU:HD12	1.45	0.95
1:F:67:ILE:HG12	1:F:78:ARG:HH22	1.30	0.95
1:B:70:ARG:HD2	1:B:78:ARG:HH21	1.33	0.94
1:F:69:LEU:HB3	1:F:77:PHE:HE2	1.30	0.94
1:E:124:LEU:O	1:E:128:GLY:N	2.01	0.93
1:G:50:MET:HA	1:G:236:GLU:HG2	1.51	0.91
1:D:121:THR:HA	1:D:124:LEU:HD21	1.54	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:ILE:HG12	1:H:78:ARG:HH22	1.37	0.89
1:A:43:VAL:HG11	1:A:46:LYS:HD3	1.52	0.88
1:B:124:LEU:O	1:B:128:GLY:N	2.06	0.88
1:B:214:PHE:O	1:B:218:PHE:N	2.05	0.88
1:F:203:ARG:NH1	1:F:274:ARG:O	2.06	0.87
1:F:124:LEU:O	1:F:128:GLY:N	2.08	0.87
1:C:121:THR:HA	1:C:124:LEU:CD2	2.04	0.87
1:D:328:LYS:HA	1:D:331:GLN:HB2	1.55	0.86
1:A:204:LYS:HE3	1:A:208:LEU:HD11	1.55	0.86
1:E:214:PHE:O	1:E:218:PHE:N	2.09	0.85
1:F:214:PHE:O	1:F:218:PHE:N	2.10	0.84
1:B:204:LYS:HE3	1:B:208:LEU:HD11	1.59	0.84
1:D:37:VAL:HG13	1:D:41:PHE:CD2	2.12	0.84
1:H:129:GLU:OE2	1:H:278:SER:HB2	1.76	0.84
1:F:78:ARG:HA	1:F:215:ASP:OD1	1.76	0.84
1:A:243:LEU:HD23	1:A:246:ASN:OD1	1.78	0.83
1:E:237:ASP:O	1:E:243:LEU:HD11	1.79	0.83
1:A:37:VAL:HG13	1:A:41:PHE:CD2	2.14	0.83
1:C:116:ILE:HD11	1:C:156:THR:OG1	1.79	0.83
1:C:55:LEU:HD13	1:C:99:ILE:HD13	1.59	0.82
1:A:38:THR:HG23	1:A:42:VAL:HG21	1.62	0.82
1:D:243:LEU:HA	1:D:246:ASN:OD1	1.79	0.82
1:F:32:SER:O	1:F:36:THR:OG1	1.97	0.82
1:B:290:LEU:HB2	1:B:291:PRO:HD3	1.61	0.81
1:C:37:VAL:HG13	1:C:41:PHE:CD2	2.15	0.81
1:F:243:LEU:HA	1:F:246:ASN:OD1	1.81	0.81
1:B:25:ILE:HG23	1:B:284:VAL:HG11	1.64	0.80
1:D:70:ARG:HD2	1:D:78:ARG:HH21	1.46	0.80
1:D:43:VAL:HG11	1:D:46:LYS:HD3	1.62	0.80
1:F:69:LEU:HB3	1:F:77:PHE:CE2	2.16	0.80
1:A:55:LEU:HD13	1:A:99:ILE:HD13	1.62	0.80
1:A:151:SER:HB2	1:A:314:ILE:HG22	1.63	0.80
1:A:102:SER:HB2	1:A:191:ASN:ND2	1.96	0.80
1:H:232:SER:HA	1:H:236:GLU:OE1	1.81	0.80
1:H:239:SER:H	1:H:243:LEU:HD12	1.47	0.80
1:A:275:VAL:HG23	1:A:276:THR:HG23	1.62	0.80
1:C:32:SER:O	1:C:36:THR:OG1	2.00	0.79
1:G:121:THR:HA	1:G:124:LEU:CD2	2.13	0.79
1:G:275:VAL:HG23	1:G:276:THR:HG23	1.64	0.79
1:B:232:SER:HA	1:B:236:GLU:OE1	1.83	0.79
1:E:232:SER:HA	1:E:236:GLU:OE1	1.81	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:VAL:CG1	1:C:46:LYS:HD3	2.12	0.79
1:E:275:VAL:HG23	1:E:276:THR:HG23	1.62	0.79
1:C:145:PHE:O	1:C:149:VAL:HG23	1.83	0.79
1:C:243:LEU:HA	1:C:246:ASN:OD1	1.82	0.79
1:D:243:LEU:HD23	1:D:246:ASN:OD1	1.82	0.79
1:E:203:ARG:NH1	1:E:274:ARG:O	2.16	0.79
1:E:256:ILE:O	1:E:260:VAL:HG23	1.83	0.79
1:H:70:ARG:HD2	1:H:78:ARG:HH21	1.48	0.79
1:C:70:ARG:HD2	1:C:78:ARG:HH21	1.45	0.79
1:A:48:PHE:CZ	1:A:247:PHE:HB3	2.12	0.79
1:D:119:ASN:HD22	1:D:122:ILE:HD11	1.49	0.78
1:A:70:ARG:HD2	1:A:78:ARG:HH21	1.47	0.78
1:D:150:LEU:O	1:D:154:VAL:N	2.12	0.78
1:F:35:MET:O	1:F:39:ASN:ND2	2.17	0.78
1:H:218:PHE:CZ	1:H:222:VAL:HG21	2.19	0.78
1:C:275:VAL:HG23	1:C:276:THR:HG23	1.63	0.78
1:D:121:THR:HA	1:D:124:LEU:CD2	2.14	0.78
1:G:55:LEU:HD13	1:G:99:ILE:HD13	1.66	0.78
1:C:109:LEU:HD13	1:C:188:MET:HG3	1.64	0.77
1:D:232:SER:HA	1:D:236:GLU:OE1	1.84	0.77
1:D:275:VAL:HG23	1:D:276:THR:HG23	1.65	0.77
1:C:243:LEU:HD23	1:C:246:ASN:OD1	1.83	0.77
1:D:37:VAL:HG13	1:D:41:PHE:HD2	1.48	0.77
1:E:32:SER:O	1:E:36:THR:OG1	2.03	0.77
1:G:32:SER:O	1:G:36:THR:OG1	2.03	0.77
1:E:290:LEU:HB2	1:E:291:PRO:HD3	1.66	0.76
1:F:29:CYS:HA	1:F:288:ASN:HD21	1.50	0.76
1:E:221:ASN:O	1:E:225:LEU:HG	1.84	0.76
1:C:247:PHE:HD2	1:C:252:LEU:HD21	1.50	0.76
1:E:204:LYS:HE3	1:E:208:LEU:CD1	2.12	0.76
1:D:121:THR:O	1:D:124:LEU:HG	1.86	0.76
1:A:151:SER:OG	1:A:311:SER:O	2.01	0.76
1:H:46:LYS:HE2	1:H:258:SER:CB	2.16	0.76
1:G:188:MET:HE3	1:G:191:ASN:HB3	1.67	0.76
1:G:310:LEU:HD22	1:G:314:ILE:HD11	1.68	0.76
1:D:188:MET:CE	1:D:191:ASN:HB3	2.15	0.75
1:C:31:SER:HB2	1:C:265:ILE:N	2.02	0.75
1:G:117:PHE:O	1:G:121:THR:HG23	1.86	0.75
1:E:243:LEU:HA	1:E:246:ASN:OD1	1.85	0.75
1:F:129:GLU:OE2	1:F:278:SER:HB2	1.86	0.75
1:A:71:ILE:HG13	1:A:72:LEU:HD22	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:LEU:O	1:E:226:PRO:HD2	1.86	0.75
1:H:221:ASN:O	1:H:225:LEU:HG	1.86	0.75
1:H:239:SER:N	1:H:243:LEU:HD12	2.00	0.75
1:B:48:PHE:HZ	1:B:247:PHE:HB3	1.52	0.74
1:H:46:LYS:HE2	1:H:258:SER:HB2	1.67	0.74
1:A:148:MET:O	1:A:152:SER:OG	2.05	0.74
1:H:275:VAL:HG23	1:H:276:THR:HG23	1.68	0.74
1:A:155:ALA:HB2	1:A:311:SER:CB	2.17	0.74
1:A:109:LEU:HD13	1:A:188:MET:HG3	1.68	0.74
1:B:91:ILE:O	1:B:95:LEU:N	2.18	0.74
1:E:247:PHE:CD2	1:E:252:LEU:HD21	2.22	0.74
1:G:108:TYR:CG	1:G:183:PRO:HB2	2.22	0.74
1:B:221:ASN:O	1:B:225:LEU:HG	1.87	0.74
1:A:290:LEU:HB2	1:A:291:PRO:HD3	1.70	0.74
1:F:256:ILE:O	1:F:260:VAL:HG23	1.87	0.74
1:G:43:VAL:CG1	1:G:46:LYS:HD3	2.16	0.74
1:H:46:LYS:HE3	1:H:54:MET:SD	2.28	0.74
1:A:188:MET:HE3	1:A:191:ASN:HB3	1.70	0.73
1:D:187:TRP:O	1:D:190:THR:OG1	2.06	0.73
1:A:71:ILE:HG13	1:A:72:LEU:CD2	2.18	0.73
1:F:204:LYS:HE3	1:F:208:LEU:CD1	2.14	0.73
1:G:71:ILE:HG13	1:G:72:LEU:HD22	1.69	0.73
1:G:145:PHE:O	1:G:149:VAL:HG23	1.89	0.73
1:H:290:LEU:HB2	1:H:291:PRO:HD3	1.70	0.73
1:B:275:VAL:HG23	1:B:276:THR:HG23	1.71	0.73
1:E:218:PHE:CZ	1:E:222:VAL:HG21	2.24	0.72
1:G:66:LEU:HB3	1:G:78:ARG:HH11	1.54	0.72
1:A:70:ARG:HD2	1:A:78:ARG:NH2	2.04	0.72
1:H:39:ASN:OD1	1:H:46:LYS:HG2	1.88	0.72
1:H:132:PHE:HE2	1:H:200:LEU:HD13	1.54	0.72
1:F:290:LEU:HB2	1:F:291:PRO:HD3	1.69	0.72
1:G:71:ILE:HG13	1:G:72:LEU:CD2	2.19	0.72
1:C:25:ILE:HG12	1:C:284:VAL:HG21	1.72	0.72
1:D:151:SER:HB2	1:D:314:ILE:HG22	1.72	0.72
1:D:71:ILE:HG13	1:D:72:LEU:HD22	1.70	0.72
1:F:317:LEU:O	1:F:321:ILE:HG12	1.89	0.72
1:H:223:LEU:O	1:H:226:PRO:HD2	1.89	0.72
1:D:117:PHE:O	1:D:121:THR:HG23	1.89	0.72
1:F:190:THR:O	1:F:193:ILE:HG13	1.90	0.72
1:H:52:PHE:O	1:H:56:PHE:N	2.23	0.72
1:A:119:ASN:HD22	1:A:122:ILE:HD11	1.54	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:PHE:O	1:A:121:THR:HG23	1.90	0.71
1:B:247:PHE:CD2	1:B:252:LEU:HD21	2.19	0.71
1:B:247:PHE:HA	1:B:251:SER:OG	1.89	0.71
1:F:149:VAL:O	1:F:153:VAL:HG23	1.90	0.71
1:G:243:LEU:HD23	1:G:246:ASN:OD1	1.89	0.71
1:C:35:MET:O	1:C:39:ASN:ND2	2.21	0.71
1:F:70:ARG:HD2	1:F:78:ARG:HH21	1.55	0.71
1:F:218:PHE:CZ	1:F:222:VAL:HG21	2.26	0.71
1:D:145:PHE:O	1:D:149:VAL:HG23	1.91	0.71
1:F:121:THR:HA	1:F:124:LEU:HD21	1.71	0.71
1:G:253:THR:HG22	1:G:257:ILE:CD1	2.20	0.71
1:F:243:LEU:HD23	1:F:246:ASN:OD1	1.90	0.71
1:C:223:LEU:O	1:C:226:PRO:HD2	1.90	0.71
1:H:190:THR:O	1:H:193:ILE:HG13	1.90	0.71
1:A:70:ARG:HD2	1:A:78:ARG:HE	1.54	0.71
1:B:203:ARG:NH1	1:B:274:ARG:O	2.23	0.71
1:F:275:VAL:HG23	1:F:276:THR:HG23	1.70	0.71
1:A:55:LEU:CD1	1:A:99:ILE:HD13	2.20	0.70
1:B:121:THR:O	1:B:124:LEU:HG	1.90	0.70
1:D:71:ILE:HG13	1:D:72:LEU:CD2	2.21	0.70
1:G:115:THR:HG22	1:G:119:ASN:OD1	1.91	0.70
1:C:116:ILE:HD11	1:C:156:THR:HG1	1.55	0.70
1:A:116:ILE:HD11	1:A:156:THR:OG1	1.91	0.70
1:D:190:THR:O	1:D:193:ILE:HG13	1.90	0.70
1:G:105:ALA:HB1	1:G:109:LEU:HD12	1.73	0.70
1:B:32:SER:O	1:B:36:THR:OG1	2.10	0.69
1:C:46:LYS:HE3	1:C:54:MET:SD	2.31	0.69
1:D:29:CYS:O	1:D:33:ILE:N	2.22	0.69
1:F:121:THR:O	1:F:124:LEU:HG	1.91	0.69
1:F:145:PHE:O	1:F:149:VAL:HG23	1.92	0.69
1:F:305:ASN:ND2	1:F:308:SER:OG	2.20	0.69
1:C:290:LEU:HB2	1:C:291:PRO:HD3	1.73	0.69
1:D:46:LYS:HE3	1:D:54:MET:SD	2.31	0.69
1:B:218:PHE:CZ	1:B:222:VAL:HG21	2.27	0.69
1:G:35:MET:O	1:G:39:ASN:ND2	2.23	0.69
1:H:243:LEU:HA	1:H:246:ASN:OD1	1.92	0.69
1:G:290:LEU:HB2	1:G:291:PRO:HD3	1.75	0.69
1:H:227:ILE:HA	1:H:230:LEU:HD12	1.74	0.69
1:H:203:ARG:NH1	1:H:274:ARG:O	2.24	0.69
1:B:121:THR:HA	1:B:124:LEU:HD21	1.75	0.69
1:E:35:MET:SD	1:E:265:ILE:HG12	2.32	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:MET:HE3	1:D:191:ASN:HB3	1.74	0.69
1:A:90:PRO:O	1:A:94:LEU:HD23	1.93	0.69
1:C:91:ILE:O	1:C:95:LEU:N	2.26	0.69
1:E:238:TRP:HA	1:E:243:LEU:HD12	1.73	0.69
1:C:204:LYS:HE3	1:C:208:LEU:CD1	2.19	0.69
1:G:48:PHE:HZ	1:G:247:PHE:HB3	1.58	0.69
1:A:151:SER:HB2	1:A:314:ILE:CG2	2.22	0.69
1:A:290:LEU:HD22	1:A:312:ILE:HA	1.74	0.69
1:E:151:SER:O	1:E:311:SER:HB2	1.93	0.69
1:G:190:THR:O	1:G:193:ILE:HG13	1.93	0.69
1:G:243:LEU:HA	1:G:246:ASN:OD1	1.92	0.69
1:C:117:PHE:O	1:C:121:THR:HG23	1.92	0.68
1:B:129:GLU:OE2	1:B:278:SER:HB2	1.93	0.68
1:C:109:LEU:CD1	1:C:188:MET:HG3	2.22	0.68
1:E:238:TRP:HA	1:E:243:LEU:CD1	2.22	0.68
1:H:68:ILE:O	1:H:72:LEU:HD23	1.93	0.68
1:F:66:LEU:HD21	1:F:214:PHE:HD1	1.58	0.68
1:C:55:LEU:CD1	1:C:99:ILE:HD13	2.24	0.68
1:G:90:PRO:O	1:G:94:LEU:HD23	1.92	0.68
1:A:190:THR:O	1:A:193:ILE:HG13	1.94	0.68
1:E:58:GLN:HG2	1:E:259:GLY:HA2	1.74	0.68
1:F:121:THR:HA	1:F:124:LEU:CD2	2.24	0.68
1:A:71:ILE:HB	1:H:240:SER:HB3	1.74	0.68
1:C:213:ASP:O	1:C:214:PHE:HB2	1.94	0.68
1:A:213:ASP:O	1:A:214:PHE:HB2	1.94	0.68
1:A:232:SER:HA	1:A:236:GLU:OE1	1.94	0.68
1:B:121:THR:HG22	1:B:192:CYS:HB3	1.76	0.68
1:B:90:PRO:O	1:B:94:LEU:N	2.23	0.67
1:E:276:THR:OG1	1:E:280:THR:HB	1.93	0.67
1:B:188:MET:O	1:B:188:MET:HE2	1.95	0.67
1:D:50:MET:HA	1:D:236:GLU:HG2	1.77	0.67
1:D:90:PRO:O	1:D:94:LEU:HD23	1.94	0.67
1:D:290:LEU:HB2	1:D:291:PRO:HD3	1.76	0.67
1:B:118:LYS:HE2	1:B:191:ASN:OD1	1.92	0.67
1:D:328:LYS:O	1:D:332:ALA:N	2.27	0.67
1:G:258:SER:O	1:G:262:SER:OG	2.11	0.67
1:E:127:TYR:OH	3:E:402:OLC:O23	2.10	0.67
1:C:247:PHE:CD2	1:C:252:LEU:HD21	2.29	0.67
1:E:239:SER:H	1:E:243:LEU:HD12	1.60	0.67
1:E:71:ILE:HG13	1:E:72:LEU:CD2	2.24	0.67
1:G:65:THR:HA	1:G:68:ILE:HD12	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:GLY:HA3	1:D:77:PHE:CZ	2.30	0.67
1:D:233:PHE:HA	1:D:238:TRP:NE1	2.11	0.67
1:E:78:ARG:HA	1:E:215:ASP:OD1	1.95	0.67
1:F:213:ASP:O	1:F:214:PHE:HB2	1.94	0.67
1:F:233:PHE:HD1	1:F:233:PHE:O	1.77	0.67
1:G:222:VAL:HA	1:G:225:LEU:HD12	1.76	0.67
1:A:289:LYS:H	1:A:289:LYS:HD2	1.59	0.66
1:B:71:ILE:HG13	1:B:72:LEU:CD2	2.25	0.66
1:B:205:ARG:O	1:B:209:THR:OG1	2.12	0.66
1:A:124:LEU:O	1:A:128:GLY:N	2.29	0.66
1:B:223:LEU:O	1:B:226:PRO:HD2	1.94	0.66
1:D:237:ASP:O	1:D:243:LEU:HD13	1.94	0.66
1:A:50:MET:HB3	1:A:236:GLU:OE2	1.95	0.66
1:C:237:ASP:O	1:C:243:LEU:HD11	1.94	0.66
1:E:247:PHE:HD2	1:E:252:LEU:HD21	1.58	0.66
1:B:121:THR:HA	1:B:124:LEU:CD2	2.25	0.66
1:D:296:GLY:O	1:D:300:PHE:HB2	1.95	0.66
1:G:221:ASN:O	1:G:225:LEU:HG	1.95	0.66
1:B:68:ILE:O	1:B:72:LEU:HD23	1.96	0.66
1:D:223:LEU:O	1:D:226:PRO:HD2	1.95	0.66
1:E:114:TYR:OH	1:E:118:LYS:HE3	1.96	0.66
1:B:204:LYS:HE3	1:B:208:LEU:CD1	2.24	0.66
1:D:68:ILE:O	1:D:72:LEU:HD23	1.95	0.66
1:E:124:LEU:HD11	1:E:196:ALA:HB2	1.76	0.66
1:B:67:ILE:HG12	1:B:78:ARG:NH2	2.08	0.66
1:C:308:SER:O	1:C:311:SER:OG	2.14	0.66
1:D:124:LEU:CD1	1:D:196:ALA:HB2	2.26	0.66
1:E:71:ILE:HG13	1:E:72:LEU:HD22	1.79	0.66
1:E:70:ARG:HD2	1:E:78:ARG:HH21	1.61	0.65
1:G:98:MET:HG3	1:G:195:SER:OG	1.95	0.65
1:D:130:VAL:HG13	1:D:135:GLY:O	1.96	0.65
1:F:115:THR:HG22	1:F:119:ASN:OD1	1.94	0.65
1:C:38:THR:HG23	1:C:42:VAL:HG21	1.79	0.65
1:C:276:THR:OG1	1:C:277:SER:N	2.29	0.65
1:F:223:LEU:O	1:F:226:PRO:HD2	1.96	0.65
1:C:37:VAL:HG13	1:C:41:PHE:HD2	1.60	0.65
1:A:296:GLY:O	1:A:300:PHE:HB2	1.97	0.65
1:A:290:LEU:O	1:A:294:LEU:N	2.22	0.65
1:D:213:ASP:O	1:D:214:PHE:HB2	1.97	0.65
1:G:213:ASP:O	1:G:214:PHE:HB2	1.95	0.65
1:A:243:LEU:HA	1:A:246:ASN:OD1	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:VAL:O	1:E:153:VAL:HG23	1.96	0.65
1:B:239:SER:N	1:B:243:LEU:HD12	2.11	0.65
1:C:218:PHE:CZ	1:C:222:VAL:HG21	2.31	0.65
1:F:58:GLN:HG2	1:F:259:GLY:HA2	1.79	0.64
1:A:229:LEU:HA	1:A:232:SER:OG	1.97	0.64
1:C:213:ASP:OD1	1:C:274:ARG:NE	2.30	0.64
1:C:28:TYR:HE2	1:C:285:GLY:HA2	1.62	0.64
1:D:239:SER:N	1:D:243:LEU:HD12	2.12	0.64
1:E:190:THR:O	1:E:193:ILE:HG13	1.95	0.64
1:G:88:TRP:HA	1:G:91:ILE:HD13	1.78	0.64
1:H:213:ASP:O	1:H:214:PHE:HB2	1.97	0.64
1:B:46:LYS:HE2	1:B:258:SER:HB2	1.78	0.64
1:A:121:THR:HA	1:A:124:LEU:CD2	2.16	0.64
1:A:188:MET:O	1:A:188:MET:HE2	1.97	0.64
1:D:109:LEU:HD13	1:D:188:MET:HG3	1.78	0.64
1:E:29:CYS:HA	1:E:288:ASN:HD21	1.62	0.64
1:G:46:LYS:HE3	1:G:54:MET:SD	2.37	0.64
1:H:205:ARG:O	1:H:209:THR:OG1	2.11	0.64
1:A:70:ARG:HD2	1:A:78:ARG:NE	2.12	0.64
1:E:68:ILE:O	1:E:72:LEU:HD23	1.98	0.64
1:F:229:LEU:O	1:F:232:SER:OG	2.14	0.64
1:B:151:SER:O	1:B:311:SER:HB2	1.97	0.64
1:F:58:GLN:HG2	1:F:259:GLY:CA	2.28	0.64
1:C:232:SER:HA	1:C:236:GLU:OE1	1.97	0.64
1:H:71:ILE:HG13	1:H:72:LEU:CD2	2.28	0.64
1:B:50:MET:HG2	1:B:236:GLU:HG2	1.80	0.64
1:G:64:ILE:O	1:G:68:ILE:HG13	1.98	0.64
1:C:222:VAL:HA	1:C:225:LEU:HD12	1.80	0.63
1:E:88:TRP:NE1	1:E:220:ASN:OD1	2.30	0.63
1:F:205:ARG:O	1:F:209:THR:OG1	2.13	0.63
1:H:149:VAL:O	1:H:153:VAL:HG23	1.98	0.63
1:C:70:ARG:HD2	1:C:78:ARG:HE	1.64	0.63
1:C:71:ILE:HG13	1:C:72:LEU:CD2	2.28	0.63
1:E:67:ILE:HA	1:E:78:ARG:NH2	2.12	0.63
1:H:71:ILE:HG13	1:H:72:LEU:HD22	1.80	0.63
1:A:113:ILE:HA	1:A:116:ILE:HD12	1.81	0.63
1:A:124:LEU:H	1:A:124:LEU:HD23	1.63	0.63
1:A:304:ARG:H	1:A:304:ARG:HD3	1.64	0.63
1:C:85:ALA:HA	1:C:219:TYR:HE2	1.62	0.63
1:D:43:VAL:CG1	1:D:46:LYS:HD3	2.28	0.63
1:E:213:ASP:O	1:E:214:PHE:HB2	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:O	1:A:311:SER:HB2	1.99	0.63
1:B:67:ILE:CG1	1:B:78:ARG:HH22	2.06	0.63
1:E:313:PHE:HA	1:E:316:PHE:HB2	1.81	0.63
1:B:213:ASP:O	1:B:214:PHE:HB2	1.99	0.62
1:G:129:GLU:OE1	1:G:277:SER:HB2	1.99	0.62
1:C:124:LEU:O	1:C:128:GLY:N	2.32	0.62
1:D:70:ARG:HD2	1:D:78:ARG:NH2	2.13	0.62
1:G:151:SER:HB2	1:G:314:ILE:HG22	1.81	0.62
1:D:109:LEU:CD1	1:D:188:MET:HG3	2.28	0.62
1:G:310:LEU:HD22	1:G:314:ILE:CD1	2.29	0.62
1:A:53:VAL:HG12	1:A:255:MET:CE	2.29	0.62
1:F:117:PHE:O	1:F:121:THR:HG23	1.99	0.62
1:D:256:ILE:O	1:D:260:VAL:HG23	1.99	0.62
1:D:276:THR:OG1	1:D:277:SER:N	2.32	0.62
1:F:93:PHE:HA	1:F:227:ILE:HD13	1.80	0.62
1:H:25:ILE:HG23	1:H:284:VAL:HG21	1.81	0.62
1:E:312:ILE:O	1:E:316:PHE:N	2.28	0.62
1:D:85:ALA:HA	1:D:219:TYR:HE2	1.65	0.62
1:A:187:TRP:O	1:A:190:THR:OG1	2.12	0.61
1:A:121:THR:HG22	1:A:192:CYS:CB	2.30	0.61
1:A:223:LEU:O	1:A:226:PRO:HD2	1.99	0.61
1:D:103:SER:O	1:D:107:GLN:HG3	1.98	0.61
1:A:204:LYS:HG3	1:A:208:LEU:CD1	2.30	0.61
1:B:150:LEU:O	1:B:154:VAL:N	2.21	0.61
1:B:70:ARG:HD2	1:B:78:ARG:NH2	2.11	0.61
1:D:66:LEU:HD21	1:D:214:PHE:HD1	1.65	0.61
1:E:145:PHE:O	1:E:149:VAL:HG23	1.99	0.61
1:F:206:ILE:HG12	1:F:216:THR:HG22	1.81	0.61
1:F:276:THR:OG1	1:F:277:SER:N	2.33	0.61
1:G:193:ILE:O	1:G:197:LEU:HG	2.01	0.61
1:G:253:THR:HG22	1:G:257:ILE:HD12	1.82	0.61
1:A:38:THR:HG23	1:A:42:VAL:CG2	2.30	0.61
1:B:25:ILE:HG23	1:B:284:VAL:CG1	2.29	0.61
1:D:114:TYR:CE2	1:D:118:LYS:HG3	2.36	0.61
1:G:239:SER:N	1:G:243:LEU:HD12	2.16	0.61
1:E:253:THR:HG22	1:E:257:ILE:CD1	2.31	0.61
1:G:37:VAL:HG13	1:G:41:PHE:CD2	2.35	0.61
1:H:307:LEU:HD22	1:H:307:LEU:H	1.66	0.61
3:C:402:OLC:C9	1:E:310:LEU:HD11	2.31	0.61
1:H:124:LEU:O	1:H:128:GLY:N	2.33	0.61
1:G:223:LEU:O	1:G:226:PRO:HD2	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ARG:HD2	1:C:78:ARG:NH2	2.16	0.60
1:A:289:LYS:N	1:A:289:LYS:HD2	2.15	0.60
1:C:206:ILE:HG12	1:C:216:THR:HG22	1.84	0.60
1:A:155:ALA:HB2	1:A:311:SER:HB2	1.83	0.60
1:A:50:MET:HA	1:A:236:GLU:HG2	1.82	0.60
1:D:204:LYS:HE3	1:D:208:LEU:CD1	2.19	0.60
1:D:48:PHE:HZ	1:D:247:PHE:HB3	1.66	0.60
1:G:55:LEU:CD1	1:G:99:ILE:HD13	2.31	0.60
1:A:109:LEU:CD1	1:A:188:MET:HG3	2.32	0.60
1:B:149:VAL:O	1:B:153:VAL:HG23	2.00	0.60
1:H:35:MET:SD	1:H:265:ILE:HG12	2.42	0.60
1:D:186:PHE:O	1:D:190:THR:HG23	2.02	0.60
1:G:202:MET:CE	1:G:273:VAL:HG21	2.31	0.60
1:G:204:LYS:HE3	1:G:208:LEU:CD1	2.20	0.60
1:G:276:THR:OG1	1:G:277:SER:N	2.33	0.60
1:F:333:GLN:HG2	1:G:45:LEU:CD1	2.32	0.60
1:A:129:GLU:OE2	1:A:278:SER:HB2	2.02	0.60
1:D:105:ALA:HB1	1:D:188:MET:HG2	1.84	0.60
1:F:118:LYS:HE2	1:F:191:ASN:OD1	2.01	0.60
1:C:57:VAL:HG13	1:C:61:VAL:HG23	1.84	0.59
1:F:240:SER:HA	1:F:244:THR:OG1	2.01	0.59
1:E:43:VAL:HG11	1:E:254:ALA:HB1	1.84	0.59
1:C:71:ILE:O	1:C:72:LEU:HD22	2.02	0.59
1:G:124:LEU:O	1:G:128:GLY:N	2.35	0.59
1:C:247:PHE:HA	1:C:251:SER:OG	2.02	0.59
1:C:259:GLY:O	1:C:263:VAL:HG23	2.02	0.59
1:D:115:THR:O	1:D:119:ASN:N	2.35	0.59
1:F:34:LEU:O	1:F:38:THR:OG1	2.12	0.59
1:G:188:MET:CE	1:G:191:ASN:HB3	2.32	0.59
1:B:308:SER:O	1:B:311:SER:OG	2.20	0.59
1:D:121:THR:HG21	1:D:192:CYS:HA	1.84	0.59
1:G:126:ALA:HB2	1:G:279:THR:HG21	1.84	0.59
1:B:46:LYS:HE2	1:B:258:SER:CB	2.33	0.59
1:D:307:LEU:H	1:D:307:LEU:HD22	1.67	0.59
1:F:221:ASN:O	1:F:225:LEU:HG	2.02	0.59
1:G:222:VAL:HA	1:G:225:LEU:CD1	2.32	0.59
1:A:43:VAL:CG1	1:A:46:LYS:HD3	2.31	0.59
1:C:229:LEU:HA	1:C:232:SER:OG	2.02	0.59
1:D:204:LYS:HG3	1:D:208:LEU:HD12	1.85	0.59
1:E:317:LEU:O	1:E:321:ILE:HG12	2.03	0.59
1:E:35:MET:O	1:E:39:ASN:ND2	2.34	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:LYS:HE3	1:E:54:MET:SD	2.42	0.59
1:E:66:LEU:HB3	1:E:78:ARG:NH1	2.18	0.59
1:B:188:MET:CE	1:B:191:ASN:HB3	2.33	0.59
1:C:227:ILE:HA	1:C:230:LEU:HD12	1.83	0.59
1:C:307:LEU:H	1:C:307:LEU:HD22	1.66	0.59
1:C:24:SER:HB2	1:C:272:CYS:HA	1.85	0.59
1:G:113:ILE:HG23	1:G:116:ILE:HD12	1.85	0.59
1:H:110:ALA:HB1	1:H:161:GLN:C	2.23	0.58
1:E:67:ILE:HG12	1:E:78:ARG:HH22	1.68	0.58
1:A:70:ARG:CD	1:A:78:ARG:HE	2.17	0.58
1:C:188:MET:CE	1:C:191:ASN:HB3	2.33	0.58
1:A:240:SER:HA	1:A:244:THR:OG1	2.04	0.58
1:B:71:ILE:HG13	1:B:72:LEU:HD22	1.85	0.58
1:D:308:SER:O	1:D:311:SER:OG	2.20	0.58
1:F:71:ILE:HG13	1:F:72:LEU:CD2	2.34	0.58
1:A:58:GLN:HE21	1:A:262:SER:HB3	1.67	0.58
1:D:73:GLY:HA3	1:D:77:PHE:HZ	1.67	0.58
1:G:225:LEU:HB2	1:G:226:PRO:HD3	1.86	0.58
1:A:119:ASN:HA	1:A:122:ILE:CD1	2.34	0.58
1:F:188:MET:HE3	1:F:191:ASN:HB3	1.86	0.58
1:G:204:LYS:HG3	1:G:208:LEU:CD1	2.34	0.58
1:H:104:LYS:HD2	1:H:107:GLN:OE1	2.04	0.58
1:A:58:GLN:HE21	1:A:262:SER:CB	2.16	0.58
1:C:150:LEU:O	1:C:154:VAL:HG23	2.03	0.58
1:E:311:SER:O	1:E:315:GLY:N	2.29	0.58
1:B:307:LEU:H	1:B:307:LEU:HD22	1.67	0.58
1:F:29:CYS:CA	1:F:288:ASN:HD21	2.17	0.58
1:G:19:ASN:O	1:G:19:ASN:ND2	2.35	0.58
1:A:85:ALA:HA	1:A:219:TYR:HE2	1.68	0.58
1:B:124:LEU:HD11	1:B:196:ALA:HB2	1.83	0.58
1:C:70:ARG:HB2	1:C:78:ARG:CZ	2.34	0.58
1:G:239:SER:H	1:G:243:LEU:HD12	1.68	0.58
1:G:307:LEU:HD22	1:G:307:LEU:H	1.68	0.57
1:F:333:GLN:HA	1:G:44:ASN:ND2	2.18	0.57
1:E:225:LEU:HB2	1:E:226:PRO:HD3	1.85	0.57
1:D:233:PHE:HA	1:D:238:TRP:HE1	1.69	0.57
1:D:276:THR:OG1	1:D:280:THR:HB	2.05	0.57
1:F:151:SER:O	1:F:311:SER:HB2	2.05	0.57
1:H:132:PHE:CE2	1:H:200:LEU:HD13	2.38	0.57
1:A:31:SER:HB2	1:A:265:ILE:HG23	1.85	0.57
1:D:115:THR:HG22	1:D:119:ASN:OD1	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:ASN:HD21	1:E:286:ALA:HB1	1.69	0.57
1:E:229:LEU:HA	1:E:232:SER:OG	2.04	0.57
1:F:88:TRP:HA	1:F:91:ILE:HD13	1.86	0.57
1:H:296:GLY:O	1:H:300:PHE:HB2	2.05	0.57
1:A:307:LEU:HD22	1:A:307:LEU:H	1.69	0.57
1:C:71:ILE:HG13	1:C:72:LEU:HD22	1.87	0.57
1:C:113:ILE:HA	1:C:116:ILE:CD1	2.35	0.57
1:C:92:SER:HB3	1:C:227:ILE:HD12	1.87	0.57
1:E:202:MET:O	1:E:206:ILE:HG13	2.05	0.57
1:E:81:ASN:N	1:E:219:TYR:OH	2.37	0.57
1:F:56:PHE:CE1	1:F:229:LEU:HG	2.40	0.57
1:A:204:LYS:HE3	1:A:208:LEU:CD1	2.32	0.57
1:B:239:SER:H	1:B:243:LEU:HD12	1.69	0.57
