



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 04:55 pm BST

PDB ID : 1AQX  
Title : GLUTATHIONE S-TRANSFERASE IN COMPLEX WITH MEISEN-HEIMER COMPLEX  
Authors : Prade, L.; Huber, R.; Manoharan, T.H.; Fahl, W.E.; Reuter, W.  
Deposited on : 1997-08-03  
Resolution : 2.00 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](mailto: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.

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

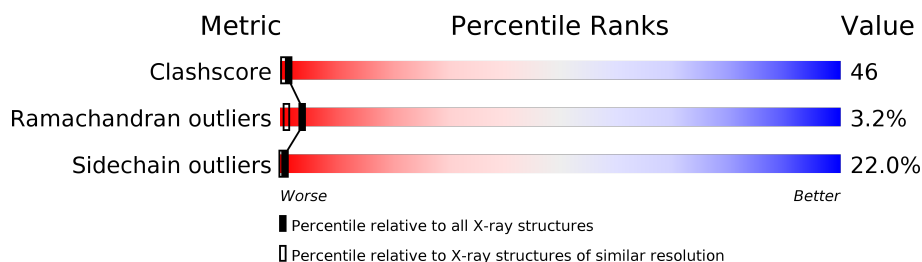
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	209	
1	B	209	
1	C	209	
1	D	209	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GTD	D	2401	-	-	X	-

## 2 Entry composition [i](#)

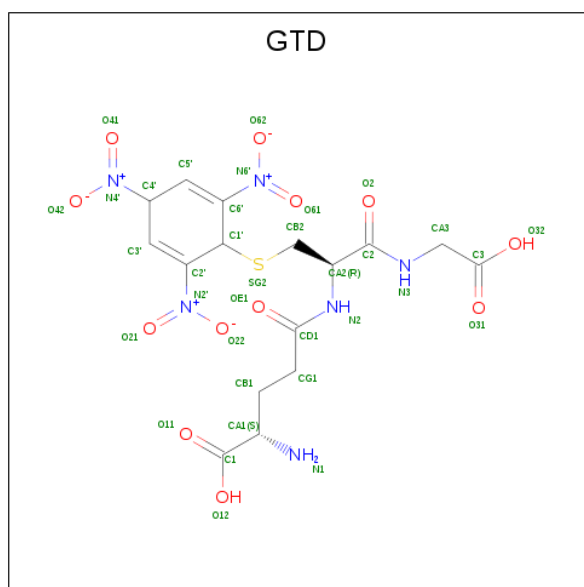
There are 4 unique types of molecules in this entry. The entry contains 7262 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1631	1047	271	307	6			
1	B	208	Total	C	N	O	S	0	0	0
			1631	1047	271	307	6			
1	C	208	Total	C	N	O	S	0	0	0
			1631	1047	271	307	6			
1	D	208	Total	C	N	O	S	0	0	0
			1631	1047	271	307	6			

- Molecule 2 is 1-(S-GLUTATHIONYL)-2,4,6-TRINITROCYCLOHEXA-2,5-DIENE (three-letter code: GTD) (formula: C<sub>16</sub>H<sub>20</sub>N<sub>6</sub>O<sub>12</sub>S).



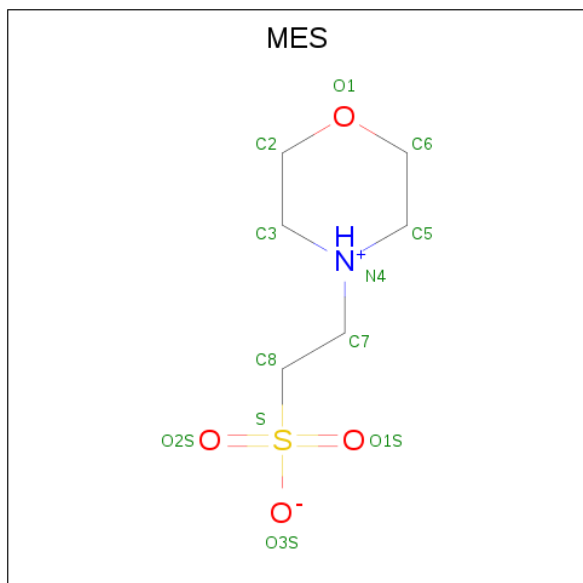
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	16	6	12	1		
2	B	1	Total	C	N	O	S	0	0
			35	16	6	12	1		

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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total	O	0	0
			135	135		
4	B	127	Total	O	0	0
			127	127		
4	C	144	Total	O	0	0
			144	144		

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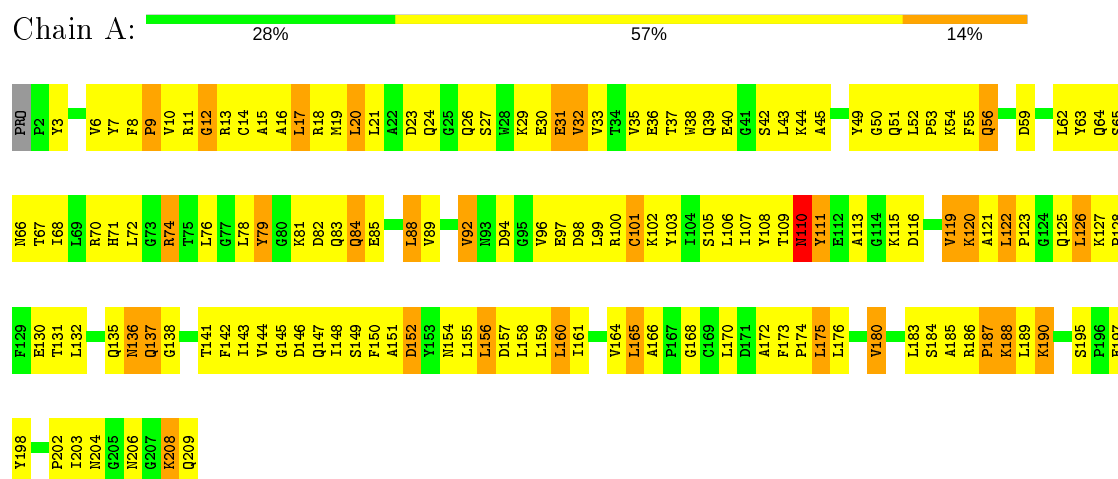
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	144	Total	O	0	0
			144	144		

### 3 Residue-property plots

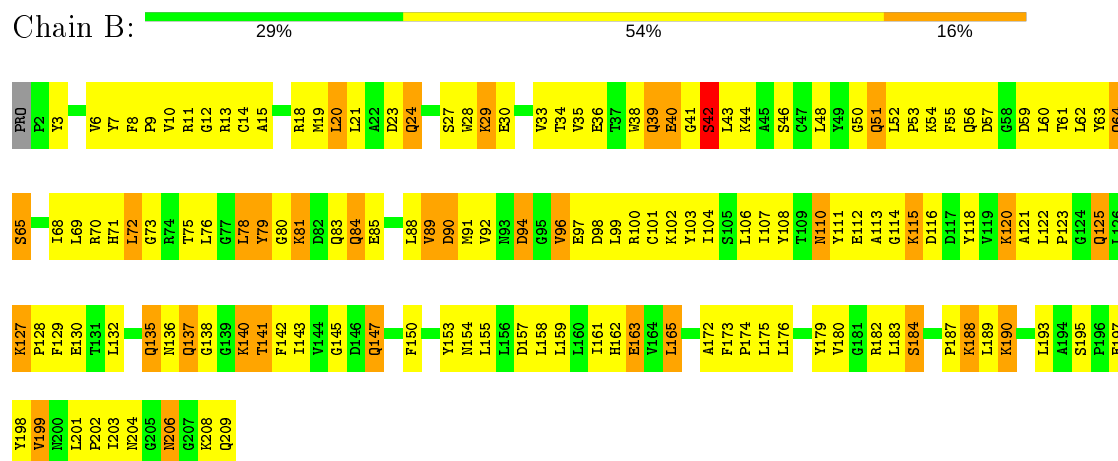
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

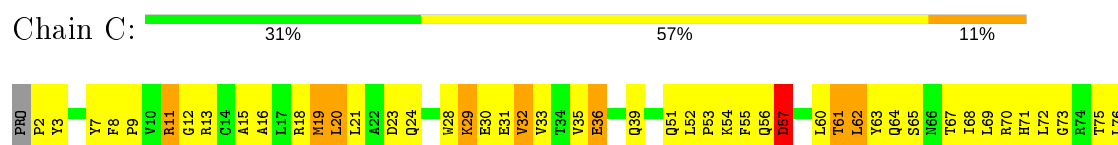
#### • Molecule 1: GLUTATHIONE S-TRANSFERASE

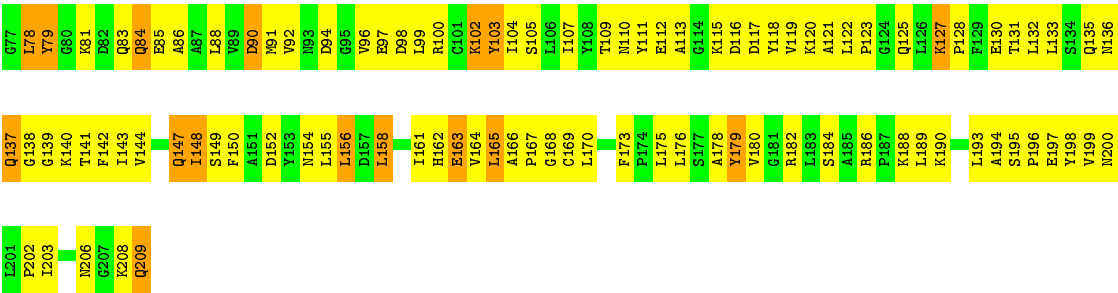


#### • Molecule 1: GLUTATHIONE S-TRANSFERASE

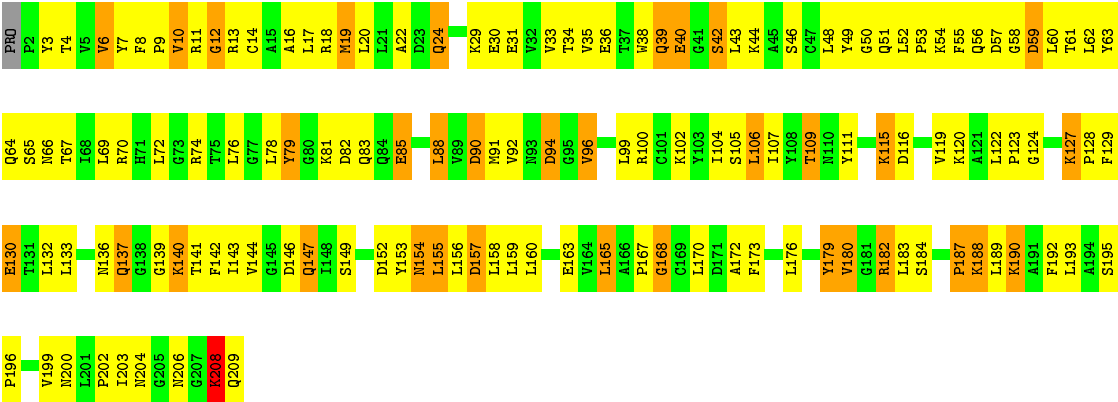
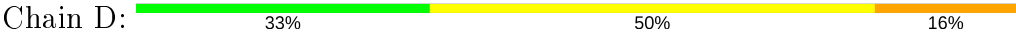


#### • Molecule 1: GLUTATHIONE S-TRANSFERASE





● Molecule 1: GLUTATHIONE S-TRANSFERASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.59 Å 72.57 Å 69.34 Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	7.00 – 2.00	Depositor
% Data completeness (in resolution range)	90.0 (7.00-2.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.5	Depositor
R, $R_{free}$	0.202 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7262	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.41	0/1665	0.68	0/2257
1	B	0.42	0/1665	0.71	0/2257
1	C	0.41	0/1665	0.70	0/2257
1	D	0.42	0/1665	0.74	0/2257
All	All	0.41	0/6660	0.71	0/9028

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1631	0	1634	169	0
1	B	1631	0	1634	145	0
1	C	1631	0	1634	151	0
1	D	1631	0	1634	171	0
2	A	35	0	17	4	0
2	B	35	0	17	4	0
2	C	35	0	17	1	0
2	D	35	0	17	10	0
3	A	12	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	13	2	0
3	C	12	0	13	0	0
3	D	12	0	13	0	0
4	A	135	0	0	20	5
4	B	127	0	0	19	1
4	C	144	0	0	17	2
4	D	144	0	0	16	4
All	All	7262	0	6656	618	6

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 46.

