



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:58 am BST

PDB ID : 3LEE
Title : Crystal structure of the human squalene synthase complexed with BPH-652
Authors : Liu, Y.-L.; Lin, F.-Y.; Oldfield, E.
Deposited on : 2010-01-14
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

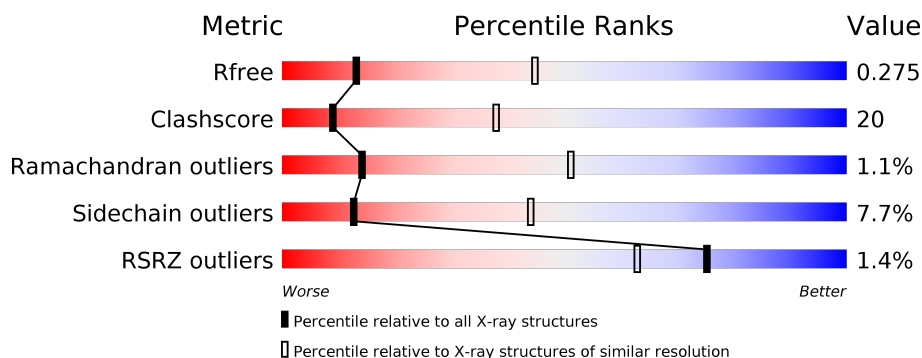
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	340	<div> <div>63%</div> <div>29%</div> <div>• 5%</div> </div>
1	B	340	<div> <div>2%</div> <div>60%</div> <div>31%</div> <div>• 5%</div> </div>
1	C	340	<div> <div>2%</div> <div>58%</div> <div>35%</div> <div>• 5%</div> </div>
1	D	340	<div> <div>2%</div> <div>57%</div> <div>32%</div> <div>6% 5%</div> </div>
1	E	340	<div> <div>56%</div> <div>34%</div> <div>• 5%</div> </div>
1	F	340	<div> <div>3%</div> <div>46%</div> <div>26%</div> <div>• 23%</div> </div>

2 Entry composition [i](#)

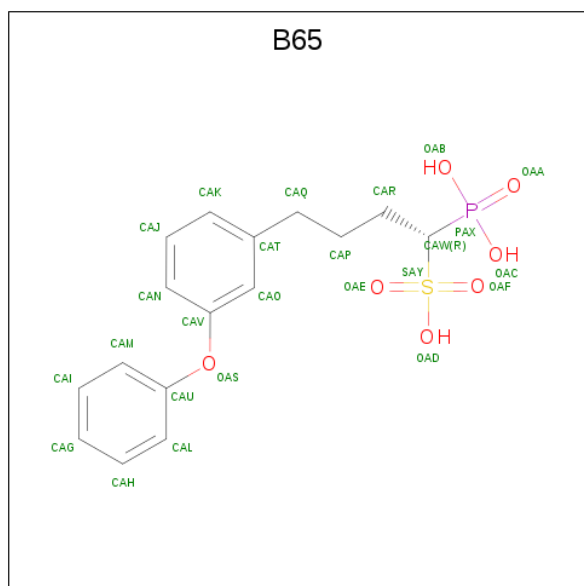
There are 4 unique types of molecules in this entry. The entry contains 15384 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Squalene synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2597	1653	438	490	16			
1	B	324	Total	C	N	O	S	0	0	0
			2600	1654	437	493	16			
1	C	324	Total	C	N	O	S	0	0	0
			2587	1647	435	489	16			
1	D	322	Total	C	N	O	S	0	0	0
			2566	1630	432	488	16			
1	E	323	Total	C	N	O	S	0	0	0
			2591	1651	436	488	16			
1	F	262	Total	C	N	O	S	0	0	0
			2099	1333	355	396	15			

- Molecule 2 is (1R)-4-(3-phenoxyphenyl)-1-phosphonobutane-1-sulfonic acid (three-letter code: B65) (formula: C₁₆H₁₉O₇PS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	O	P	S	0	0
			25	16	7	1	1		
2	B	1	Total	C	O	P	S	0	0
			25	16	7	1	1		
2	C	1	Total	C	O	P	S	0	0
			25	16	7	1	1		
2	D	1	Total	C	O	P	S	0	0
			25	16	7	1	1		
2	E	1	Total	C	O	P	S	0	0
			25	16	7	1	1		
2	F	1	Total	C	O	P	S	0	0
			25	16	7	1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

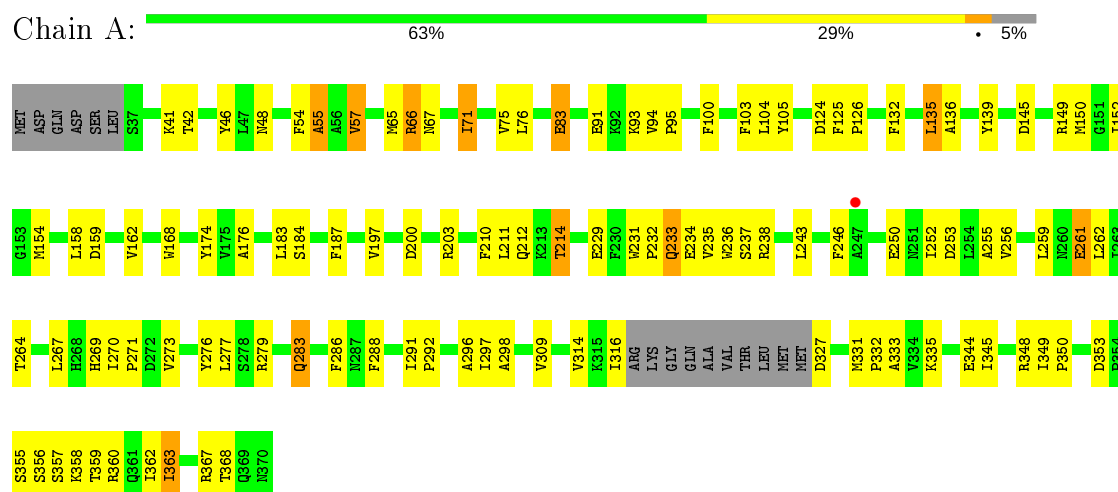
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O	0	0
			36	36		
4	B	46	Total	O	0	0
			46	46		
4	C	37	Total	O	0	0
			37	37		
4	D	28	Total	O	0	0
			28	28		
4	E	20	Total	O	0	0
			20	20		
4	F	21	Total	O	0	0
			21	21		