1:A:119:ASN:HD22	1:A:122:ILE:CD1	2.17	0.57
1:B:227:ILE:CA	1:B:230:LEU:HD12	2.19	0.56
1:E:304:ARG:HG3	1:E:309:ILE:HD11	1.87	0.56
1:F:142:LEU:HD13	1:F:142:LEU:O	2.05	0.56
1:C:57:VAL:CG1	1:C:61:VAL:HG23	2.35	0.56
1:F:46:LYS:NZ	1:F:54:MET:SD	2.71	0.56
1:B:202:MET:CE	1:B:273:VAL:HG21	2.35	0.56
1:F:43:VAL:HG11	1:F:254:ALA:HB1	1.86	0.56
1:H:112:PRO:O	1:H:116:ILE:HG13	2.06	0.56
1:A:276:THR:OG1	1:A:277:SER:N	2.38	0.56
1:A:46:LYS:HE3	1:A:54:MET:SD	2.46	0.56
1:B:182:ASN:N	1:B:183:PRO:HD2	2.20	0.56
1:C:190:THR:O	1:C:193:ILE:HG13	2.05	0.56
1:C:35:MET:SD	1:C:265:ILE:HG12	2.45	0.56
1:F:67:ILE:CG1	1:F:78:ARG:HH22	2.12	0.56
1:B:190:THR:O	1:B:193:ILE:HG13	2.05	0.56
1:D:247:PHE:HA	1:D:251:SER:OG	2.05	0.56
1:B:244:THR:HA	1:B:247:PHE:CE1	2.40	0.56
1:F:182:ASN:N	1:F:183:PRO:HD2	2.21	0.56
1:F:102:SER:HB2	1:F:191:ASN:ND2	2.21	0.56
1:G:100:TYR:HE1	1:G:235:VAL:HG11	1.71	0.56
1:D:188:MET:HE3	1:D:188:MET:HA	1.87	0.56
1:E:193:ILE:O	1:E:197:LEU:HG	2.06	0.56
1:G:232:SER:HA	1:G:236:GLU:OE1	2.06	0.56
1:A:114:TYR:CE2	1:A:118:LYS:HG3	2.40	0.56
1:A:121:THR:CA	1:A:124:LEU:HD21	2.19	0.56
1:B:151:SER:HB2	1:B:314:ILE:HG22	1.88	0.56
1:C:71:ILE:C	1:C:72:LEU:HD22	2.26	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:ASN:ND2	1:F:286:ALA:HB1	2.20	0.56
1:G:233:PHE:O	1:G:233:PHE:HD1	1.89	0.56
1:H:81:ASN:N	1:H:219:TYR:OH	2.38	0.55
1:C:70:ARG:CD	1:C:78:ARG:HE	2.19	0.55
1:F:130:VAL:HG22	1:F:135:GLY:O	2.06	0.55
1:A:70:ARG:HD2	1:A:78:ARG:CZ	2.36	0.55
1:C:62:CYS:SG	1:C:263:VAL:HA	2.46	0.55
1:F:29:CYS:HA	1:F:288:ASN:ND2	2.20	0.55
1:G:204:LYS:HG3	1:G:208:LEU:HD12	1.89	0.55
1:H:121:THR:O	1:H:124:LEU:HG	2.06	0.55
1:H:93:PHE:CA	1:H:227:ILE:HD13	2.37	0.55
1:H:253:THR:HG22	1:H:257:ILE:CD1	2.36	0.55
1:A:188:MET:CE	1:A:191:ASN:HB3	2.35	0.55
1:B:71:ILE:O	1:B:72:LEU:HD22	2.07	0.55
1:E:147:LEU:HD23	1:E:150:LEU:HD12	1.87	0.55
1:B:202:MET:HG2	1:B:206:ILE:CD1	2.36	0.55
1:E:142:LEU:HD13	1:E:146:LEU:HG	1.87	0.55
1:F:332:ALA:O	1:G:44:ASN:ND2	2.39	0.55
1:A:43:VAL:CG1	1:A:254:ALA:HB1	2.37	0.55
1:A:155:ALA:N	1:A:311:SER:HB3	2.21	0.55
1:C:90:PRO:O	1:C:94:LEU:HD23	2.06	0.55
1:F:188:MET:CE	1:F:191:ASN:HB3	2.36	0.55
1:B:193:ILE:O	1:B:197:LEU:HG	2.07	0.55
1:C:253:THR:O	1:C:257:ILE:HG13	2.06	0.55
1:C:202:MET:CE	1:C:273:VAL:HG21	2.37	0.55
1:D:109:LEU:HG	1:D:184:GLY:HA3	1.88	0.55
1:E:206:ILE:HG12	1:E:216:THR:HG22	1.87	0.55
1:B:227:ILE:O	1:B:230:LEU:HB2	2.07	0.55
1:E:90:PRO:O	1:E:94:LEU:HD23	2.07	0.55
1:C:270:GLY:HA2	1:C:273:VAL:CG2	2.37	0.55
1:D:212:LYS:O	1:D:215:ASP:HB2	2.07	0.55
1:E:112:PRO:HB2	1:E:156:THR:OG1	2.06	0.55
1:G:150:LEU:O	1:G:154:VAL:HG23	2.07	0.55
1:B:233:PHE:HD1	1:B:233:PHE:O	1.89	0.55
1:G:202:MET:O	1:G:206:ILE:HG13	2.06	0.55
1:G:25:ILE:HG23	1:G:284:VAL:HG11	1.89	0.55
1:A:204:LYS:HG3	1:A:208:LEU:HD12	1.87	0.54
1:B:138:THR:HG22	1:B:140:MET:H	1.72	0.54
1:C:221:ASN:O	1:C:225:LEU:HG	2.07	0.54
1:D:98:MET:HG3	1:D:195:SER:OG	2.07	0.54
1:A:308:SER:O	1:A:311:SER:OG	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:GLY:O	1:B:300:PHE:HB2	2.06	0.54
1:C:57:VAL:O	1:C:61:VAL:N	2.31	0.54
1:F:307:LEU:H	1:F:307:LEU:HD22	1.72	0.54
1:A:130:VAL:HG22	1:A:135:GLY:O	2.06	0.54
1:A:35:MET:O	1:A:39:ASN:ND2	2.30	0.54
1:E:93:PHE:CA	1:E:227:ILE:HD13	2.37	0.54
1:H:243:LEU:HD23	1:H:246:ASN:OD1	2.07	0.54
1:B:208:LEU:O	1:F:83:THR:OG1	2.16	0.54
1:D:148:MET:O	1:D:152:SER:OG	2.25	0.54
3:D:402:OLC:O23	3:D:402:OLC:O19	2.22	0.54
1:E:67:ILE:HA	1:E:78:ARG:HH22	1.72	0.54
1:F:110:ALA:HB1	1:F:161:GLN:C	2.28	0.54
1:H:247:PHE:HB2	1:H:251:SER:OG	2.07	0.54
1:C:238:TRP:HA	1:C:243:LEU:HD12	1.89	0.54
1:G:202:MET:HE2	1:G:273:VAL:HG21	1.89	0.54
1:G:37:VAL:HG13	1:G:41:PHE:HD2	1.70	0.54
1:B:35:MET:HG2	1:B:39:ASN:ND2	2.22	0.54
1:D:218:PHE:CZ	1:D:222:VAL:HG21	2.43	0.54
1:E:52:PHE:HZ	1:E:100:TYR:HD1	1.55	0.54
1:E:270:GLY:HA2	1:E:273:VAL:HG22	1.89	0.54
1:E:56:PHE:CE1	1:E:229:LEU:HG	2.43	0.54
1:F:39:ASN:OD1	1:F:46:LYS:HE2	2.08	0.54
1:C:202:MET:HG2	1:C:206:ILE:CD1	2.38	0.54
1:F:25:ILE:HG23	1:F:284:VAL:HG21	1.89	0.54
1:A:253:THR:HG22	1:A:257:ILE:CD1	2.38	0.54
1:A:94:LEU:HB3	1:A:198:PHE:HB2	1.90	0.54
1:B:276:THR:OG1	1:B:277:SER:N	2.38	0.54
1:C:93:PHE:O	1:C:97:LEU:HB2	2.08	0.54
1:E:61:VAL:HG21	1:E:256:ILE:HG23	1.89	0.54
1:A:114:TYR:OH	1:A:118:LYS:HE3	2.08	0.53
1:A:121:THR:HG22	1:A:192:CYS:HB3	1.90	0.53
1:A:32:SER:O	1:A:36:THR:OG1	2.19	0.53
1:C:35:MET:HG2	1:C:39:ASN:ND2	2.23	0.53
1:G:144:SER:HB3	1:G:322:TYR:HB2	1.90	0.53
1:G:48:PHE:CZ	1:G:247:PHE:HB3	2.39	0.53
1:B:202:MET:O	1:B:206:ILE:HG13	2.07	0.53
1:B:290:LEU:HB2	1:B:291:PRO:CD	2.37	0.53
1:F:203:ARG:CZ	1:F:207:LYS:HD2	2.38	0.53
1:F:271:TRP:O	1:F:275:VAL:HG22	2.07	0.53
1:H:215:ASP:OD1	1:H:215:ASP:N	2.40	0.53
1:H:52:PHE:CE2	1:H:231:PHE:HB3	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:HG22	1:A:140:MET:H	1.73	0.53
1:B:254:ALA:HA	1:B:257:ILE:HD12	1.89	0.53
1:H:270:GLY:HA2	1:H:273:VAL:CG2	2.39	0.53
1:D:25:ILE:HG23	1:D:284:VAL:HG21	1.90	0.53
1:G:279:THR:O	1:G:283:MET:N	2.40	0.53
1:D:121:THR:HG22	1:D:192:CYS:HB3	1.90	0.53
1:E:91:ILE:O	1:E:95:LEU:N	2.41	0.53
1:F:290:LEU:HD22	1:F:312:ILE:HA	1.90	0.53
1:G:121:THR:HG22	1:G:192:CYS:CB	2.38	0.53
1:B:66:LEU:CD2	1:B:214:PHE:HD1	2.21	0.53
1:C:187:TRP:O	1:C:190:THR:OG1	2.16	0.53
1:A:46:LYS:NZ	1:A:255:MET:HG3	2.24	0.53
1:B:256:ILE:O	1:B:260:VAL:HG23	2.09	0.53
1:D:25:ILE:HG23	1:D:284:VAL:HG11	1.91	0.53
1:D:35:MET:HG2	1:D:39:ASN:ND2	2.23	0.53
1:E:121:THR:O	1:E:124:LEU:HG	2.09	0.53
1:E:93:PHE:HA	1:E:227:ILE:HD13	1.91	0.53
1:D:121:THR:HG22	1:D:192:CYS:CB	2.38	0.53
1:E:276:THR:OG1	1:E:277:SER:N	2.35	0.53
1:F:202:MET:SD	1:F:220:ASN:ND2	2.81	0.53
1:F:52:PHE:O	1:F:56:PHE:N	2.38	0.53
1:G:204:LYS:CE	1:G:208:LEU:HD11	2.20	0.53
1:A:212:LYS:O	1:A:215:ASP:HB2	2.10	0.52
1:D:46:LYS:NZ	1:D:255:MET:HG3	2.24	0.52
1:G:256:ILE:O	1:G:260:VAL:HG23	2.07	0.52
1:B:227:ILE:HA	1:B:230:LEU:CD1	2.20	0.52
1:C:133:PHE:HZ	1:C:203:ARG:HG3	1.75	0.52
1:C:98:MET:HG3	1:C:195:SER:OG	2.09	0.52
1:D:119:ASN:HD22	1:D:122:ILE:CD1	2.20	0.52
1:D:204:LYS:HG3	1:D:208:LEU:CD1	2.39	0.52
1:E:119:ASN:HA	1:E:122:ILE:CD1	2.39	0.52
1:G:212:LYS:O	1:G:215:ASP:HB2	2.10	0.52
1:G:87:ASN:HB3	1:G:205:ARG:CZ	2.39	0.52
1:H:317:LEU:O	1:H:321:ILE:HG12	2.08	0.52
1:A:221:ASN:O	1:A:225:LEU:HG	2.09	0.52
1:C:56:PHE:CE1	1:C:225:LEU:HB3	2.44	0.52
1:D:262:SER:O	1:D:265:ILE:HG13	2.08	0.52
1:E:253:THR:HG22	1:E:257:ILE:HD11	1.92	0.52
1:G:121:THR:HG22	1:G:192:CYS:HB3	1.90	0.52
1:G:269:SER:O	1:G:273:VAL:HG22	2.09	0.52
1:H:114:TYR:O	1:H:118:LYS:HB2	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:PHE:CZ	1:B:247:PHE:HB3	2.38	0.52
1:H:100:TYR:CE1	1:H:235:VAL:HG21	2.45	0.52
1:H:276:THR:OG1	1:H:277:SER:N	2.42	0.52
1:A:35:MET:HG2	1:A:39:ASN:ND2	2.25	0.52
1:B:43:VAL:HG11	1:B:254:ALA:HB1	1.90	0.52
1:B:151:SER:OG	1:B:311:SER:O	2.20	0.52
1:E:154:VAL:HB	1:E:311:SER:HB3	1.91	0.52
1:G:253:THR:HG22	1:G:257:ILE:HD11	1.92	0.52
1:B:240:SER:HA	1:B:244:THR:OG1	2.10	0.52
1:E:58:GLN:HG2	1:E:259:GLY:CA	2.38	0.52
1:H:93:PHE:HA	1:H:227:ILE:HD13	1.92	0.52
1:A:206:ILE:HG12	1:A:216:THR:HG22	1.90	0.52
1:D:150:LEU:O	1:D:154:VAL:HG23	2.09	0.52
1:E:100:TYR:HE1	1:E:235:VAL:HG11	1.73	0.52
1:G:66:LEU:HD21	1:G:214:PHE:HD1	1.74	0.52
1:E:275:VAL:HG23	1:E:276:THR:N	2.25	0.52
1:E:289:LYS:N	1:E:289:LYS:CD	2.72	0.52
1:H:142:LEU:HD13	1:H:142:LEU:O	2.10	0.52
1:D:94:LEU:HB3	1:D:198:PHE:HB2	1.92	0.52
1:E:138:THR:HG22	1:E:140:MET:H	1.74	0.52
1:E:214:PHE:HA	1:E:217:MET:HB3	1.92	0.52
1:H:114:TYR:OH	1:H:118:LYS:HE3	2.09	0.52
1:A:115:THR:O	1:A:119:ASN:N	2.41	0.52
1:A:127:TYR:OH	1:A:142:LEU:HD22	2.10	0.52
1:B:25:ILE:HG12	1:B:284:VAL:HG21	1.91	0.52
1:B:288:ASN:O	1:B:291:PRO:HD2	2.10	0.52
1:B:332:ALA:O	1:C:45:LEU:HD12	2.10	0.52
1:E:142:LEU:O	1:E:142:LEU:HD13	2.10	0.52
1:F:53:VAL:HG12	1:F:255:MET:CE	2.40	0.52
1:F:71:ILE:HG13	1:F:72:LEU:HD22	1.91	0.52
1:A:259:GLY:O	1:A:263:VAL:HG23	2.10	0.51
1:A:71:ILE:C	1:A:72:LEU:HD22	2.30	0.51
1:B:179:ALA:O	1:B:183:PRO:HD3	2.10	0.51
1:B:124:LEU:CD1	1:B:196:ALA:HB2	2.39	0.51
1:C:56:PHE:HA	1:C:228:LEU:CD1	2.40	0.51
1:G:202:MET:HG2	1:G:206:ILE:CD1	2.40	0.51
1:H:270:GLY:HA2	1:H:273:VAL:HG22	1.92	0.51
1:B:71:ILE:C	1:B:72:LEU:HD22	2.30	0.51
1:G:222:VAL:O	1:G:226:PRO:HD3	2.10	0.51
1:A:67:ILE:HG12	1:A:78:ARG:HH12	1.75	0.51
1:C:188:MET:HE3	1:C:191:ASN:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:LEU:HD21	1:D:114:TYR:CG	2.44	0.51
1:D:290:LEU:CD1	1:D:315:GLY:HA3	2.40	0.51
1:F:333:GLN:HG2	1:G:45:LEU:HD13	1.90	0.51
1:C:254:ALA:HA	1:C:257:ILE:HD12	1.92	0.51
1:D:182:ASN:N	1:D:183:PRO:HD2	2.26	0.51
1:D:204:LYS:CE	1:D:208:LEU:HD11	2.20	0.51
1:H:57:VAL:HA	1:H:60:LEU:HB3	1.93	0.51
1:C:101:THR:O	1:C:105:ALA:N	2.40	0.51
1:C:120:LEU:HD23	1:C:123:ILE:HD12	1.91	0.51
1:C:118:LYS:O	1:C:121:THR:OG1	2.24	0.51
1:E:193:ILE:HD12	1:E:197:LEU:HD12	1.92	0.51
1:F:227:ILE:CA	1:F:230:LEU:HD12	2.31	0.51
1:A:186:PHE:O	1:A:190:THR:HG23	2.11	0.51
1:A:202:MET:O	1:A:206:ILE:HG13	2.10	0.51
1:C:269:SER:O	1:C:273:VAL:HG22	2.10	0.51
1:H:32:SER:O	1:H:36:THR:OG1	2.23	0.51
1:A:182:ASN:N	1:A:183:PRO:HD2	2.25	0.51
1:A:213:ASP:OD1	1:A:274:ARG:NE	2.42	0.51
1:D:181:PHE:C	1:D:183:PRO:HD2	2.31	0.51
1:F:253:THR:HG22	1:F:257:ILE:CD1	2.41	0.51
1:H:307:LEU:N	1:H:307:LEU:HD22	2.26	0.51
1:B:180:SER:O	1:B:183:PRO:HG2	2.11	0.51
1:D:54:MET:HG2	1:D:58:GLN:OE1	2.11	0.51
1:F:214:PHE:HA	1:F:217:MET:HB3	1.92	0.51
1:F:284:VAL:HG12	1:F:288:ASN:OD1	2.11	0.51
1:G:202:MET:HG2	1:G:206:ILE:HD11	1.93	0.51
1:G:43:VAL:HG11	1:G:254:ALA:HB1	1.93	0.51
1:G:292:ILE:HG23	3:G:401:OLC:H8	1.93	0.51
1:G:35:MET:HG2	1:G:39:ASN:ND2	2.26	0.51
1:G:71:ILE:C	1:G:72:LEU:HD22	2.30	0.51
1:H:218:PHE:CE1	1:H:222:VAL:HG21	2.46	0.51
1:E:66:LEU:CD2	1:E:214:PHE:HD1	2.24	0.51
1:G:43:VAL:CG1	1:G:254:ALA:HB1	2.41	0.51
1:C:113:ILE:HA	1:C:116:ILE:HD12	1.93	0.51
1:B:116:ILE:HD11	1:B:156:THR:OG1	2.11	0.50
1:B:69:LEU:HB3	1:B:77:PHE:HE2	1.76	0.50
1:C:109:LEU:HG	1:C:184:GLY:HA3	1.94	0.50
1:D:225:LEU:HB2	1:D:226:PRO:HD3	1.93	0.50
1:D:43:VAL:HG13	1:D:254:ALA:HB1	1.93	0.50
1:G:25:ILE:HG12	1:G:284:VAL:HG21	1.93	0.50
1:H:253:THR:HG22	1:H:257:ILE:HD11	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:65:THR:HA	1:H:68:ILE:HD12	1.94	0.50
1:A:150:LEU:O	1:A:154:VAL:N	2.20	0.50
1:B:333:GLN:HG2	1:C:45:LEU:HB2	1.93	0.50
1:C:148:MET:O	1:C:152:SER:OG	2.22	0.50
1:C:239:SER:H	1:C:243:LEU:HD12	1.76	0.50
1:C:276:THR:OG1	1:C:280:THR:HB	2.11	0.50
1:C:63:THR:O	1:C:67:ILE:HG13	2.12	0.50
1:D:317:LEU:O	1:D:321:ILE:HG12	2.11	0.50
1:E:90:PRO:O	1:E:94:LEU:HB2	2.11	0.50
1:G:233:PHE:HA	1:G:238:TRP:NE1	2.27	0.50
1:G:31:SER:HB2	1:G:265:ILE:N	2.26	0.50
1:G:114:TYR:OH	1:G:118:LYS:HE3	2.10	0.50
1:G:124:LEU:HD23	1:G:124:LEU:H	1.75	0.50
1:H:271:TRP:O	1:H:275:VAL:HG22	2.11	0.50
1:A:145:PHE:O	1:A:149:VAL:HG23	2.11	0.50
1:C:133:PHE:CZ	1:C:203:ARG:HG3	2.47	0.50
1:D:66:LEU:HB3	1:D:78:ARG:NH1	2.27	0.50
1:E:271:TRP:O	1:E:275:VAL:HG22	2.12	0.50
1:H:27:SER:HB3	1:H:268:CYS:SG	2.51	0.50
1:H:151:SER:O	1:H:311:SER:HB2	2.12	0.50
1:A:149:VAL:O	1:A:153:VAL:HG23	2.12	0.50
1:A:225:LEU:HB2	1:A:226:PRO:HD3	1.94	0.50
1:B:43:VAL:CG1	1:B:254:ALA:HB1	2.42	0.50
1:E:121:THR:HG22	1:E:192:CYS:HB3	1.93	0.50
1:E:212:LYS:O	1:E:215:ASP:HB2	2.12	0.50
1:A:105:ALA:HB1	1:A:188:MET:HG2	1.94	0.50
1:D:119:ASN:HA	1:D:122:ILE:CD1	2.42	0.50
1:F:71:ILE:O	1:F:72:LEU:HD22	2.12	0.50
1:C:124:LEU:HD23	1:C:124:LEU:H	1.75	0.50
1:C:237:ASP:O	1:C:243:LEU:CD1	2.59	0.50
1:C:29:CYS:HA	1:C:288:ASN:OD1	2.12	0.50
1:D:43:VAL:CG1	1:D:254:ALA:HB1	2.41	0.50
1:E:182:ASN:N	1:E:183:PRO:HD2	2.26	0.50
1:F:202:MET:O	1:F:206:ILE:HG13	2.11	0.50
1:A:19:ASN:HA	1:A:271:TRP:CZ2	2.46	0.50
1:E:55:LEU:HA	1:E:58:GLN:HB2	1.94	0.50
1:F:121:THR:HG22	1:F:192:CYS:HB3	1.94	0.50
1:G:114:TYR:CE2	1:G:118:LYS:HG3	2.47	0.50
1:C:55:LEU:CD1	1:C:99:ILE:HG21	2.42	0.49
1:E:71:ILE:C	1:E:72:LEU:HD22	2.32	0.49
1:G:144:SER:CB	1:G:322:TYR:HB2	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:THR:HA	1:H:124:LEU:HD21	1.92	0.49
1:H:150:LEU:O	1:H:154:VAL:HG23	2.12	0.49
1:B:193:ILE:HD12	1:B:197:LEU:HD12	1.93	0.49
1:B:69:LEU:HB3	1:B:77:PHE:CE2	2.47	0.49
1:C:181:PHE:C	1:C:183:PRO:HD2	2.32	0.49
1:C:95:LEU:HD12	1:C:198:PHE:CE1	2.47	0.49
1:D:25:ILE:CG2	1:D:284:VAL:HG21	2.42	0.49
1:E:181:PHE:HD2	1:E:185:TYR:HE2	1.60	0.49
1:E:148:MET:HE1	1:E:318:SER:HB3	1.93	0.49
1:G:127:TYR:OH	1:G:142:LEU:HD23	2.12	0.49
1:C:138:THR:HG22	1:C:140:MET:H	1.77	0.49
1:D:142:LEU:O	1:D:142:LEU:HD13	2.13	0.49
1:G:199:VAL:O	1:G:278:SER:OG	2.08	0.49
1:H:91:ILE:O	1:H:95:LEU:N	2.43	0.49
1:A:271:TRP:O	1:A:275:VAL:HG22	2.12	0.49
1:A:31:SER:O	1:A:35:MET:N	2.34	0.49
1:D:126:ALA:HB2	1:D:279:THR:HG21	1.95	0.49
1:H:121:THR:HA	1:H:124:LEU:CD2	2.42	0.49
1:A:155:ALA:HB2	1:A:311:SER:OG	2.12	0.49
1:B:102:SER:O	1:B:106:LEU:HG	2.12	0.49
1:B:127:TYR:HA	1:B:130:VAL:HG23	1.94	0.49
1:C:59:SER:HB3	1:C:221:ASN:O	2.12	0.49
1:D:221:ASN:O	1:D:225:LEU:HG	2.12	0.49
1:F:288:ASN:O	1:F:291:PRO:HD2	2.13	0.49
1:F:68:ILE:O	1:F:72:LEU:HB2	2.12	0.49
1:H:113:ILE:HA	1:H:116:ILE:HD12	1.95	0.49
1:C:142:LEU:HD13	1:C:142:LEU:O	2.12	0.49
1:D:127:TYR:OH	1:D:142:LEU:HD23	2.12	0.49
1:E:104:LYS:HD2	1:E:107:GLN:OE1	2.13	0.49
1:G:28:TYR:HE2	1:G:285:GLY:HA2	1.77	0.49
1:A:71:ILE:O	1:A:72:LEU:HD22	2.12	0.49
1:B:59:SER:C	1:B:225:LEU:HD21	2.33	0.49
1:B:317:LEU:O	1:B:321:ILE:HG12	2.12	0.49
1:C:61:VAL:HG21	1:C:256:ILE:HG23	1.92	0.49
1:D:243:LEU:O	1:D:246:ASN:HB2	2.12	0.49
1:F:270:GLY:HA2	1:F:273:VAL:HG22	1.94	0.49
1:A:237:ASP:O	1:A:243:LEU:CD1	2.60	0.49
1:A:30:GLY:O	1:A:34:LEU:N	2.37	0.49
1:C:262:SER:O	1:C:265:ILE:HG13	2.12	0.49
1:C:29:CYS:O	1:C:33:ILE:N	2.37	0.49
1:C:320:ILE:O	1:C:324:VAL:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:MET:HA	1:C:236:GLU:HG2	1.93	0.49
1:F:68:ILE:O	1:F:72:LEU:HD23	2.12	0.49
1:H:109:LEU:CD1	1:H:188:MET:HG3	2.42	0.49
1:E:121:THR:HG21	1:E:192:CYS:HA	1.93	0.49
1:A:141:GLU:HB3	1:A:145:PHE:CZ	2.48	0.49
1:C:213:ASP:O	1:C:214:PHE:CB	2.61	0.49
1:H:237:ASP:O	1:H:243:LEU:CD1	2.60	0.49
1:A:113:ILE:HA	1:A:116:ILE:CD1	2.43	0.48
1:A:31:SER:HB2	1:A:265:ILE:N	2.28	0.48
1:A:67:ILE:HA	1:A:78:ARG:NH1	2.28	0.48
1:B:247:PHE:HA	1:B:251:SER:HG	1.78	0.48
1:B:58:GLN:HG2	1:B:259:GLY:HA2	1.95	0.48
1:C:182:ASN:N	1:C:183:PRO:HD2	2.27	0.48
1:F:132:PHE:CE2	1:F:200:LEU:HD13	2.48	0.48
1:F:146:LEU:O	1:F:149:VAL:HB	2.13	0.48
1:C:70:ARG:HB2	1:C:78:ARG:NE	2.28	0.48
1:D:149:VAL:O	1:D:153:VAL:HG23	2.12	0.48
1:F:43:VAL:CG1	1:F:254:ALA:HB1	2.43	0.48
1:F:27:SER:HB3	1:F:268:CYS:SG	2.53	0.48
1:G:109:LEU:CD1	1:G:188:MET:HG3	2.43	0.48
1:G:133:PHE:CZ	1:G:203:ARG:HG3	2.48	0.48
1:G:310:LEU:HD13	3:G:402:OLC:H18B	1.95	0.48
1:H:101:THR:O	1:H:105:ALA:N	2.35	0.48
1:A:290:LEU:HD11	1:A:315:GLY:HA3	1.95	0.48
1:B:229:LEU:O	1:B:232:SER:OG	2.25	0.48
1:B:202:MET:HE3	1:B:273:VAL:HG21	1.96	0.48
1:F:188:MET:O	1:F:188:MET:HE2	2.13	0.48
1:A:121:THR:HG21	1:A:192:CYS:HA	1.96	0.48
1:C:121:THR:HG22	1:C:192:CYS:SG	2.52	0.48
1:D:239:SER:OG	1:D:243:LEU:HG	2.13	0.48
1:E:111:VAL:N	1:E:112:PRO:HD2	2.28	0.48
1:F:275:VAL:HG23	1:F:276:THR:N	2.29	0.48
1:G:290:LEU:O	1:G:293:ALA:N	2.46	0.48
1:C:222:VAL:O	1:C:226:PRO:HD3	2.14	0.48
1:D:130:VAL:HG22	1:D:135:GLY:O	2.14	0.48
1:E:270:GLY:HA2	1:E:273:VAL:CG2	2.43	0.48
1:G:56:PHE:O	1:G:60:LEU:N	2.46	0.48
1:G:66:LEU:HB3	1:G:78:ARG:NH1	2.23	0.48
1:G:95:LEU:O	1:G:98:MET:HB3	2.13	0.48
1:H:119:ASN:HD21	1:H:286:ALA:HB1	1.78	0.48
1:D:121:THR:CG2	1:D:192:CYS:HA	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:LYS:N	1:E:289:LYS:HD3	2.29	0.48
1:F:81:ASN:HB2	1:F:219:TYR:OH	2.13	0.48
1:F:253:THR:HG22	1:F:257:ILE:HD11	1.96	0.48
1:G:114:TYR:CZ	1:G:118:LYS:HG3	2.49	0.48
1:A:197:LEU:O	1:A:201:ILE:HG13	2.14	0.48
1:C:228:LEU:O	1:C:232:SER:N	2.42	0.48
1:F:181:PHE:C	1:F:183:PRO:HD2	2.34	0.48
1:H:67:ILE:CG1	1:H:78:ARG:HH22	2.18	0.48
1:B:58:GLN:HG2	1:B:259:GLY:CA	2.43	0.48
1:C:130:VAL:O	1:C:134:GLY:HA2	2.14	0.48
1:G:148:MET:O	1:G:152:SER:OG	2.13	0.48
1:G:202:MET:HE3	1:G:273:VAL:HG21	1.96	0.48
1:H:111:VAL:N	1:H:112:PRO:HD2	2.29	0.48
1:B:46:LYS:HE3	1:B:54:MET:SD	2.54	0.48
1:C:106:LEU:HD21	1:C:114:TYR:CD2	2.49	0.48
1:D:275:VAL:HG23	1:D:276:THR:N	2.28	0.48
1:F:304:ARG:H	1:F:304:ARG:HD3	1.78	0.48
1:G:268:CYS:O	1:G:272:CYS:N	2.39	0.48
1:H:55:LEU:HA	1:H:58:GLN:HB2	1.96	0.48
1:A:296:GLY:HA2	1:A:300:PHE:HD2	1.79	0.48
1:B:273:VAL:HG13	1:B:281:TYR:CG	2.49	0.48
1:E:102:SER:HB2	1:E:191:ASN:ND2	2.28	0.48
1:E:202:MET:HG2	1:E:206:ILE:CD1	2.44	0.48
1:F:93:PHE:CA	1:F:227:ILE:HD13	2.43	0.48
1:C:50:MET:HB3	1:C:236:GLU:OE2	2.14	0.47
1:H:182:ASN:N	1:H:183:PRO:HD2	2.28	0.47
1:B:271:TRP:O	1:B:275:VAL:HG22	2.14	0.47
1:B:86:LYS:HD2	1:B:86:LYS:HA	1.65	0.47
1:B:90:PRO:O	1:B:94:LEU:HD23	2.14	0.47
1:C:296:GLY:O	1:C:300:PHE:HB2	2.13	0.47
1:D:27:SER:HB3	1:D:268:CYS:SG	2.54	0.47
1:F:19:ASN:HA	1:F:271:TRP:CZ2	2.48	0.47
1:F:296:GLY:O	1:F:300:PHE:HB2	2.14	0.47
1:H:214:PHE:O	1:H:218:PHE:N	2.24	0.47
1:C:113:ILE:HG23	1:C:116:ILE:HD12	1.96	0.47
1:C:151:SER:HB2	1:C:314:ILE:HG22	1.96	0.47
1:E:35:MET:CE	2:E:401:GDD:O2A	2.62	0.47
1:F:133:PHE:CZ	1:F:203:ARG:HG3	2.49	0.47
1:A:37:VAL:HG22	1:A:41:PHE:CE2	2.49	0.47
1:C:56:PHE:HA	1:C:228:LEU:HD13	1.95	0.47
1:F:188:MET:HA	1:F:188:MET:HE2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:275:VAL:HG23	1:G:276:THR:N	2.29	0.47
1:H:305:ASN:OD1	1:H:308:SER:OG	2.30	0.47
1:B:202:MET:HE1	1:B:273:VAL:HG21	1.97	0.47
1:C:127:TYR:OH	1:C:142:LEU:HD23	2.13	0.47
1:C:129:GLU:OE1	1:C:277:SER:HB2	2.14	0.47
1:C:35:MET:HG2	1:C:39:ASN:HD21	1.80	0.47
1:E:119:ASN:HD22	1:E:122:ILE:HD11	1.80	0.47
1:E:202:MET:CE	1:E:273:VAL:HG21	2.44	0.47
1:G:142:LEU:O	1:G:142:LEU:HD13	2.15	0.47
1:B:104:LYS:HD2	1:B:107:GLN:OE1	2.15	0.47
1:F:111:VAL:N	1:F:112:PRO:HD2	2.30	0.47
1:F:197:LEU:O	1:F:201:ILE:HD12	2.15	0.47
1:H:233:PHE:O	1:H:233:PHE:HD1	1.96	0.47
1:B:19:ASN:N	1:B:19:ASN:OD1	2.47	0.47
1:B:78:ARG:HA	1:B:215:ASP:OD1	2.15	0.47
1:B:61:VAL:O	1:B:65:THR:OG1	2.27	0.47
1:E:243:LEU:HD23	1:E:246:ASN:OD1	2.15	0.47
1:E:35:MET:HE3	2:E:401:GDD:O1A	2.15	0.47
1:B:111:VAL:N	1:B:112:PRO:HD2	2.29	0.47
1:B:142:LEU:O	1:B:142:LEU:HD13	2.14	0.47
1:C:193:ILE:O	1:C:197:LEU:HG	2.14	0.47
1:E:227:ILE:O	1:E:230:LEU:HB2	2.15	0.47
1:F:66:LEU:CD2	1:F:214:PHE:HD1	2.25	0.47
1:F:269:SER:O	1:F:273:VAL:HG22	2.15	0.47
1:A:275:VAL:HG23	1:A:276:THR:N	2.30	0.47
1:D:138:THR:HG22	1:D:140:MET:H	1.80	0.47
1:D:237:ASP:O	1:D:243:LEU:CD1	2.63	0.47
1:D:71:ILE:C	1:D:72:LEU:HD22	2.35	0.47
1:E:29:CYS:CA	1:E:288:ASN:HD21	2.27	0.47
1:G:237:ASP:O	1:G:243:LEU:CD1	2.63	0.47
1:A:328:LYS:HD3	1:A:328:LYS:HA	1.59	0.47
1:D:239:SER:O	1:D:243:LEU:N	2.44	0.47
1:D:66:LEU:HB3	1:D:78:ARG:HH11	1.80	0.47
1:E:50:MET:CE	1:E:243:LEU:HD13	2.45	0.47