All (618) 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:C:92:VAL:HG11	1:C:143:ILE:HG12	1.36	1.06
1:B:110:ASN:HD21	1:B:113:ALA:HB3	1.25	1.01
1:D:36:GLU:HA	1:D:39:GLN:HB2	1.46	0.98
1:B:120:LYS:HE3	1:B:121:ALA:HB2	1.48	0.95
1:D:81:LYS:HD2	1:D:147:GLN:HE21	1.38	0.89
1:A:99:LEU:HD23	1:A:158:LEU:HD21	1.52	0.89
1:C:163:GLU:OE1	1:C:167:PRO:HA	1.73	0.88
1:A:111:TYR:HB3	1:A:208:LYS:HE3	1.57	0.87
1:C:19:MET:HE1	1:C:156:LEU:HD23	1.58	0.86
1:A:10:VAL:HG12	1:A:202:PRO:HG2	1.55	0.85
1:B:38:TRP:HE1	1:B:44:LYS:HE2	1.39	0.85
1:B:71:HIS:O	1:B:75:THR:HG23	1.77	0.85
1:D:6:VAL:HG21	1:D:54:LYS:HD3	1.58	0.84
1:A:7:TYR:HE2	1:A:10:VAL:HG23	1.41	0.84
1:C:136:ASN:O	1:C:138:GLY:N	2.10	0.84
1:C:35:VAL:O	1:C:39:GLN:HG3	1.78	0.84
1:A:159:LEU:HD22	1:A:170:LEU:HD21	1.61	0.83
1:B:14:CYS:SG	1:B:53:PRO:HB3	2.19	0.82
1:B:110:ASN:ND2	1:B:113:ALA:HB3	1.94	0.81
1:D:100:ARG:HH21	1:D:154:ASN:ND2	1.77	0.81
1:C:92:VAL:O	1:C:96:VAL:HG23	1.80	0.81
1:D:6:VAL:HB	1:D:54:LYS:HB3	1.61	0.81
1:C:90:ASP:HB3	1:D:67:THR:HG23	1.61	0.80
1:D:35:VAL:O	1:D:39:GLN:HB2	1.82	0.80
1:C:3:TYR:HD1	1:C:57:ASP:HB2	1.45	0.80
1:B:100:ARG:O	1:B:104:ILE:HG13	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:HH21	1:A:154:ASN:ND2	1.80	0.79
1:A:7:TYR:HA	1:A:52:LEU:HD13	1.63	0.79
1:C:130:GLU:OE1	1:C:173:PHE:HB3	1.83	0.78
1:D:130:GLU:HG2	1:D:173:PHE:HB3	1.64	0.78
1:C:31:GLU:O	1:C:32:VAL:O	2.02	0.78
1:D:136:ASN:O	1:D:137:GLN:HB2	1.81	0.78
1:C:65:SER:HA	1:C:68:ILE:HD12	1.66	0.78
1:D:184:SER:O	1:D:190:LYS:HB2	1.84	0.77
1:D:96:VAL:HG22	1:D:158:LEU:HD22	1.66	0.77
1:D:10:VAL:HG21	2:D:2401:GTD:O62	1.85	0.77
1:A:10:VAL:HG21	2:A:2101:GTD:O62	1.85	0.77
1:D:44:LYS:O	1:D:50:GLY:HA2	1.85	0.76
1:B:129:PHE:HA	1:B:132:LEU:HD12	1.67	0.76
1:C:142:PHE:HB3	1:C:152:ASP:OD2	1.86	0.76
1:A:96:VAL:HG13	1:A:158:LEU:HD22	1.68	0.75
1:C:3:TYR:CD1	1:C:57:ASP:HB2	2.21	0.75
1:B:184:SER:O	1:B:190:LYS:HB2	1.87	0.75
1:B:163:GLU:OE1	1:B:163:GLU:HA	1.87	0.74
1:C:88:LEU:HD22	4:C:3507:HOH:O	1.86	0.74
1:C:11:ARG:HG3	1:C:203:ILE:HA	1.69	0.73
1:D:52:LEU:HB3	1:D:53:PRO:HA	1.69	0.73
1:A:7:TYR:CE2	1:A:10:VAL:HG23	2.22	0.72
1:A:110:ASN:HD21	1:A:113:ALA:HB3	1.52	0.72
1:A:156:LEU:HA	4:A:3254:HOH:O	1.90	0.72
1:D:44:LYS:HE2	2:D:2401:GTD:O32	1.89	0.72
1:A:110:ASN:ND2	1:A:113:ALA:HB3	2.04	0.72
1:D:203:ILE:CD1	1:D:209:GLN:HE21	2.03	0.71
1:A:51:GLN:HG2	2:A:2101:GTD:C2	2.20	0.71
1:D:147:GLN:CD	1:D:147:GLN:H	1.94	0.71
1:B:38:TRP:NE1	1:B:44:LYS:HE2	2.05	0.71
1:C:100:ARG:HH21	1:C:154:ASN:ND2	1.89	0.70
1:C:131:THR:O	1:C:135:GLN:HG3	1.91	0.70
1:A:142:PHE:HB3	1:A:152:ASP:OD2	1.92	0.70
1:C:96:VAL:HG21	1:C:155:LEU:HB2	1.74	0.70
1:D:82:ASP:OD1	1:D:85:GLU:HB2	1.92	0.69
1:D:81:LYS:NZ	1:D:147:GLN:HG3	2.07	0.69
1:C:130:GLU:OE1	1:C:176:LEU:HG	1.92	0.69
1:C:182:ARG:HB3	4:C:3314:HOH:O	1.92	0.69
1:C:143:ILE:HG23	1:C:144:VAL:HG23	1.75	0.69
1:A:49:TYR:N	4:A:3003:HOH:O	2.26	0.68
1:C:2:PRO:O	1:C:57:ASP:HA	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:LEU:HD11	1:D:176:LEU:HD22	1.74	0.68
1:A:202:PRO:HB2	1:A:204:ASN:O	1.94	0.68
1:A:35:VAL:O	1:A:39:GLN:HG3	1.92	0.68
1:B:106:LEU:HD11	1:B:115:LYS:HA	1.74	0.68
1:C:107:ILE:O	1:C:206:ASN:ND2	2.26	0.68
1:D:143:ILE:HG13	1:D:143:ILE:O	1.91	0.68
1:D:14:CYS:SG	1:D:53:PRO:HB3	2.34	0.68
1:C:36:GLU:HA	1:C:39:GLN:HE21	1.58	0.68
1:C:20:LEU:O	1:C:20:LEU:HD23	1.93	0.67
1:C:196:PRO:O	1:C:200:ASN:HB2	1.93	0.67
1:D:179:TYR:O	1:D:183:LEU:HD13	1.94	0.67
1:B:136:ASN:O	1:B:138:GLY:N	2.26	0.67
1:A:203:ILE:HG22	1:A:204:ASN:ND2	2.10	0.67
1:B:107:ILE:O	1:B:107:ILE:HG22	1.93	0.67
1:D:13:ARG:CD	2:D:2401:GTD:HB11	2.25	0.67
1:C:121:ALA:O	1:C:125:GLN:HG2	1.95	0.67
1:A:159:LEU:CD2	1:A:170:LEU:HD21	2.24	0.67
1:C:99:LEU:HD12	1:C:102:LYS:HD2	1.78	0.66
1:C:98:ASP:OD2	1:D:64:GLN:NE2	2.24	0.66
1:D:14:CYS:O	1:D:18:ARG:HD2	1.96	0.66
1:D:19:MET:HB2	1:D:189:LEU:HD11	1.77	0.66
1:D:99:LEU:HD23	1:D:158:LEU:HD21	1.78	0.66
1:B:10:VAL:HG21	2:B:2201:GTD:O62	1.96	0.66
1:C:99:LEU:HD23	1:C:158:LEU:HD21	1.78	0.66
1:A:127:LYS:N	1:A:128:PRO:HD2	2.10	0.66
1:A:99:LEU:HG	1:A:158:LEU:HD11	1.77	0.66
1:B:136:ASN:C	1:B:138:GLY:H	1.99	0.66
1:A:83:GLN:OE1	1:B:75:THR:HG22	1.96	0.66
1:D:24:GLN:NE2	1:D:78:LEU:HD21	2.11	0.65
1:C:56:GLN:NE2	1:C:61:THR:HB	2.12	0.65
1:D:36:GLU:HA	1:D:39:GLN:CB	2.24	0.65
1:A:81:LYS:HG2	1:A:85:GLU:OE1	1.97	0.65
1:B:197:GLU:HG3	4:B:3382:HOH:O	1.95	0.65
1:D:107:ILE:O	1:D:206:ASN:ND2	2.28	0.65
1:A:9:PRO:HD3	1:A:33:VAL:O	1.96	0.65
1:D:81:LYS:HZ2	1:D:147:GLN:HG3	1.62	0.65
1:C:184:SER:O	1:C:190:LYS:HB2	1.96	0.65
1:D:179:TYR:HA	1:D:182:ARG:NH2	2.11	0.65
1:C:110:ASN:OD1	1:C:113:ALA:HB3	1.97	0.64
1:C:143:ILE:HD13	1:C:155:LEU:CD2	2.28	0.64
1:A:7:TYR:O	1:A:33:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:MET:SD	1:C:189:LEU:HD11	2.37	0.64
1:A:111:TYR:CB	1:A:208:LYS:HE3	2.28	0.64
1:B:72:LEU:O	1:B:76:LEU:HB2	1.97	0.64
1:B:20:LEU:HD23	1:B:20:LEU:C	2.17	0.63
1:B:111:TYR:O	1:B:115:LYS:HB3	1.98	0.63
1:A:78:LEU:HB3	1:A:149:SER:HA	1.80	0.63
1:A:10:VAL:HA	1:A:202:PRO:HD2	1.80	0.63
1:D:7:TYR:CE2	1:D:14:CYS:HB2	2.34	0.63
1:A:78:LEU:HD22	1:A:148:ILE:HG23	1.79	0.63
1:B:193:LEU:HD23	1:B:198:TYR:CE1	2.34	0.63
1:C:91:MET:HE2	1:D:62:LEU:HD23	1.80	0.63
1:B:103:TYR:CZ	1:B:107:ILE:HG13	2.35	0.62
1:B:136:ASN:ND2	1:B:142:PHE:O	2.32	0.62
1:C:209:GLN:N	1:C:209:GLN:HE21	1.97	0.62
1:B:51:GLN:HB3	2:B:2201:GTD:O2	1.99	0.62
1:C:55:PHE:O	1:C:56:GLN:HG2	1.98	0.62
1:A:174:PRO:HG3	1:C:197:GLU:HA	1.82	0.62
1:A:176:LEU:O	1:A:180:VAL:HG22	1.98	0.62
1:B:7:TYR:CE2	1:B:10:VAL:HG23	2.34	0.62
1:B:106:LEU:CD1	1:B:115:LYS:HA	2.29	0.62
1:B:13:ARG:HD3	1:B:65:SER:OG	1.98	0.62
1:A:55:PHE:CB	1:A:68:ILE:HD13	2.29	0.62
1:C:60:LEU:HG	1:C:61:THR:N	2.14	0.62
1:B:188:LYS:HD2	4:B:3198:HOH:O	2.00	0.62
1:B:29:LYS:HG2	4:B:3380:HOH:O	2.00	0.62
1:C:100:ARG:HH21	1:C:154:ASN:HD21	1.48	0.62
1:D:203:ILE:HD13	1:D:209:GLN:HG2	1.81	0.62
1:C:206:ASN:CG	1:C:208:LYS:HG3	2.21	0.61
1:D:156:LEU:HD12	1:D:156:LEU:O	1.99	0.61
1:D:6:VAL:HG13	1:D:31:GLU:HB3	1.82	0.61
1:B:6:VAL:HB	1:B:54:LYS:HB3	1.82	0.61
1:D:9:PRO:HD3	1:D:33:VAL:O	2.00	0.61
1:D:49:TYR:HD2	4:D:3021:HOH:O	1.82	0.61
1:A:43:LEU:HD23	4:A:3355:HOH:O	1.98	0.61
4:A:3244:HOH:O	1:B:70:ARG:HD2	2.00	0.61
1:C:161:ILE:HG22	1:C:203:ILE:HD13	1.81	0.61
1:C:56:GLN:CD	1:C:61:THR:HB	2.21	0.61
1:D:172:ALA:HB2	4:D:3306:HOH:O	2.00	0.61
1:B:135:GLN:HG3	4:B:3553:HOH:O	1.99	0.61
1:B:182:ARG:O	1:B:182:ARG:HG2	1.99	0.61
1:D:196:PRO:O	1:D:200:ASN:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASP:OD1	1:A:147:GLN:HG3	2.01	0.61
1:A:23:ASP:OD1	1:A:189:LEU:HB2	2.01	0.61
1:C:178:ALA:O	1:C:182:ARG:HG2	2.01	0.61
1:C:78:LEU:HD11	1:C:148:ILE:HG23	1.83	0.61
1:C:78:LEU:CD1	1:C:148:ILE:HG23	2.31	0.60
1:A:120:LYS:HD3	4:A:3542:HOH:O	1.99	0.60
1:A:128:PRO:O	1:A:132:LEU:HG	2.01	0.60
1:A:130:GLU:CD	1:A:175:LEU:HD12	2.20	0.60
1:A:137:GLN:HA	1:A:137:GLN:NE2	2.15	0.60
1:B:102:LYS:HG3	4:B:3331:HOH:O	2.00	0.60
1:B:14:CYS:O	1:B:18:ARG:HD2	2.01	0.60
1:D:156:LEU:HD22	1:D:183:LEU:HB3	1.81	0.60
1:D:142:PHE:HE2	1:D:146:ASP:O	1.85	0.60
1:C:56:GLN:HG2	1:C:61:THR:HB	1.83	0.60
1:D:11:ARG:HG3	1:D:202:PRO:O	2.01	0.60
1:A:107:ILE:O	1:A:206:ASN:ND2	2.35	0.59
1:B:96:VAL:HG23	1:B:129:PHE:CE2	2.37	0.59
1:A:92:VAL:HG12	1:A:151:ALA:HB1	1.83	0.59
1:A:11:ARG:HA	1:A:18:ARG:HH12	1.68	0.59
1:B:107:ILE:O	1:B:206:ASN:OD1	2.21	0.59
1:C:52:LEU:HB3	1:C:53:PRO:HA	1.84	0.59
1:D:96:VAL:HG21	1:D:155:LEU:HB2	1.84	0.59
1:A:190:LYS:NZ	1:A:190:LYS:HB2	2.18	0.59
1:C:165:LEU:HB2	1:C:209:GLN:O	2.02	0.59
1:B:165:LEU:HA	4:B:3070:HOH:O	2.02	0.59
1:C:30:GLU:O	1:C:31:GLU:HG2	2.03	0.59
1:B:97:GLU:OE2	1:B:101:CYS:SG	2.61	0.58
4:A:3057:HOH:O	1:B:94:ASP:HB3	2.02	0.58
1:A:97:GLU:O	1:A:101:CYS:HB2	2.03	0.58
1:A:50:GLY:O	1:A:51:GLN:HG3	2.03	0.58
1:C:163:GLU:CD	1:C:168:GLY:H	2.07	0.58
1:A:9:PRO:O	1:A:202:PRO:HD2	2.04	0.58
1:A:92:VAL:O	1:A:96:VAL:HG23	2.04	0.58
1:B:143:ILE:HG12	4:B:3422:HOH:O	2.04	0.58
1:A:156:LEU:HG	1:A:160:LEU:HD22	1.86	0.58
1:B:73:GLY:HA2	1:B:78:LEU:HB2	1.85	0.58
1:B:79:TYR:HD1	1:B:79:TYR:O	1.87	0.58
1:C:19:MET:CE	1:C:156:LEU:HD23	2.32	0.58
1:C:186:ARG:O	1:C:190:LYS:N	2.35	0.58
1:A:55:PHE:HB2	1:A:68:ILE:HD13	1.85	0.58
1:D:189:LEU:O	1:D:193:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:SER:H	2:D:2401:GTD:C1	2.17	0.58
1:D:130:GLU:OE1	1:D:130:GLU:HA	2.04	0.57
1:A:137:GLN:HG3	1:A:141:THR:HG21	1.85	0.57
1:D:203:ILE:HG22	1:D:204:ASN:ND2	2.19	0.57
1:B:84:GLN:N	1:B:84:GLN:HE21	2.02	0.57
1:D:100:ARG:NH2	1:D:154:ASN:ND2	2.49	0.57
1:D:92:VAL:HG22	1:D:132:LEU:HD13	1.86	0.57
1:A:14:CYS:HA	1:A:17:LEU:HD21	1.86	0.57
1:B:107:ILE:CG2	1:B:107:ILE:O	2.53	0.57
1:C:11:ARG:HB2	1:C:15:ALA:HB2	1.87	0.57
1:A:121:ALA:O	1:A:125:GLN:HG2	2.05	0.56
1:A:98:ASP:O	1:A:102:LYS:HD2	2.06	0.56
1:A:16:ALA:HB3	4:A:3089:HOH:O	2.04	0.56
1:B:20:LEU:HB2	1:B:153:TYR:CD2	2.40	0.56