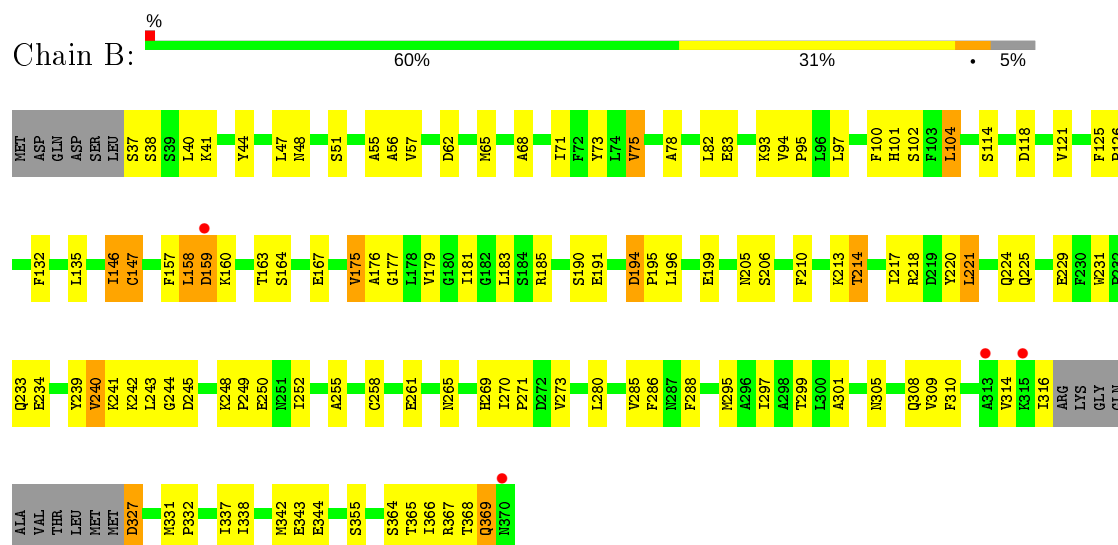
3 Residue-property plots

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

• Molecule 1: Squalene synthetase

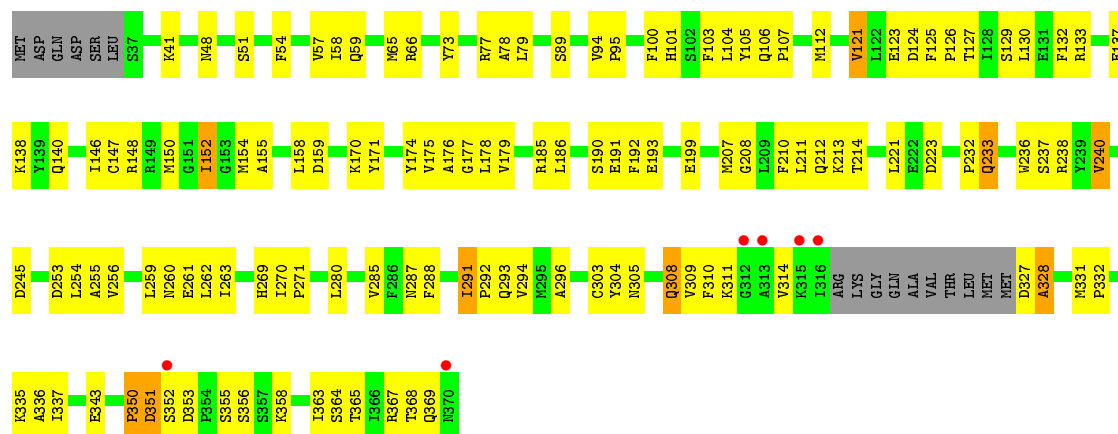


• Molecule 1: Squalene synthetase

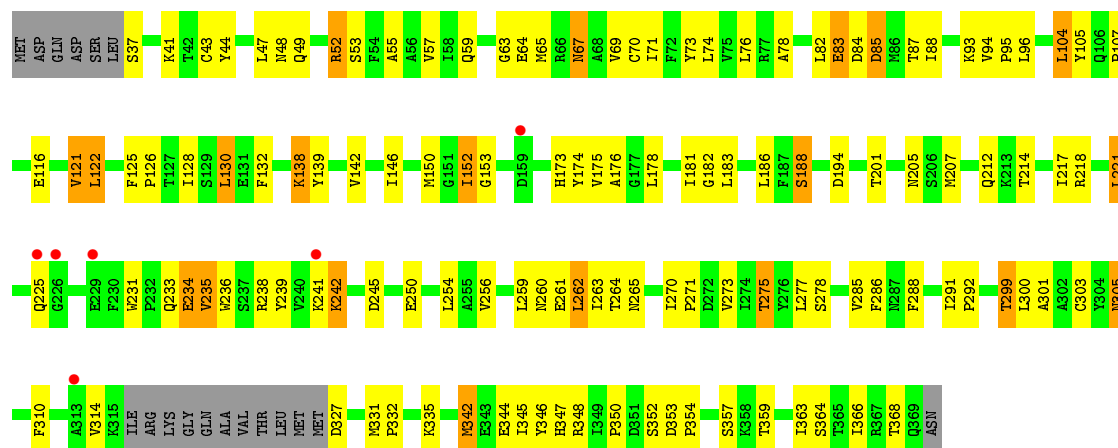


• Molecule 1: Squalene synthetase

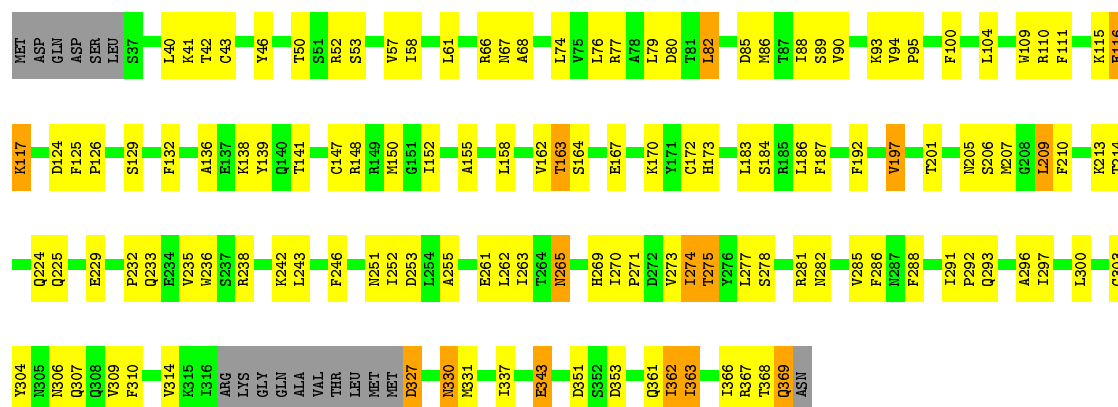




• Molecule 1: Squalene synthetase

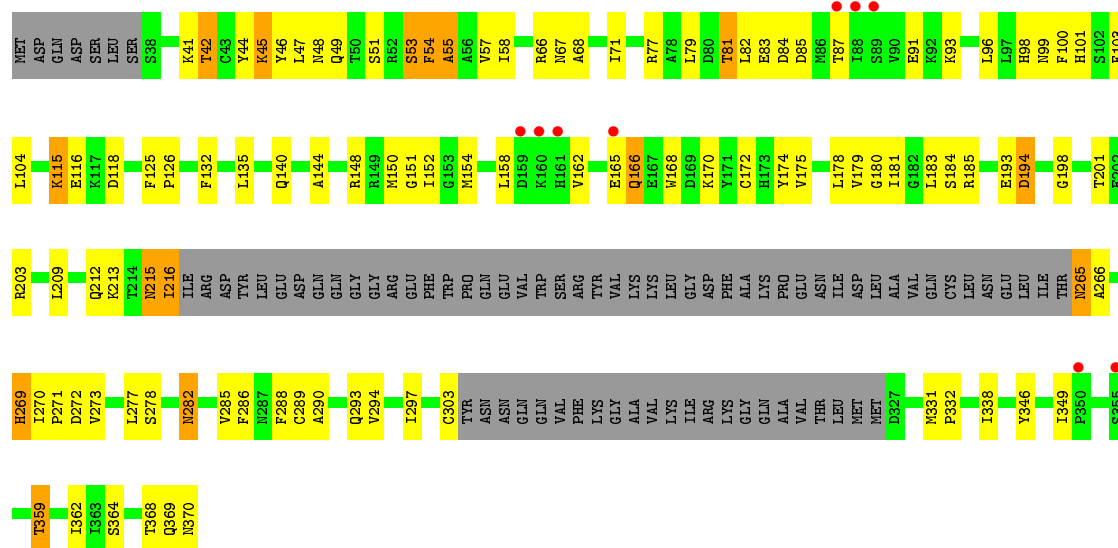


• Molecule 1: Squalene synthetase



• Molecule 1: Squalene synthetase

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.66Å 153.42Å 92.90Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	29.58 – 3.20 29.58 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.58-3.20) 99.5 (29.58-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.191 , 0.276 0.192 , 0.275	Depositor DCC
R_{free} test set	1973 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15384	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, B65

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	0.32	0/2651	0.41	0/3590
1	B	0.30	0/2654	0.40	0/3594
1	C	0.30	0/2641	0.40	0/3579
1	D	0.29	0/2620	0.40	0/3554
1	E	0.29	0/2645	0.40	0/3582
1	F	0.29	0/2140	0.39	0/2893
All	All	0.30	0/15351	0.40	0/20792

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	52	ARG	Peptide
1	E	52	ARG	Peptide

