



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:58 AM UTC

PDB ID : 3LEE / pdb_00003lee
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 types of validation reports are described at

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

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

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

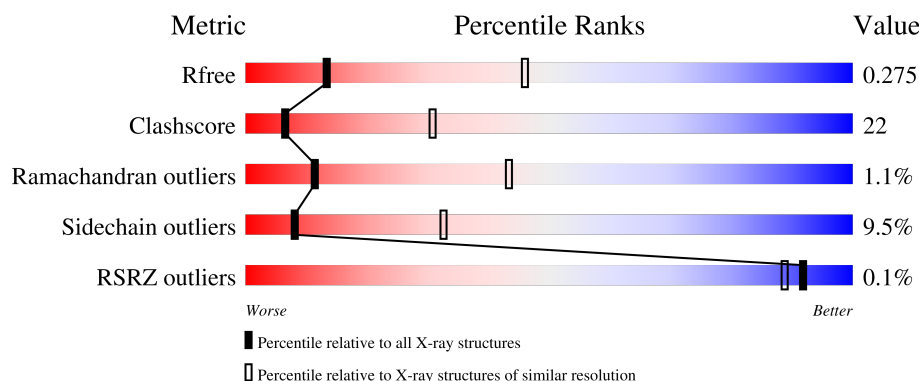
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	340	
1	B	340	
1	C	340	
1	D	340	
1	E	340	

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Mol	Chain	Length	Quality of chain
1	F	340	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (44%), yellow (28%), orange (5%), and grey (23%).

2 Entry composition [i](#)

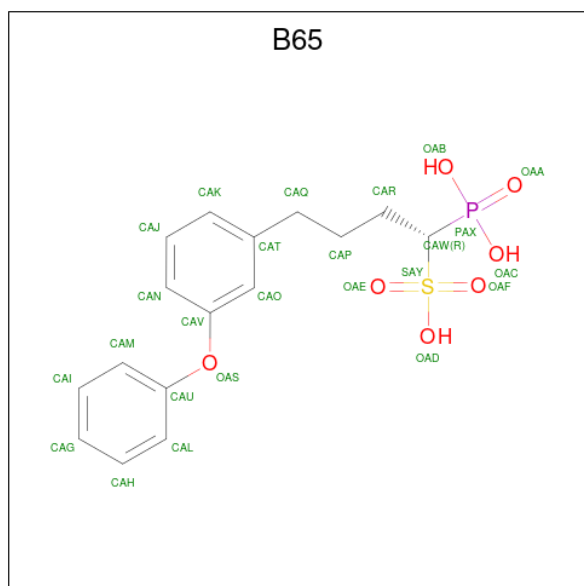
There are 4 unique types of molecules in this entry. The entry contains 15384 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

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

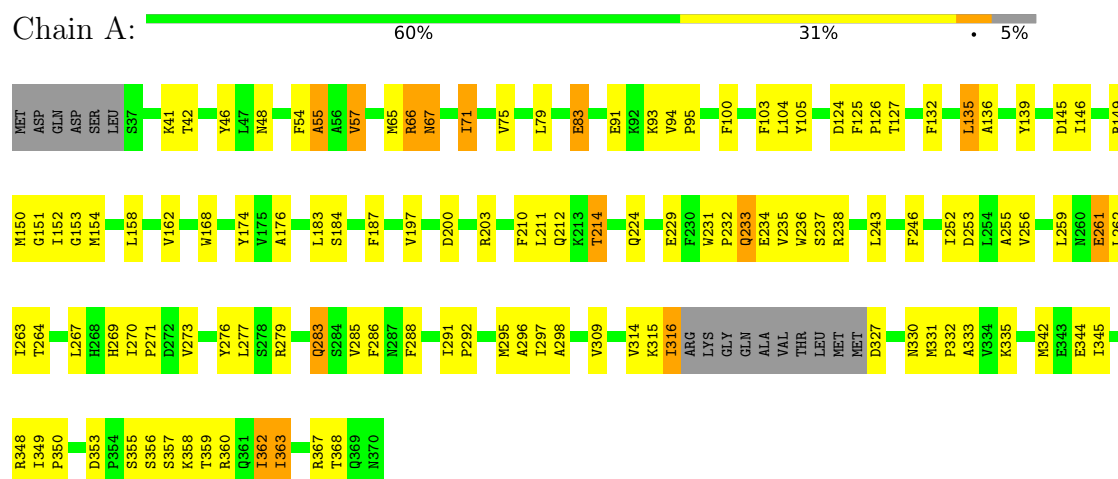
- Molecule 4 is water.