1:B:183:LEU:O	1:B:189:LEU:HD23	2.05	0.56
1:D:7:TYR:CD2	1:D:14:CYS:HB2	2.40	0.56
1:B:28:TRP:CZ2	3:B:2600:MES:H32	2.41	0.56
1:D:20:LEU:HD23	1:D:20:LEU:C	2.25	0.56
1:A:158:LEU:HA	1:A:161:ILE:HD11	1.87	0.56
1:A:70:ARG:HG2	1:A:150:PHE:CZ	2.41	0.56
1:B:63:TYR:HB3	4:B:3132:HOH:O	2.06	0.56
1:A:67:THR:HG23	1:B:90:ASP:HB3	1.87	0.56
1:A:148:ILE:HD11	4:A:3327:HOH:O	2.05	0.56
1:A:96:VAL:HG21	1:A:155:LEU:HB2	1.88	0.56
1:C:116:ASP:O	1:C:120:LYS:HG3	2.06	0.56
1:D:38:TRP:HZ2	2:D:2401:GTD:O32	1.89	0.56
1:C:111:TYR:HB3	1:C:112:GLU:OE2	2.05	0.56
1:D:115:LYS:O	1:D:115:LYS:HD2	2.06	0.56
1:A:128:PRO:HB3	1:B:48:LEU:O	2.06	0.56
1:C:127:LYS:HG3	4:C:3499:HOH:O	2.05	0.56
1:D:72:LEU:O	1:D:76:LEU:HB2	2.05	0.56
1:A:45:ALA:HB3	4:A:3400:HOH:O	2.05	0.56
1:B:38:TRP:HZ2	1:B:50:GLY:O	1.89	0.55
1:C:136:ASN:C	1:C:138:GLY:H	2.09	0.55
1:A:109:THR:O	1:A:109:THR:HG22	2.06	0.55
1:A:111:TYR:O	1:A:111:TYR:CD1	2.60	0.55
1:A:11:ARG:HB3	1:A:15:ALA:HB2	1.87	0.55
1:A:71:HIS:HA	1:A:74:ARG:HD2	1.88	0.55
1:D:159:LEU:CD1	1:D:176:LEU:HD22	2.36	0.55
1:D:46:SER:HB3	4:D:3307:HOH:O	2.06	0.55
1:D:40:GLU:OE2	1:D:42:SER:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ALA:HB3	4:D:3096:HOH:O	2.05	0.55
1:D:187:PRO:HB2	4:D:3273:HOH:O	2.06	0.55
1:B:206:ASN:N	1:B:206:ASN:HD22	2.03	0.55
1:B:50:GLY:C	1:B:51:GLN:HG2	2.26	0.55
1:C:56:GLN:CG	1:C:61:THR:HB	2.37	0.55
1:B:51:GLN:HG3	4:B:3347:HOH:O	2.06	0.55
1:B:99:LEU:HD13	1:B:125:GLN:CG	2.37	0.55
1:A:11:ARG:HA	1:A:18:ARG:NH1	2.21	0.54
1:B:176:LEU:O	1:B:180:VAL:HB	2.08	0.54
1:B:206:ASN:HD22	1:B:206:ASN:H	1.55	0.54
1:C:73:GLY:HA2	1:C:78:LEU:HB2	1.89	0.54
1:D:195:SER:O	1:D:199:VAL:HG23	2.07	0.54
1:D:203:ILE:HD12	1:D:209:GLN:HE21	1.72	0.54
1:B:138:GLY:O	1:B:140:LYS:HE2	2.07	0.54
1:A:38:TRP:HA	4:A:3037:HOH:O	2.07	0.54
1:C:142:PHE:CD2	1:C:148:ILE:HD12	2.43	0.54
1:D:100:ARG:HH21	1:D:154:ASN:HD22	1.53	0.54
1:B:127:LYS:HA	1:B:173:PHE:CE1	2.43	0.54
1:C:96:VAL:HG22	1:C:155:LEU:HD13	1.90	0.54
1:A:160:LEU:O	1:A:164:VAL:HG23	2.07	0.54
1:C:148:ILE:HG13	1:C:149:SER:H	1.73	0.53
1:C:67:THR:HG23	1:D:90:ASP:HB3	1.90	0.53
1:A:37:THR:HG22	1:A:43:LEU:HD13	1.90	0.53
1:A:96:VAL:HG13	1:A:158:LEU:CD2	2.38	0.53
1:A:119:VAL:HG22	1:A:166:ALA:HB2	1.89	0.53
1:A:79:TYR:HD1	1:A:79:TYR:O	1.91	0.53
1:B:97:GLU:O	1:B:101:CYS:SG	2.64	0.53
1:C:24:GLN:NE2	4:C:3151:HOH:O	2.41	0.53
1:A:8:PHE:O	1:A:10:VAL:N	2.36	0.53
1:C:148:ILE:HG13	1:C:149:SER:N	2.24	0.53
1:D:10:VAL:CG1	1:D:202:PRO:HG2	2.38	0.53
1:A:107:ILE:HD13	1:A:111:TYR:HD2	1.73	0.53
1:A:156:LEU:HD13	1:A:183:LEU:HB3	1.90	0.53
1:B:106:LEU:O	1:B:111:TYR:HB2	2.09	0.53
1:A:64:GLN:O	1:A:68:ILE:HG13	2.09	0.53
1:B:122:LEU:N	1:B:123:PRO:CD	2.72	0.53
1:C:96:VAL:CG2	1:C:155:LEU:HB2	2.38	0.53
1:C:70:ARG:HG2	1:C:79:TYR:OH	2.08	0.52
1:D:63:TYR:O	1:D:64:GLN:HB2	2.09	0.52
1:D:183:LEU:O	1:D:189:LEU:HD23	2.09	0.52
1:C:100:ARG:HH11	1:C:100:ARG:HG3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:SER:HB3	4:C:3186:HOH:O	2.08	0.52
1:A:156:LEU:O	1:A:160:LEU:HD22	2.10	0.52
1:C:70:ARG:HG3	1:C:150:PHE:CZ	2.45	0.52
1:C:208:LYS:C	1:C:209:GLN:HG3	2.30	0.52
1:C:60:LEU:HD11	1:D:88:LEU:HD21	1.91	0.52
1:A:20:LEU:C	1:A:20:LEU:HD23	2.30	0.52
1:C:72:LEU:O	1:C:76:LEU:HB2	2.09	0.52
1:D:100:ARG:O	1:D:104:ILE:HG13	2.10	0.52
1:D:13:ARG:HD2	2:D:2401:GTD:HB11	1.91	0.52
1:A:116:ASP:HB3	4:A:3246:HOH:O	2.09	0.52
1:A:17:LEU:HA	1:A:20:LEU:HB3	1.91	0.52
1:B:129:PHE:HD2	4:B:3422:HOH:O	1.93	0.52
1:B:99:LEU:HD13	1:B:125:GLN:HG2	1.90	0.52
1:D:51:GLN:HB3	2:D:2401:GTD:O2	2.10	0.52
1:B:11:ARG:HB2	1:B:202:PRO:O	2.10	0.52
1:D:4:THR:HA	1:D:29:LYS:O	2.10	0.52
1:A:38:TRP:CE2	1:A:44:LYS:HB2	2.45	0.51
1:C:176:LEU:O	1:C:180:VAL:HG23	2.10	0.51
1:D:106:LEU:HD12	1:D:111:TYR:HA	1.91	0.51
1:B:111:TYR:O	1:B:111:TYR:CD1	2.63	0.51
1:C:133:LEU:HD12	1:C:176:LEU:HD23	1.92	0.51
1:A:184:SER:O	1:A:190:LYS:HB2	2.11	0.51
1:C:104:ILE:HG21	4:C:3270:HOH:O	2.09	0.51
1:C:20:LEU:C	1:C:20:LEU:HD23	2.30	0.51
1:D:156:LEU:HB2	1:D:183:LEU:HD23	1.92	0.51
1:A:115:LYS:HE3	1:A:165:LEU:HD12	1.92	0.51
1:A:7:TYR:CD1	1:A:53:PRO:HB3	2.46	0.51
1:B:63:TYR:O	1:B:64:GLN:HB2	2.09	0.51
1:C:194:ALA:HB1	4:C:3533:HOH:O	2.09	0.51
1:D:107:ILE:HG22	1:D:206:ASN:HD21	1.76	0.51
1:A:137:GLN:HB2	1:A:141:THR:OG1	2.11	0.51
1:B:61:THR:O	1:B:62:LEU:HG	2.11	0.51
1:B:80:GLY:HA2	4:B:3396:HOH:O	2.11	0.51
1:C:132:LEU:HD21	1:D:48:LEU:HD21	1.93	0.51
1:D:109:THR:HA	4:D:3444:HOH:O	2.11	0.51
1:D:10:VAL:HG13	1:D:202:PRO:HG2	1.92	0.51
1:A:70:ARG:HB3	1:A:79:TYR:HE2	1.76	0.51
1:B:195:SER:O	1:B:199:VAL:HB	2.11	0.51
1:C:142:PHE:N	1:C:142:PHE:CD1	2.79	0.51
1:C:86:ALA:O	1:C:90:ASP:HB2	2.11	0.51
1:A:19:MET:HB3	1:A:189:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASP:OD1	1:A:85:GLU:N	2.43	0.51
1:D:156:LEU:O	1:D:160:LEU:HG	2.11	0.51
1:A:107:ILE:HD13	1:A:111:TYR:CD2	2.46	0.51
1:A:72:LEU:O	1:A:76:LEU:HB2	2.10	0.51
1:B:155:LEU:HG	1:B:159:LEU:HD12	1.93	0.51
1:D:133:LEU:HD22	1:D:139:GLY:HA2	1.91	0.50
1:A:20:LEU:O	1:A:24:GLN:HG2	2.11	0.50
1:B:118:TYR:OH	1:B:162:HIS:NE2	2.38	0.50
1:B:55:PHE:O	1:B:61:THR:HA	2.10	0.50
1:C:133:LEU:O	1:C:139:GLY:N	2.44	0.50
1:D:116:ASP:O	1:D:120:LYS:HG3	2.11	0.50
1:C:111:TYR:O	1:C:115:LYS:HB2	2.10	0.50
1:C:147:GLN:NE2	1:C:148:ILE:O	2.44	0.50
1:D:106:LEU:CD1	1:D:111:TYR:HA	2.42	0.50
1:D:115:LYS:HD3	1:D:165:LEU:CD1	2.42	0.50
1:D:66:ASN:HD22	1:D:69:LEU:HD12	1.77	0.50
1:C:127:LYS:N	1:C:128:PRO:CD	2.74	0.50
1:D:36:GLU:OE1	1:D:36:GLU:N	2.45	0.50
1:D:58:GLY:HA3	4:D:3296:HOH:O	2.10	0.50
1:A:89:VAL:HG13	1:A:151:ALA:HB2	1.93	0.50
1:A:180:VAL:HG12	4:A:3254:HOH:O	2.12	0.50
1:B:13:ARG:HD3	1:B:65:SER:HG	1.77	0.50
1:B:96:VAL:HG21	1:B:155:LEU:HB2	1.92	0.50
1:C:158:LEU:O	1:C:158:LEU:HG	2.11	0.50
1:D:10:VAL:HG11	1:D:204:ASN:O	2.12	0.50
1:D:127:LYS:HB3	1:D:128:PRO:HD3	1.94	0.50
1:C:9:PRO:O	1:C:202:PRO:HD2	2.11	0.50
1:D:116:ASP:O	1:D:120:LYS:CG	2.60	0.50
1:A:16:ALA:HB3	4:A:3085:HOH:O	2.12	0.50
1:B:163:GLU:CA	1:B:163:GLU:OE1	2.59	0.50
1:C:206:ASN:ND2	1:C:208:LYS:HG3	2.27	0.50
1:D:140:LYS:HB2	4:D:3259:HOH:O	2.12	0.50
2:C:2301:GTD:N1	4:C:3348:HOH:O	2.35	0.49
1:D:19:MET:CE	1:D:157:ASP:HB2	2.42	0.49
1:D:159:LEU:HD22	1:D:170:LEU:HD21	1.93	0.49
1:A:31:GLU:O	1:A:32:VAL:C	2.50	0.49
1:C:63:TYR:O	1:C:64:GLN:HB2	2.11	0.49
1:D:106:LEU:O	1:D:111:TYR:N	2.45	0.49
1:B:79:TYR:CD1	1:B:79:TYR:O	2.65	0.49
1:C:21:LEU:HD11	1:C:72:LEU:HD11	1.95	0.49
1:D:55:PHE:O	1:D:56:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:THR:HG21	1:D:91:MET:HB2	1.94	0.49
1:D:99:LEU:HA	1:D:102:LYS:HG3	1.94	0.49
1:A:161:ILE:HG22	1:A:203:ILE:HD13	1.94	0.49
1:A:38:TRP:CZ2	1:A:44:LYS:HB2	2.47	0.49
1:D:20:LEU:HD23	1:D:20:LEU:O	2.12	0.49
1:D:22:ALA:O	1:D:188:LYS:HB2	2.12	0.49
1:C:84:GLN:CD	1:D:60:LEU:HD13	2.31	0.49
1:D:100:ARG:HH21	1:D:154:ASN:HD21	1.57	0.49
1:D:105:SER:O	1:D:109:THR:HG23	2.12	0.49
1:B:20:LEU:O	1:B:24:GLN:HB2	2.13	0.49
1:B:3:TYR:HB2	1:B:28:TRP:HB2	1.94	0.49
1:C:39:GLN:NE2	4:C:3104:HOH:O	2.45	0.49
1:C:7:TYR:HA	1:C:52:LEU:HD13	1.95	0.49
1:A:37:THR:HG22	1:A:43:LEU:CD1	2.43	0.49
1:B:65:SER:H	2:B:2201:GTD:C1	2.26	0.49
1:D:18:ARG:HD3	4:D:3060:HOH:O	2.12	0.49
1:C:127:LYS:HE2	1:C:127:LYS:HA	1.94	0.49
1:A:15:ALA:O	1:A:19:MET:HG3	2.13	0.48
1:A:65:SER:H	2:A:2101:GTD:C1	2.26	0.48
1:A:13:ARG:HD3	1:A:65:SER:OG	2.12	0.48
1:C:137:GLN:HG3	1:C:141:THR:HG21	1.95	0.48
1:A:45:ALA:HB2	4:A:3469:HOH:O	2.12	0.48
1:B:107:ILE:HG21	1:B:204:ASN:CG	2.33	0.48
1:D:156:LEU:HD22	1:D:183:LEU:HD23	1.94	0.48
1:B:106:LEU:HD22	1:B:118:TYR:CD1	2.48	0.48
1:D:92:VAL:CG2	1:D:132:LEU:HD13	2.43	0.48
1:B:90:ASP:O	1:B:94:ASP:OD1	2.31	0.48
1:C:156:LEU:O	1:C:156:LEU:HG	2.12	0.48
1:C:85:GLU:HG3	1:C:144:VAL:CG1	2.44	0.48
1:A:172:ALA:HB1	4:A:3101:HOH:O	2.13	0.48
1:A:63:TYR:O	1:A:64:GLN:HB2	2.12	0.48
1:C:190:LYS:HG2	1:C:190:LYS:O	2.12	0.48
1:C:84:GLN:NE2	1:D:60:LEU:HD13	2.29	0.48
1:B:203:ILE:HG12	4:B:3093:HOH:O	2.12	0.48
1:C:142:PHE:HD2	1:C:148:ILE:HD12	1.78	0.48
1:D:115:LYS:HD3	1:D:165:LEU:HD12	1.95	0.48
1:D:64:GLN:HB2	1:D:67:THR:OG1	2.13	0.48
1:B:20:LEU:HD23	1:B:21:LEU:N	2.28	0.48
1:D:35:VAL:HG23	1:D:36:GLU:OE1	2.13	0.48
1:D:147:GLN:N	1:D:147:GLN:CD	2.63	0.48
1:C:84:GLN:OE1	1:D:60:LEU:HD13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ASP:O	1:B:161:ILE:HG23	2.14	0.47
1:D:122:LEU:HB3	1:D:123:PRO:HD3	1.96	0.47
1:D:136:ASN:CG	1:D:136:ASN:O	2.52	0.47
1:D:141:THR:HA	4:D:3325:HOH:O	2.13	0.47
1:A:126:LEU:HD13	1:A:173:PHE:CE2	2.49	0.47
1:A:21:LEU:O	1:A:26:GLN:HB2	2.14	0.47
1:B:11:ARG:HD3	1:B:198:TYR:CE2	2.50	0.47
1:D:43:LEU:O	1:D:43:LEU:HD12	2.13	0.47
1:D:24:GLN:HG2	1:D:76:LEU:HD13	1.96	0.47
1:B:11:ARG:HG2	1:B:15:ALA:HB2	1.95	0.47
1:B:19:MET:HG2	1:B:189:LEU:CD1	2.44	0.47
1:A:131:THR:O	1:A:135:GLN:HB2	2.14	0.47
1:B:136:ASN:C	1:B:138:GLY:N	2.66	0.47
1:B:193:LEU:O	1:B:199:VAL:HG23	2.14	0.47
1:B:64:GLN:O	1:B:68:ILE:HG13	2.14	0.47