1:G:273:VAL:HG12	1:G:281:TYR:HB3	1.96	0.47
1:A:30:GLY:O	1:A:34:LEU:HB2	2.14	0.47
1:D:129:GLU:OE1	1:D:277:SER:HB2	2.15	0.47
1:A:114:TYR:CZ	1:A:118:LYS:HG3	2.50	0.46
1:A:290:LEU:HB2	1:A:291:PRO:CD	2.43	0.46
1:C:212:LYS:N	1:C:215:ASP:OD2	2.48	0.46
1:C:310:LEU:HD22	1:C:314:ILE:CD1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:SER:HA	1:D:244:THR:OG1	2.14	0.46
1:E:247:PHE:HD2	1:E:252:LEU:HD11	1.80	0.46
1:F:119:ASN:HD21	1:F:286:ALA:HB1	1.79	0.46
1:H:127:TYR:OH	1:H:142:LEU:HD23	2.15	0.46
1:A:213:ASP:O	1:A:214:PHE:CB	2.63	0.46
1:B:275:VAL:HG23	1:B:276:THR:N	2.30	0.46
1:C:194:THR:O	1:C:198:PHE:HB3	2.15	0.46
1:E:205:ARG:O	1:E:209:THR:OG1	2.28	0.46
1:B:177:ALA:O	1:B:179:ALA:N	2.45	0.46
1:B:90:PRO:O	1:B:94:LEU:HB2	2.14	0.46
1:D:121:THR:HA	1:D:124:LEU:CG	2.45	0.46
1:G:311:SER:O	1:G:315:GLY:N	2.36	0.46
1:H:59:SER:C	1:H:225:LEU:HD21	2.36	0.46
1:H:43:VAL:HG23	1:H:257:ILE:HG21	1.96	0.46
1:A:247:PHE:HA	1:A:251:SER:OG	2.16	0.46
1:B:188:MET:HE3	1:B:191:ASN:HB3	1.97	0.46
1:C:201:ILE:O	1:C:204:LYS:N	2.48	0.46
1:C:212:LYS:O	1:C:215:ASP:HB2	2.14	0.46
1:A:65:THR:HA	1:A:68:ILE:HD12	1.97	0.46
1:A:77:PHE:CD1	1:A:77:PHE:N	2.83	0.46
1:B:121:THR:HG21	1:B:192:CYS:HA	1.96	0.46
1:B:56:PHE:CE1	1:B:225:LEU:HB3	2.50	0.46
1:C:196:ALA:O	1:C:200:LEU:HG	2.15	0.46
1:C:222:VAL:HA	1:C:225:LEU:CD1	2.44	0.46
1:C:71:ILE:HG13	1:C:72:LEU:HD23	1.97	0.46
1:H:204:LYS:HG3	1:H:208:LEU:CD1	2.45	0.46
1:B:214:PHE:HA	1:B:217:MET:HB3	1.97	0.46
1:B:39:ASN:OD1	1:B:46:LYS:HE2	2.16	0.46
1:C:195:SER:O	1:C:199:VAL:HG13	2.15	0.46
1:C:59:SER:O	1:C:221:ASN:HB3	2.16	0.46
1:F:19:ASN:N	1:F:19:ASN:OD1	2.47	0.46
1:H:151:SER:HB2	1:H:314:ILE:HG22	1.98	0.46
1:A:98:MET:HG3	1:A:195:SER:OG	2.16	0.46
1:C:146:LEU:HD22	1:E:150:LEU:CD1	2.45	0.46
1:D:108:TYR:CG	1:D:183:PRO:HB2	2.50	0.46
1:G:300:PHE:CE2	3:G:401:OLC:O19	2.69	0.46
1:B:237:ASP:O	1:B:243:LEU:CD1	2.64	0.46
3:A:403:OLC:H14	1:B:310:LEU:HD11	1.98	0.46
1:B:71:ILE:HG13	1:B:72:LEU:HD23	1.97	0.46
1:C:108:TYR:HB2	1:C:184:GLY:HA2	1.98	0.46
1:D:32:SER:O	1:D:36:THR:OG1	2.27	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:SER:HA	1:F:236:GLU:OE1	2.16	0.46
1:G:108:TYR:CD2	1:G:183:PRO:HB2	2.50	0.46
1:G:151:SER:O	1:G:311:SER:HB2	2.16	0.46
1:H:329:LYS:O	1:H:332:ALA:HB3	2.16	0.46
1:A:115:THR:HG22	1:A:119:ASN:OD1	2.16	0.46
1:A:222:VAL:HA	1:A:225:LEU:CD1	2.46	0.46
1:B:31:SER:HB2	1:B:265:ILE:N	2.31	0.46
1:B:310:LEU:O	1:B:314:ILE:HG13	2.15	0.46
1:C:86:LYS:HD2	1:C:86:LYS:HA	1.68	0.46
1:D:215:ASP:N	1:D:215:ASP:OD1	2.48	0.46
1:D:46:LYS:HZ3	1:D:255:MET:HG3	1.80	0.46
1:F:54:MET:O	1:F:58:GLN:HG3	2.16	0.46
1:H:275:VAL:HG23	1:H:276:THR:N	2.31	0.46
1:C:307:LEU:HD22	1:C:307:LEU:N	2.30	0.46
1:A:204:LYS:CE	1:A:208:LEU:HD11	2.38	0.45
1:B:202:MET:HG2	1:B:206:ILE:HD11	1.97	0.45
1:D:46:LYS:HA	1:D:46:LYS:HD2	1.73	0.45
1:E:222:VAL:O	1:E:226:PRO:HD3	2.16	0.45
1:E:129:GLU:OE2	1:E:278:SER:HB2	2.15	0.45
1:G:115:THR:O	1:G:119:ASN:N	2.47	0.45
1:G:120:LEU:O	1:G:124:LEU:HD23	2.15	0.45
1:G:201:ILE:O	1:G:204:LYS:HB3	2.15	0.45
1:H:19:ASN:HA	1:H:271:TRP:HZ2	1.81	0.45
1:H:38:THR:HG23	1:H:42:VAL:HG21	1.98	0.45
1:C:310:LEU:HD22	1:C:314:ILE:HD11	1.97	0.45
1:E:259:GLY:HA2	1:E:262:SER:OG	2.16	0.45
1:F:188:MET:HE2	1:F:188:MET:CA	2.46	0.45
1:G:148:MET:O	1:G:152:SER:N	2.47	0.45
1:G:188:MET:HA	1:G:188:MET:CE	2.46	0.45
1:G:71:ILE:O	1:G:72:LEU:HD22	2.17	0.45
1:H:262:SER:HA	1:H:265:ILE:HG13	1.97	0.45
1:H:88:TRP:HA	1:H:91:ILE:HD13	1.99	0.45
1:A:146:LEU:O	1:A:149:VAL:HB	2.16	0.45
1:C:103:SER:O	1:C:107:GLN:HG3	2.17	0.45
1:C:275:VAL:HG23	1:C:276:THR:N	2.31	0.45
1:B:333:GLN:HA	1:C:44:ASN:ND2	2.31	0.45
1:D:116:ILE:O	1:D:120:LEU:N	2.46	0.45
1:D:288:ASN:O	1:D:291:PRO:HD2	2.16	0.45
1:E:147:LEU:HD13	1:E:317:LEU:HD23	1.97	0.45
1:E:71:ILE:O	1:E:72:LEU:HD22	2.16	0.45
1:G:317:LEU:O	1:G:321:ILE:HG12	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:PHE:O	1:G:56:PHE:N	2.46	0.45
1:G:88:TRP:HA	1:G:91:ILE:CD1	2.44	0.45
1:H:206:ILE:HG12	1:H:216:THR:HG22	1.98	0.45
1:H:31:SER:HB2	1:H:264:GLY:HA3	1.97	0.45
1:A:150:LEU:O	1:A:154:VAL:HG23	2.17	0.45
1:A:37:VAL:HG13	1:A:41:PHE:HD2	1.74	0.45
1:C:96:VAL:HG13	1:C:228:LEU:HD23	1.97	0.45
1:F:332:ALA:O	1:G:45:LEU:HD12	2.17	0.45
1:H:213:ASP:HB3	1:H:267:TYR:CE1	2.51	0.45
1:H:66:LEU:HB3	1:H:78:ARG:NH1	2.31	0.45
1:B:88:TRP:NE1	1:B:220:ASN:OD1	2.49	0.45
1:D:252:LEU:O	1:D:256:ILE:HG13	2.16	0.45
1:D:96:VAL:HG12	1:D:231:PHE:CD2	2.51	0.45
1:F:53:VAL:HA	1:F:56:PHE:HB3	1.99	0.45
1:G:219:TYR:O	1:G:223:LEU:HD13	2.16	0.45
1:H:145:PHE:O	1:H:149:VAL:HG23	2.17	0.45
1:B:307:LEU:HD22	1:B:307:LEU:N	2.31	0.45
1:B:81:ASN:HB2	1:B:84:ASP:HB2	1.99	0.45
1:E:151:SER:HB2	1:E:314:ILE:HG22	1.98	0.45
1:E:19:ASN:OD1	1:E:19:ASN:N	2.48	0.45
1:E:307:LEU:HD22	1:E:307:LEU:H	1.81	0.45
1:E:154:VAL:HG12	1:E:307:LEU:O	2.16	0.45
1:E:67:ILE:CG1	1:E:78:ARG:HH22	2.30	0.45
1:F:213:ASP:O	1:F:214:PHE:CB	2.61	0.45
1:G:213:ASP:O	1:G:214:PHE:CB	2.65	0.45
1:A:262:SER:O	1:A:265:ILE:HG13	2.16	0.45
1:C:105:ALA:HB1	1:C:188:MET:HG2	1.99	0.45
1:C:279:THR:O	1:C:283:MET:N	2.48	0.45
1:D:310:LEU:HD22	1:D:314:ILE:HD11	1.99	0.45
1:E:98:MET:SD	1:E:195:SER:HA	2.56	0.45
1:E:25:ILE:HG23	1:E:284:VAL:HG21	1.99	0.45
1:F:86:LYS:HA	1:F:86:LYS:HD2	1.63	0.45
1:F:90:PRO:O	1:F:94:LEU:HD23	2.16	0.45
1:G:25:ILE:HG23	1:G:284:VAL:HG21	1.98	0.45
1:H:238:TRP:CD1	1:H:238:TRP:N	2.85	0.45
1:A:112:PRO:O	1:A:116:ILE:HG13	2.16	0.45
1:D:247:PHE:HD2	1:D:252:LEU:HD21	1.82	0.45
1:D:290:LEU:HD11	1:D:315:GLY:HA3	1.98	0.45
1:F:105:ALA:HB1	1:F:188:MET:HG2	1.99	0.45
1:H:181:PHE:C	1:H:183:PRO:HD2	2.37	0.45
1:H:213:ASP:O	1:H:214:PHE:CB	2.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:CG2	1:A:192:CYS:HA	2.46	0.45
1:A:204:LYS:HG3	1:A:208:LEU:HD11	1.98	0.45
1:C:202:MET:O	1:C:206:ILE:HG13	2.17	0.45
1:C:270:GLY:HA2	1:C:273:VAL:HG22	1.98	0.45
1:D:307:LEU:N	1:D:307:LEU:HD22	2.30	0.45
1:E:66:LEU:HD21	1:E:214:PHE:HD1	1.81	0.45
1:E:58:GLN:HE21	1:E:262:SER:HB3	1.81	0.45
1:F:71:ILE:C	1:F:72:LEU:HD22	2.37	0.45
1:B:181:PHE:C	1:B:183:PRO:HD2	2.38	0.44
1:C:19:ASN:ND2	1:C:19:ASN:O	2.50	0.44
1:D:73:GLY:CA	1:D:77:PHE:HZ	2.29	0.44
1:E:223:LEU:C	1:E:226:PRO:HD2	2.36	0.44
1:F:102:SER:HB2	1:F:191:ASN:HD21	1.81	0.44
1:H:19:ASN:HB2	1:H:271:TRP:NE1	2.32	0.44
1:A:62:CYS:SG	1:A:263:VAL:HA	2.57	0.44
1:B:24:SER:HB3	1:B:275:VAL:HG21	1.98	0.44
1:B:56:PHE:HA	1:B:228:LEU:HD13	1.99	0.44
1:B:66:LEU:HB3	1:B:78:ARG:HH11	1.83	0.44
1:C:223:LEU:C	1:C:226:PRO:HD2	2.38	0.44
1:D:116:ILE:HD11	1:D:156:THR:OG1	2.17	0.44
1:D:124:LEU:HD12	1:D:125:ILE:HG13	1.99	0.44
1:D:151:SER:O	1:D:311:SER:HB2	2.18	0.44
1:E:124:LEU:CD1	1:E:196:ALA:HB2	2.45	0.44
1:E:247:PHE:HA	1:E:251:SER:OG	2.17	0.44
1:H:53:VAL:HG12	1:H:255:MET:HE3	1.99	0.44
1:A:111:VAL:N	1:A:112:PRO:HD2	2.32	0.44
1:B:204:LYS:HE3	1:B:208:LEU:CG	2.48	0.44
1:C:111:VAL:N	1:C:112:PRO:HD2	2.32	0.44
1:F:188:MET:HA	1:F:188:MET:CE	2.48	0.44
1:F:202:MET:HG2	1:F:206:ILE:CD1	2.48	0.44
1:A:259:GLY:HA2	1:A:262:SER:OG	2.17	0.44
1:A:284:VAL:HG12	1:A:288:ASN:ND2	2.31	0.44
1:C:202:MET:HE1	1:C:273:VAL:HG21	1.98	0.44
1:B:332:ALA:HB1	1:C:45:LEU:CD1	2.47	0.44
1:D:217:MET:HG3	1:D:266:SER:HB3	2.00	0.44
1:E:46:LYS:HA	1:E:46:LYS:HD2	1.67	0.44
1:F:270:GLY:HA2	1:F:273:VAL:CG2	2.47	0.44
1:G:307:LEU:HD22	1:G:307:LEU:N	2.32	0.44
1:A:307:LEU:N	1:A:307:LEU:HD22	2.32	0.44
1:A:314:ILE:HD11	3:A:402:OLC:H15A	2.00	0.44
1:B:132:PHE:CE2	1:B:200:LEU:HD13	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:ILE:HA	1:F:230:LEU:CD1	2.32	0.44
1:B:121:THR:HG22	1:B:192:CYS:CB	2.45	0.44
1:B:66:LEU:HD21	1:B:214:PHE:HD1	1.82	0.44
1:C:108:TYR:HB2	1:C:184:GLY:CA	2.48	0.44
1:D:253:THR:O	1:D:257:ILE:HG13	2.17	0.44
1:F:98:MET:O	1:F:191:ASN:ND2	2.51	0.44
1:F:305:ASN:HB2	1:F:308:SER:H	1.83	0.44
1:G:138:THR:HG22	1:G:140:MET:H	1.83	0.44
1:G:25:ILE:HG23	1:G:284:VAL:CG1	2.48	0.44
1:A:86:LYS:HA	1:A:86:LYS:HD2	1.62	0.44
1:E:306:PHE:CZ	1:E:310:LEU:HG	2.52	0.44
1:F:202:MET:O	1:F:206:ILE:N	2.46	0.44
1:F:276:THR:OG1	1:F:280:THR:HB	2.18	0.44
1:H:37:VAL:HG13	1:H:41:PHE:CD2	2.52	0.44
1:A:43:VAL:HG11	1:A:254:ALA:HB1	1.98	0.44
1:B:222:VAL:O	1:B:226:PRO:HD3	2.17	0.44
1:B:237:ASP:O	1:B:243:LEU:HD13	2.17	0.44
1:C:95:LEU:O	1:C:98:MET:HB3	2.17	0.44
1:E:58:GLN:HE21	1:E:262:SER:CB	2.30	0.44
1:F:59:SER:C	1:F:225:LEU:HD21	2.38	0.44
1:A:114:TYR:O	1:A:118:LYS:HB2	2.18	0.44
1:A:121:THR:CG2	1:A:192:CYS:SG	3.06	0.44
1:B:332:ALA:O	1:C:44:ASN:ND2	2.49	0.44
1:C:70:ARG:HD2	1:C:78:ARG:NE	2.30	0.44
1:E:35:MET:HE3	2:E:401:GDD:PA	2.58	0.44
1:H:71:ILE:C	1:H:72:LEU:HD22	2.38	0.44
1:C:61:VAL:CG2	1:C:256:ILE:HG23	2.48	0.43
1:D:211:PHE:HE2	1:D:219:TYR:CD1	2.35	0.43
1:E:213:ASP:O	1:E:214:PHE:CB	2.64	0.43
1:F:101:THR:HB	1:F:191:ASN:HB2	1.99	0.43
1:F:31:SER:HB2	1:F:265:ILE:HG23	2.00	0.43
1:F:290:LEU:HD11	1:F:315:GLY:HA3	2.00	0.43
1:A:116:ILE:HD11	1:A:156:THR:CB	2.48	0.43
1:B:233:PHE:CD1	1:B:233:PHE:O	2.71	0.43
1:B:61:VAL:HG21	1:B:256:ILE:HG23	1.99	0.43
1:C:92:SER:CB	1:C:227:ILE:HD12	2.48	0.43
1:E:233:PHE:O	1:E:233:PHE:HD1	2.01	0.43
1:E:239:SER:OG	1:E:242:ASN:HB2	2.19	0.43
1:F:124:LEU:CD1	1:F:196:ALA:HB2	2.47	0.43
1:F:307:LEU:N	1:F:307:LEU:HD22	2.32	0.43
1:G:187:TRP:O	1:G:190:THR:OG1	2.29	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:205:ARG:HA	1:H:208:LEU:HB2	2.00	0.43
1:H:253:THR:O	1:H:257:ILE:HG13	2.17	0.43
1:D:206:ILE:HG12	1:D:216:THR:HG22	1.99	0.43
1:H:56:PHE:HA	1:H:228:LEU:HD13	2.01	0.43
1:A:324:VAL:O	1:A:327:GLN:HB2	2.18	0.43
1:D:36:THR:HG21	1:D:292:ILE:HD13	2.00	0.43
1:E:202:MET:HG2	1:E:206:ILE:HD11	2.01	0.43
1:C:102:SER:HB2	1:C:191:ASN:ND2	2.34	0.43
1:G:130:VAL:HG13	1:G:135:GLY:O	2.18	0.43
1:G:108:TYR:CD1	1:G:183:PRO:HB2	2.53	0.43
1:G:182:ASN:N	1:G:183:PRO:HD2	2.33	0.43
1:G:35:MET:HG2	1:G:39:ASN:HD21	1.83	0.43
1:A:289:LYS:CD	1:A:289:LYS:N	2.82	0.43
1:B:28:TYR:HE2	1:B:285:GLY:HA2	1.83	0.43
1:C:148:MET:HE3	1:C:287:LEU:HD23	2.01	0.43
1:E:220:ASN:O	1:E:224:ALA:CB	2.67	0.43
1:F:29:CYS:CB	1:F:288:ASN:HD21	2.31	0.43
1:H:37:VAL:HG13	1:H:41:PHE:HB2	2.01	0.43
1:A:102:SER:HB2	1:A:191:ASN:HD21	1.82	0.43
1:B:115:THR:HG22	1:B:119:ASN:HD21	1.82	0.43
1:B:115:THR:HG22	1:B:119:ASN:ND2	2.34	0.43
1:G:295:SER:HB3	3:G:401:OLC:H9	2.00	0.43
1:G:29:CYS:SG	1:G:288:ASN:ND2	2.81	0.43
1:G:151:SER:HA	1:G:311:SER:HA	2.00	0.43
1:F:333:GLN:CG	1:G:45:LEU:HD13	2.48	0.43
1:A:151:SER:HB2	1:A:314:ILE:CB	2.49	0.43
1:B:132:PHE:HE2	1:B:200:LEU:HD13	1.83	0.43
1:B:29:CYS:HA	1:B:288:ASN:OD1	2.18	0.43
1:B:52:PHE:O	1:B:56:PHE:N	2.45	0.43
1:D:232:SER:O	1:D:236:GLU:HB2	2.19	0.43
1:D:19:ASN:HB2	1:D:271:TRP:NE1	2.34	0.43
1:E:228:LEU:O	1:E:232:SER:N	2.52	0.43
1:G:120:LEU:HD23	1:G:123:ILE:HD12	2.01	0.43
1:A:121:THR:HG22	1:A:192:CYS:SG	2.59	0.43
1:A:296:GLY:HA2	1:A:300:PHE:CD2	2.54	0.43
1:C:258:SER:O	1:C:262:SER:N	2.39	0.43
1:D:19:ASN:O	1:D:19:ASN:ND2	2.49	0.43
1:D:66:LEU:O	1:D:70:ARG:N	2.48	0.43
1:D:95:LEU:O	1:D:98:MET:HB3	2.19	0.43
1:E:181:PHE:HD2	1:E:185:TYR:CE2	2.37	0.43
1:E:290:LEU:HB2	1:E:291:PRO:CD	2.42	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:313:PHE:HA	1:F:316:PHE:HB2	2.00	0.43
1:G:186:PHE:O	1:G:190:THR:HG23	2.19	0.43
1:H:290:LEU:HD22	1:H:312:ILE:HA	2.00	0.43
1:A:130:VAL:O	1:A:134:GLY:HA2	2.18	0.43
1:B:239:SER:OG	1:B:243:LEU:HG	2.19	0.43
1:C:117:PHE:HB2	1:C:188:MET:SD	2.59	0.43
1:D:155:ALA:HB2	1:D:311:SER:CB	2.49	0.43
1:E:102:SER:HG	1:E:114:TYR:HH	1.66	0.43
1:F:91:ILE:O	1:F:95:LEU:N	2.51	0.43
1:G:116:ILE:HD11	1:G:156:THR:OG1	2.19	0.43
1:H:22:PRO:HA	1:H:25:ILE:HD12	1.99	0.43
1:A:121:THR:O	1:A:124:LEU:HG	2.19	0.42
1:A:253:THR:HG22	1:A:257:ILE:HD11	1.99	0.42
1:C:202:MET:HG2	1:C:206:ILE:HD12	2.01	0.42
1:C:202:MET:HE3	1:C:273:VAL:HG21	2.01	0.42
1:D:117:PHE:HB2	1:D:188:MET:SD	2.58	0.42
1:D:247:PHE:CD2	1:D:252:LEU:HD21	2.54	0.42
1:F:88:TRP:CD1	1:F:219:TYR:HB3	2.54	0.42
1:G:129:GLU:OE2	1:G:278:SER:HB2	2.18	0.42
1:D:52:PHE:O	1:D:56:PHE:N	2.48	0.42
1:E:56:PHE:O	1:E:60:LEU:N	2.52	0.42
1:F:142:LEU:CD1	1:F:146:LEU:HD11	2.49	0.42
1:G:188:MET:O	1:G:188:MET:HE2	2.18	0.42
1:H:146:LEU:O	1:H:149:VAL:HB	2.19	0.42
1:H:129:GLU:CD	1:H:278:SER:HB2	2.39	0.42
1:C:67:ILE:HA	1:C:78:ARG:HH12	1.85	0.42
1:E:203:ARG:CZ	1:E:207:LYS:HD2	2.48	0.42
1:G:238:TRP:HA	1:G:243:LEU:HD12	2.01	0.42
1:H:269:SER:O	1:H:273:VAL:HG22	2.19	0.42
1:A:95:LEU:O	1:A:98:MET:HB3	2.19	0.42
1:A:99:ILE:O	1:A:103:SER:N	2.31	0.42
1:F:227:ILE:HA	1:F:230:LEU:HB2	2.00	0.42
1:A:119:ASN:HD21	1:A:286:ALA:HB1	1.84	0.42
1:A:23:ILE:H	1:A:23:ILE:HG13	1.69	0.42
1:C:130:VAL:HG22	1:C:135:GLY:O	2.20	0.42
1:G:252:LEU:O	1:G:256:ILE:HG13	2.19	0.42
1:G:308:SER:O	1:G:311:SER:OG	2.30	0.42
1:G:63:THR:O	1:G:67:ILE:HG13	2.19	0.42
1:A:71:ILE:CB	1:H:240:SER:HB3	2.46	0.42
1:A:148:MET:O	1:A:152:SER:N	2.46	0.42
1:B:211:PHE:CD2	1:B:215:ASP:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:THR:HG21	1:B:292:ILE:HD13	2.02	0.42
1:C:317:LEU:O	1:C:321:ILE:HG12	2.19	0.42
1:D:19:ASN:HB2	1:D:271:TRP:CE2	2.53	0.42
1:D:213:ASP:O	1:D:214:PHE:CB	2.66	0.42
1:F:19:ASN:HB2	1:F:271:TRP:NE1	2.34	0.42
1:G:239:SER:O	1:G:243:LEU:N	2.44	0.42
1:C:225:LEU:HB2	1:C:226:PRO:HD3	2.02	0.42
1:D:232:SER:OG	1:D:238:TRP:HZ2	2.02	0.42
1:D:328:LYS:HG2	1:D:331:GLN:OE1	2.20	0.42
1:G:123:ILE:O	1:G:127:TYR:HD1	2.01	0.42
1:E:86:LYS:HD2	1:E:86:LYS:HA	1.57	0.42
1:E:95:LEU:O	1:E:98:MET:HB3	2.20	0.42
1:F:233:PHE:CD1	1:F:233:PHE:O	2.66	0.42
1:F:66:LEU:HD21	1:F:214:PHE:CD1	2.48	0.42
1:F:89:PHE:HA	1:F:223:LEU:HD23	2.02	0.42
1:A:253:THR:O	1:A:257:ILE:HG13	2.20	0.42
1:D:289:LYS:HA	1:D:289:LYS:HD3	1.92	0.42
1:F:124:LEU:HD12	1:F:125:ILE:N	2.34	0.42
1:G:227:ILE:HA	1:G:230:LEU:HD12	2.02	0.42
1:G:324:VAL:O	1:G:327:GLN:HB3	2.19	0.42
1:H:19:ASN:HB2	1:H:271:TRP:CE2	2.55	0.42
1:C:259:GLY:HA2	1:C:262:SER:OG	2.19	0.42
1:C:31:SER:HB2	1:C:264:GLY:C	2.39	0.42
1:D:310:LEU:HD22	1:D:314:ILE:CD1	2.50	0.42
1:H:67:ILE:HG12	1:H:78:ARG:NH2	2.20	0.42
1:B:117:PHE:HA	1:B:120:LEU:HD12	2.01	0.41
1:B:213:ASP:O	1:B:214:PHE:CB	2.66	0.41
1:B:315:GLY:O	1:B:318:SER:HB3	2.19	0.41
1:C:20:SER:O	1:C:23:ILE:HD12	2.20	0.41
1:C:248:SER:N	1:C:251:SER:OG	2.52	0.41
1:C:46:LYS:HG3	1:C:46:LYS:O	2.19	0.41
1:D:111:VAL:N	1:D:112:PRO:HD2	2.35	0.41
1:G:146:LEU:O	1:G:149:VAL:HB	2.19	0.41
1:G:204:LYS:HG3	1:G:208:LEU:HD11	2.01	0.41
1:G:244:THR:HA	1:G:247:PHE:CE1	2.55	0.41
1:A:105:ALA:O	1:A:109:LEU:HB2	2.19	0.41
3:C:401:OLC:H13	1:E:314:ILE:HD11	2.01	0.41
1:E:239:SER:N	1:E:243:LEU:HD12	2.30	0.41
1:H:37:VAL:O	1:H:41:PHE:N	2.35	0.41
1:A:130:VAL:HG13	1:A:135:GLY:O	2.20	0.41
1:A:228:LEU:O	1:A:232:SER:N	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:SER:OG	1:A:242:ASN:HB2	2.20	0.41
1:F:88:TRP:NE1	1:F:220:ASN:OD1	2.50	0.41
1:F:237:ASP:O	1:F:243:LEU:CD1	2.69	0.41
1:B:60:LEU:HG	1:B:64:ILE:HD13	2.01	0.41
1:C:148:MET:CE	1:C:287:LEU:HD23	2.50	0.41
1:D:151:SER:HB2	1:D:314:ILE:CG2	2.46	0.41
1:D:247:PHE:CG	1:D:247:PHE:O	2.73	0.41
1:E:46:LYS:CE	1:E:54:MET:SD	3.08	0.41
1:F:213:ASP:HB3	1:F:267:TYR:CE1	2.55	0.41
1:F:290:LEU:HB2	1:F:291:PRO:CD	2.46	0.41
1:G:126:ALA:HA	1:G:279:THR:OG1	2.20	0.41
1:H:138:THR:HG22	1:H:140:MET:H	1.85	0.41
1:H:214:PHE:HA	1:H:217:MET:HB3	2.02	0.41
1:H:237:ASP:O	1:H:243:LEU:HD13	2.19	0.41
1:B:212:LYS:O	1:B:215:ASP:HB2	2.21	0.41
1:C:239:SER:N	1:C:243:LEU:HD12	2.34	0.41
1:C:73:GLY:HA3	1:C:77:PHE:CZ	2.54	0.41
1:E:221:ASN:ND2	2:E:401:GDD:O6	2.54	0.41
1:G:271:TRP:O	1:G:275:VAL:HG22	2.21	0.41
1:H:117:PHE:O	1:H:121:THR:HG23	2.20	0.41
1:H:232:SER:O	1:H:236:GLU:HB2	2.20	0.41
1:A:120:LEU:O	1:A:124:LEU:HD23	2.21	0.41
1:A:67:ILE:HA	1:A:78:ARG:HH12	1.85	0.41
1:B:204:LYS:HG3	1:B:208:LEU:HD12	2.02	0.41
1:B:213:ASP:HB3	1:B:267:TYR:CE1	2.56	0.41
1:B:50:MET:HB3	1:B:236:GLU:OE2	2.20	0.41
1:E:82:LYS:HA	1:E:85:ALA:CB	2.50	0.41
1:F:316:PHE:HD1	1:F:316:PHE:HA	1.78	0.41
1:H:102:SER:O	1:H:106:LEU:HG	2.21	0.41
1:H:112:PRO:HB2	1:H:156:THR:OG1	2.21	0.41
1:H:109:LEU:HD12	1:H:188:MET:HG3	2.03	0.41
1:H:132:PHE:CE2	1:H:200:LEU:HB3	2.56	0.41
1:A:37:VAL:HG22	1:A:41:PHE:HE2	1.84	0.41
1:B:66:LEU:HB3	1:B:78:ARG:NH1	2.35	0.41
1:C:56:PHE:CA	1:C:228:LEU:HD13	2.51	0.41
1:C:290:LEU:HB2	1:C:291:PRO:CD	2.46	0.41
1:D:124:LEU:HD11	1:D:196:ALA:HB2	2.00	0.41
1:E:253:THR:HG22	1:E:257:ILE:HD12	2.01	0.41
1:H:38:THR:HA	1:H:42:VAL:HG23	2.03	0.41
1:A:38:THR:HA	1:A:42:VAL:HG23	2.03	0.41
1:B:93:PHE:O	1:B:97:LEU:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:VAL:O	1:C:278:SER:OG	2.31	0.41
1:D:289:LYS:HG3	2:D:401:GDD:O6A	2.21	0.41
1:E:227:ILE:CA	1:E:230:LEU:HD12	2.32	0.41
1:F:117:PHE:HA	1:F:120:LEU:HB2	2.03	0.41
1:F:35:MET:SD	1:F:265:ILE:HG12	2.60	0.41
1:H:19:ASN:HA	1:H:271:TRP:CZ2	2.56	0.41
1:H:305:ASN:HB2	1:H:308:SER:H	1.86	0.41
1:H:316:PHE:HA	1:H:316:PHE:HD1	1.77	0.41
1:B:56:PHE:CE1	1:B:225:LEU:O	2.73	0.41
1:D:23:ILE:HG13	1:D:23:ILE:H	1.74	0.41
1:E:177:ALA:O	1:E:179:ALA:N	2.46	0.41
1:E:29:CYS:HA	1:E:288:ASN:ND2	2.34	0.41
1:F:31:SER:HB2	1:F:265:ILE:N	2.36	0.41
1:H:220:ASN:O	1:H:224:ALA:CB	2.69	0.41
1:H:310:LEU:HA	1:H:310:LEU:HD23	1.84	0.41
1:B:238:TRP:N	1:B:238:TRP:CD1	2.88	0.41
1:B:289:LYS:HA	1:B:289:LYS:HD3	1.93	0.41
1:B:92:SER:O	1:B:96:VAL:HG23	2.21	0.41
1:C:72:LEU:HA	1:C:72:LEU:HD13	1.97	0.41
1:D:290:LEU:HD13	1:D:315:GLY:HA3	2.03	0.41
1:G:111:VAL:N	1:G:112:PRO:HD2	2.36	0.41
1:G:109:LEU:HD13	1:G:188:MET:HG3	2.03	0.41
1:B:323:ALA:O	1:B:327:GLN:HG3	2.21	0.41
1:C:148:MET:HB2	1:C:318:SER:OG	2.21	0.41
1:F:27:SER:HG	1:F:271:TRP:HZ3	1.67	0.41
1:C:191:ASN:O	1:C:195:SER:HB2	2.21	0.40
1:C:227:ILE:O	1:C:230:LEU:HB2	2.20	0.40
1:C:36:THR:HG21	1:C:292:ILE:HD13	2.03	0.40
1:D:270:GLY:HA2	1:D:273:VAL:HG22	2.03	0.40
1:D:279:THR:O	1:D:283:MET:N	2.54	0.40
1:E:218:PHE:CE2	1:E:222:VAL:HG21	2.56	0.40
1:E:252:LEU:HD23	1:E:255:MET:SD	2.61	0.40
1:F:306:PHE:O	1:F:310:LEU:HB2	2.20	0.40
1:F:333:GLN:HA	1:G:44:ASN:HD21	1.85	0.40
1:H:70:ARG:HD2	1:H:78:ARG:NH2	2.24	0.40
1:B:128:GLY:O	1:B:132:PHE:HD2	2.04	0.40
1:B:69:LEU:O	1:B:77:PHE:CE2	2.74	0.40
1:F:52:PHE:CE2	1:F:231:PHE:HB3	2.56	0.40
1:C:273:VAL:HG12	1:C:281:TYR:HB3	2.02	0.40
1:E:289:LYS:HD2	1:E:289:LYS:HA	1.68	0.40
1:H:265:ILE:HD12	1:H:266:SER:N	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:O	1:B:149:VAL:HB	2.22	0.40
1:F:268:CYS:O	1:F:272:CYS:N	2.43	0.40
1:B:92:SER:HB3	1:B:224:ALA:HA	2.04	0.40
1:B:324:VAL:HA	1:B:327:GLN:HB2	2.04	0.40
1:C:193:ILE:CD1	1:C:194:THR:HG23	2.52	0.40
1:D:295:SER:HB3	3:D:402:OLC:H5	2.03	0.40
1:E:247:PHE:CD2	1:E:252:LEU:HD11	2.56	0.40
1:E:202:MET:HE1	1:E:273:VAL:HG21	2.04	0.40
1:F:19:ASN:HA	1:F:271:TRP:HZ2	1.85	0.40
1:F:231:PHE:HA	1:F:234:CYS:HB2	2.02	0.40
1:G:201:ILE:O	1:G:204:LYS:N	2.55	0.40
1:G:28:TYR:HE2	1:G:285:GLY:CA	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:THR:OG1	1:H:208:LEU:O[1_545]	2.02	0.18