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	2597	0	2533	84	0
1	B	2600	0	2537	106	0
1	C	2587	0	2513	113	0
1	D	2566	0	2472	116	0
1	E	2591	0	2537	116	0
1	F	2099	0	2068	86	0
2	A	25	0	17	1	0
2	B	25	0	17	2	0
2	C	25	0	17	1	0
2	D	25	0	17	1	0
2	E	25	0	17	0	0
2	F	25	0	17	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	36	0	0	1	0
4	B	46	0	0	6	0
4	C	37	0	0	7	0
4	D	28	0	0	2	0
4	E	20	0	0	1	0
4	F	21	0	0	5	0
All	All	15384	0	14762	606	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (606) 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:B:65:MET:CE	1:B:285:VAL:HG22	1.76	1.15
1:A:150:MET:CE	1:A:154:MET:HE3	1.79	1.12
1:E:94:VAL:HG23	1:E:95:PRO:HD3	1.35	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:PHE:O	1:B:214:THR:HG23	1.57	1.04
1:B:65:MET:HE1	1:B:285:VAL:HG22	1.32	1.03
1:D:277:LEU:C	1:D:331:MET:HE3	1.81	1.01
1:C:343:GLU:OE2	1:C:367:ARG:NH2	1.96	0.99
1:A:150:MET:HE2	1:A:154:MET:HE3	1.03	0.99
1:C:207:MET:CE	1:C:293:GLN:HE21	1.77	0.96
1:C:240:VAL:HG21	1:C:245:ASP:HB2	1.45	0.96
1:C:207:MET:HE3	1:C:293:GLN:HE21	1.32	0.92
1:C:221:LEU:HD12	1:C:310:PHE:O	1.71	0.90
1:A:367:ARG:O	1:C:66:ARG:NH2	2.04	0.90
1:B:118:ASP:O	1:B:121:VAL:HG12	1.72	0.90
1:D:57:VAL:HG11	1:D:288:PHE:HA	1.55	0.89
1:D:327:ASP:OD1	1:E:327:ASP:N	2.05	0.89
1:C:176:ALA:CB	1:C:212:GLN:HB2	2.02	0.88
1:D:65:MET:HE1	1:D:285:VAL:HG22	1.53	0.87
1:B:221:LEU:O	1:B:225:GLN:HG2	1.74	0.87
1:B:240:VAL:HG22	4:B:402:HOH:O	1.74	0.87
1:B:65:MET:HE1	1:B:285:VAL:CG2	2.05	0.87
1:B:65:MET:HE2	1:B:285:VAL:HG22	1.56	0.86
1:D:291:ILE:HB	1:D:292:PRO:HD3	1.57	0.86
1:D:142:VAL:HG11	1:D:186:LEU:HD13	1.59	0.85
1:D:314:VAL:HG23	4:D:385:HOH:O	1.76	0.85
1:E:94:VAL:HG23	1:E:95:PRO:CD	2.06	0.84
1:B:48:ASN:ND2	1:B:55:ALA:HB1	1.92	0.84
1:B:65:MET:CE	1:B:285:VAL:CG2	2.56	0.84
1:D:130:LEU:O	1:D:130:LEU:HD12	1.78	0.84
1:F:144:ALA:HB1	4:F:373:HOH:O	1.79	0.83
1:F:369:GLN:OE1	4:F:374:HOH:O	1.97	0.81
1:B:240:VAL:HG21	1:B:245:ASP:HB2	1.62	0.81
1:A:150:MET:HE2	1:A:154:MET:CE	1.99	0.81
1:B:163:THR:HG23	1:B:164:SER:H	1.45	0.81
1:F:57:VAL:HG11	1:F:288:PHE:HA	1.62	0.81
1:F:277:LEU:C	1:F:331:MET:HE3	2.01	0.80
1:A:291:ILE:HB	1:A:292:PRO:HD3	1.62	0.79
1:B:179:VAL:O	1:B:183:LEU:HD12	1.83	0.79
1:C:79:LEU:HD13	1:C:100:PHE:CG	2.18	0.78
1:C:191:GLU:OE2	1:F:370:ASN:HB2	1.81	0.78
1:E:148:ARG:O	1:E:152:ILE:HD13	1.84	0.78
1:A:41:LYS:HA	1:B:368:THR:HG21	1.66	0.78
1:D:286:PHE:HE1	1:D:331:MET:HE1	1.50	0.77
1:E:277:LEU:C	1:E:331:MET:HE1	2.05	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:VAL:HG21	1:B:245:ASP:CB	2.15	0.76
1:D:57:VAL:CG1	1:D:288:PHE:HA	2.16	0.76
1:D:44:TYR:CD2	1:F:368:THR:HG22	2.20	0.76
1:C:176:ALA:HB2	1:C:212:GLN:HB2	1.67	0.76
1:C:57:VAL:HG11	1:C:288:PHE:HA	1.68	0.76
1:C:269:HIS:HD2	4:C:398:HOH:O	1.69	0.74
1:A:233:GLN:HG3	1:A:234:GLU:N	2.01	0.74
1:E:368:THR:HG21	1:F:41:LYS:HA	1.69	0.73
1:A:210:PHE:O	1:A:214:THR:HG23	1.88	0.73
1:F:277:LEU:HB3	1:F:331:MET:HE1	1.70	0.73
1:E:109:TRP:CH2	1:E:111:PHE:HB2	2.23	0.72
1:D:264:THR:HG21	1:D:359:THR:OG1	1.89	0.72
1:D:188:SER:OG	1:D:194:ASP:O	2.07	0.71
1:C:221:LEU:CD1	1:C:310:PHE:O	2.38	0.71
1:C:78:ALA:HB2	1:C:121:VAL:HG13	1.72	0.71
1:D:173:HIS:ND1	1:D:205:ASN:ND2	2.39	0.70
1:D:65:MET:CE	1:D:285:VAL:HG22	2.21	0.70
1:B:159:ASP:OD1	1:B:159:ASP:C	2.31	0.69
1:B:316:ILE:O	1:B:316:ILE:HG22	1.90	0.69
1:F:93:LYS:HD3	1:F:158:LEU:HD21	1.73	0.69
1:A:150:MET:CE	1:A:154:MET:CE	2.64	0.69
1:C:280:LEU:HD13	1:C:285:VAL:HG12	1.75	0.69
1:D:277:LEU:C	1:D:331:MET:CE	2.61	0.69
2:B:451:B65:HAPA	2:B:451:B65:OAA	1.92	0.68
1:D:175:VAL:HG13	1:D:212:GLN:HE21	1.58	0.68
1:A:200:ASP:OD2	1:A:279:ARG:NH2	2.26	0.68
1:F:172:CYS:HB2	1:F:209:LEU:HD22	1.73	0.68
1:F:277:LEU:HB3	1:F:331:MET:CE	2.24	0.68
1:C:155:ALA:HA	1:C:158:LEU:HD12	1.76	0.68
1:F:277:LEU:CB	1:F:331:MET:HE3	2.23	0.68
1:D:264:THR:HG22	1:D:359:THR:HG23	1.75	0.67
1:E:269:HIS:O	1:E:273:VAL:HG23	1.94	0.67
1:D:76:LEU:HD12	2:D:451:B65:HAM	1.77	0.67
1:F:278:SER:N	1:F:331:MET:HE3	2.09	0.67
1:E:214:THR:HG22	1:E:300:LEU:HD11	1.75	0.67
1:C:327:ASP:HA	4:C:375:HOH:O	1.95	0.66
1:B:41:LYS:HA	1:C:368:THR:HG21	1.77	0.66
1:F:290:ALA:O	1:F:294:VAL:HG23	1.95	0.66
1:E:94:VAL:CG2	1:E:95:PRO:HD3	2.22	0.66
1:B:163:THR:HG23	1:B:164:SER:N	2.10	0.66
1:B:210:PHE:O	1:B:214:THR:CG2	2.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:MET:HB3	1:B:332:PRO:HD3	1.78	0.66
1:D:364:SER:O	1:D:368:THR:HG23	1.96	0.66
1:E:136:ALA:HB3	1:E:138:LYS:HG3	1.77	0.65
1:D:278:SER:N	1:D:331:MET:HE3	2.10	0.65
1:C:148:ARG:O	1:C:152:ILE:HD13	1.95	0.65
1:C:294:VAL:HG13	1:C:337:ILE:HG21	1.78	0.65
1:F:174:TYR:HA	1:F:178:LEU:HD12	1.79	0.65
1:B:94:VAL:HB	1:B:95:PRO:HD3	1.78	0.65
1:C:112:MET:SD	1:C:123:GLU:HG2	2.37	0.65
1:A:277:LEU:HB3	1:A:331:MET:HE1	1.78	0.65
1:E:46:TYR:O	1:E:50:THR:HG23	1.96	0.65
1:D:342:MET:HA	1:D:342:MET:CE	2.26	0.64
1:E:286:PHE:CE1	1:E:331:MET:HE2	2.32	0.64
1:B:159:ASP:OD1	1:B:160:LYS:N	2.31	0.64
1:E:163:THR:HG23	1:E:167:GLU:HG3	1.80	0.64
1:E:232:PRO:HB2	1:E:235:VAL:HG23	1.79	0.64
1:D:221:LEU:HD12	1:D:310:PHE:O	1.97	0.64
1:E:278:SER:HA	1:E:331:MET:HE3	1.79	0.64
1:C:309:VAL:HG12	1:C:309:VAL:O	1.97	0.63
2:F:451:B65:OAE	4:F:377:HOH:O	2.12	0.63
1:D:263:ILE:HG12	1:D:300:LEU:HD22	1.79	0.63
1:E:94:VAL:CG2	1:E:95:PRO:CD	2.77	0.63
1:A:277:LEU:C	1:A:331:MET:HE3	2.19	0.63
1:F:84:ASP:OD2	4:F:377:HOH:O	2.15	0.63
1:A:105:TYR:OH	4:A:24:HOH:O	2.14	0.63
1:C:260:ASN:ND2	1:C:304:TYR:CD1	2.67	0.63
1:B:181:ILE:O	1:B:185:ARG:HG3	1.99	0.63
1:B:249:PRO:HA	1:B:252:ILE:HD13	1.79	0.63
1:B:183:LEU:HD22	1:B:288:PHE:CE2	2.32	0.63
1:D:235:VAL:HG11	1:D:262:LEU:HD11	1.80	0.62
1:E:309:VAL:HG12	1:E:309:VAL:O	1.98	0.62
1:C:54:PHE:CD1	2:C:451:B65:HAH	2.34	0.62
1:D:65:MET:O	1:D:69:VAL:HG23	1.98	0.62
1:A:94:VAL:HB	1:A:95:PRO:HD3	1.81	0.62
1:D:125:PHE:N	1:D:126:PRO:HD2	2.14	0.62
1:F:150:MET:HG2	1:F:174:TYR:O	2.00	0.62
1:B:327:ASP:HB3	1:B:337:ILE:HD11	1.81	0.62
1:F:175:VAL:CG2	1:F:212:GLN:NE2	2.63	0.62
1:D:142:VAL:CG1	1:D:186:LEU:HD13	2.30	0.61
1:E:368:THR:O	1:E:369:GLN:C	2.39	0.61
1:F:277:LEU:CB	1:F:331:MET:CE	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:LEU:HD22	1:E:150:MET:SD	2.39	0.61
1:D:93:LYS:HA	1:D:96:LEU:HD12	1.83	0.61
1:D:44:TYR:CD2	1:F:368:THR:CG2	2.84	0.61
1:E:343:GLU:OE1	1:E:367:ARG:NH1	2.30	0.61
1:D:175:VAL:HG13	1:D:212:GLN:NE2	2.16	0.60
1:E:79:LEU:O	1:E:82:LEU:HB2	2.01	0.60
1:F:57:VAL:CG1	1:F:288:PHE:HA	2.30	0.60
1:C:221:LEU:HD12	1:C:310:PHE:C	2.21	0.60
1:D:85:ASP:OD2	1:D:87:THR:OG1	2.15	0.60
1:A:253:ASP:O	1:A:256:VAL:HG22	2.02	0.60
1:A:264:THR:HG23	1:A:359:THR:HA	1.82	0.60
1:D:85:ASP:HB3	1:D:88:ILE:HD12	1.82	0.60
1:F:175:VAL:HG21	1:F:212:GLN:HE21	1.65	0.60
1:B:239:TYR:OH	1:B:261:GLU:OE1	2.17	0.60
1:D:270:ILE:N	1:D:271:PRO:HD2	2.16	0.60
1:B:177:GLY:HA3	1:B:205:ASN:ND2	2.16	0.60
1:C:255:ALA:HB1	1:C:310:PHE:CE1	2.37	0.60
1:F:277:LEU:C	1:F:331:MET:CE	2.70	0.60
1:A:71:ILE:N	1:A:71:ILE:HD13	2.14	0.60
1:F:104:LEU:HD23	1:F:132:PHE:CE1	2.37	0.60
1:C:269:HIS:CD2	4:C:398:HOH:O	2.49	0.60
1:C:57:VAL:CG1	1:C:288:PHE:HA	2.31	0.60
1:F:271:PRO:HA	1:F:369:GLN:HE22	1.67	0.60
1:F:44:TYR:OH	1:F:67:ASN:OD1	2.17	0.60
1:C:125:PHE:N	1:C:126:PRO:CD	2.65	0.59
1:E:293:GLN:O	1:E:297:ILE:CD1	2.49	0.59
1:A:57:VAL:HG11	1:A:288:PHE:HA	1.85	0.59
1:E:255:ALA:HB1	1:E:310:PHE:CZ	2.37	0.59
1:C:79:LEU:HG	1:C:154:MET:CE	2.32	0.59
1:E:43:CYS:O	1:E:74:LEU:HD11	2.01	0.59
1:B:342:MET:CE	1:B:342:MET:HA	2.33	0.59
1:F:175:VAL:HG23	1:F:212:GLN:NE2	2.18	0.59
1:C:240:VAL:HG21	1:C:245:ASP:CB	2.28	0.59
1:D:55:ALA:O	1:D:59:GLN:HG3	2.03	0.59
1:B:125:PHE:N	1:B:126:PRO:CD	2.66	0.59
1:B:157:PHE:CE2	1:B:160:LYS:HE3	2.38	0.59
1:D:291:ILE:HB	1:D:292:PRO:CD	2.31	0.59
1:E:286:PHE:HE1	1:E:331:MET:CE	2.14	0.59
1:B:255:ALA:HB1	1:B:310:PHE:CZ	2.38	0.58
1:C:237:SER:OG	4:C:376:HOH:O	2.16	0.58
1:E:363:ILE:O	1:E:367:ARG:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLN:HA	1:A:236:TRP:CE2	2.39	0.58
1:C:309:VAL:HG22	1:C:314:VAL:HG21	1.85	0.58
1:A:132:PHE:O	1:A:135:LEU:HB2	2.03	0.58
1:E:172:CYS:CB	1:E:209:LEU:HD22	2.34	0.58
1:B:40:LEU:HD21	1:B:44:TYR:HE2	1.68	0.58
1:E:100:PHE:HD2	1:E:147:CYS:SG	2.27	0.58
1:E:362:ILE:O	1:E:362:ILE:HD13	2.03	0.58
1:A:57:VAL:CG1	1:A:288:PHE:HA	2.34	0.58
1:A:316:ILE:N	1:A:316:ILE:HD13	2.18	0.58
1:D:264:THR:CG2	1:D:359:THR:OG1	2.52	0.58
1:C:79:LEU:HG	1:C:154:MET:HE1	1.85	0.57
1:D:342:MET:HA	1:D:342:MET:HE2	1.86	0.57
1:B:190:SER:O	1:B:191:GLU:HB2	2.03	0.57
1:D:176:ALA:HB2	1:D:212:GLN:HE21	1.69	0.57
1:D:277:LEU:O	1:D:331:MET:CE	2.52	0.57
1:D:130:LEU:C	1:D:130:LEU:HD12	2.24	0.57
1:E:297:ILE:N	1:E:297:ILE:HD12	2.20	0.57
1:A:238:ARG:NH2	1:A:261:GLU:OE1	2.36	0.57
1:C:48:ASN:HD21	1:C:59:GLN:NE2	2.02	0.57
1:A:259:LEU:HD21	1:A:309:VAL:HG21	1.85	0.56
1:F:125:PHE:N	1:F:126:PRO:CD	2.68	0.56
1:B:71:ILE:O	1:B:75:VAL:HG13	2.06	0.56
1:B:295:MET:O	1:B:299:THR:HG23	2.05	0.56
1:D:368:THR:HG21	1:E:41:LYS:HA	1.88	0.56
1:A:279:ARG:NH1	1:D:194:ASP:OD1	2.38	0.56
1:B:309:VAL:HG22	1:B:314:VAL:HG21	1.87	0.56
1:D:277:LEU:HB3	1:D:331:MET:HE1	1.87	0.56
1:B:51:SER:HB2	1:B:73:TYR:CZ	2.40	0.56