1:A:14:CYS:O	1:A:17:LEU:HG	2.14	0.47
1:C:16:ALA:HB3	4:C:3303:HOH:O	2.14	0.47
1:C:64:GLN:HB2	1:C:67:THR:OG1	2.14	0.47
1:A:159:LEU:HD12	4:A:3254:HOH:O	2.14	0.47
1:D:107:ILE:HG21	1:D:204:ASN:OD1	2.14	0.47
1:D:24:GLN:HE21	1:D:78:LEU:HD21	1.76	0.47
1:D:155:LEU:HD23	1:D:179:TYR:OH	2.15	0.47
1:B:44:LYS:O	1:B:50:GLY:HA2	2.15	0.47
1:A:185:ALA:HB2	4:A:3129:HOH:O	2.15	0.46
1:A:82:ASP:OD1	1:A:84:GLN:N	2.48	0.46
1:D:7:TYR:OH	1:D:12:GLY:HA3	2.15	0.46
1:A:159:LEU:HB3	1:A:180:VAL:HG11	1.97	0.46
1:A:10:VAL:CG1	1:A:202:PRO:HG2	2.38	0.46
1:B:36:GLU:HA	1:B:39:GLN:HB2	1.97	0.46
1:B:7:TYR:CE1	1:B:53:PRO:HD3	2.50	0.46
1:D:156:LEU:CD1	1:D:180:VAL:HG22	2.45	0.46
1:D:35:VAL:HG23	1:D:36:GLU:CD	2.36	0.46
1:C:71:HIS:O	1:C:75:THR:OG1	2.30	0.46
1:D:44:LYS:HG2	1:D:44:LYS:O	2.15	0.46
1:A:92:VAL:HG21	1:A:143:ILE:CG1	2.45	0.46
1:B:33:VAL:HG21	1:B:52:LEU:HD11	1.97	0.46
1:C:63:TYR:CD1	1:C:63:TYR:N	2.83	0.46
1:B:104:ILE:O	1:B:108:TYR:HD2	1.98	0.46
1:C:103:TYR:C	1:C:103:TYR:CD1	2.88	0.46
1:A:19:MET:O	1:A:23:ASP:HB2	2.16	0.46
1:A:52:LEU:HB3	1:A:53:PRO:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ALA:O	1:B:174:PRO:HD3	2.16	0.46
1:B:81:LYS:HG2	1:B:85:GLU:CD	2.35	0.46
1:D:3:TYR:HA	1:D:56:GLN:O	2.15	0.46
1:A:168:GLY:HA2	4:A:3338:HOH:O	2.14	0.46
1:A:66:ASN:OD1	1:A:97:GLU:OE1	2.34	0.46
1:C:142:PHE:CE2	1:C:148:ILE:HB	2.50	0.46
1:C:97:GLU:O	1:C:97:GLU:HG3	2.16	0.46
1:D:167:PRO:HB3	4:D:3483:HOH:O	2.14	0.46
1:D:19:MET:HE2	1:D:157:ASP:HB2	1.98	0.46
1:A:100:ARG:NH2	1:A:154:ASN:ND2	2.57	0.46
1:B:41:GLY:O	1:B:43:LEU:N	2.49	0.46
1:B:97:GLU:O	1:B:97:GLU:HG3	2.16	0.46
1:D:14:CYS:SG	1:D:53:PRO:CB	3.04	0.46
1:A:122:LEU:O	1:A:125:GLN:N	2.46	0.45
1:A:99:LEU:HD23	1:A:158:LEU:CD2	2.36	0.45
1:B:127:LYS:N	1:B:128:PRO:CD	2.78	0.45
1:C:165:LEU:HA	4:C:3140:HOH:O	2.16	0.45
1:A:51:GLN:HB2	4:A:3346:HOH:O	2.15	0.45
1:B:6:VAL:HG21	1:B:54:LYS:HD3	1.98	0.45
1:C:78:LEU:HD12	1:C:148:ILE:O	2.16	0.45
1:C:195:SER:CB	4:C:3172:HOH:O	2.65	0.45
1:D:147:GLN:HB2	4:D:3067:HOH:O	2.16	0.45
1:A:156:LEU:HG	1:A:160:LEU:CD2	2.47	0.45
1:A:208:LYS:H	1:A:208:LYS:HG2	1.51	0.45
1:B:13:ARG:HG3	4:B:3241:HOH:O	2.16	0.45
1:B:182:ARG:HD3	4:B:3068:HOH:O	2.15	0.45
1:C:8:PHE:HA	1:C:33:VAL:O	2.17	0.45
1:C:137:GLN:HG3	1:C:141:THR:CG2	2.47	0.45
1:D:10:VAL:CG2	2:D:2401:GTD:O62	2.62	0.45
1:C:91:MET:HB2	1:D:67:THR:HG21	1.99	0.45
1:D:51:GLN:HG2	2:D:2401:GTD:O31	2.16	0.45
1:A:89:VAL:HG23	1:A:144:VAL:HG11	1.98	0.45
1:B:29:LYS:HA	4:B:3380:HOH:O	2.17	0.45
1:B:69:LEU:HB3	1:B:150:PHE:CD2	2.51	0.45
1:D:143:ILE:O	1:D:144:VAL:HG23	2.16	0.45
1:D:38:TRP:CZ2	2:D:2401:GTD:O32	2.69	0.45
1:A:143:ILE:O	1:A:143:ILE:HD12	2.17	0.45
1:C:209:GLN:N	1:C:209:GLN:NE2	2.64	0.45
1:D:6:VAL:CB	1:D:54:LYS:HB3	2.39	0.45
1:A:92:VAL:HG21	1:A:143:ILE:HG13	1.98	0.45
1:B:6:VAL:HG12	1:B:52:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:HG2	1:B:150:PHE:CZ	2.51	0.45
1:D:79:TYR:HD1	1:D:79:TYR:O	2.00	0.45
1:B:52:LEU:CD2	1:B:54:LYS:HB2	2.47	0.44
1:D:57:ASP:O	1:D:58:GLY:C	2.53	0.44
1:D:56:GLN:NE2	1:D:61:THR:OG1	2.50	0.44
1:D:38:TRP:CZ3	1:D:44:LYS:HA	2.52	0.44
1:C:166:ALA:N	1:C:167:PRO:HD3	2.32	0.44
1:D:141:THR:HB	1:D:142:PHE:H	1.57	0.44
1:D:142:PHE:CE2	1:D:146:ASP:O	2.68	0.44
1:A:197:GLU:OE1	3:A:2500:MES:H32	2.17	0.44
1:C:143:ILE:HD13	1:C:155:LEU:HD22	2.00	0.44
1:A:11:ARG:HD3	1:A:198:TYR:CE2	2.52	0.44
1:B:28:TRP:HE1	1:B:30:GLU:CD	2.21	0.44
1:B:28:TRP:CE2	3:B:2600:MES:H32	2.52	0.44
1:D:96:VAL:HG23	1:D:129:PHE:CZ	2.52	0.44
1:A:78:LEU:O	1:A:149:SER:HB2	2.17	0.44
1:B:130:GLU:HG3	1:B:130:GLU:O	2.16	0.44
1:B:6:VAL:O	1:B:7:TYR:HB2	2.17	0.44
1:C:60:LEU:HD21	1:C:62:LEU:CD2	2.48	0.44
1:C:99:LEU:HA	1:C:102:LYS:HE2	1.99	0.44
1:A:99:LEU:CD2	1:A:158:LEU:HD21	2.37	0.44
1:A:79:TYR:CD1	1:A:79:TYR:O	2.69	0.44
1:A:127:LYS:N	1:A:128:PRO:CD	2.79	0.43
1:B:20:LEU:HD11	1:B:78:LEU:HD23	2.00	0.43
1:D:19:MET:CE	1:D:153:TYR:O	2.65	0.43
1:D:10:VAL:HG11	1:D:204:ASN:C	2.37	0.43
1:A:190:LYS:HZ2	1:A:190:LYS:HB2	1.82	0.43
1:B:56:GLN:NE2	1:B:60:LEU:O	2.51	0.43
1:C:23:ASP:HB2	1:C:189:LEU:HB2	2.00	0.43
1:D:19:MET:HB3	1:D:192:PHE:CE2	2.53	0.43
1:D:70:ARG:HD2	4:D:3024:HOH:O	2.17	0.43
1:B:23:ASP:HB2	1:B:189:LEU:HB2	1.99	0.43
1:C:3:TYR:HB2	1:C:28:TRP:HB2	2.00	0.43
1:C:64:GLN:O	1:C:67:THR:HB	2.18	0.43
1:A:88:LEU:HD22	1:A:88:LEU:HA	1.82	0.43
1:D:18:ARG:HB3	1:D:192:PHE:HZ	1.84	0.43
1:A:71:HIS:HA	1:A:74:ARG:HH11	1.84	0.43
1:A:84:GLN:O	1:A:84:GLN:HG3	2.18	0.43
1:B:13:ARG:HH22	1:B:97:GLU:CD	2.21	0.43
1:B:62:LEU:HD11	1:B:71:HIS:CD2	2.53	0.43
1:C:169:CYS:SG	1:C:170:LEU:HD23	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PRO:CG	1:C:197:GLU:HA	2.48	0.43
1:A:11:ARG:O	1:A:12:GLY:C	2.57	0.43
1:C:100:ARG:HG3	1:C:100:ARG:NH1	2.32	0.43
1:C:11:ARG:CG	1:C:203:ILE:HA	2.46	0.43
1:C:62:LEU:HD13	1:C:67:THR:HG22	2.01	0.43
1:D:156:LEU:HD13	1:D:180:VAL:HG22	2.01	0.43
1:D:163:GLU:OE1	1:D:168:GLY:N	2.47	0.43
1:B:13:ARG:NH1	1:B:97:GLU:OE1	2.47	0.43
1:C:8:PHE:HB3	1:C:9:PRO:HD2	2.01	0.43
1:A:122:LEU:O	1:A:123:PRO:C	2.57	0.43
1:A:190:LYS:HD3	4:A:3029:HOH:O	2.19	0.43
1:A:30:GLU:HG2	3:A:2500:MES:H21	2.00	0.43
1:B:206:ASN:ND2	1:B:206:ASN:H	2.16	0.43
1:C:163:GLU:OE2	1:C:168:GLY:N	2.45	0.43
1:A:132:LEU:HB2	1:A:143:ILE:HD11	2.01	0.43
1:B:123:PRO:HD2	4:B:3097:HOH:O	2.17	0.43
1:B:35:VAL:HG13	1:B:36:GLU:OE1	2.19	0.43
1:D:107:ILE:HG23	1:D:208:LYS:CB	2.49	0.43
1:D:29:LYS:HD3	1:D:30:GLU:O	2.19	0.43
1:A:136:ASN:O	1:A:138:GLY:N	2.52	0.42
1:A:78:LEU:HD22	1:A:148:ILE:CG2	2.48	0.42
1:A:187:PRO:HB2	1:A:188:LYS:HE3	2.01	0.42
1:A:67:THR:O	1:A:71:HIS:HB3	2.19	0.42
1:C:208:LYS:O	1:C:209:GLN:HG3	2.18	0.42
1:D:33:VAL:HG12	1:D:34:THR:O	2.19	0.42
1:B:20:LEU:CD1	1:B:78:LEU:HD23	2.49	0.42
1:C:88:LEU:O	1:C:92:VAL:HG23	2.19	0.42
1:D:14:CYS:HG	1:D:53:PRO:HB3	1.84	0.42
1:D:59:ASP:OD1	1:D:59:ASP:N	2.50	0.42
1:A:7:TYR:CA	1:A:52:LEU:HD13	2.42	0.42
1:D:31:GLU:HG2	4:D:3189:HOH:O	2.19	0.42
1:A:3:TYR:HB3	1:A:56:GLN:O	2.18	0.42
1:B:92:VAL:HG22	4:B:3422:HOH:O	2.19	0.42
1:C:122:LEU:N	1:C:123:PRO:CD	2.83	0.42
1:C:8:PHE:HB3	1:C:9:PRO:CD	2.49	0.42
1:D:92:VAL:HG22	1:D:132:LEU:CD1	2.49	0.42
1:A:11:ARG:HH11	1:A:203:ILE:HG12	1.85	0.42
1:B:147:GLN:CD	1:B:147:GLN:H	2.23	0.42
1:D:124:GLY:O	1:D:128:PRO:HD3	2.19	0.42
1:D:182:ARG:NH1	4:D:3325:HOH:O	2.51	0.42
1:D:96:VAL:HG22	1:D:158:LEU:CD2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ILE:HG22	1:C:107:ILE:O	2.20	0.42
1:A:100:ARG:HE	1:A:154:ASN:HD21	1.68	0.42
1:A:54:LYS:HA	1:A:62:LEU:O	2.20	0.42
1:A:174:PRO:CD	1:C:197:GLU:HA	2.50	0.42
1:D:130:GLU:HG3	1:D:173:PHE:HD1	1.84	0.42
1:A:156:LEU:HB2	1:A:183:LEU:HD23	2.01	0.42
1:C:115:LYS:O	1:C:119:VAL:HG23	2.19	0.42
1:C:78:LEU:HD12	1:C:148:ILE:C	2.41	0.42
1:D:142:PHE:HB3	1:D:152:ASP:OD2	2.20	0.42
1:D:81:LYS:HZ2	1:D:147:GLN:CG	2.32	0.42
1:A:137:GLN:CB	1:A:141:THR:OG1	2.67	0.42
1:B:10:VAL:CG2	2:B:2201:GTD:O62	2.67	0.42
1:B:40:GLU:OE1	1:B:42:SER:HB3	2.20	0.42
1:B:81:LYS:HG2	1:B:85:GLU:OE1	2.20	0.41
1:D:11:ARG:O	1:D:12:GLY:C	2.58	0.41
1:A:55:PHE:HB3	1:A:68:ILE:HD13	2.00	0.41
1:D:81:LYS:HZ3	1:D:147:GLN:HG3	1.82	0.41
1:B:206:ASN:ND2	1:B:208:LYS:H	2.17	0.41
1:D:43:LEU:HA	1:D:46:SER:OG	2.19	0.41
1:C:83:GLN:HG2	1:D:74:ARG:HD3	2.02	0.41
1:A:130:GLU:OE1	1:A:175:LEU:HB2	2.20	0.41
1:A:84:GLN:CD	1:B:60:LEU:HD13	2.40	0.41
1:B:94:ASP:OD1	1:B:94:ASP:N	2.52	0.41
1:C:29:LYS:CG	1:C:30:GLU:O	2.68	0.41
1:D:11:ARG:O	1:D:12:GLY:O	2.39	0.41
1:D:130:GLU:CG	1:D:173:PHE:HB3	2.41	0.41
1:D:94:ASP:HB3	4:D:3112:HOH:O	2.19	0.41
1:A:110:ASN:HD21	1:A:113:ALA:CB	2.27	0.41
1:B:175:LEU:O	4:B:3009:HOH:O	2.22	0.41
1:B:137:GLN:HB2	1:B:141:THR:OG1	2.21	0.41
1:B:88:LEU:HD23	1:B:91:MET:CE	2.51	0.41
1:C:175:LEU:O	1:C:179:TYR:HB3	2.20	0.41
1:C:69:LEU:HD12	4:C:3214:HOH:O	2.19	0.41
1:C:76:LEU:HD22	4:C:3269:HOH:O	2.21	0.41
1:A:107:ILE:HG22	1:A:108:TYR:CD2	2.55	0.41
1:C:103:TYR:HB2	1:C:118:TYR:OH	2.20	0.41
1:C:198:TYR:HA	4:C:3043:HOH:O	2.20	0.41
1:C:199:VAL:HG12	1:C:199:VAL:O	2.19	0.41
1:A:119:VAL:CG2	1:A:166:ALA:HB2	2.51	0.41
1:B:141:THR:HB	1:B:142:PHE:H	1.44	0.41
1:B:29:LYS:NZ	4:B:3492:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:VAL:HG12	1:B:52:LEU:CD1	2.50	0.41
1:A:143:ILE:HG22	1:A:152:ASP:CG	2.41	0.41
1:A:64:GLN:OE1	2:A:2101:GTD:N1	2.54	0.41
1:B:180:VAL:O	1:B:180:VAL:CG1	2.69	0.41
1:C:131:THR:O	1:C:135:GLN:CG	2.66	0.41
1:A:136:ASN:C	1:A:138:GLY:H	2.23	0.40
1:A:157:ASP:O	1:A:161:ILE:HG12	2.21	0.40
1:B:85:GLU:O	1:B:89:VAL:HB	2.21	0.40
1:C:83:GLN:HB2	4:C:3260:HOH:O	2.22	0.40
1:D:8:PHE:CE2	1:D:52:LEU:HB2	2.55	0.40
1:A:6:VAL:O	1:A:52:LEU:HD22	2.21	0.40
1:B:8:PHE:HB3	1:B:9:PRO:HD2	2.01	0.40
1:C:16:ALA:HB3	4:C:3229:HOH:O	2.21	0.40
1:A:107:ILE:HG22	1:A:206:ASN:HD21	1.87	0.40
1:A:109:THR:O	1:A:110:ASN:HB2	2.21	0.40
1:B:190:LYS:HG3	1:B:190:LYS:O	2.20	0.40
1:B:103:TYR:CE2	1:B:161:ILE:HD12	2.57	0.40
1:D:17:LEU:HD12	1:D:17:LEU:C	2.42	0.40