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	286/337 (85%)	275 (96%)	11 (4%)	0	100	100
1	B	291/337 (86%)	281 (97%)	10 (3%)	0	100	100
1	C	288/337 (86%)	277 (96%)	11 (4%)	0	100	100
1	D	288/337 (86%)	277 (96%)	11 (4%)	0	100	100
1	E	292/337 (87%)	279 (96%)	13 (4%)	0	100	100
1	F	288/337 (86%)	277 (96%)	11 (4%)	0	100	100
1	G	290/337 (86%)	277 (96%)	13 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	288/337 (86%)	277 (96%)	11 (4%)	0	100	100
All	All	2311/2696 (86%)	2220 (96%)	91 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	262/289 (91%)	254 (97%)	8 (3%)	40	71
1	B	265/289 (92%)	260 (98%)	5 (2%)	57	80
1	C	263/289 (91%)	258 (98%)	5 (2%)	57	80
1	D	263/289 (91%)	258 (98%)	5 (2%)	57	80
1	E	265/289 (92%)	259 (98%)	6 (2%)	50	76
1	F	263/289 (91%)	257 (98%)	6 (2%)	50	76
1	G	264/289 (91%)	256 (97%)	8 (3%)	41	71
1	H	263/289 (91%)	257 (98%)	6 (2%)	50	76
All	All	2108/2312 (91%)	2059 (98%)	49 (2%)	50	76