1:C:327:ASP:O	4:C:384:HOH:O	2.18	0.56
1:B:175:VAL:HG23	1:B:175:VAL:O	2.04	0.56
1:C:232:PRO:HD2	1:C:262:LEU:HD21	1.88	0.56
1:C:351:ASP:C	1:C:353:ASP:H	2.08	0.56
1:F:175:VAL:CG2	1:F:212:GLN:HE21	2.19	0.56
1:E:297:ILE:H	1:E:297:ILE:HD12	1.70	0.56
1:A:246:PHE:CE1	1:A:255:ALA:HA	2.41	0.55
1:D:233:GLN:O	1:D:235:VAL:N	2.34	0.55
1:D:271:PRO:HD3	1:D:366:ILE:HG12	1.87	0.55
1:E:293:GLN:O	1:E:297:ILE:HD13	2.06	0.55
1:D:233:GLN:C	1:D:235:VAL:H	2.10	0.55
1:B:68:ALA:HA	1:B:135:LEU:HD22	1.88	0.55
1:D:235:VAL:HG11	1:D:262:LEU:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ARG:NH2	1:E:261:GLU:OE1	2.39	0.55
1:A:54:PHE:O	1:A:55:ALA:C	2.44	0.55
1:D:152:ILE:HG22	1:D:153:GLY:N	2.21	0.55
1:F:68:ALA:HA	1:F:135:LEU:HD21	1.88	0.55
1:A:93:LYS:HD2	1:A:158:LEU:HD11	1.89	0.55
1:A:264:THR:HA	1:A:267:LEU:HD12	1.89	0.55
1:A:270:ILE:N	1:A:271:PRO:CD	2.69	0.55
1:D:242:LYS:HB3	1:D:245:ASP:OD2	2.07	0.55
1:D:260:ASN:O	1:D:264:THR:HG23	2.07	0.55
1:E:172:CYS:HB2	1:E:209:LEU:HD22	1.89	0.55
1:F:193:GLU:O	1:F:194:ASP:HB2	2.07	0.55
1:C:129:SER:OG	1:C:133:ARG:NH1	2.40	0.54
1:D:346:TYR:HB2	1:D:363:ILE:HD13	1.89	0.54
1:E:286:PHE:CE1	1:E:331:MET:CE	2.90	0.54
1:A:183:LEU:HD13	1:A:288:PHE:HE2	1.72	0.54
1:B:344:GLU:HG2	4:B:410:HOH:O	2.07	0.54
1:E:368:THR:HG22	1:F:44:TYR:CD2	2.42	0.54
1:A:291:ILE:CB	1:A:292:PRO:HD3	2.34	0.54
1:A:368:THR:HG21	1:C:41:LYS:HA	1.89	0.54
1:E:116:GLU:O	1:E:117:LYS:C	2.45	0.54
1:D:88:ILE:HB	1:D:93:LYS:HE3	1.90	0.54
1:F:172:CYS:HA	1:F:175:VAL:HG22	1.88	0.54
1:E:88:ILE:HG22	1:E:93:LYS:HB2	1.89	0.54
1:B:229:GLU:HG2	1:B:243:LEU:HD23	1.89	0.53
1:C:238:ARG:NH2	1:C:261:GLU:OE2	2.41	0.53
1:D:181:ILE:HG23	1:D:201:THR:HG22	1.90	0.53
1:E:136:ALA:HB3	1:E:138:LYS:CG	2.38	0.53
1:C:150:MET:HG3	1:C:174:TYR:O	2.08	0.53
1:E:252:ILE:HG23	1:E:253:ASP:N	2.24	0.53
1:D:233:GLN:HA	1:D:236:TRP:NE1	2.23	0.53
1:E:155:ALA:HA	1:E:158:LEU:HD12	1.90	0.53
1:E:270:ILE:N	1:E:271:PRO:CD	2.71	0.53
1:F:100:PHE:HA	1:F:103:PHE:CD2	2.44	0.53
1:A:327:ASP:O	1:A:333:ALA:HB1	2.09	0.53
1:E:263:ILE:HG12	1:E:300:LEU:HD22	1.91	0.53
1:D:262:LEU:O	1:D:265:ASN:HB3	2.09	0.53
1:A:71:ILE:O	1:A:75:VAL:HG23	2.09	0.53
1:B:297:ILE:HD13	1:B:338:ILE:HG23	1.90	0.53
1:E:94:VAL:N	1:E:95:PRO:HD2	2.24	0.53
1:A:150:MET:HG3	1:A:174:TYR:O	2.10	0.52
1:C:207:MET:HE3	1:C:293:GLN:NE2	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ASN:ND2	1:C:304:TYR:CE1	2.77	0.52
1:A:331:MET:HG3	1:A:335:LYS:HD2	1.91	0.52
1:C:100:PHE:HD2	1:C:147:CYS:SG	2.33	0.52
1:E:125:PHE:N	1:E:126:PRO:CD	2.72	0.52
1:C:363:ILE:HG22	1:C:363:ILE:O	2.09	0.52
1:E:214:THR:HG22	1:E:300:LEU:CD1	2.39	0.52
1:E:286:PHE:HE1	1:E:331:MET:HE1	1.75	0.52
1:F:181:ILE:HD13	1:F:201:THR:HB	1.91	0.52
1:A:200:ASP:OD2	1:A:203:ARG:HD2	2.10	0.52
1:A:277:LEU:CB	1:A:331:MET:HE1	2.39	0.52
1:D:94:VAL:HB	1:D:95:PRO:HD3	1.90	0.52
1:D:65:MET:CE	1:D:285:VAL:CG2	2.88	0.52
1:D:85:ASP:HA	1:D:116:GLU:OE2	2.10	0.52
1:F:68:ALA:HA	1:F:135:LEU:CD2	2.40	0.52
1:F:277:LEU:HB2	1:F:331:MET:HE3	1.92	0.51
1:A:283:GLN:CA	1:A:283:GLN:HE21	2.22	0.51
1:B:48:ASN:HD21	1:B:55:ALA:HB1	1.74	0.51
1:B:65:MET:HE2	1:B:285:VAL:CG2	2.30	0.51
1:F:87:THR:HG21	1:F:115:LYS:HE2	1.91	0.51
1:A:283:GLN:NE2	1:A:283:GLN:HA	2.26	0.51
1:C:293:GLN:O	1:C:296:ALA:HB3	2.11	0.51
1:E:210:PHE:O	1:E:214:THR:HG23	2.10	0.51
1:C:73:TYR:C	1:C:73:TYR:CD2	2.84	0.51
1:E:277:LEU:HB3	1:E:331:MET:HE1	1.92	0.51
1:E:368:THR:HG22	1:F:44:TYR:HB2	1.92	0.51
1:D:71:ILE:HG21	1:D:132:PHE:HB2	1.92	0.51
1:A:286:PHE:HE1	1:A:331:MET:CE	2.24	0.51
1:B:242:LYS:O	1:B:245:ASP:HB2	2.11	0.51
1:C:104:LEU:HD23	1:C:132:PHE:CE1	2.46	0.50
1:E:201:THR:O	1:E:205:ASN:HB2	2.11	0.50
1:B:163:THR:HA	1:B:233:GLN:HB3	1.93	0.50
1:A:104:LEU:HD13	1:A:132:PHE:CE1	2.46	0.50
1:A:184:SER:HB3	1:A:276:TYR:OH	2.12	0.50
1:B:308:GLN:O	1:B:308:GLN:HG3	2.11	0.50
1:F:184:SER:HB3	1:F:198:GLY:HA2	1.92	0.50
1:E:129:SER:O	1:E:132:PHE:HB3	2.11	0.50
1:E:309:VAL:HG22	1:E:314:VAL:HG11	1.93	0.50
1:A:344:GLU:O	1:A:348:ARG:HG3	2.11	0.50
1:F:104:LEU:HD23	1:F:132:PHE:CZ	2.46	0.50
1:B:179:VAL:HG12	1:B:183:LEU:HD11	1.93	0.50
1:C:94:VAL:N	1:C:95:PRO:HD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:TYR:CD1	1:E:186:LEU:HD23	2.46	0.50
1:C:137:GLU:O	1:C:138:LYS:C	2.50	0.50
1:D:368:THR:HA	1:E:66:ARG:HH22	1.76	0.50
1:B:194:ASP:HB2	4:B:397:HOH:O	2.12	0.49
1:B:270:ILE:HB	1:B:271:PRO:HD3	1.93	0.49
1:E:79:LEU:HD13	1:E:100:PHE:CG	2.47	0.49
1:B:224:GLN:HE22	1:B:243:LEU:HG	1.76	0.49
1:D:256:VAL:HG11	1:D:305:ASN:HD22	1.76	0.49
2:B:451:B65:CAP	2:B:451:B65:OAA	2.61	0.49
1:F:265:ASN:OD1	1:F:266:ALA:N	2.45	0.49
1:F:77:ARG:HD2	2:F:451:B65:HAJ	1.93	0.49
1:B:78:ALA:HB2	1:B:121:VAL:HG22	1.95	0.49
1:B:94:VAL:HB	1:B:95:PRO:CD	2.42	0.49
1:A:136:ALA:HB3	1:A:139:TYR:CD2	2.48	0.49
1:B:125:PHE:N	1:B:126:PRO:HD2	2.28	0.49
1:C:104:LEU:HD23	1:C:132:PHE:CD1	2.48	0.49
1:C:291:ILE:HB	1:C:292:PRO:HD3	1.94	0.49
1:D:299:THR:O	1:D:303:CYS:HB2	2.13	0.49
1:E:277:LEU:O	1:E:331:MET:HE1	2.11	0.49
1:B:57:VAL:HG23	1:B:288:PHE:HD1	1.78	0.49
1:B:62:ASP:O	1:B:65:MET:HG2	2.13	0.49
1:D:301:ALA:O	1:D:348:ARG:NH2	2.46	0.49
1:D:256:VAL:HG11	1:D:305:ASN:ND2	2.27	0.49
1:F:175:VAL:HG21	1:F:212:GLN:NE2	2.27	0.48
1:A:233:GLN:HA	1:A:236:TRP:NE1	2.28	0.48
1:C:233:GLN:HA	1:C:236:TRP:NE1	2.28	0.48
1:D:78:ALA:O	1:D:122:LEU:HD21	2.13	0.48
1:B:365:THR:O	1:B:369:GLN:HB2	2.12	0.48
1:B:73:TYR:CD1	1:B:73:TYR:C	2.86	0.48
1:D:125:PHE:N	1:D:126:PRO:CD	2.75	0.48
1:D:286:PHE:CE1	1:D:331:MET:HE1	2.39	0.48
1:B:240:VAL:HG21	1:B:245:ASP:HB3	1.94	0.48
1:B:82:LEU:O	1:B:93:LYS:HE2	2.12	0.48
1:A:100:PHE:HA	1:A:103:PHE:CD2	2.48	0.48
1:E:170:LYS:O	1:E:173:HIS:HB3	2.14	0.48
1:E:46:TYR:HB2	1:E:74:LEU:HD21	1.96	0.48
1:B:240:VAL:CG2	1:B:245:ASP:HB2	2.40	0.48
1:F:132:PHE:CZ	1:F:140:GLN:HG2	2.49	0.48
1:C:287:ASN:O	1:C:291:ILE:HD12	2.14	0.48
1:C:351:ASP:O	1:C:353:ASP:N	2.44	0.48
1:D:138:LYS:HD2	1:D:139:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:MET:SD	1:D:273:VAL:HG13	2.54	0.48
1:E:309:VAL:CG1	1:E:309:VAL:O	2.61	0.48
1:B:248:LYS:HB3	1:B:250:GLU:OE2	2.14	0.48
1:B:342:MET:HA	1:B:342:MET:HE2	1.96	0.48
1:C:78:ALA:CB	1:C:121:VAL:HG13	2.42	0.48
1:D:259:LEU:HD21	1:D:303:CYS:O	2.13	0.48
1:B:93:LYS:O	1:B:97:LEU:HG	2.14	0.48
1:B:100:PHE:O	1:B:101:HIS:C	2.51	0.48
1:D:331:MET:HB3	1:D:332:PRO:HD3	1.95	0.48
1:F:79:LEU:HD22	1:F:154:MET:SD	2.54	0.48
1:B:146:ILE:HA	1:B:146:ILE:HD13	1.69	0.47
1:C:174:TYR:HA	1:C:178:LEU:HD12	1.96	0.47
1:A:277:LEU:CB	1:A:331:MET:CE	2.93	0.47
1:B:240:VAL:CG2	1:B:245:ASP:CB	2.90	0.47
1:C:365:THR:O	1:C:369:GLN:HB2	2.14	0.47
1:E:277:LEU:C	1:E:331:MET:CE	2.79	0.47
1:E:361:GLN:HG3	1:E:362:ILE:N	2.29	0.47
1:F:154:MET:O	1:F:158:LEU:HD12	2.14	0.47
1:F:77:ARG:O	1:F:81:THR:OG1	2.32	0.47
1:A:125:PHE:N	1:A:126:PRO:CD	2.77	0.47
1:C:177:GLY:HA2	1:C:208:GLY:HA3	1.96	0.47
1:C:176:ALA:O	1:C:179:VAL:HB	2.13	0.47
1:E:270:ILE:HB	1:E:366:ILE:HD11	1.95	0.47
1:A:298:ALA:HB1	1:A:316:ILE:CG2	2.44	0.47
1:D:347:HIS:ND1	1:D:347:HIS:O	2.47	0.47
1:E:282:ASN:HB3	1:E:285:VAL:HB	1.97	0.47
1:A:145:ASP:O	1:A:149:ARG:HG3	2.14	0.47
1:A:235:VAL:HG11	1:A:262:LEU:HD21	1.96	0.47
1:B:183:LEU:HD22	1:B:288:PHE:HE2	1.74	0.47
1:B:316:ILE:CG2	1:B:316:ILE:O	2.59	0.47
1:B:47:LEU:O	1:B:51:SER:HB3	2.14	0.47
1:A:162:VAL:HG11	1:A:168:TRP:HA	1.97	0.47
1:A:67:ASN:N	1:A:67:ASN:HD22	2.12	0.47
1:B:265:ASN:OD1	1:B:265:ASN:C	2.54	0.47
1:B:342:MET:HG3	1:B:366:ILE:HG21	1.96	0.47
1:C:78:ALA:HA	1:C:121:VAL:HG11	1.96	0.47
1:E:90:VAL:O	1:E:94:VAL:HG22	2.14	0.47
1:E:233:GLN:HA	1:E:236:TRP:NE1	2.29	0.47
1:E:89:SER:O	1:E:93:LYS:N	2.48	0.47
1:C:355:SER:O	1:C:356:SER:C	2.53	0.47
1:F:265:ASN:C	1:F:265:ASN:OD1	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:451:B65:OAE	2:A:451:B65:OAC	2.32	0.46
1:D:239:TYR:O	1:D:254:LEU:HD23	2.15	0.46
1:B:270:ILE:N	1:B:271:PRO:CD	2.78	0.46
1:C:327:ASP:O	1:C:328:ALA:HB3	2.14	0.46
1:A:298:ALA:HB1	1:A:316:ILE:HG23	1.98	0.46
1:D:88:ILE:HG22	1:D:93:LYS:HB2	1.97	0.46
1:E:125:PHE:N	1:E:126:PRO:HD2	2.30	0.46
1:E:163:THR:OG1	1:E:164:SER:N	2.46	0.46
1:F:125:PHE:N	1:F:126:PRO:HD2	2.29	0.46
1:A:76:LEU:HD22	1:A:150:MET:HE1	1.96	0.46
1:B:100:PHE:O	1:B:102:SER:N	2.48	0.46
1:B:196:LEU:HA	1:B:199:GLU:HG3	1.97	0.46
1:F:132:PHE:CZ	1:F:140:GLN:CG	2.99	0.46
1:F:269:HIS:O	1:F:273:VAL:HG23	2.16	0.46
1:A:362:ILE:O	1:A:362:ILE:HD12	2.15	0.46
1:B:241:LYS:N	4:B:402:HOH:O	2.38	0.46
1:E:293:GLN:O	1:E:297:ILE:HD12	2.16	0.46
1:F:270:ILE:N	1:F:271:PRO:CD	2.78	0.46
1:E:246:PHE:CD1	1:E:255:ALA:HB2	2.50	0.46
1:E:367:ARG:HD2	1:F:48:ASN:ND2	2.31	0.46
1:D:146:ILE:HG23	1:D:178:LEU:HB3	1.98	0.46
1:E:236:TRP:CE2	1:E:243:LEU:HB2	2.50	0.46
1:C:259:LEU:HD21	1:C:303:CYS:O	2.16	0.46
1:D:122:LEU:HA	1:D:122:LEU:HD13	1.78	0.46
1:E:46:TYR:OH	1:E:124:ASP:OD2	2.26	0.46
1:B:217:ILE:O	1:B:218:ARG:C	2.53	0.46
1:D:73:TYR:C	1:D:73:TYR:CD1	2.90	0.46
1:F:101:HIS:CE1	1:F:148:ARG:HD3	2.50	0.46
1:B:229:GLU:CG	1:B:243:LEU:HD23	2.46	0.45
1:B:255:ALA:HB1	1:B:310:PHE:CE2	2.51	0.45
1:C:262:LEU:O	1:C:263:ILE:C	2.53	0.45
1:C:213:LYS:NZ	1:C:269:HIS:HE1	2.13	0.45