All (6) 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)
4:A:3493:HOH:O	4:D:3102:HOH:O[2_656]	1.46	0.74
4:A:3209:HOH:O	4:D:3360:HOH:O[2_656]	1.81	0.39
4:B:3380:HOH:O	4:D:3121:HOH:O[1_455]	1.83	0.37
4:A:3152:HOH:O	4:C:3294:HOH:O[1_554]	1.96	0.24
4:A:3446:HOH:O	4:C:3299:HOH:O[1_554]	2.06	0.14
4:A:3285:HOH:O	4:D:3325:HOH:O[2_646]	2.13	0.07

## 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	206/209 (99%)	189 (92%)	8 (4%)	9 (4%)	2	0
1	B	206/209 (99%)	191 (93%)	7 (3%)	8 (4%)	3	1
1	C	206/209 (99%)	192 (93%)	10 (5%)	4 (2%)	8	3
1	D	206/209 (99%)	188 (91%)	13 (6%)	5 (2%)	6	2
All	All	824/836 (99%)	760 (92%)	38 (5%)	26 (3%)	4	1

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	137	GLN
1	B	137	GLN
1	C	32	VAL
1	C	137	GLN
1	A	12	GLY
1	A	32	VAL
1	B	12	GLY
1	B	42	SER
1	C	12	GLY
1	D	12	GLY
1	D	137	GLN
1	C	57	ASP
1	B	64	GLN
1	D	208	LYS
1	A	42	SER
1	A	111	TYR
1	A	187	PRO
1	B	110	ASN
1	B	187	PRO
1	D	168	GLY
1	A	9	PRO
1	B	145	GLY
1	A	145	GLY
1	B	114	GLY
1	D	187	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/176 (99%)	138 (79%)	37 (21%)	1	0
1	B	175/176 (99%)	129 (74%)	46 (26%)	0	0
1	C	175/176 (99%)	138 (79%)	37 (21%)	1	0
1	D	175/176 (99%)	141 (81%)	34 (19%)	1	0
All	All	700/704 (99%)	546 (78%)	154 (22%)	1	0