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ILE
1	A	77	PHE
1	A	124	LEU
1	A	142	LEU
1	A	188	MET
1	A	289	LYS
1	A	304	ARG
1	A	310	LEU
1	B	78	ARG
1	B	188	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	233	PHE
1	B	304	ARG
1	B	310	LEU
1	C	19	ASN
1	C	124	LEU
1	C	188	MET
1	C	304	ARG
1	C	310	LEU
1	D	19	ASN
1	D	188	MET
1	D	215	ASP
1	D	304	ARG
1	D	310	LEU
1	E	78	ARG
1	E	188	MET
1	E	233	PHE
1	E	289	LYS
1	E	304	ARG
1	E	310	LEU
1	F	142	LEU
1	F	160	GLN
1	F	188	MET
1	F	233	PHE
1	F	304	ARG
1	F	310	LEU
1	G	19	ASN
1	G	124	LEU
1	G	142	LEU
1	G	188	MET
1	G	233	PHE
1	G	262	SER
1	G	304	ARG
1	G	310	LEU
1	H	142	LEU
1	H	188	MET
1	H	215	ASP
1	H	233	PHE
1	H	304	ARG
1	H	310	LEU

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

Mol	Chain	Res	Type
1	A	58	GLN
1	A	119	ASN
1	B	19	ASN
1	E	288	ASN
1	F	288	ASN
1	F	305	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 carbohydrates in this entry.

5.6 Ligand geometry

11 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	GDD	A	401	-	35,42,42	0.82	1 (2%)	47,65,65	1.75	7 (14%)
3	OLC	A	403	-	24,24,24	0.68	0	25,25,25	0.73	0
2	GDD	E	401	-	35,42,42	0.79	1 (2%)	47,65,65	1.68	5 (10%)
3	OLC	D	402	-	24,24,24	0.61	0	25,25,25	0.80	0
3	OLC	G	401	-	24,24,24	0.77	0	25,25,25	0.89	1 (4%)
3	OLC	E	402	-	24,24,24	0.68	0	25,25,25	0.77	0
3	OLC	G	402	-	24,24,24	0.78	0	25,25,25	0.64	0
3	OLC	C	401	-	24,24,24	0.67	0	25,25,25	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	OLC	A	402	-	24,24,24	0.75	0	25,25,25	0.72	0
2	GDD	D	401	-	35,42,42	0.80	1 (2%)	47,65,65	1.69	5 (10%)
3	OLC	C	402	-	24,24,24	0.81	0	25,25,25	0.71	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	GDD	A	401	-	-	7/19/59/59	0/4/4/4
3	OLC	A	403	-	-	3/24/24/24	-
2	GDD	E	401	-	-	10/19/59/59	0/4/4/4
3	OLC	D	402	-	-	8/24/24/24	-
3	OLC	G	401	-	-	10/24/24/24	-
3	OLC	E	402	-	-	4/24/24/24	-
3	OLC	G	402	-	-	7/24/24/24	-
3	OLC	C	401	-	-	8/24/24/24	-
3	OLC	A	402	-	-	7/24/24/24	-
2	GDD	D	401	-	-	6/19/59/59	0/4/4/4
3	OLC	C	402	-	-	5/24/24/24	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GDD	C6-N1	3.21	1.38	1.33
2	E	401	GDD	C6-N1	3.20	1.38	1.33
2	D	401	GDD	C6-N1	3.19	1.38	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	GDD	C5-C6-N1	-8.30	112.08	123.43
2	A	401	GDD	C5-C6-N1	-8.29	112.09	123.43
2	D	401	GDD	C5-C6-N1	-8.28	112.10	123.43
2	D	401	GDD	C6-N1-C2	5.85	125.22	115.93
2	E	401	GDD	C6-N1-C2	5.84	125.22	115.93
2	A	401	GDD	C6-N1-C2	5.81	125.16	115.93
2	A	401	GDD	O3A-PB-O1B	3.05	108.63	102.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	GDD	N3-C2-N1	-2.88	123.38	127.22
2	E	401	GDD	N3-C2-N1	-2.87	123.39	127.22
2	A	401	GDD	N3-C2-N1	-2.81	123.48	127.22
2	E	401	GDD	C6-C5-C4	-2.62	118.29	120.80
2	A	401	GDD	C6-C5-C4	-2.59	118.33	120.80
2	D	401	GDD	C6-C5-C4	-2.46	118.44	120.80
2	A	401	GDD	PB-O1B-C11	2.36	128.86	119.74
2	D	401	GDD	C2-N3-C4	-2.30	112.73	115.36
3	G	401	OLC	O20-C1-O19	-2.26	117.88	123.59
2	A	401	GDD	C2-N3-C4	-2.24	112.79	115.36
2	E	401	GDD	C2-N3-C4	-2.23	112.81	115.36