1:E:330:ASN:N	1:E:330:ASN:HD22	2.14	0.45
1:B:343:GLU:OE2	1:B:367:ARG:NH1	2.35	0.45
1:C:65:MET:CE	1:C:192:PHE:CD2	2.99	0.45
1:C:270:ILE:N	1:C:271:PRO:CD	2.79	0.45
1:E:255:ALA:HB1	1:E:310:PHE:CE1	2.51	0.45
1:E:286:PHE:CZ	1:E:331:MET:HE2	2.51	0.45
1:E:41:LYS:NZ	4:E:377:HOH:O	2.49	0.45
1:A:183:LEU:HD13	1:A:288:PHE:CE2	2.50	0.45
1:D:256:VAL:HG13	1:D:305:ASN:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:ILE:CD1	1:E:297:ILE:H	2.29	0.45
1:F:165:GLU:O	1:F:166:GLN:C	2.53	0.45
1:C:127:THR:O	1:C:130:LEU:HB3	2.17	0.45
1:E:291:ILE:HB	1:E:292:PRO:HD3	1.98	0.45
1:A:345:ILE:HG21	1:A:363:ILE:HD11	1.98	0.45
1:A:65:MET:O	1:A:66:ARG:C	2.54	0.45
1:B:240:VAL:CG2	4:B:402:HOH:O	2.48	0.45
1:F:118:ASP:N	1:F:118:ASP:OD1	2.49	0.45
1:B:164:SER:HA	1:B:234:GLU:HB2	1.98	0.45
1:C:170:LYS:O	1:C:171:TYR:C	2.55	0.45
1:D:181:ILE:CG2	1:D:201:THR:HG22	2.46	0.45
1:D:301:ALA:HA	1:D:345:ILE:HD11	1.99	0.45
1:D:303:CYS:SG	1:D:314:VAL:HG11	2.56	0.45
1:D:82:LEU:O	1:D:84:ASP:N	2.50	0.45
1:F:168:TRP:CZ2	1:F:216:ILE:HD11	2.52	0.45
1:A:176:ALA:CB	1:A:212:GLN:HB2	2.47	0.45
1:B:194:ASP:CG	1:B:195:PRO:HD2	2.37	0.45
1:C:363:ILE:CG2	1:C:363:ILE:O	2.65	0.45
1:E:57:VAL:HB	1:E:288:PHE:HA	1.99	0.45
1:F:53:SER:C	1:F:55:ALA:N	2.69	0.45
1:C:294:VAL:HG13	1:C:337:ILE:CG2	2.46	0.45
1:D:176:ALA:HB2	1:D:212:GLN:NE2	2.31	0.45
1:D:271:PRO:O	1:D:275:THR:HG23	2.17	0.45
1:C:132:PHE:CD2	1:C:132:PHE:C	2.91	0.44
1:C:210:PHE:O	1:C:214:THR:HG22	2.17	0.44
1:D:105:TYR:O	1:D:107:PRO:HD3	2.16	0.44
1:E:172:CYS:HB3	1:E:209:LEU:HD22	1.98	0.44
1:E:206:SER:O	1:E:207:MET:C	2.55	0.44
1:E:251:ASN:O	1:E:252:ILE:C	2.55	0.44
1:C:233:GLN:O	1:C:237:SER:OG	2.30	0.44
1:E:213:LYS:NZ	1:E:269:HIS:CE1	2.85	0.44
1:B:213:LYS:HZ1	1:B:269:HIS:HE1	1.65	0.44
1:C:233:GLN:HA	1:C:236:TRP:CE2	2.52	0.44
1:E:58:ILE:O	1:E:61:LEU:HB2	2.17	0.44
1:F:180:GLY:HA2	1:F:183:LEU:HD12	1.99	0.44
1:F:82:LEU:O	1:F:83:GLU:C	2.55	0.44
1:B:280:LEU:HD13	1:B:286:PHE:HA	1.98	0.44
1:C:105:TYR:O	1:C:107:PRO:HD3	2.17	0.44
1:C:138:LYS:CD	4:C:372:HOH:O	2.66	0.44
1:C:309:VAL:CG1	1:C:309:VAL:O	2.63	0.44
1:B:56:ALA:HB1	1:C:336:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ALA:HB1	4:B:410:HOH:O	2.17	0.44
1:C:331:MET:HE2	1:C:335:LYS:HD2	2.00	0.44
1:D:41:LYS:HA	1:F:368:THR:HG21	2.00	0.44
1:D:277:LEU:HB3	1:D:331:MET:CE	2.48	0.44
1:D:342:MET:HA	1:D:342:MET:HE3	1.97	0.44
1:D:347:HIS:O	1:D:347:HIS:CG	2.71	0.44
1:D:67:ASN:OD1	1:D:67:ASN:N	2.49	0.44
1:F:282:ASN:HB3	1:F:285:VAL:HG23	2.00	0.44
1:C:358:LYS:O	1:C:358:LYS:HD3	2.18	0.44
1:D:88:ILE:HB	1:D:93:LYS:CE	2.46	0.44
1:F:179:VAL:O	1:F:183:LEU:HG	2.17	0.44
1:A:283:GLN:CA	1:A:283:GLN:NE2	2.81	0.44
1:C:190:SER:O	1:C:191:GLU:HB2	2.18	0.44
1:D:238:ARG:NH2	1:D:261:GLU:OE1	2.51	0.44
1:A:184:SER:HB2	1:A:197:VAL:HG12	1.99	0.44
1:A:231:TRP:HA	1:A:232:PRO:HD3	1.83	0.44
1:B:94:VAL:CB	1:B:95:PRO:HD3	2.45	0.44
1:F:359:THR:HA	1:F:362:ILE:HG22	2.00	0.44
1:A:331:MET:N	1:A:332:PRO:CD	2.81	0.43
1:D:182:GLY:O	1:D:186:LEU:HB2	2.18	0.43
1:D:270:ILE:O	1:D:273:VAL:N	2.51	0.43
1:E:40:LEU:HD21	1:E:67:ASN:HD21	1.82	0.43
1:A:233:GLN:O	1:A:237:SER:HB3	2.18	0.43
1:A:48:ASN:ND2	1:B:367:ARG:HD2	2.33	0.43
1:E:262:LEU:O	1:E:265:ASN:HB3	2.17	0.43
1:F:297:ILE:HD13	1:F:338:ILE:HG12	1.99	0.43
1:C:104:LEU:CD2	1:C:132:PHE:CE1	3.01	0.43
1:E:183:LEU:O	1:E:187:PHE:CG	2.71	0.43
1:E:263:ILE:HD13	1:E:304:TYR:HA	2.00	0.43
1:B:146:ILE:HG22	1:B:147:CYS:N	2.33	0.43
1:B:269:HIS:O	1:B:273:VAL:HG23	2.18	0.43
1:C:133:ARG:HA	1:C:140:GLN:NE2	2.33	0.43
1:E:233:GLN:HA	1:E:236:TRP:CD1	2.54	0.43
1:A:184:SER:HA	1:A:187:PHE:CD2	2.53	0.43
1:A:233:GLN:CG	1:A:234:GLU:N	2.78	0.43
1:B:220:TYR:C	1:B:220:TYR:CD2	2.90	0.43
1:D:69:VAL:HG13	1:D:183:LEU:HD21	2.01	0.43
1:D:314:VAL:N	4:D:385:HOH:O	2.28	0.43
1:F:289:CYS:O	1:F:293:GLN:HG2	2.19	0.43
1:B:231:TRP:HZ3	1:B:258:CYS:HG	1.67	0.43
1:C:101:HIS:HA	1:C:104:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:GLN:C	1:C:310:PHE:H	2.21	0.43
1:D:43:CYS:O	1:D:74:LEU:HD11	2.19	0.43
1:F:215:ASN:HD22	1:F:215:ASN:N	2.16	0.43
1:A:210:PHE:O	1:A:214:THR:CG2	2.62	0.43
1:A:269:HIS:O	1:A:273:VAL:HG23	2.17	0.43
1:C:54:PHE:HB3	1:C:58:ILE:CD1	2.49	0.43
1:C:78:ALA:HB2	1:C:121:VAL:CG1	2.45	0.43
1:D:264:THR:HG22	1:D:359:THR:CG2	2.46	0.43
1:F:162:VAL:HG11	1:F:168:TRP:CD1	2.54	0.43
1:F:346:TYR:O	1:F:349:ILE:HG13	2.18	0.43
1:B:213:LYS:NZ	1:B:265:ASN:OD1	2.52	0.43
1:B:57:VAL:HG23	1:B:288:PHE:CD1	2.54	0.43
1:C:146:ILE:O	1:C:150:MET:HB2	2.19	0.43
1:F:47:LEU:HD11	1:F:58:ILE:HD12	2.00	0.43
1:C:287:ASN:O	1:C:291:ILE:CD1	2.67	0.43
1:C:304:TYR:O	1:C:305:ASN:CB	2.67	0.43
1:E:109:TRP:CE3	1:E:110:ARG:N	2.87	0.43
1:B:177:GLY:CA	1:B:205:ASN:HD22	2.30	0.43
1:C:294:VAL:CG1	1:C:337:ILE:HG21	2.45	0.43
1:E:277:LEU:CB	1:E:331:MET:HE1	2.49	0.43
1:A:124:ASP:CG	1:A:124:ASP:O	2.58	0.42
1:A:349:ILE:HD12	1:A:360:ARG:HG2	2.01	0.42
1:A:350:PRO:HG2	1:A:353:ASP:HB2	2.00	0.42
1:E:236:TRP:CG	1:E:243:LEU:HD13	2.54	0.42
1:F:57:VAL:HG12	1:F:288:PHE:HD1	1.83	0.42
1:C:193:GLU:OE1	1:C:193:GLU:HA	2.19	0.42
1:E:192:PHE:CD2	1:E:282:ASN:ND2	2.87	0.42
1:E:210:PHE:HE2	1:E:297:ILE:HD12	1.83	0.42
1:C:175:VAL:CG1	1:C:212:GLN:NE2	2.82	0.42
1:E:224:GLN:HE21	1:E:229:GLU:HG2	1.84	0.42
1:E:303:CYS:O	1:E:306:ASN:CB	2.68	0.42
1:A:229:GLU:HG2	1:A:243:LEU:HD23	2.01	0.42
1:C:331:MET:N	1:C:332:PRO:HD2	2.34	0.42
1:D:234:GLU:O	1:D:235:VAL:HG23	2.20	0.42
1:E:93:LYS:HD3	1:E:158:LEU:HD11	2.01	0.42
1:C:124:ASP:CG	1:C:124:ASP:O	2.58	0.42
1:E:184:SER:HB3	1:E:197:VAL:O	2.20	0.42
1:E:331:MET:HE2	1:E:331:MET:HB2	1.92	0.42
1:A:349:ILE:CD1	1:A:360:ARG:HG2	2.50	0.42
1:A:345:ILE:CG2	1:A:363:ILE:HD11	2.49	0.42
1:D:76:LEU:HD22	1:D:150:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LEU:HD13	1:C:100:PHE:CB	2.50	0.42
1:F:93:LYS:HD3	1:F:158:LEU:CD2	2.47	0.42
1:D:277:LEU:CB	1:D:331:MET:CE	2.98	0.42
1:D:47:LEU:HA	1:D:74:LEU:HD21	2.02	0.42
1:C:199:GLU:OE2	1:F:203:ARG:NH2	2.41	0.42
1:D:231:TRP:CE3	1:D:262:LEU:CD2	3.03	0.42
1:D:291:ILE:CB	1:D:292:PRO:CD	2.97	0.42
1:E:139:TYR:HD1	1:E:186:LEU:HD23	1.85	0.42
1:D:104:LEU:HB3	1:D:132:PHE:CE2	2.55	0.41
1:E:274:ILE:O	1:E:275:THR:C	2.59	0.41
1:A:283:GLN:HE21	1:A:283:GLN:HA	1.85	0.41
1:C:364:SER:O	1:C:367:ARG:N	2.52	0.41
1:B:93:LYS:HD2	1:B:158:LEU:HD21	2.02	0.41
1:B:94:VAL:CB	1:B:95:PRO:CD	2.97	0.41
1:C:79:LEU:HG	1:C:154:MET:HE2	2.02	0.41
1:D:121:VAL:HG22	1:D:128:ILE:CD1	2.49	0.41
1:D:63:GLY:O	1:D:64:GLU:C	2.58	0.41
1:E:162:VAL:HG12	1:E:232:PRO:HA	2.01	0.41
1:F:185:ARG:NH1	4:F:384:HOH:O	2.52	0.41
1:F:42:THR:O	1:F:45:LYS:HB3	2.21	0.41
1:B:179:VAL:HG12	1:B:183:LEU:CD1	2.50	0.41
1:D:291:ILE:CB	1:D:292:PRO:HD3	2.39	0.41
1:E:85:ASP:C	1:E:86:MET:HE3	2.41	0.41
1:C:125:PHE:N	1:C:126:PRO:HD2	2.34	0.41
1:E:148:ARG:O	1:E:152:ILE:CD1	2.63	0.41
1:E:252:ILE:HD11	1:E:307:GLN:HB2	2.03	0.41
1:C:138:LYS:HD2	4:C:372:HOH:O	2.21	0.41
1:C:48:ASN:HD21	1:C:59:GLN:HE22	1.67	0.41
1:D:350:PRO:HG2	1:D:353:ASP:HB2	2.02	0.41
1:F:53:SER:O	1:F:54:PHE:C	2.59	0.41
1:A:211:LEU:HD23	1:A:296:ALA:HB2	2.02	0.41
1:E:351:ASP:C	1:E:353:ASP:H	2.23	0.41
1:E:77:ARG:O	1:E:80:ASP:N	2.53	0.41
1:A:42:THR:HG22	1:A:46:TYR:CE2	2.55	0.41
1:B:343:GLU:OE2	1:B:367:ARG:HD3	2.20	0.41
1:C:103:PHE:HA	1:C:106:GLN:HB2	2.02	0.41
1:C:207:MET:HE1	1:C:293:GLN:HG3	2.03	0.41
1:E:68:ALA:HB1	1:E:186:LEU:HD22	2.01	0.41
1:E:327:ASP:HB3	1:E:337:ILE:HD11	2.02	0.41
1:F:151:GLY:O	1:F:152:ILE:C	2.59	0.41
1:F:209:LEU:O	1:F:213:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:PHE:CE1	1:F:331:MET:HE1	2.55	0.41
1:A:358:LYS:O	1:A:362:ILE:HG22	2.21	0.41
1:A:200:ASP:OD2	1:A:203:ARG:HB2	2.20	0.41
1:B:48:ASN:ND2	1:B:55:ALA:CB	2.74	0.41
1:C:176:ALA:HB3	1:C:212:GLN:HB2	1.99	0.41
1:D:48:ASN:ND2	1:D:55:ALA:HB1	2.36	0.41
1:E:293:GLN:O	1:E:296:ALA:HB3	2.21	0.41
1:E:330:ASN:N	1:E:330:ASN:ND2	2.70	0.41
1:F:46:TYR:HA	1:F:49:GLN:HG2	2.03	0.41
1:B:224:GLN:NE2	1:B:244:GLY:HA2	2.36	0.40
1:C:255:ALA:HB1	1:C:310:PHE:CZ	2.56	0.40
1:D:214:THR:O	1:D:217:ILE:HB	2.21	0.40
1:D:83:GLU:O	1:D:83:GLU:HG2	2.20	0.40
1:A:83:GLU:HA	1:A:93:LYS:HD3	2.03	0.40
1:B:213:LYS:NZ	1:B:269:HIS:HE1	2.20	0.40
1:C:150:MET:O	1:C:154:MET:HG3	2.22	0.40
1:C:175:VAL:HG12	1:C:212:GLN:NE2	2.36	0.40
1:C:350:PRO:O	1:C:351:ASP:C	2.59	0.40
1:F:85:ASP:OD2	1:F:116:GLU:HG2	2.21	0.40
1:D:150:MET:HG2	1:D:174:TYR:O	2.21	0.40
1:D:270:ILE:O	1:D:271:PRO:C	2.59	0.40
1:D:70:CYS:O	1:D:74:LEU:HG	2.21	0.40
1:E:252:ILE:CG2	1:E:253:ASP:N	2.83	0.40
1:B:104:LEU:HB3	1:B:132:PHE:CE2	2.57	0.40
1:C:304:TYR:O	1:C:305:ASN:HB2	2.21	0.40
1:F:270:ILE:N	1:F:271:PRO:HD2	2.36	0.40
1:F:277:LEU:HD21	1:F:289:CYS:HB3	2.02	0.40
1:F:331:MET:HB3	1:F:332:PRO:HD3	2.04	0.40
1:F:96:LEU:HD23	1:F:96:LEU:HA	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/340 (94%)	304 (95%)	14 (4%)	2 (1%)	25	64
1	B	320/340 (94%)	297 (93%)	19 (6%)	4 (1%)	12	47
1	C	320/340 (94%)	292 (91%)	25 (8%)	3 (1%)	17	56
1	D	318/340 (94%)	298 (94%)	15 (5%)	5 (2%)	9	43
1	E	319/340 (94%)	293 (92%)	24 (8%)	2 (1%)	25	64
1	F	256/340 (75%)	222 (87%)	30 (12%)	4 (2%)	9	43
All	All	1853/2040 (91%)	1706 (92%)	127 (7%)	20 (1%)	14	51