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	20	LEU
1	A	27	SER
1	A	29	LYS
1	A	31	GLU
1	A	36	GLU
1	A	40	GLU
1	A	56	GLN
1	A	59	ASP
1	A	74	ARG
1	A	79	TYR
1	A	84	GLN
1	A	88	LEU
1	A	92	VAL
1	A	94	ASP
1	A	101	CYS
1	A	103	TYR
1	A	105	SER
1	A	106	LEU
1	A	110	ASN
1	A	119	VAL
1	A	120	LYS
1	A	122	LEU
1	A	126	LEU
1	A	136	ASN
1	A	152	ASP
1	A	156	LEU
1	A	160	LEU
1	A	165	LEU
1	A	175	LEU

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Mol	Chain	Res	Type
1	A	180	VAL
1	A	186	ARG
1	A	188	LYS
1	A	190	LYS
1	A	195	SER
1	A	208	LYS
1	A	209	GLN
1	B	20	LEU
1	B	24	GLN
1	B	27	SER
1	B	29	LYS
1	B	34	THR
1	B	39	GLN
1	B	40	GLU
1	B	42	SER
1	B	46	SER
1	B	51	GLN
1	B	57	ASP
1	B	59	ASP
1	B	65	SER
1	B	72	LEU
1	B	78	LEU
1	B	79	TYR
1	B	81	LYS
1	B	83	GLN
1	B	84	GLN
1	B	89	VAL
1	B	90	ASP
1	B	94	ASP
1	B	96	VAL
1	B	98	ASP
1	B	112	GLU
1	B	115	LYS
1	B	116	ASP
1	B	120	LYS
1	B	125	GLN
1	B	127	LYS
1	B	135	GLN
1	B	140	LYS
1	B	141	THR
1	B	147	GLN
1	B	154	ASN

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Mol	Chain	Res	Type
1	B	158	LEU
1	B	163	GLU
1	B	165	LEU
1	B	179	TYR
1	B	184	SER
1	B	188	LYS
1	B	190	LYS
1	B	199	VAL
1	B	201	LEU
1	B	206	ASN
1	B	209	GLN
1	C	11	ARG
1	C	13	ARG
1	C	18	ARG
1	C	19	MET
1	C	20	LEU
1	C	29	LYS
1	C	36	GLU
1	C	51	GLN
1	C	54	LYS
1	C	57	ASP
1	C	61	THR
1	C	62	LEU
1	C	78	LEU
1	C	79	TYR
1	C	81	LYS
1	C	84	GLN
1	C	90	ASP
1	C	94	ASP
1	C	102	LYS
1	C	103	TYR
1	C	105	SER
1	C	109	THR
1	C	117	ASP
1	C	127	LYS
1	C	140	LYS
1	C	147	GLN
1	C	148	ILE
1	C	156	LEU
1	C	158	LEU
1	C	162	HIS
1	C	163	GLU