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GDD	C5'-O5'-PA-O3A
2	A	401	GDD	O51-C11-O1B-PB
2	E	401	GDD	C5'-O5'-PA-O3A
2	E	401	GDD	C11-O1B-PB-O2B
2	E	401	GDD	O51-C11-O1B-PB
3	G	401	OLC	C2-C1-O20-C21
3	G	401	OLC	O19-C1-O20-C21
3	G	402	OLC	O20-C21-C22-C24
3	C	401	OLC	O20-C21-C22-C24
3	C	401	OLC	O20-C21-C22-O23
2	D	401	GDD	O51-C11-O1B-PB
3	G	402	OLC	O20-C21-C22-O23
3	A	402	OLC	O20-C21-C22-C24
3	C	401	OLC	C1-C2-C3-C4
3	A	402	OLC	O20-C21-C22-O23
2	E	401	GDD	C11-O1B-PB-O3A
2	D	401	GDD	O4'-C4'-C5'-O5'
3	C	402	OLC	C5-C6-C7-C8
3	D	402	OLC	C5-C6-C7-C8
3	G	402	OLC	C12-C13-C14-C15
3	G	402	OLC	C5-C6-C7-C8
3	D	402	OLC	C14-C15-C16-C17
3	G	401	OLC	C3-C4-C5-C6
3	A	402	OLC	C5-C6-C7-C8
3	C	401	OLC	C13-C14-C15-C16
3	G	402	OLC	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	401	OLC	C13-C14-C15-C16
3	G	401	OLC	C2-C3-C4-C5
3	A	402	OLC	C14-C15-C16-C17
3	C	402	OLC	C6-C7-C8-C9
3	C	402	OLC	C13-C14-C15-C16
2	D	401	GDD	O51-C51-C61-O6A
3	A	402	OLC	C3-C4-C5-C6
3	G	401	OLC	C1-C2-C3-C4
2	D	401	GDD	C4'-C5'-O5'-PA
3	E	402	OLC	C4-C5-C6-C7
3	G	402	OLC	C1-C2-C3-C4
3	C	401	OLC	C5-C6-C7-C8
2	E	401	GDD	C4'-C5'-O5'-PA
3	D	402	OLC	C1-C2-C3-C4
2	E	401	GDD	PB-O3A-PA-O5'
3	D	402	OLC	C22-C21-O20-C1
3	D	402	OLC	C2-C3-C4-C5
3	G	401	OLC	C5-C6-C7-C8
3	E	402	OLC	C5-C6-C7-C8
2	E	401	GDD	C11-O1B-PB-O3B
2	A	401	GDD	C5'-O5'-PA-O1A
2	A	401	GDD	C5'-O5'-PA-O2A
2	E	401	GDD	C5'-O5'-PA-O1A
3	A	402	OLC	C2-C3-C4-C5
3	A	402	OLC	C10-C11-C12-C13
2	D	401	GDD	C3'-C4'-C5'-O5'
3	G	402	OLC	C4-C5-C6-C7
3	G	401	OLC	C10-C11-C12-C13
3	D	402	OLC	C9-C10-C11-C12
3	G	401	OLC	C15-C16-C17-C18
3	A	403	OLC	C7-C8-C9-C10
2	A	401	GDD	C4'-C5'-O5'-PA
3	A	403	OLC	C9-C10-C11-C12
2	E	401	GDD	PA-O3A-PB-O3B
3	C	401	OLC	C7-C8-C9-C10
3	E	402	OLC	C14-C15-C16-C17
3	D	402	OLC	C7-C8-C9-C10
3	G	401	OLC	C6-C7-C8-C9
2	E	401	GDD	O4'-C4'-C5'-O5'
3	C	402	OLC	C9-C10-C11-C12
3	A	403	OLC	C14-C15-C16-C17
3	D	402	OLC	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	401	OLC	C2-C3-C4-C5
2	A	401	GDD	PB-O3A-PA-O1A
2	A	401	GDD	PB-O3A-PA-O2A
3	C	401	OLC	C9-C10-C11-C12
2	D	401	GDD	C5'-O5'-PA-O1A
3	E	402	OLC	O20-C1-C2-C3
3	C	402	OLC	C7-C8-C9-C10

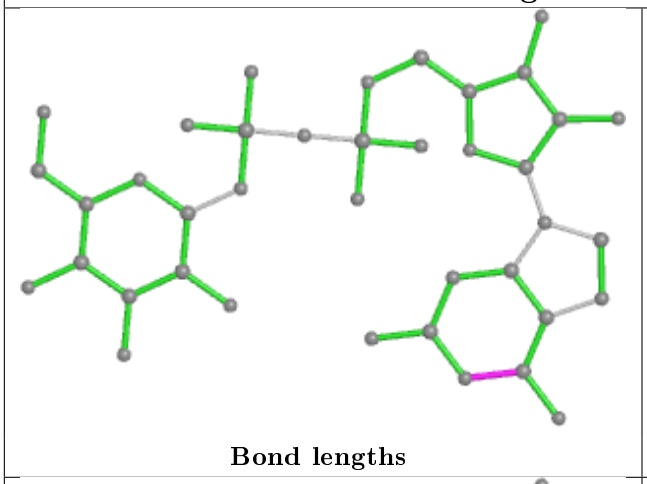
There are no ring outliers.

10 monomers are involved in 16 short contacts:

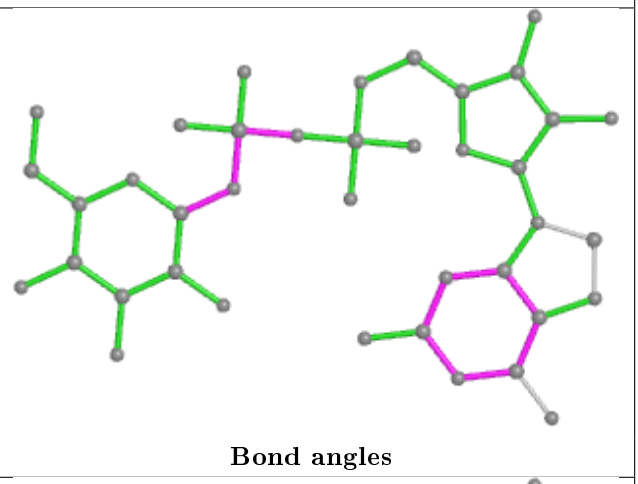
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	OLC	1	0
2	E	401	GDD	4	0
3	D	402	OLC	2	0
3	G	401	OLC	3	0
3	E	402	OLC	1	0
3	G	402	OLC	1	0
3	C	401	OLC	1	0
3	A	402	OLC	1	0
2	D	401	GDD	1	0
3	C	402	OLC	1	0

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.