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA
1	E	117	LYS
1	F	54	PHE
1	C	352	SER
1	D	52	ARG
1	D	83	GLU
1	D	234	GLU
1	C	328	ALA
1	D	235	VAL
1	F	55	ALA
1	B	176	ALA
1	B	305	ASN
1	B	369	GLN
1	C	350	PRO
1	F	194	ASP
1	D	85	ASP
1	A	66	ARG
1	F	66	ARG
1	E	274	ILE
1	B	240	VAL

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	282/303 (93%)	263 (93%)	19 (7%)	16	50
1	B	284/303 (94%)	265 (93%)	19 (7%)	16	50
1	C	280/303 (92%)	261 (93%)	19 (7%)	16	49
1	D	277/303 (91%)	250 (90%)	27 (10%)	8	31
1	E	283/303 (93%)	262 (93%)	21 (7%)	13	46
1	F	232/303 (77%)	211 (91%)	21 (9%)	9	34
All	All	1638/1818 (90%)	1512 (92%)	126 (8%)	13	44

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	A	71	ILE
1	A	83	GLU
1	A	91	GLU
1	A	135	LEU
1	A	152	ILE
1	A	159	ASP
1	A	214	THR
1	A	233	GLN
1	A	250	GLU
1	A	252	ILE
1	A	261	GLU
1	A	283	GLN
1	A	297	ILE
1	A	314	VAL
1	A	355	SER
1	A	356	SER
1	A	357	SER
1	A	363	ILE
1	B	37	SER
1	B	38	SER
1	B	75	VAL
1	B	83	GLU
1	B	104	LEU
1	B	114	SER
1	B	146	ILE
1	B	147	CYS
1	B	158	LEU
1	B	159	ASP
1	B	167	GLU

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Mol	Chain	Res	Type
1	B	175	VAL
1	B	194	ASP
1	B	206	SER
1	B	214	THR
1	B	221	LEU
1	B	327	ASP
1	B	355	SER
1	B	364	SER
1	C	51	SER
1	C	77	ARG
1	C	89	SER
1	C	121	VAL
1	C	152	ILE
1	C	159	ASP
1	C	185	ARG
1	C	186	LEU
1	C	211	LEU
1	C	223	ASP
1	C	233	GLN
1	C	240	VAL
1	C	253	ASP
1	C	254	LEU
1	C	256	VAL
1	C	291	ILE
1	C	308	GLN
1	C	311	LYS
1	C	351	ASP
1	D	37	SER
1	D	49	GLN
1	D	53	SER
1	D	67	ASN
1	D	104	LEU
1	D	121	VAL
1	D	122	LEU
1	D	130	LEU
1	D	138	LYS
1	D	152	ILE
1	D	188	SER
1	D	218	ARG
1	D	221	LEU
1	D	225	GLN
1	D	241	LYS

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Mol	Chain	Res	Type
1	D	242	LYS
1	D	250	GLU
1	D	262	LEU
1	D	275	THR
1	D	299	THR
1	D	305	ASN
1	D	335	LYS
1	D	342	MET
1	D	344	GLU
1	D	352	SER
1	D	354	PRO
1	D	357	SER
1	E	42	THR
1	E	53	SER
1	E	82	LEU
1	E	104	LEU
1	E	115	LYS
1	E	116	GLU
1	E	141	THR
1	E	163	THR
1	E	197	VAL
1	E	209	LEU
1	E	225	GLN
1	E	242	LYS
1	E	265	ASN
1	E	275	THR
1	E	281	ARG
1	E	327	ASP
1	E	330	ASN
1	E	343	GLU
1	E	362	ILE
1	E	363	ILE
1	E	369	GLN
1	F	42	THR
1	F	45	LYS
1	F	51	SER
1	F	53	SER
1	F	71	ILE
1	F	81	THR
1	F	91	GLU
1	F	98	HIS
1	F	99	ASN

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Mol	Chain	Res	Type
1	F	115	LYS
1	F	166	GLN
1	F	170	LYS
1	F	215	ASN
1	F	216	ILE
1	F	265	ASN
1	F	269	HIS
1	F	272	ASP
1	F	282	ASN
1	F	303	CYS
1	F	359	THR
1	F	364	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	212	GLN
1	A	283	GLN
1	A	308	GLN
1	B	48	ASN
1	B	49	GLN
1	B	205	ASN
1	B	224	GLN
1	B	269	HIS
1	B	287	ASN
1	C	59	GLN
1	C	134	ASN
1	C	173	HIS
1	C	205	ASN
1	C	212	GLN
1	C	224	GLN
1	C	233	GLN
1	C	260	ASN
1	C	268	HIS
1	C	269	HIS
1	C	293	GLN
1	C	306	ASN
1	C	347	HIS
1	C	361	GLN
1	D	48	ASN
1	D	49	GLN

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Mol	Chain	Res	Type
1	D	99	ASN
1	D	120	GLN
1	D	205	ASN
1	D	212	GLN
1	D	215	ASN
1	D	225	GLN
1	D	269	HIS
1	D	287	ASN
1	D	305	ASN
1	E	59	GLN
1	E	99	ASN
1	E	106	GLN
1	E	224	GLN
1	E	225	GLN
1	E	265	ASN
1	E	269	HIS
1	E	330	ASN
1	F	98	HIS
1	F	140	GLN
1	F	212	GLN
1	F	215	ASN
1	F	282	ASN
1	F	283	GLN
1	F	369	GLN
1	F	370	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

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	B65	F	451	3	24,26,26	0.89	2 (8%)	32,37,37	0.72	1 (3%)
2	B65	B	451	3	24,26,26	0.79	1 (4%)	32,37,37	0.87	2 (6%)
2	B65	A	451	3	24,26,26	0.80	0	32,37,37	0.85	1 (3%)
2	B65	C	451	3	24,26,26	0.82	0	32,37,37	0.93	2 (6%)
2	B65	E	451	3	24,26,26	0.86	0	32,37,37	0.92	2 (6%)
2	B65	D	451	3	24,26,26	0.83	0	32,37,37	0.86	1 (3%)

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	B65	F	451	3	-	2/15/22/22	0/2/2/2
2	B65	B	451	3	-	4/15/22/22	0/2/2/2
2	B65	A	451	3	-	3/15/22/22	0/2/2/2
2	B65	C	451	3	-	3/15/22/22	0/2/2/2
2	B65	E	451	3	-	6/15/22/22	0/2/2/2
2	B65	D	451	3	-	2/15/22/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	451	B65	PAX-OAC	-2.25	1.51	1.54
2	F	451	B65	PAX-OAB	-2.07	1.51	1.54
2	B	451	B65	PAX-OAB	-2.03	1.51	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	451	B65	CAV-OAS-CAU	3.10	126.05	118.80
2	A	451	B65	OAC-PAX-OAB	2.58	114.58	107.64
2	E	451	B65	CAV-OAS-CAU	2.56	124.79	118.80
2	B	451	B65	CAP-CAR-CAW	2.55	117.22	112.81
2	E	451	B65	OAC-PAX-OAB	2.42	114.13	107.64
2	D	451	B65	OAC-PAX-OAB	2.37	114.01	107.64
2	C	451	B65	OAC-PAX-OAB	2.28	113.77	107.64
2	F	451	B65	OAC-PAX-OAB	2.08	113.22	107.64
2	B	451	B65	CAV-OAS-CAU	2.01	123.50	118.80

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	451	B65	CAP-CAR-CAW-PAX
2	B	451	B65	CAR-CAW-PAX-OAC
2	E	451	B65	CAR-CAW-PAX-OAB
2	E	451	B65	CAR-CAW-PAX-OAC
2	E	451	B65	CAR-CAW-PAX-OAA
2	F	451	B65	CAQ-CAP-CAR-CAW
2	B	451	B65	CAQ-CAP-CAR-CAW
2	C	451	B65	CAR-CAP-CAQ-CAT
2	B	451	B65	CAR-CAW-PAX-OAA
2	A	451	B65	CAR-CAW-PAX-OAA
2	D	451	B65	CAR-CAW-PAX-OAA
2	A	451	B65	CAR-CAP-CAQ-CAT
2	A	451	B65	CAR-CAW-SAY-OAE
2	C	451	B65	CAR-CAW-SAY-OAE
2	E	451	B65	CAR-CAW-SAY-OAE
2	D	451	B65	CAR-CAP-CAQ-CAT
2	E	451	B65	CAP-CAR-CAW-SAY
2	E	451	B65	CAR-CAP-CAQ-CAT
2	C	451	B65	CAR-CAW-PAX-OAA
2	F	451	B65	CAR-CAP-CAQ-CAT

There are no ring outliers.