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Mol	Chain	Res	Type
1	C	164	VAL
1	C	165	LEU
1	C	179	TYR
1	C	188	LYS
1	C	193	LEU
1	C	209	GLN
1	D	6	VAL
1	D	10	VAL
1	D	19	MET
1	D	24	GLN
1	D	39	GLN
1	D	40	GLU
1	D	42	SER
1	D	59	ASP
1	D	79	TYR
1	D	83	GLN
1	D	85	GLU
1	D	88	LEU
1	D	90	ASP
1	D	94	ASP
1	D	96	VAL
1	D	106	LEU
1	D	109	THR
1	D	115	LYS
1	D	119	VAL
1	D	127	LYS
1	D	130	GLU
1	D	140	LYS
1	D	147	GLN
1	D	149	SER
1	D	154	ASN
1	D	155	LEU
1	D	157	ASP
1	D	165	LEU
1	D	179	TYR
1	D	180	VAL
1	D	182	ARG
1	D	188	LYS
1	D	190	LYS
1	D	208	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	93	ASN
1	A	110	ASN
1	A	136	ASN
1	A	137	GLN
1	A	154	ASN
1	A	204	ASN
1	B	56	GLN
1	B	66	ASN
1	B	71	HIS
1	B	84	GLN
1	B	93	ASN
1	B	110	ASN
1	B	135	GLN
1	B	147	GLN
1	B	154	ASN
1	B	206	ASN
1	C	24	GLN
1	C	39	GLN
1	C	66	ASN
1	C	83	GLN
1	C	93	ASN
1	C	154	ASN
1	C	204	ASN
1	C	209	GLN
1	D	56	GLN
1	D	66	ASN
1	D	83	GLN
1	D	93	ASN
1	D	125	GLN
1	D	154	ASN
1	D	209	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

8 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
3	MES	B	2600	-	12,12,12	2.92	5 (41%)	14,16,16	2.03	4 (28%)
3	MES	A	2500	-	12,12,12	2.87	5 (41%)	14,16,16	2.04	5 (35%)
3	MES	D	2800	-	12,12,12	2.83	5 (41%)	14,16,16	1.91	4 (28%)
2	GTD	D	2401	-	20,35,35	1.41	4 (20%)	17,48,48	0.74	0
3	MES	C	2700	-	12,12,12	2.87	5 (41%)	14,16,16	1.89	4 (28%)
2	GTD	B	2201	-	20,35,35	1.51	4 (20%)	17,48,48	0.63	0
2	GTD	A	2101	-	20,35,35	1.50	4 (20%)	17,48,48	0.63	0
2	GTD	C	2301	-	20,35,35	1.51	4 (20%)	17,48,48	0.63	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
3	MES	B	2600	-	-	3/6/14/14	0/1/1/1
3	MES	A	2500	-	-	3/6/14/14	0/1/1/1
3	MES	D	2800	-	-	4/6/14/14	0/1/1/1
2	GTD	D	2401	-	-	7/25/55/55	0/1/1/1
3	MES	C	2700	-	-	4/6/14/14	0/1/1/1
2	GTD	B	2201	-	-	2/25/55/55	0/1/1/1
2	GTD	A	2101	-	-	2/25/55/55	0/1/1/1
2	GTD	C	2301	-	-	2/25/55/55	0/1/1/1



All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2600	MES	O3S-S	5.73	1.67	1.47
3	A	2500	MES	O3S-S	5.71	1.67	1.47
3	D	2800	MES	O3S-S	5.67	1.67	1.47
3	C	2700	MES	O3S-S	5.62	1.67	1.47
3	C	2700	MES	O2S-S	4.91	1.59	1.45
3	D	2800	MES	O2S-S	4.89	1.59	1.45
3	B	2600	MES	O2S-S	4.86	1.59	1.45
3	A	2500	MES	O2S-S	4.81	1.59	1.45
3	B	2600	MES	O1S-S	4.77	1.59	1.45
3	D	2800	MES	O1S-S	4.71	1.58	1.45
3	A	2500	MES	O1S-S	4.68	1.58	1.45
3	C	2700	MES	O1S-S	4.66	1.58	1.45
2	B	2201	GTD	C4'-C5'	-3.43	1.40	1.50
2	C	2301	GTD	C4'-C5'	-3.41	1.40	1.50
2	A	2101	GTD	C4'-C5'	-3.41	1.40	1.50
2	D	2401	GTD	C4'-C5'	-3.25	1.40	1.50
2	D	2401	GTD	C4'-C3'	-3.22	1.40	1.50
2	C	2301	GTD	C4'-C3'	-3.14	1.41	1.50
2	A	2101	GTD	C4'-C3'	-3.13	1.41	1.50
2	B	2201	GTD	C4'-C3'	-3.12	1.41	1.50
2	C	2301	GTD	CB2-SG2	2.64	1.84	1.82
2	B	2201	GTD	CB2-SG2	2.61	1.84	1.82
2	A	2101	GTD	CB2-SG2	2.53	1.84	1.82
3	C	2700	MES	C5-N4	2.50	1.53	1.46
3	A	2500	MES	C5-N4	2.41	1.53	1.46
3	B	2600	MES	C5-N4	2.36	1.53	1.46
3	C	2700	MES	C3-N4	2.30	1.53	1.46
3	D	2800	MES	C5-N4	2.28	1.53	1.46
3	A	2500	MES	C3-N4	2.27	1.53	1.46
3	B	2600	MES	C3-N4	2.22	1.53	1.46
3	D	2800	MES	C3-N4	2.21	1.53	1.46
2	C	2301	GTD	C3'-C2'	2.17	1.41	1.34
2	B	2201	GTD	C3'-C2'	2.16	1.41	1.34
2	A	2101	GTD	C3'-C2'	2.16	1.41	1.34
2	D	2401	GTD	C5'-C6'	2.08	1.41	1.34
2	D	2401	GTD	C3'-C2'	2.08	1.41	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2500	MES	O2S-S-C8	4.52	112.35	106.92
3	B	2600	MES	O2S-S-C8	4.03	111.77	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2800	MES	O2S-S-C8	3.81	111.50	106.92
3	C	2700	MES	O2S-S-C8	3.54	111.17	106.92
3	C	2700	MES	O1S-S-C8	2.94	110.45	106.92
3	B	2600	MES	C5-N4-C3	2.93	115.43	108.83
3	D	2800	MES	O1S-S-C8	2.88	110.39	106.92
3	C	2700	MES	O3S-S-C8	2.86	110.39	105.77
3	A	2500	MES	O3S-S-C8	2.84	110.36	105.77
3	B	2600	MES	O3S-S-C8	2.82	110.32	105.77
3	D	2800	MES	C5-N4-C3	2.81	115.16	108.83
3	A	2500	MES	O1S-S-C8	2.74	110.21	106.92
3	B	2600	MES	O1S-S-C8	2.73	110.20	106.92
3	D	2800	MES	O3S-S-C8	2.60	109.98	105.77
3	A	2500	MES	C5-N4-C3	2.60	114.69	108.83
3	C	2700	MES	C5-N4-C3	2.41	114.26	108.83
3	A	2500	MES	O3S-S-O2S	-2.07	106.21	111.27

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2600	MES	C7-C8-S-O1S
3	B	2600	MES	C7-C8-S-O3S
3	A	2500	MES	C7-C8-S-O1S
3	A	2500	MES	C7-C8-S-O3S
3	D	2800	MES	C7-C8-S-O1S
3	D	2800	MES	C7-C8-S-O3S
2	C	2301	GTD	C2-CA2-CB2-SG2
2	D	2401	GTD	C2-CA2-CB2-SG2
3	C	2700	MES	C8-C7-N4-C5
3	C	2700	MES	C7-C8-S-O1S
3	C	2700	MES	C7-C8-S-O2S
3	C	2700	MES	C7-C8-S-O3S
2	B	2201	GTD	C2-CA2-CB2-SG2
2	A	2101	GTD	C2-CA2-CB2-SG2
2	C	2301	GTD	N2-CA2-CB2-SG2
2	D	2401	GTD	N2-CA2-CB2-SG2
2	B	2201	GTD	N2-CA2-CB2-SG2
2	A	2101	GTD	N2-CA2-CB2-SG2
3	B	2600	MES	C7-C8-S-O2S
3	A	2500	MES	C7-C8-S-O2S
3	D	2800	MES	C7-C8-S-O2S
2	D	2401	GTD	N1-CA1-CB1-CG1

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Mol	Chain	Res	Type	Atoms
2	D	2401	GTD	C3-CA3-N3-C2
3	D	2800	MES	C8-C7-N4-C3
2	D	2401	GTD	O2-C2-CA2-N2
2	D	2401	GTD	N3-C2-CA2-N2
2	D	2401	GTD	CA2-CB2-SG2-C1'

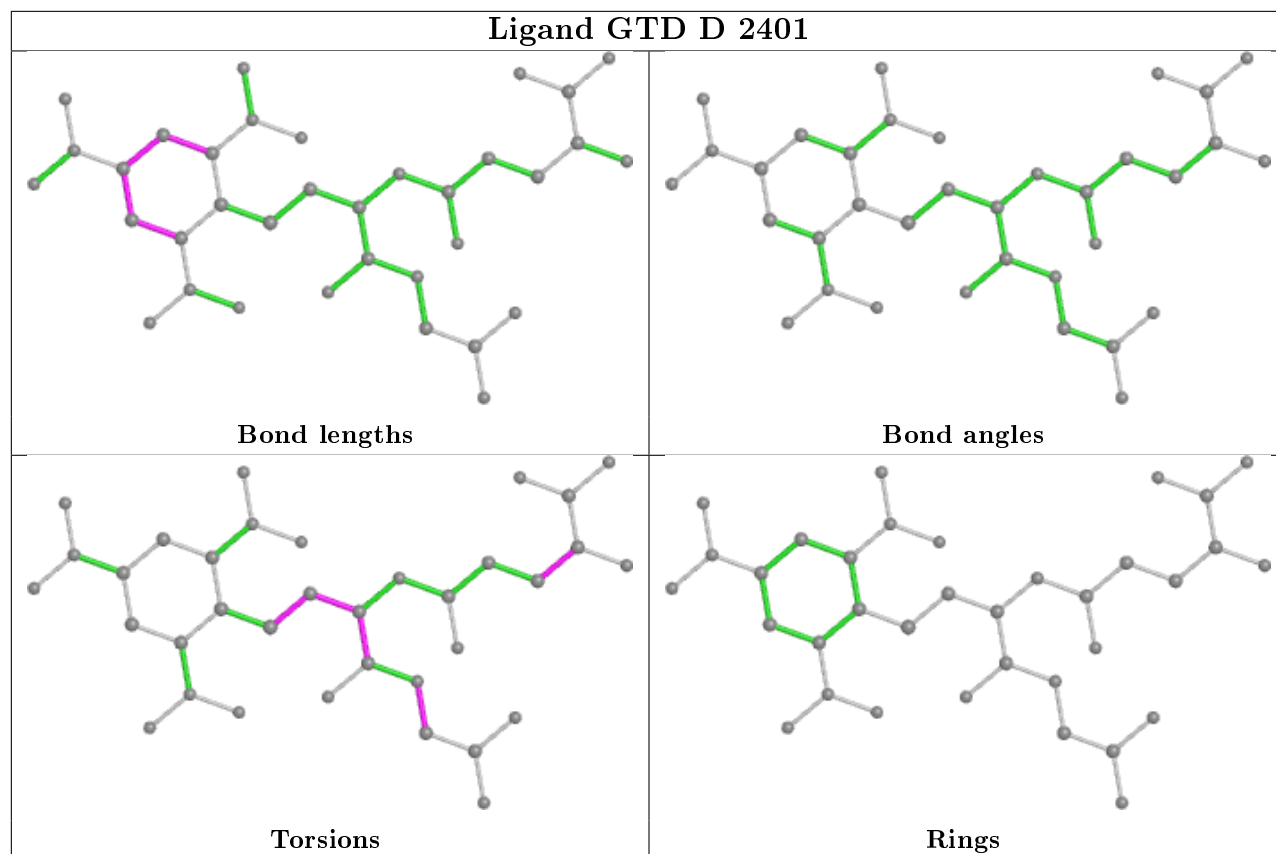
There are no ring outliers.