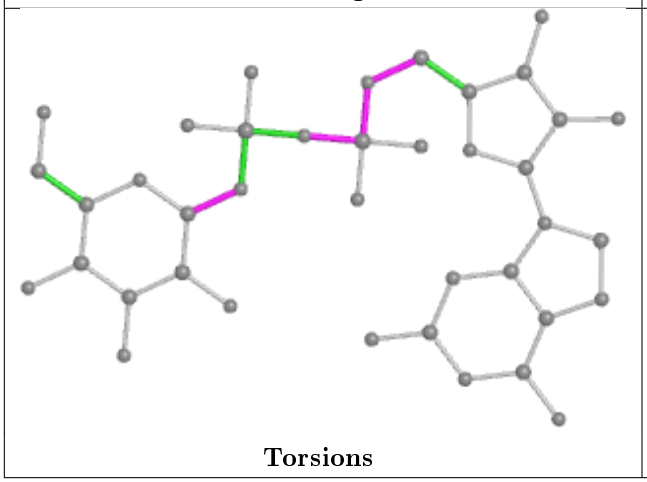
Ligand GDD A 401



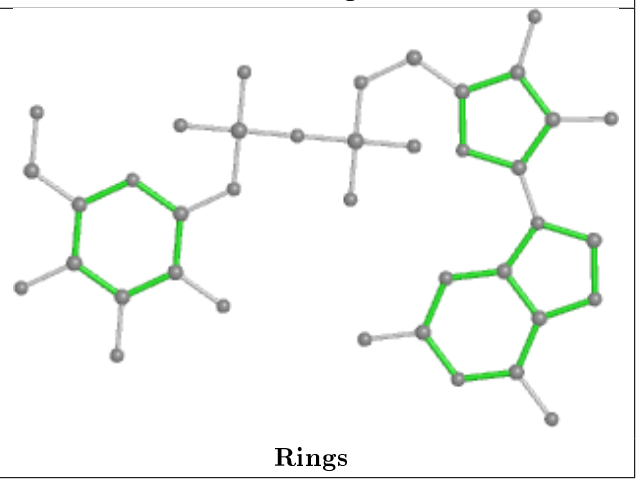
Bond lengths



Bond angles

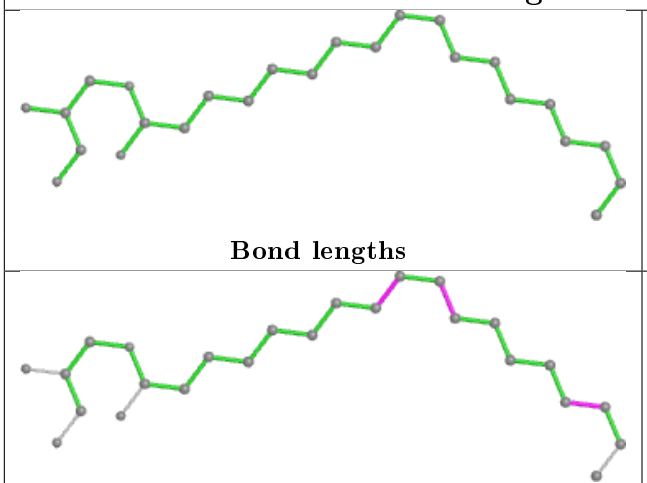


Torsions

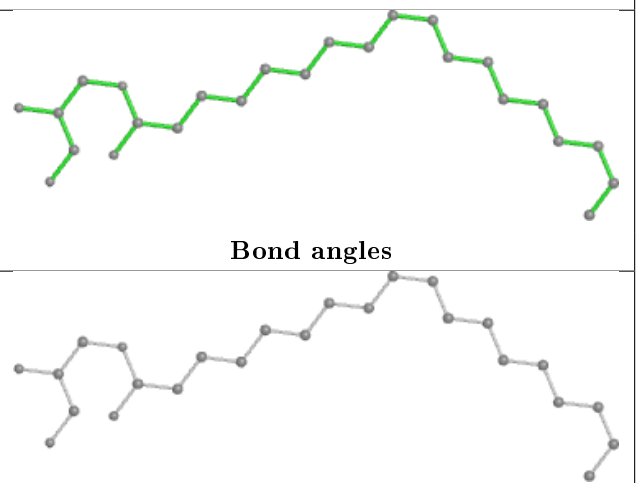


Rings

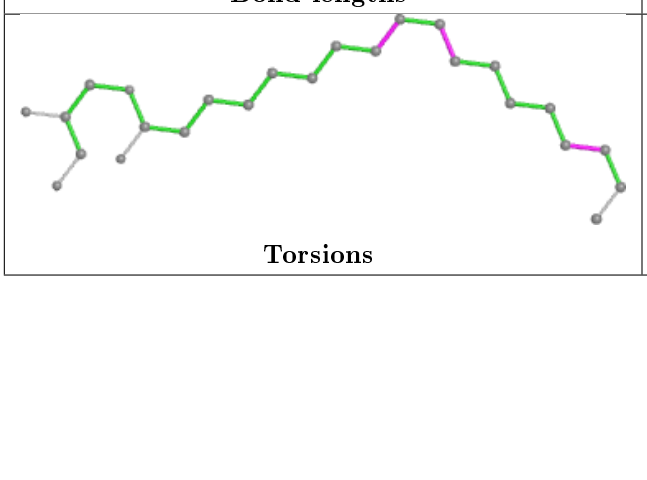
Ligand OLC A 403



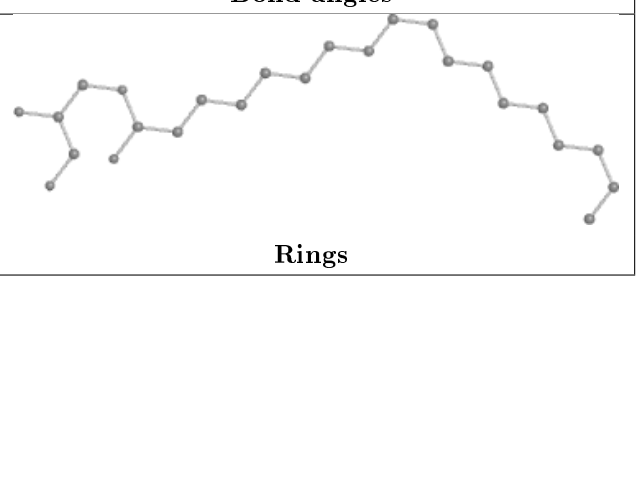
Bond lengths



Bond angles

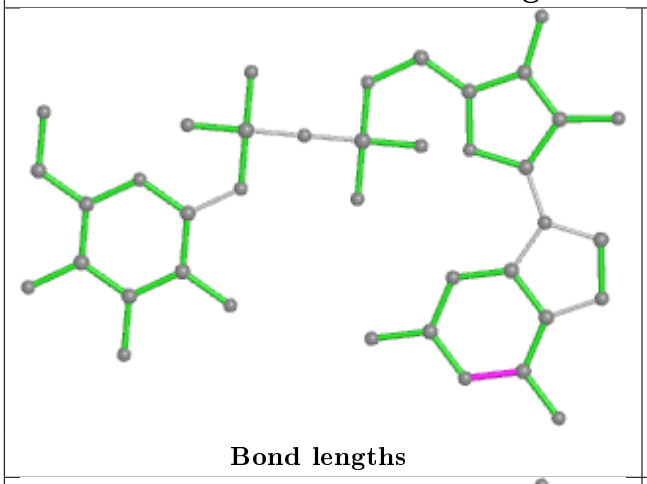


Torsions

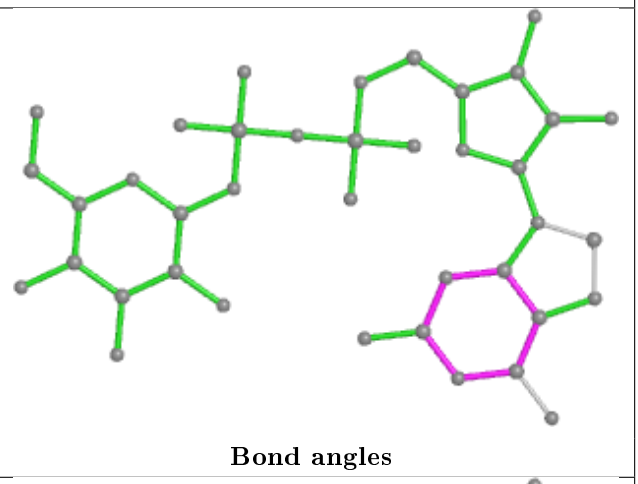


Rings

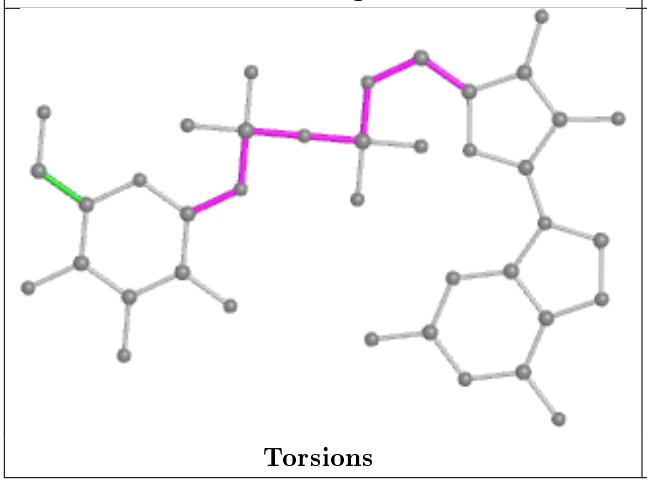
Ligand GDD E 401



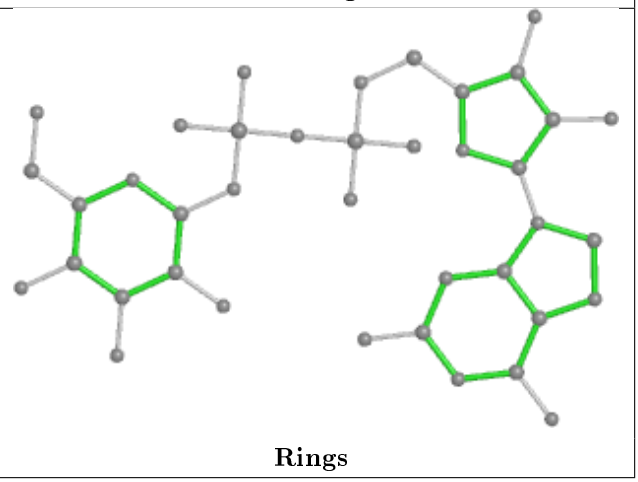
Bond lengths



Bond angles

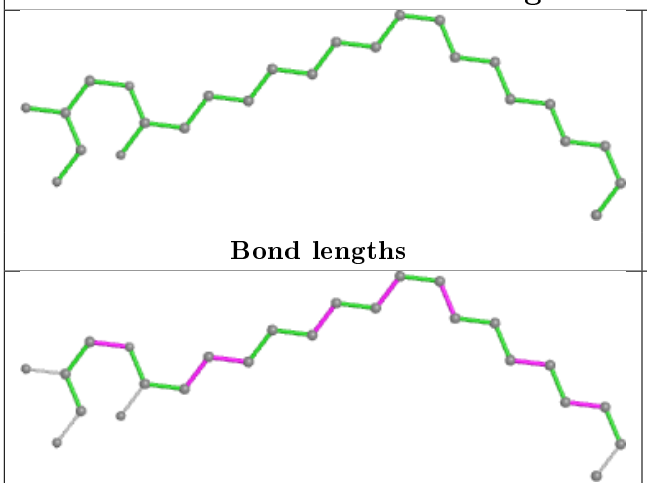


Torsions

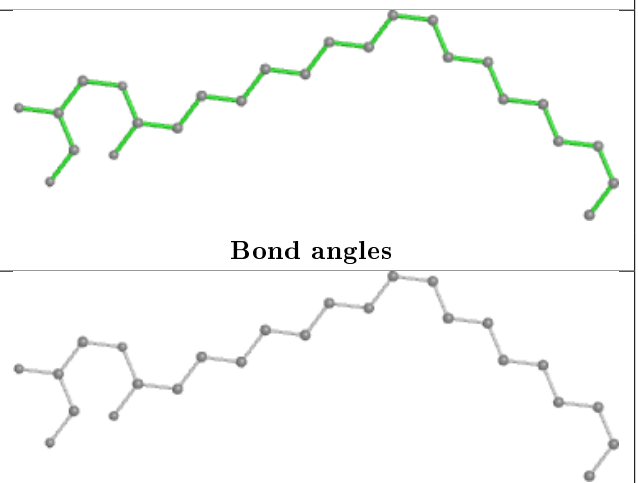


Rings

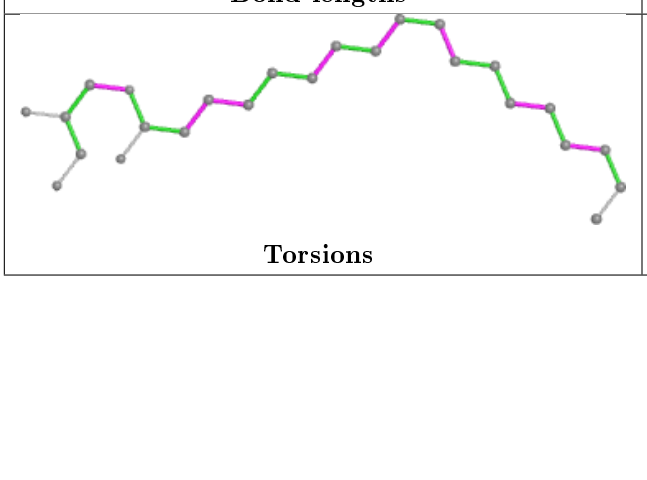
Ligand OLC D 402



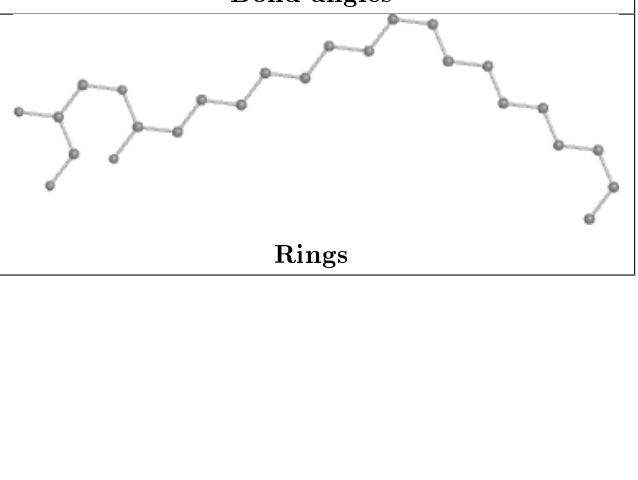
Bond lengths



Bond angles

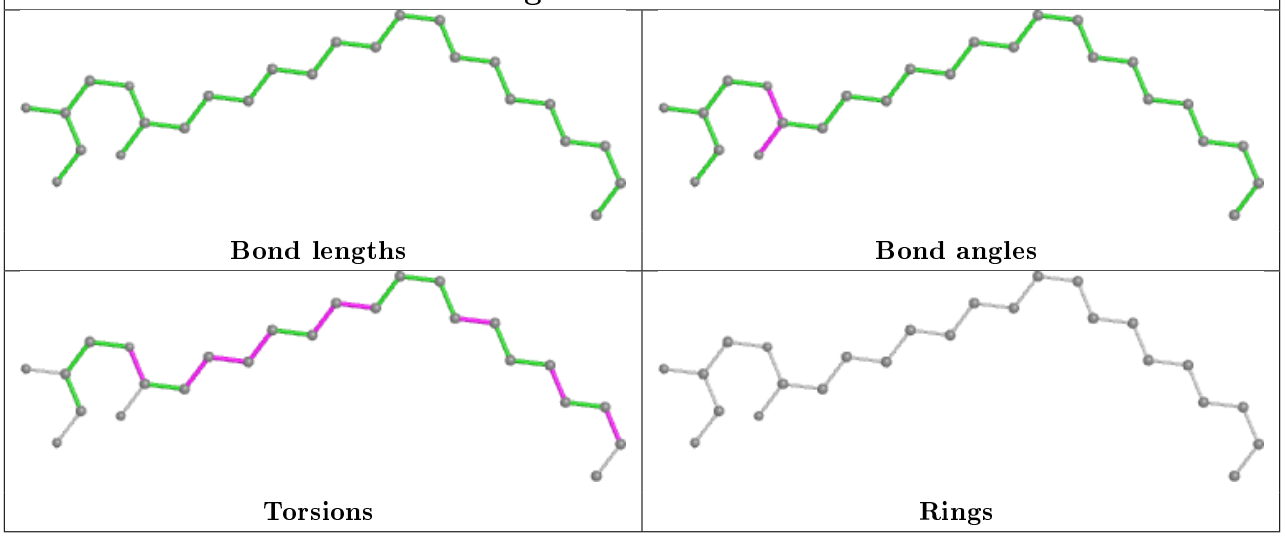


Torsions

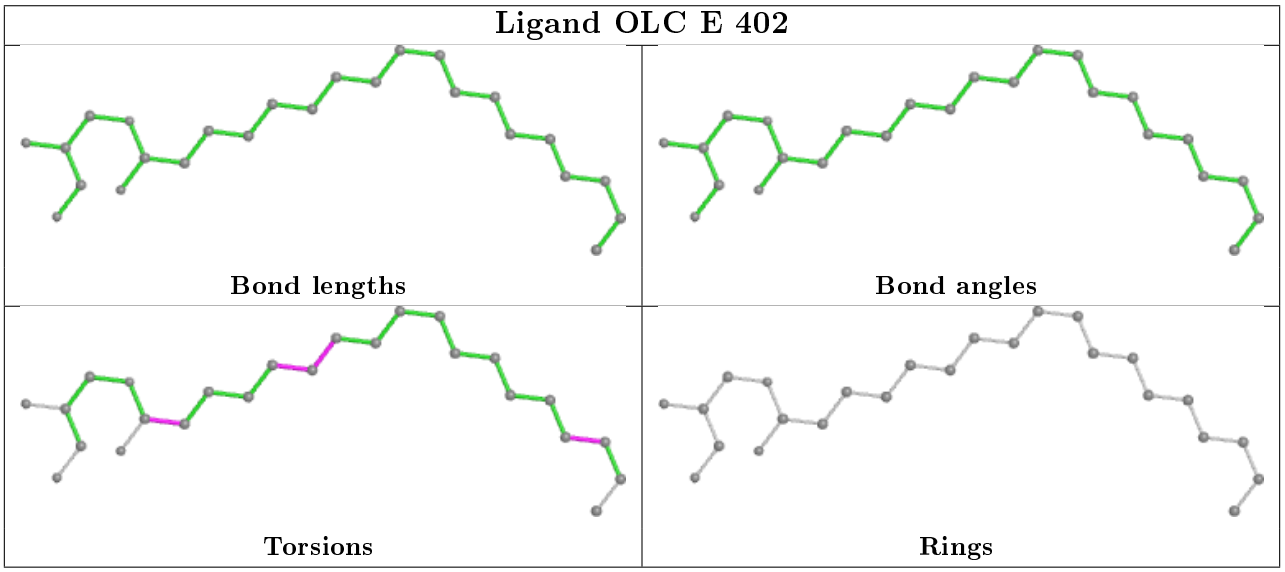


Rings

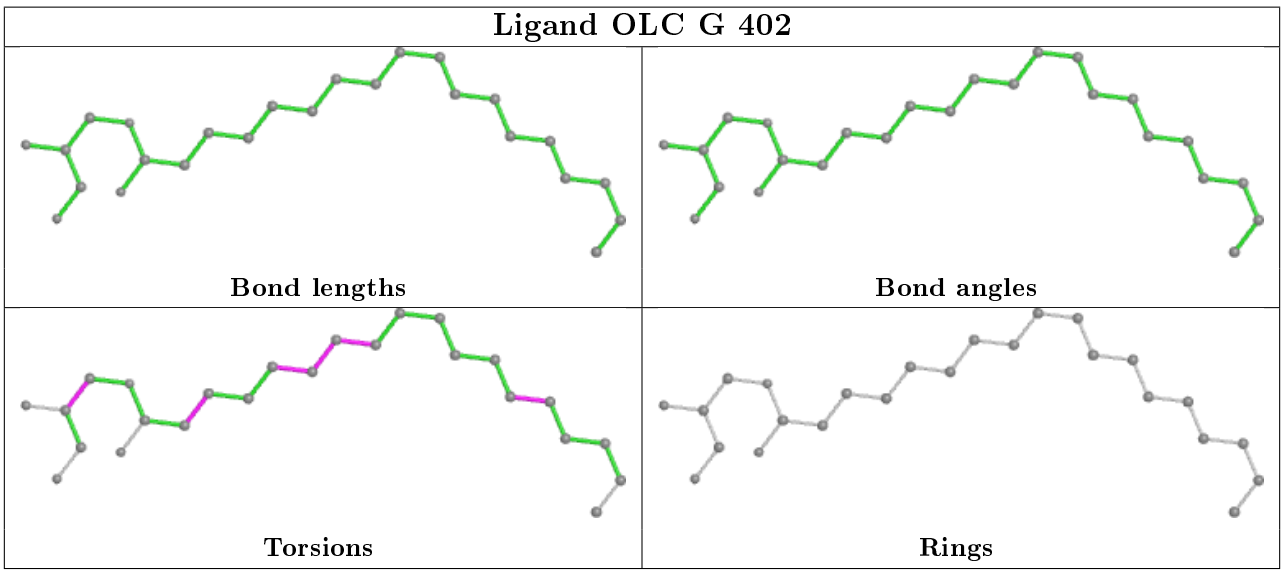
Ligand OLC G 401



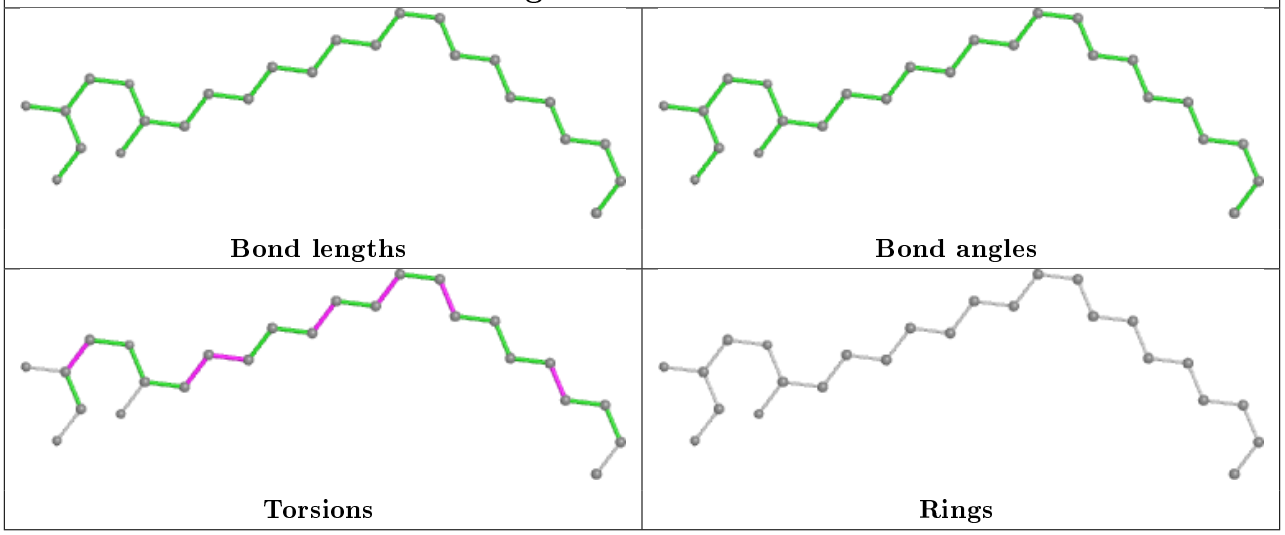
Ligand OLC E 402



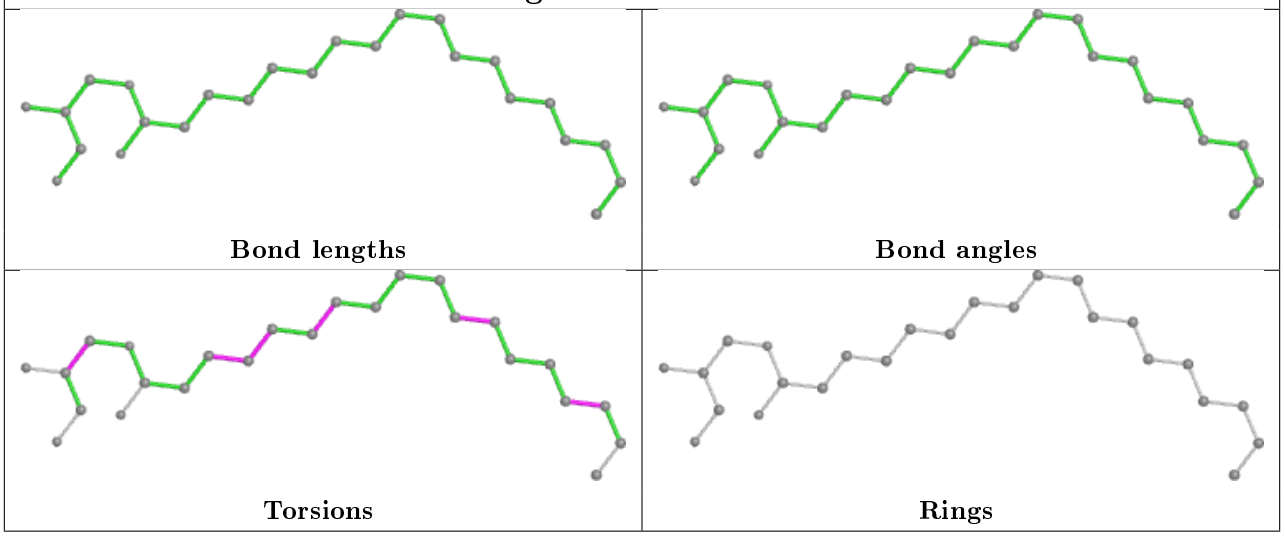
Ligand OLC G 402



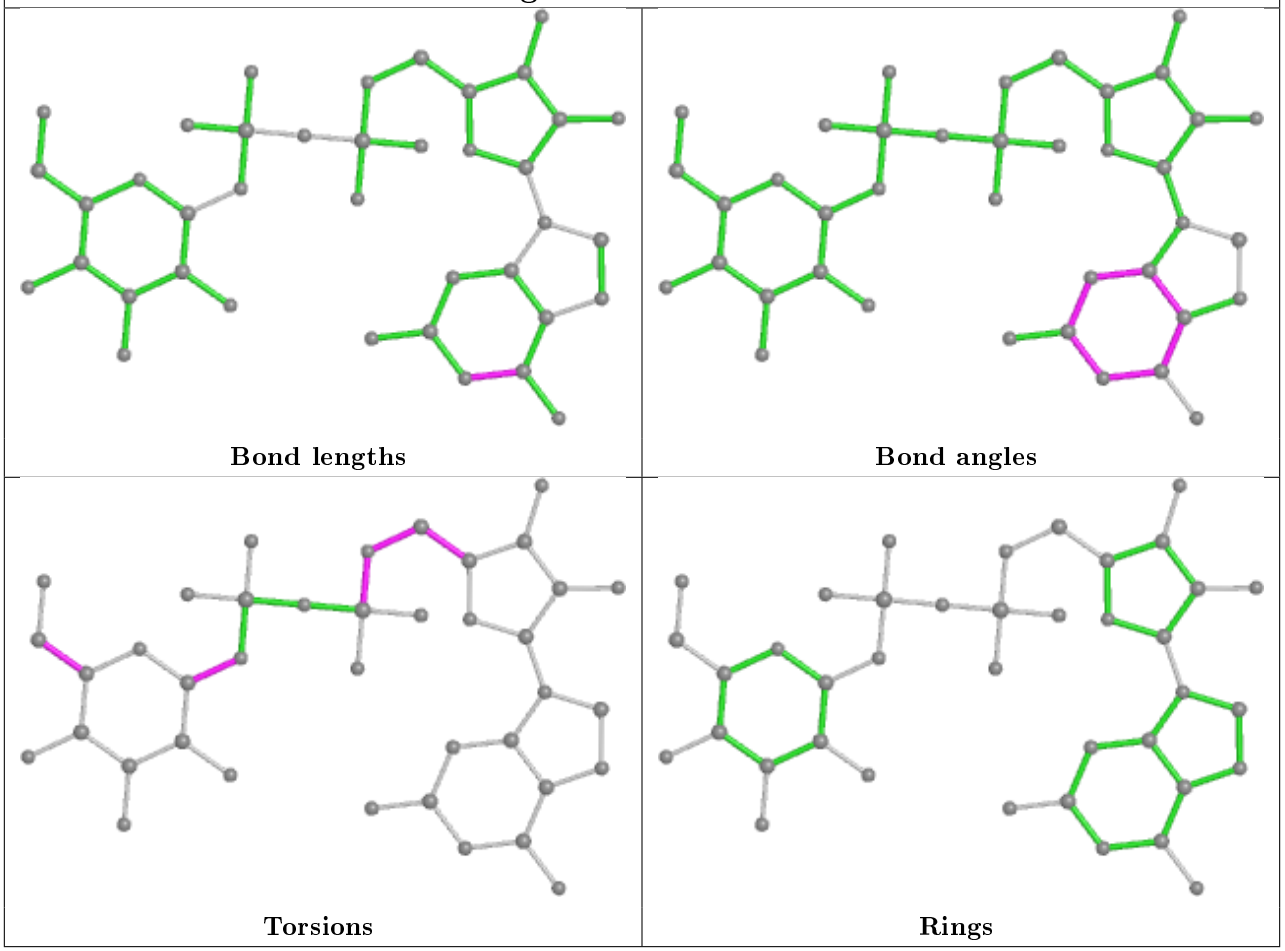
Ligand OLC C 401



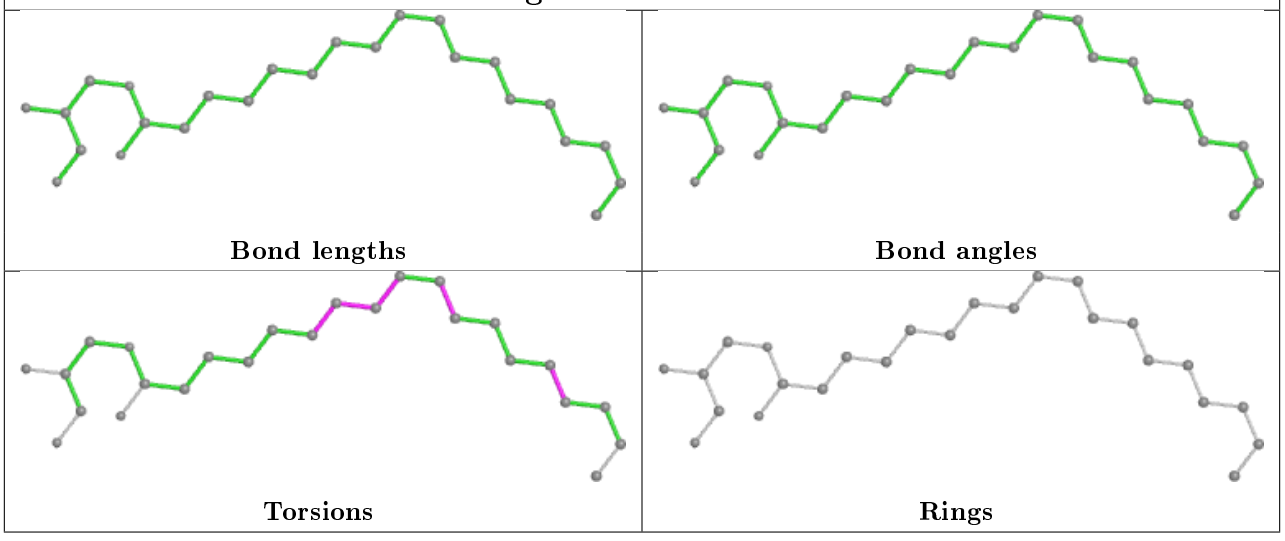
Ligand OLC A 402



Ligand GDD D 401



Ligand OLC C 402



5.7 Other polymers (i)

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	292/337 (86%)	-0.44	6 (2%)	63	48	56, 78, 111, 138	0
1	B	297/337 (88%)	-0.37	4 (1%)	77	63	54, 81, 128, 159	0
1	C	294/337 (87%)	-0.38	4 (1%)	75	61	58, 78, 114, 144	0
1	D	294/337 (87%)	-0.36	7 (2%)	59	42	55, 81, 112, 148	0
1	E	298/337 (88%)	-0.38	8 (2%)	54	38	55, 81, 130, 159	0
1	F	294/337 (87%)	-0.40	1 (0%)	94	88	58, 79, 127, 149	0
1	G	296/337 (87%)	-0.49	1 (0%)	94	88	58, 75, 109, 133	0
1	H	294/337 (87%)	-0.35	5 (1%)	70	55	58, 81, 125, 159	0
All	All	2359/2696 (87%)	-0.39	36 (1%)	73	60	54, 79, 121, 159	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	ASP	5.7
1	H	47	ASP	4.9
1	D	240	SER	4.7
1	E	331	GLN	4.0
1	D	237	ASP	3.9
1	D	244	THR	3.4
1	C	333	GLN	3.4
1	A	245	ASN	3.0
1	E	47	ASP	2.8
1	E	246	ASN	2.8
1	H	244	THR	2.8
1	A	240	SER	2.8
1	C	240	SER	2.7
1	H	242	ASN	2.7
1	B	48	PHE	2.7
1	D	241	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	245	ASN	2.6
1	H	249	ASN	2.6
1	A	135	GLY	2.6
1	D	239	SER	2.5
1	B	79	SER	2.5
1	E	48	PHE	2.5
1	C	244	THR	2.4
1	A	241	VAL	2.3
1	G	245	ASN	2.3
1	B	180	SER	2.3
1	C	245	ASN	2.2
1	E	236	GLU	2.2
1	H	331	GLN	2.2
1	A	237	ASP	2.1
1	E	247	PHE	2.1
1	D	333	GLN	2.1
1	F	331	GLN	2.1
1	E	244	THR	2.0
1	D	132	PHE	2.0
1	A	132	PHE	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, 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
2	GDD	A	401	39/39	0.84	0.17	77,109,140,149	0
3	OLC	E	402	25/25	0.84	0.48	57,90,114,118	0
2	GDD	D	401	39/39	0.84	0.22	77,100,121,129	64

Continued on next page...

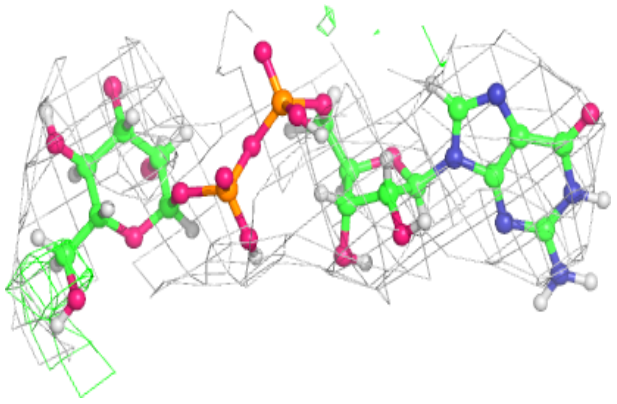
Continued from previous page...