5 monomers are involved in 7 short contacts:

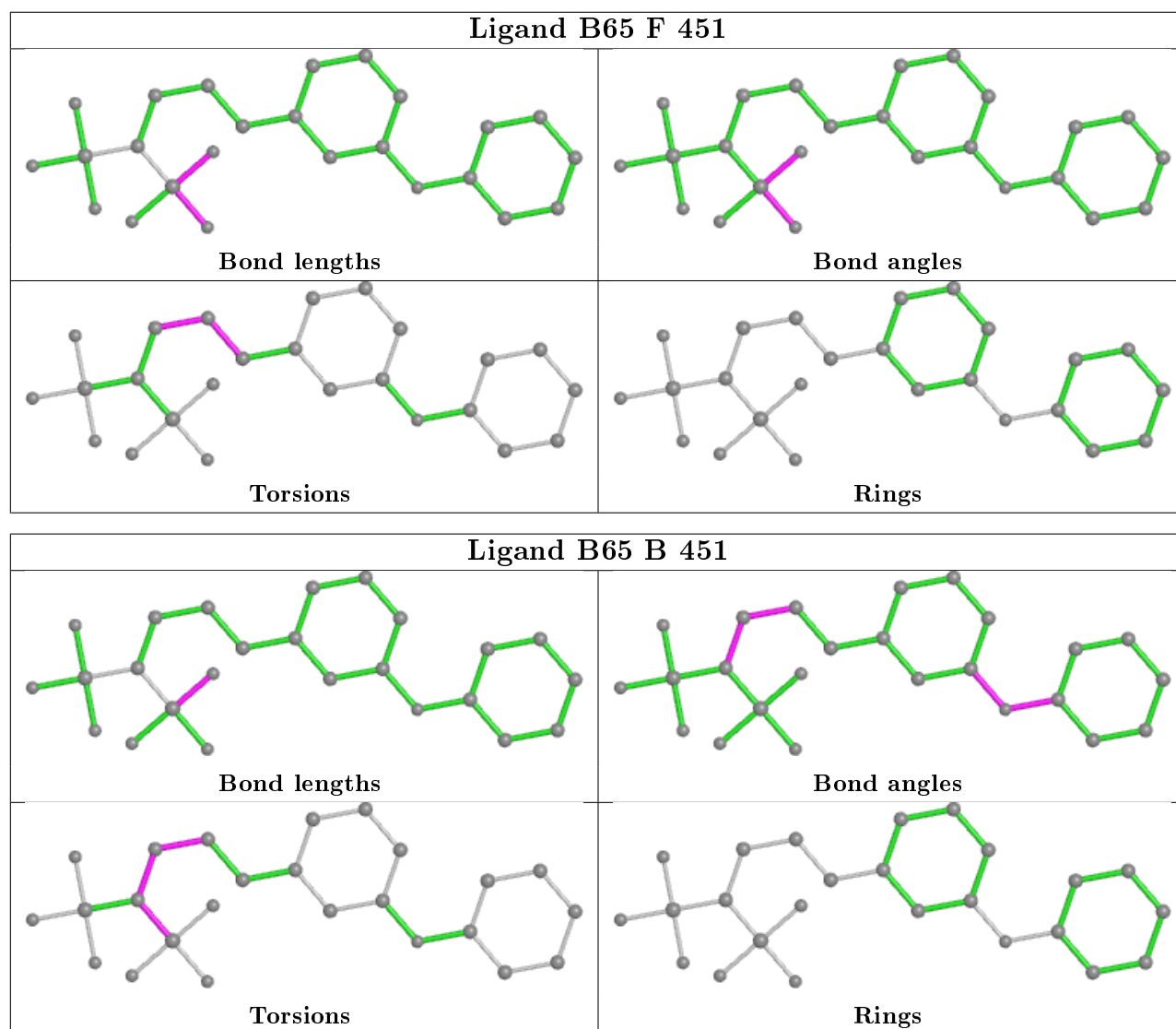
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	451	B65	2	0
2	B	451	B65	2	0
2	A	451	B65	1	0

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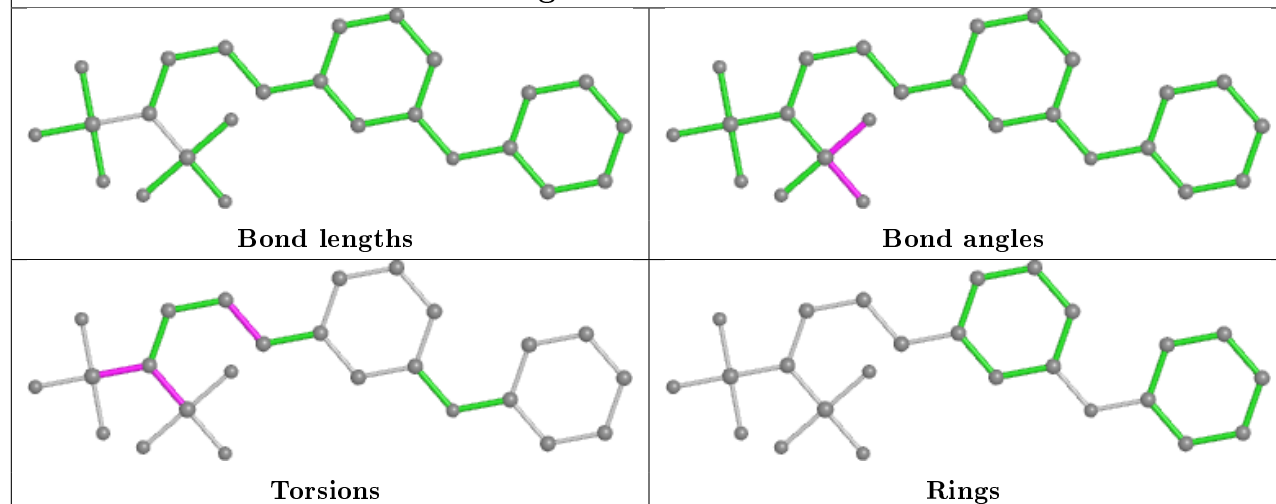
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	451	B65	1	0
2	D	451	B65	1	0

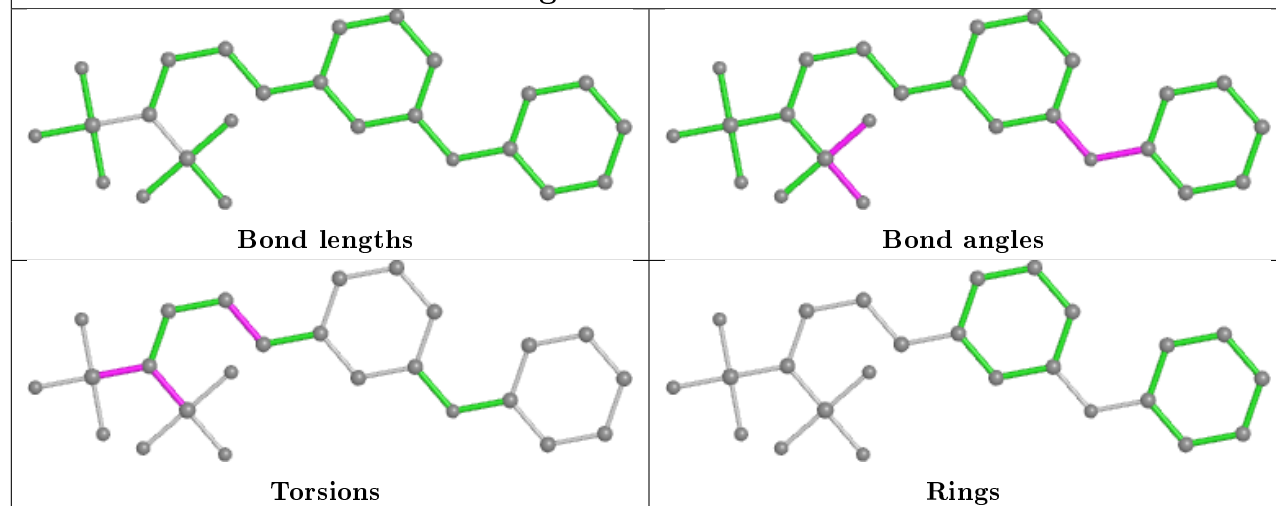
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



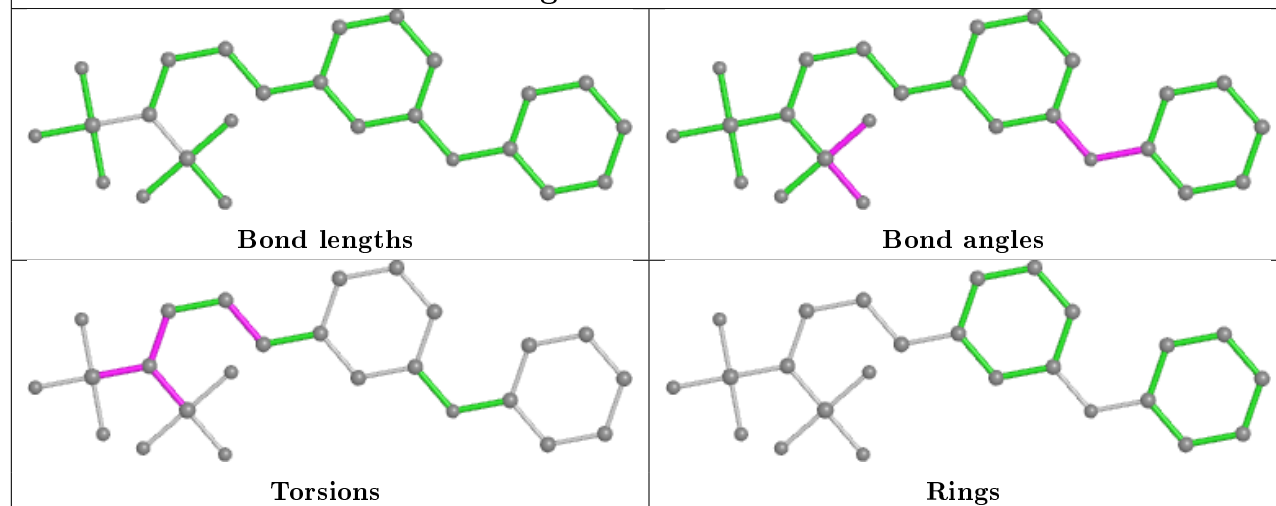
Ligand B65 A 451

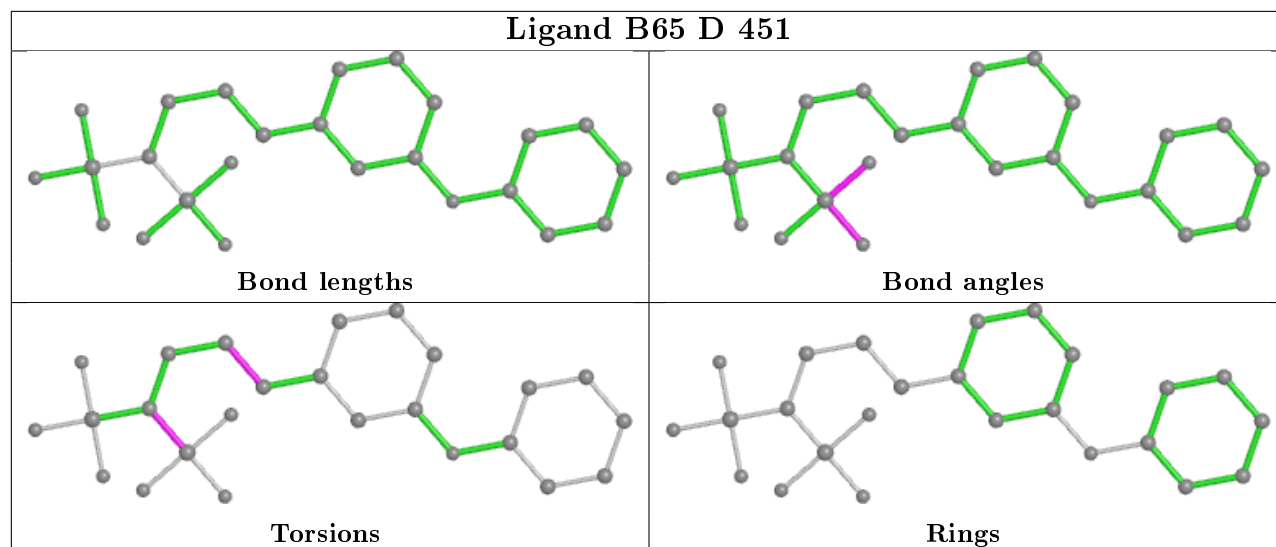


Ligand B65 C 451



Ligand B65 E 451





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	324/340 (95%)	-0.56	1 (0%) 94 92	26, 41, 72, 96	0
1	B	324/340 (95%)	-0.44	4 (1%) 79 67	26, 44, 72, 99	0
1	C	324/340 (95%)	-0.42	6 (1%) 66 53	24, 43, 120, 232	0
1	D	322/340 (94%)	-0.33	6 (1%) 66 53	27, 53, 120, 152	0
1	E	323/340 (95%)	-0.39	0 100 100	32, 61, 105, 123	0
1	F	262/340 (77%)	-0.14	9 (3%) 45 29	28, 65, 106, 118	0
All	All	1879/2040 (92%)	-0.39	26 (1%) 75 63	24, 50, 102, 232	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	316	ILE	3.6
1	D	225	GLN	3.5
1	F	161	HIS	3.3
1	F	160	LYS	3.2
1	D	159	ASP	3.0
1	C	313	ALA	2.9
1	B	313	ALA	2.9
1	C	312	GLY	2.9
1	B	159	ASP	2.8
1	D	241	LYS	2.6
1	D	229	GLU	2.5
1	C	352	SER	2.5
1	F	165	GLU	2.4
1	B	315	LYS	2.4
1	D	226	GLY	2.4
1	F	159	ASP	2.3
1	F	88	ILE	2.3
1	B	370	ASN	2.3
1	F	350	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	370	ASN	2.2
1	F	89	SER	2.2
1	C	315	LYS	2.1
1	A	247	ALA	2.1
1	F	355	SER	2.1
1	F	87	THR	2.1
1	D	313	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