6 monomers are involved in 23 short contacts:

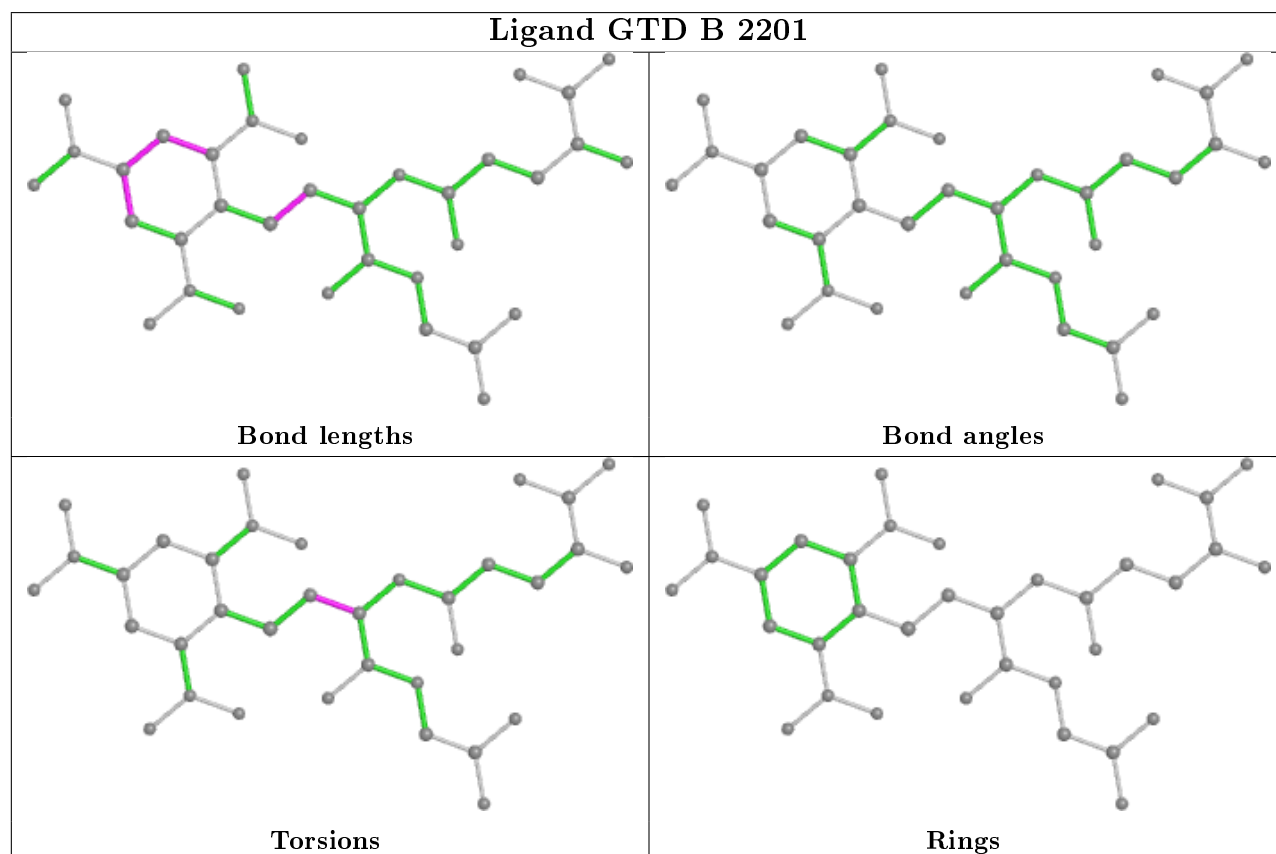
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2600	MES	2	0
3	A	2500	MES	2	0
2	D	2401	GTD	10	0
2	B	2201	GTD	4	0
2	A	2101	GTD	4	0
2	C	2301	GTD	1	0

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

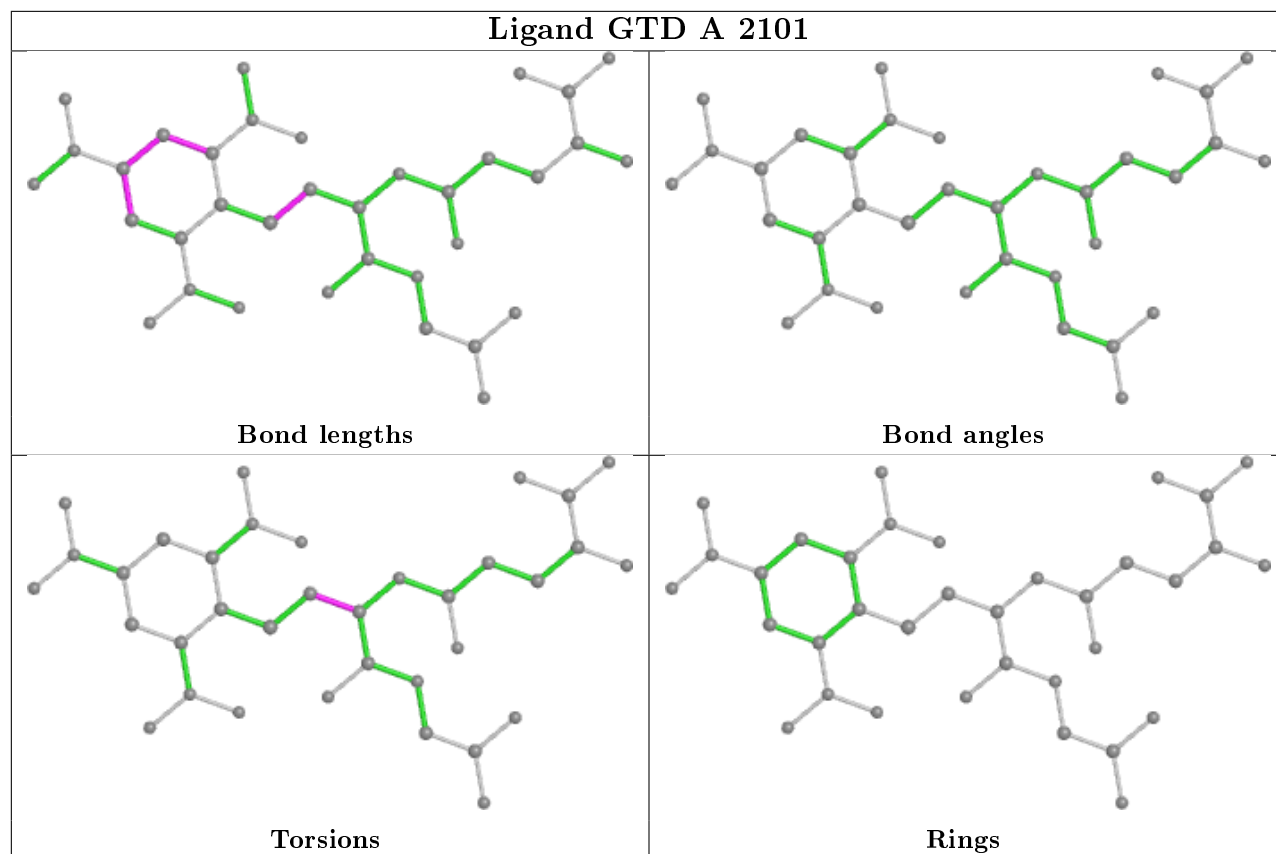
## Ligand GTD D 2401



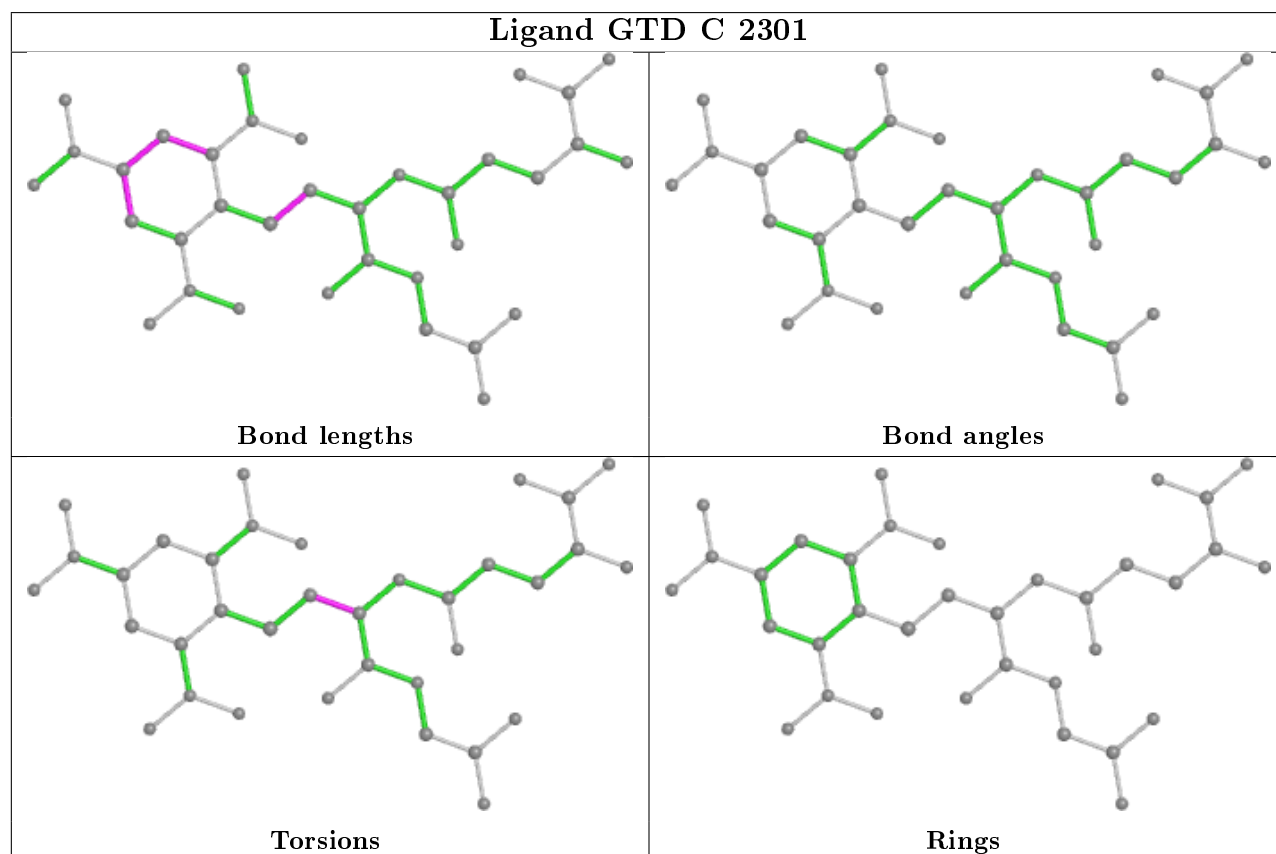
## Ligand GTD B 2201



## Ligand GTD A 2101



## Ligand GTD C 2301



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.