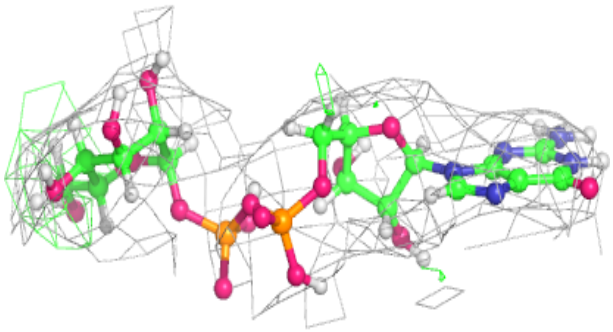
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OLC	G	402	25/25	0.86	0.62	45,89,131,154	0
3	OLC	D	402	25/25	0.86	0.47	64,87,108,121	0
3	OLC	C	402	25/25	0.86	0.48	56,90,108,111	0
2	GDD	E	401	39/39	0.87	0.16	93,126,152,161	0
3	OLC	G	401	25/25	0.89	0.66	63,95,145,164	0
3	OLC	A	403	25/25	0.90	0.31	56,85,105,112	0
3	OLC	A	402	25/25	0.90	0.47	37,73,112,115	0
3	OLC	C	401	25/25	0.91	0.44	51,84,115,127	0

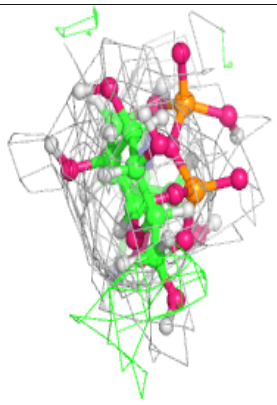
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDD A 401:

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

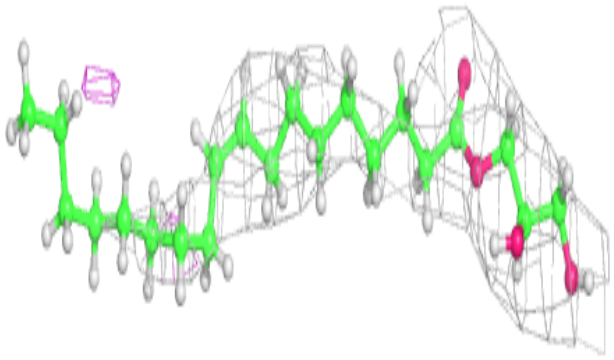


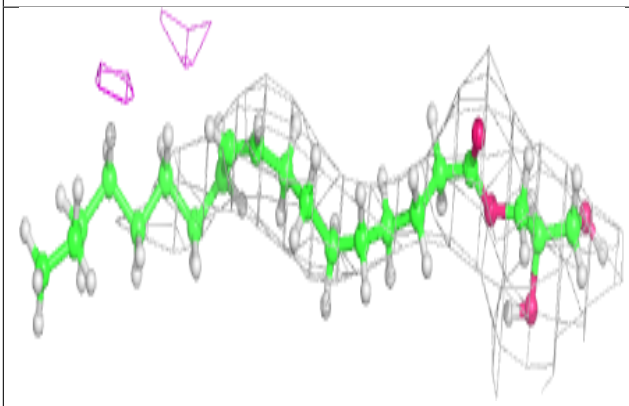


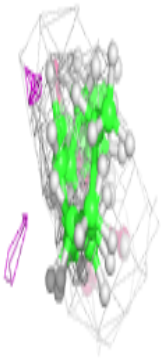


Electron density around OLC E 402:

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

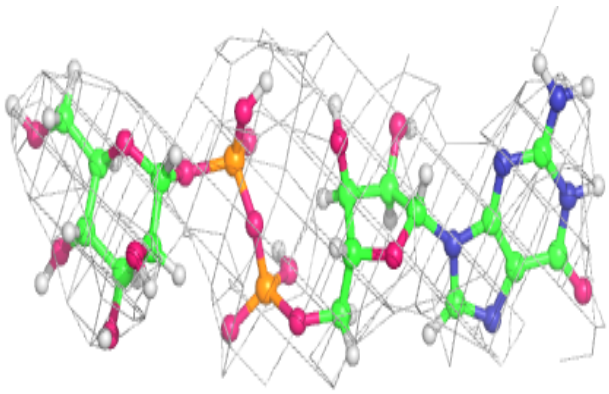


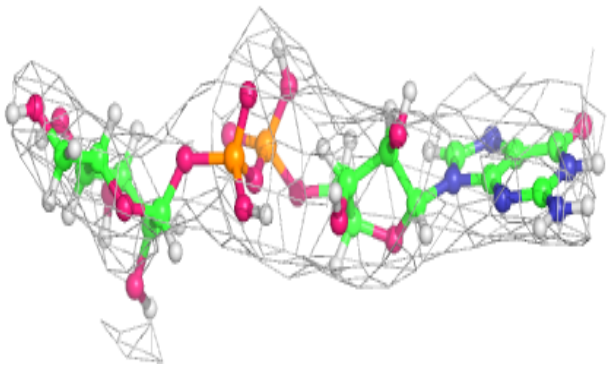


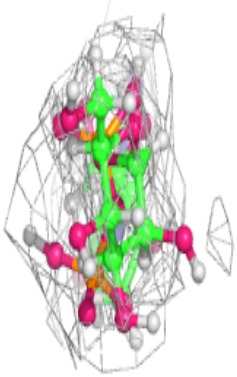


Electron density around GDD D 401:

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

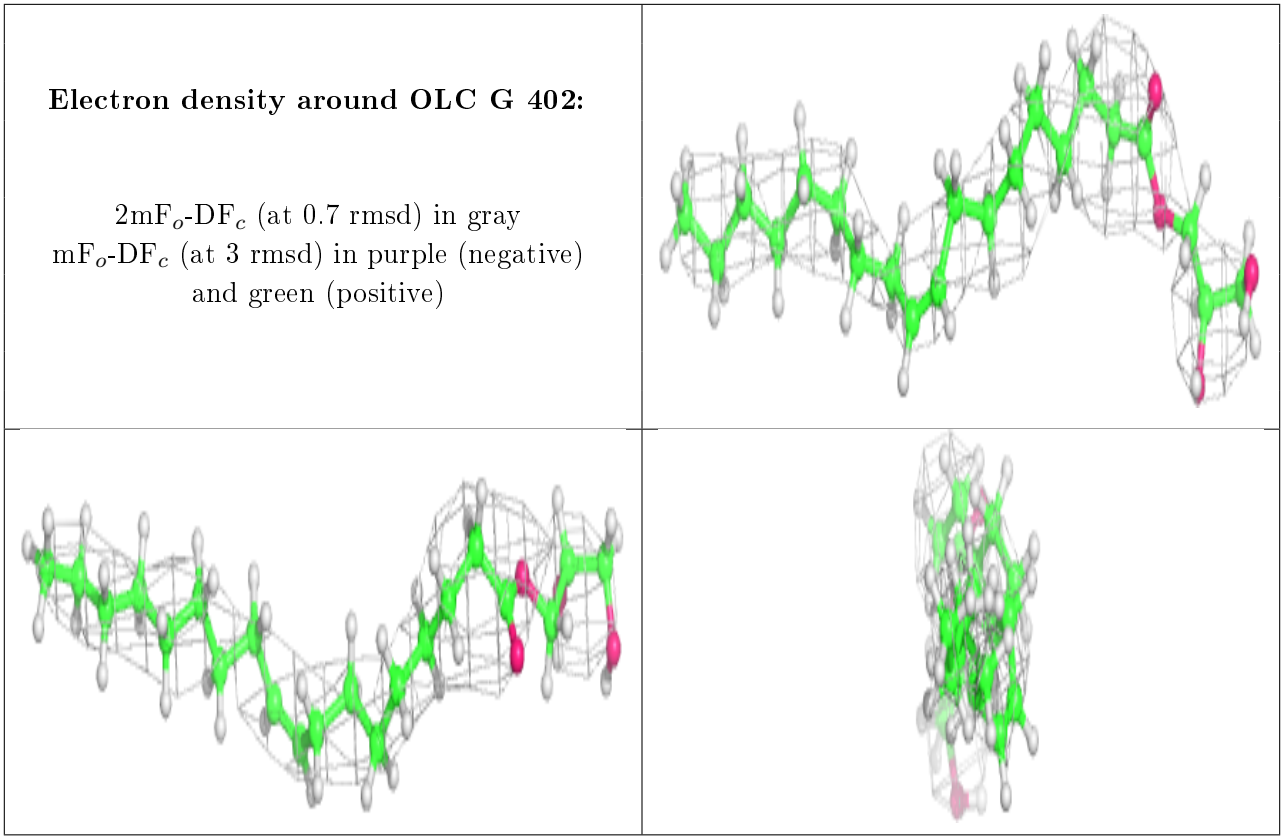






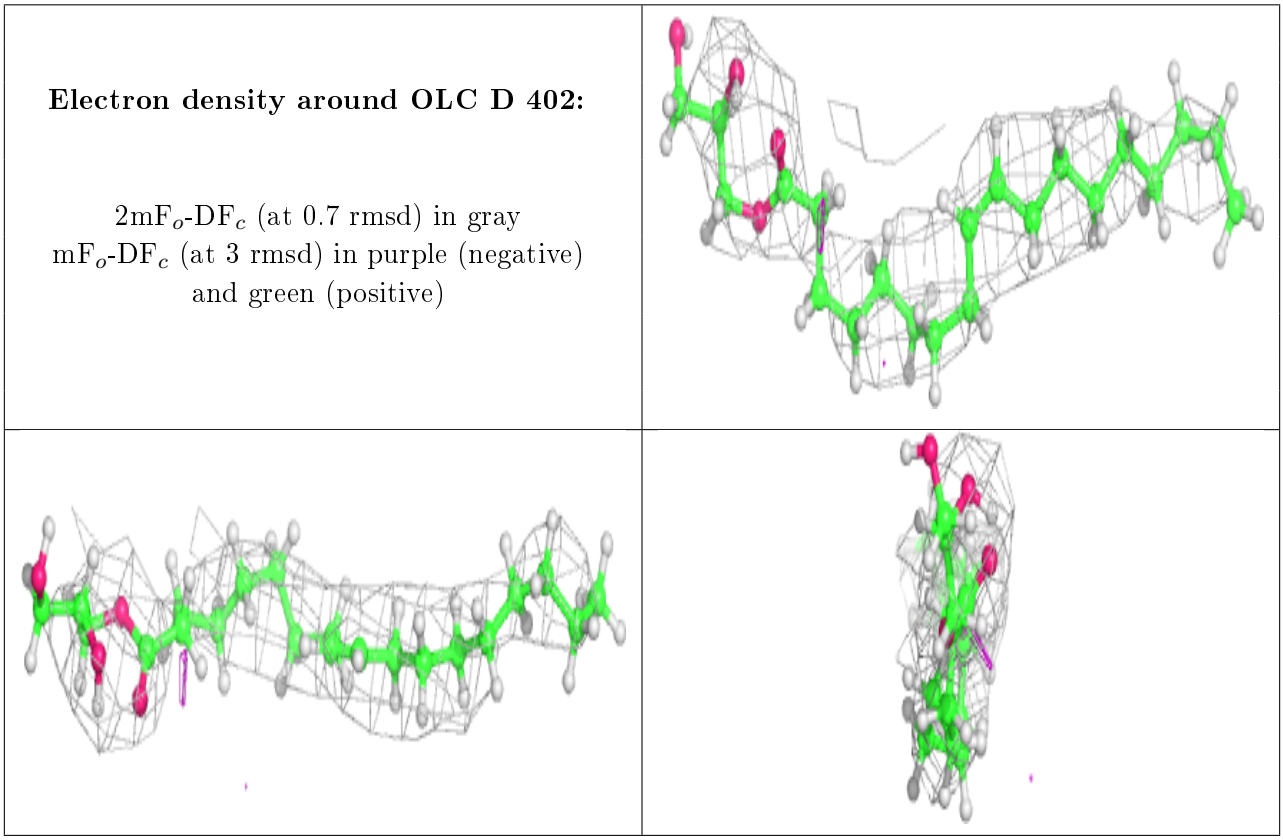
Electron density around OLC G 402:

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



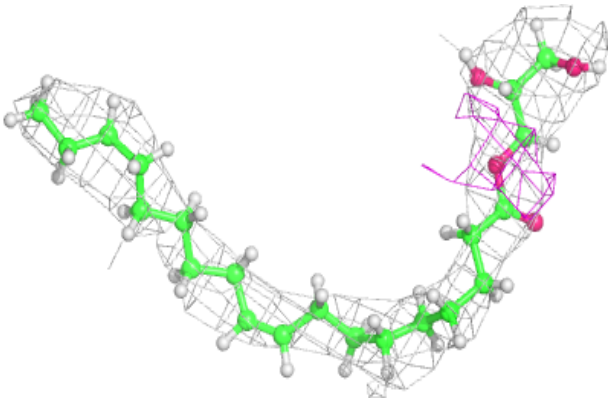
Electron density around OLC D 402:

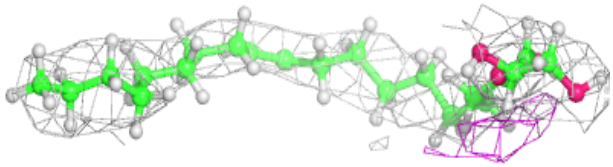
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

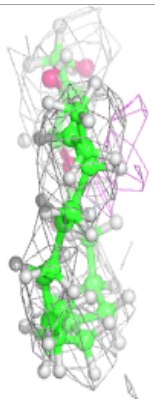


Electron density around OLC C 402:

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

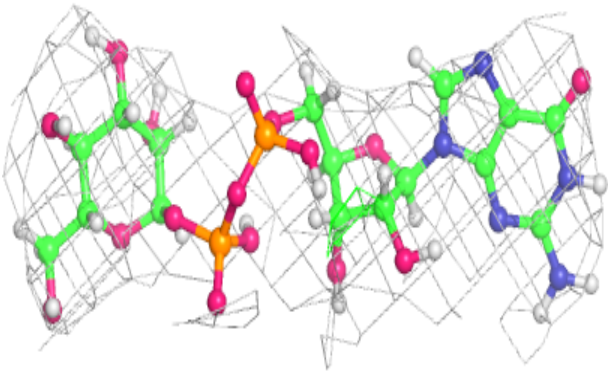


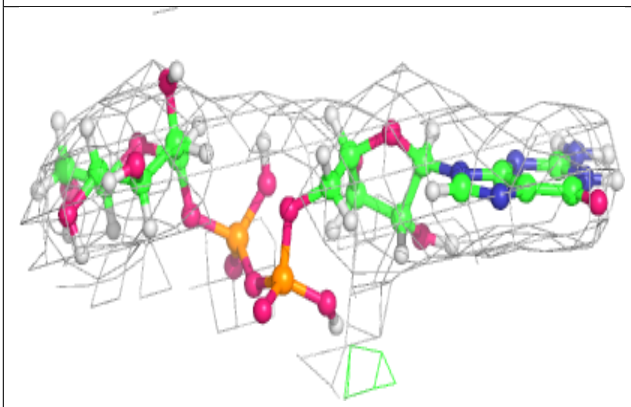


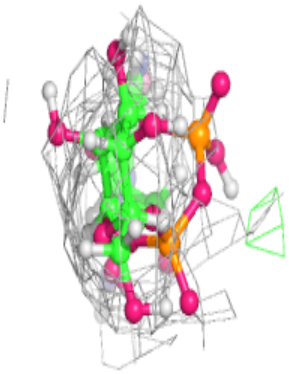


Electron density around GDD E 401:

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

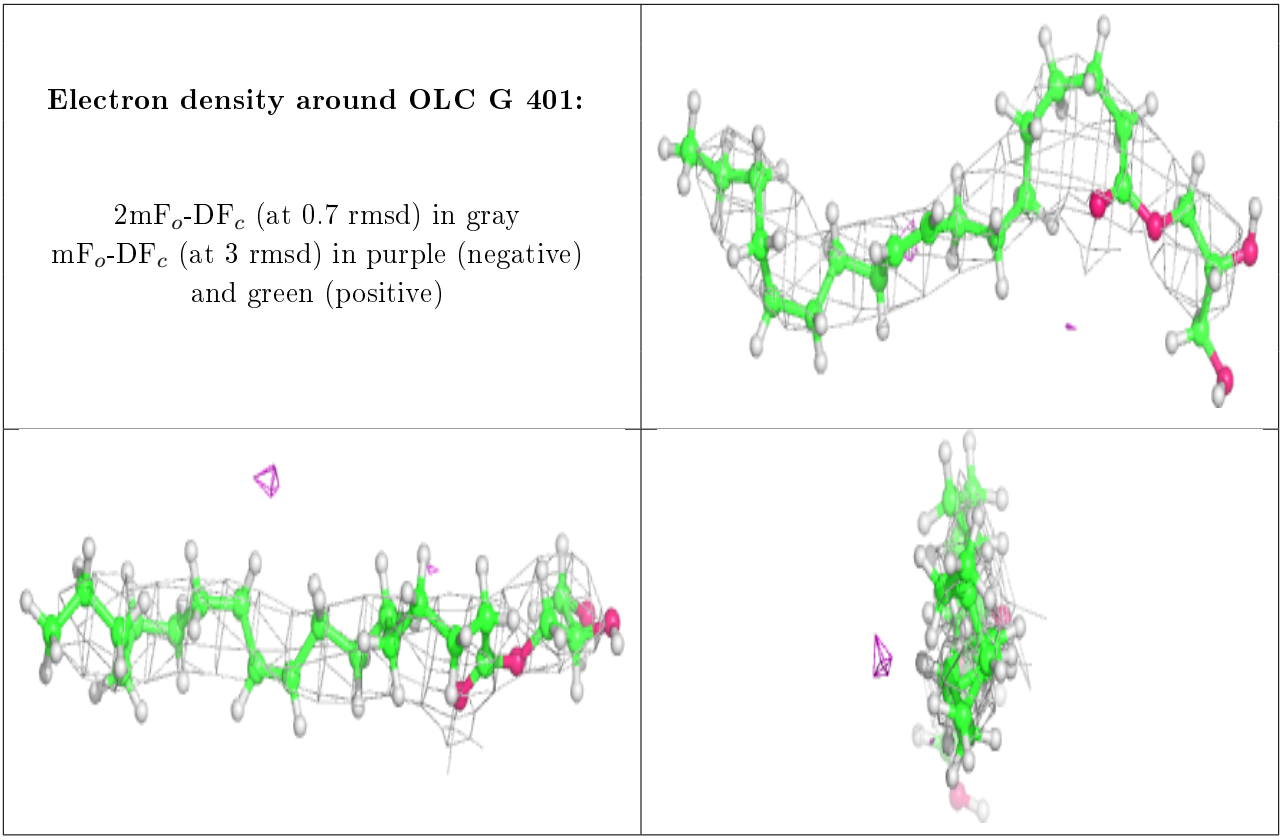






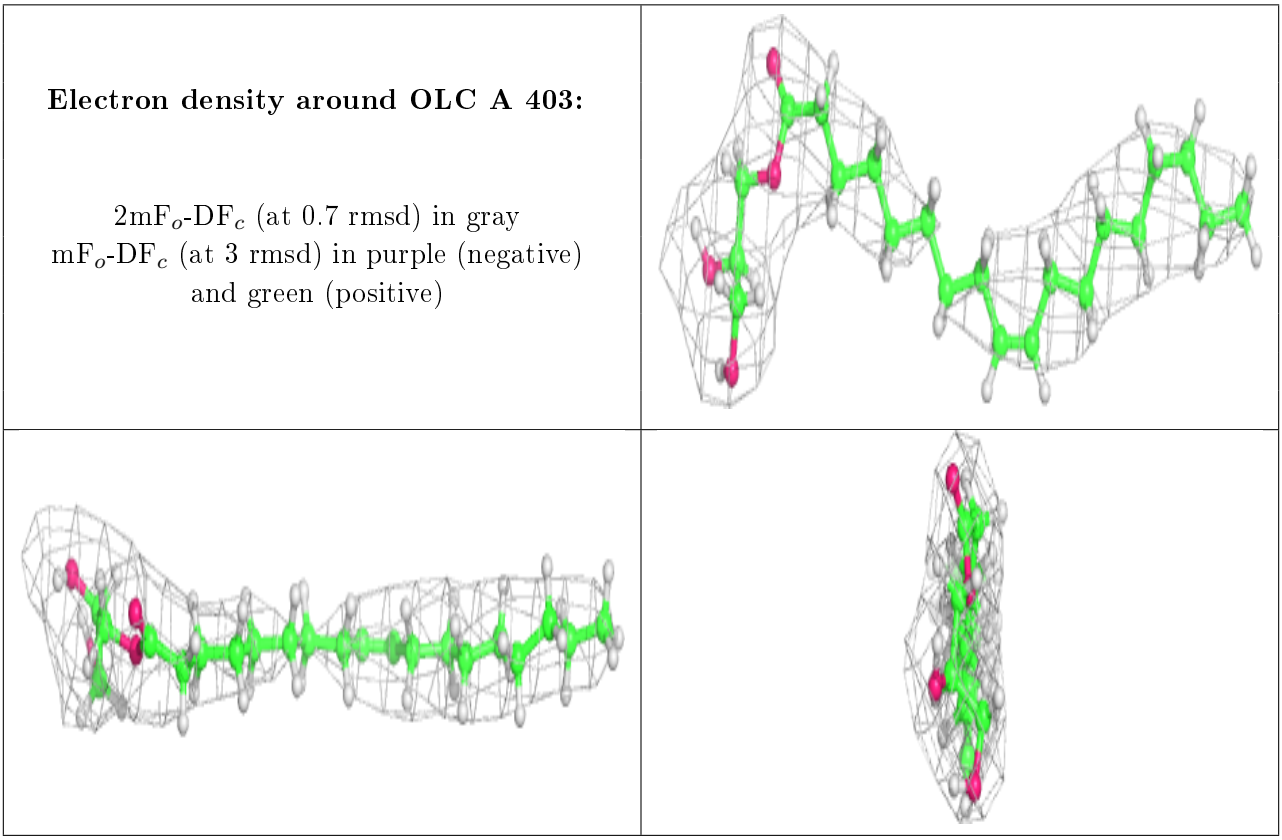
Electron density around OLC G 401:

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



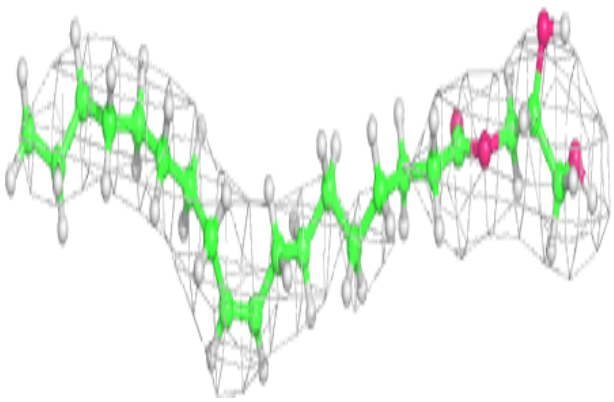
Electron density around OLC A 403:

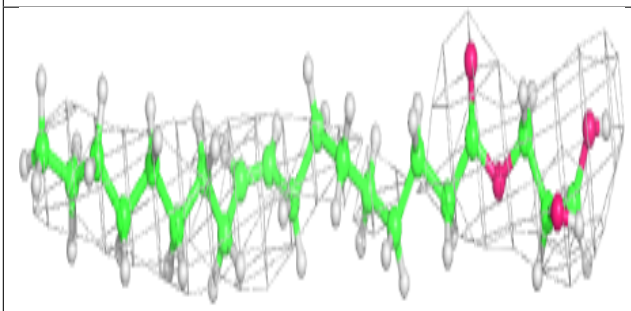
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

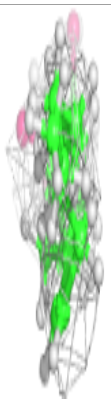


Electron density around OLC A 402:

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

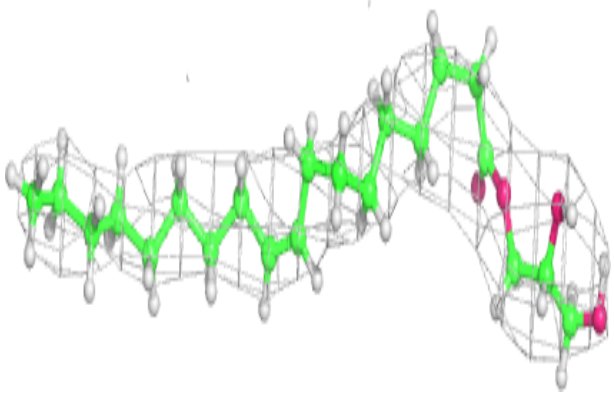


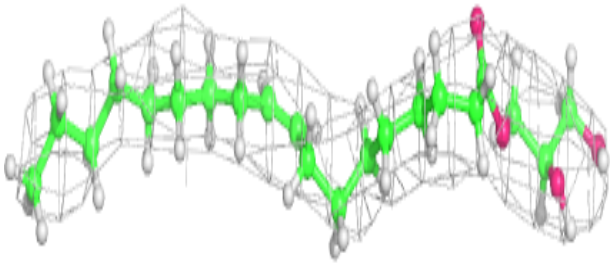


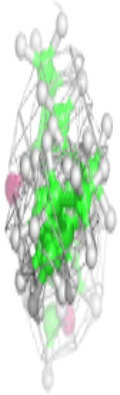


Electron density around OLC C 401:

$2mF_o$-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.