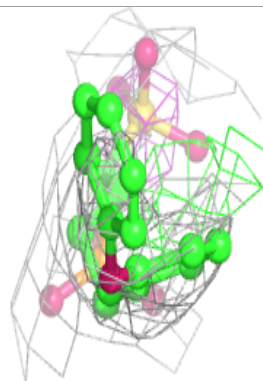
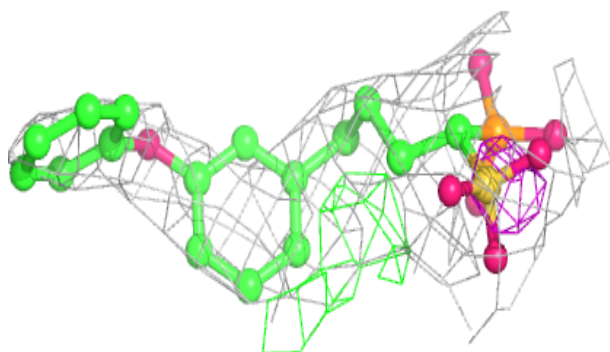
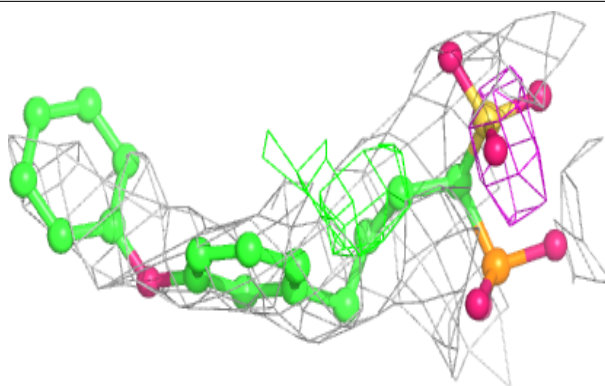
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	B65	F	451	25/25	0.86	0.26	89,97,109,109	0
3	MG	E	452	1/1	0.88	0.13	81,81,81,81	0
2	B65	C	451	25/25	0.88	0.25	68,78,92,93	0
2	B65	E	451	25/25	0.92	0.26	79,84,87,87	0
3	MG	F	452	1/1	0.92	0.06	81,81,81,81	0
2	B65	B	451	25/25	0.93	0.19	64,76,83,85	0
3	MG	B	452	1/1	0.93	0.10	37,37,37,37	0
2	B65	D	451	25/25	0.93	0.19	60,77,91,91	0
3	MG	D	452	1/1	0.94	0.09	34,34,34,34	0
3	MG	C	452	1/1	0.96	0.24	52,52,52,52	0
2	B65	A	451	25/25	0.96	0.18	64,72,78,78	0
3	MG	A	452	1/1	0.99	0.09	40,40,40,40	0

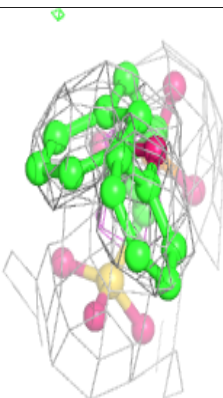
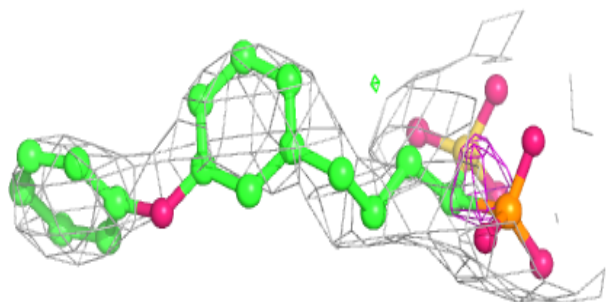
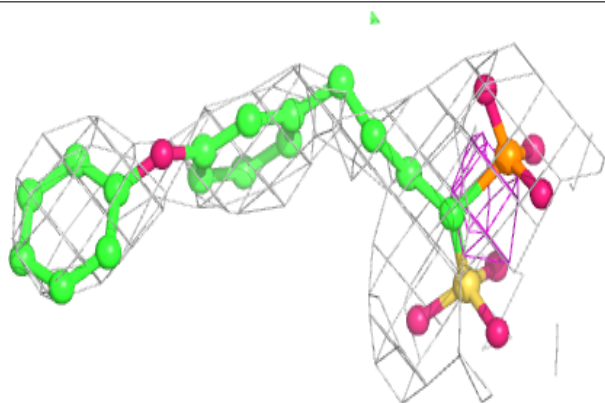
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B65 F 451:

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

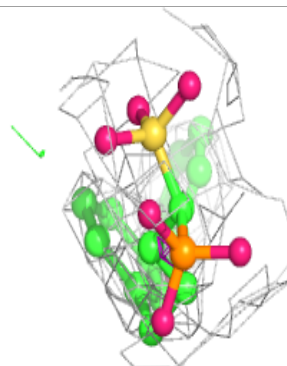
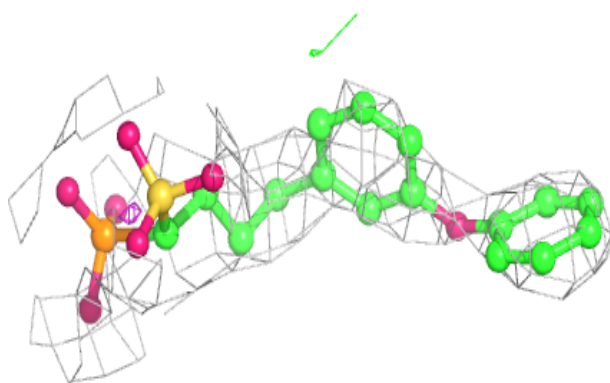
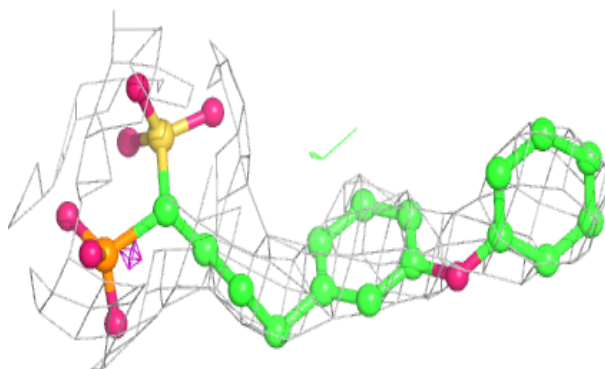
**Electron density around B65 C 451:**

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

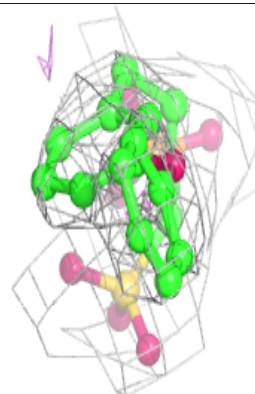
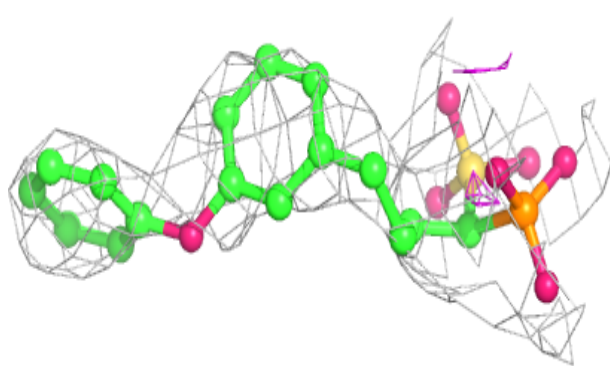
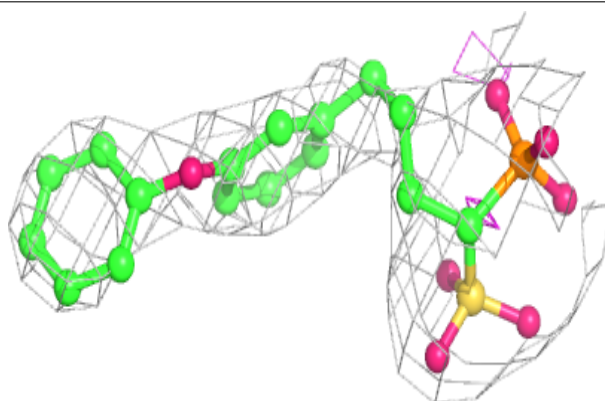


Electron density around B65 E 451:

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

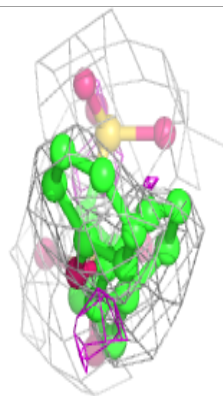
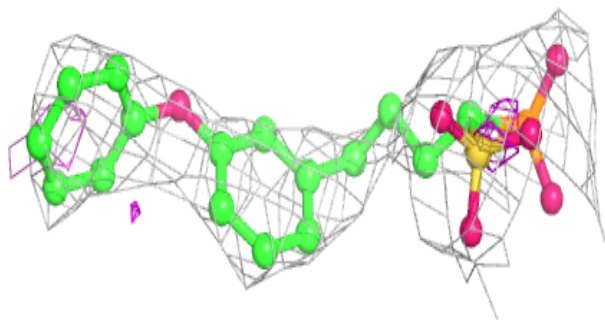
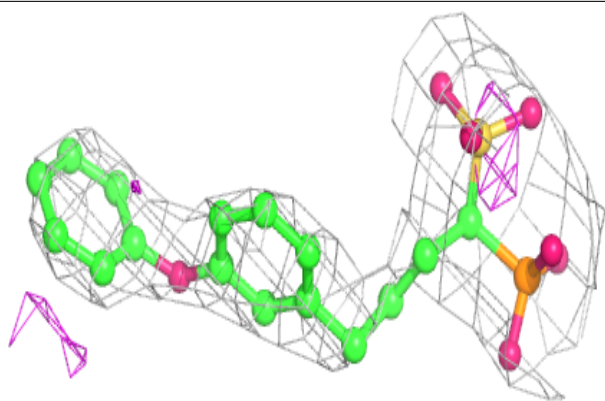
**Electron density around B65 B 451:**

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

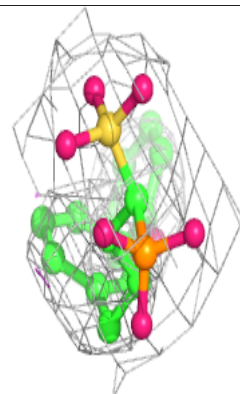
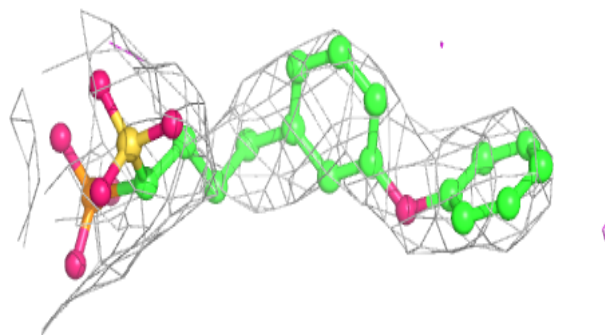
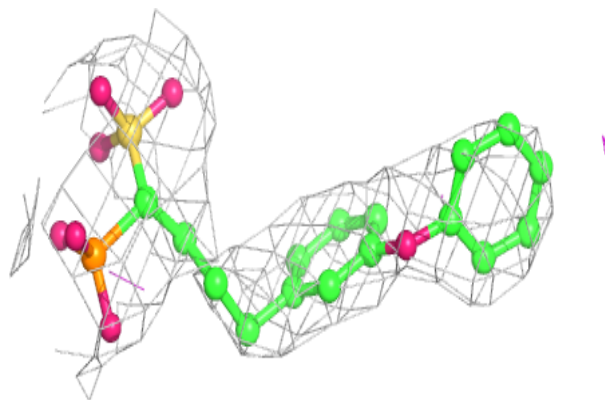


Electron density around B65 D 451:

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

**Electron density around B65 A 451:**

$2mF_o-DF_c$ (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.