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		

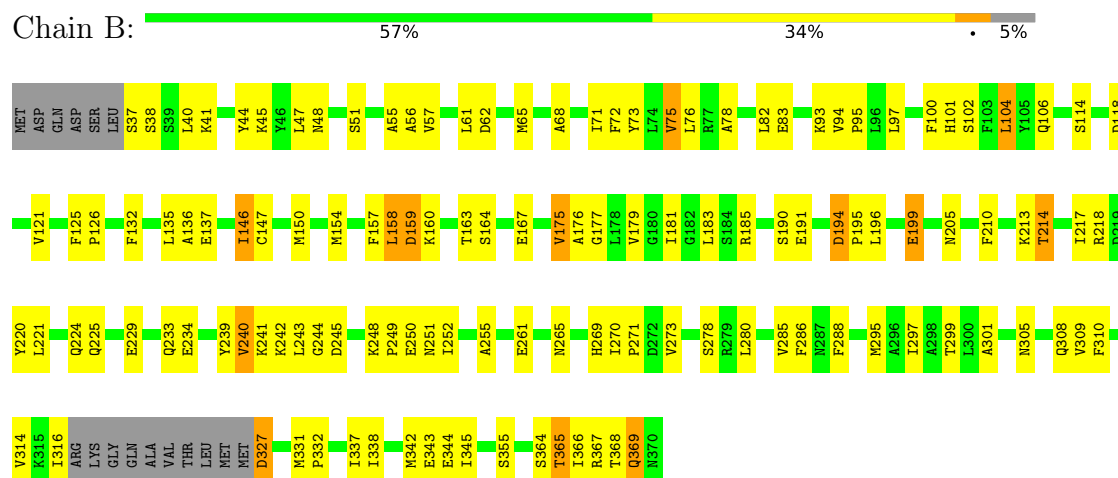
3 Residue-property plots

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

• Molecule 1: Squalene synthetase

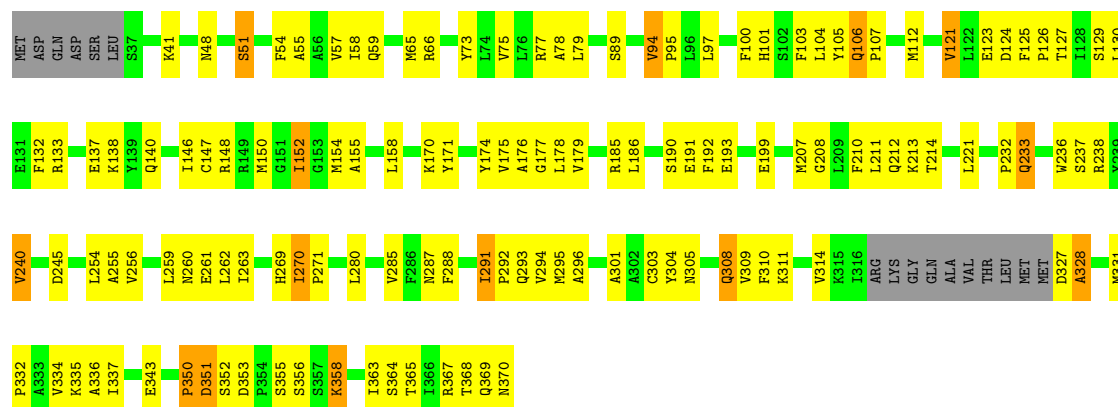


• Molecule 1: Squalene synthetase

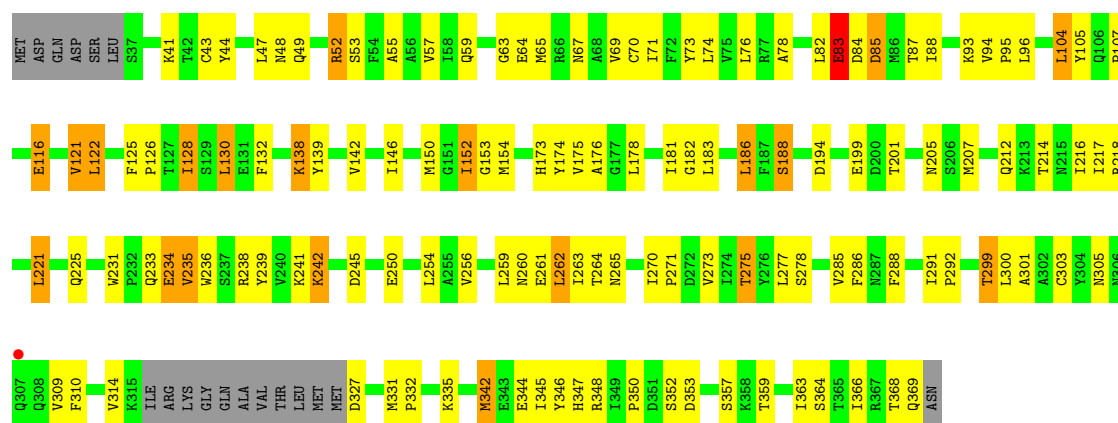


• Molecule 1: Squalene synthetase

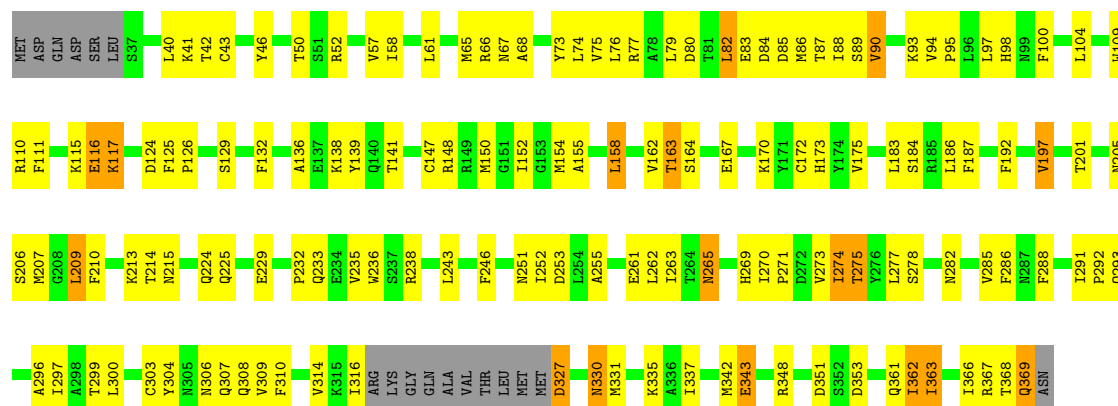




• Molecule 1: Squalene synthetase



• Molecule 1: Squalene synthetase



• Molecule 1: Squalene synthetase



E344	N285	E202	K115	MET
E345	A266	R203	ASP E116	ASP GLN
Y346	H269	M207	K117	ASP
H347	L270	G208	D118	SER
R348	P271	L209	V121	LEU
I349	D272			SER
T359	V273	Q212	F125	S38
		K213	F126	
I362	L277	T214	P126	K41
S363	S278	N215	T127	T42
		I216	I128	C43
	N282	ILE		Y44
	Q283	ARG	F132	K45
	S284	ASP	L135	Y46
T368	V285	TYR	L135	L47
Q369	F286	LEU	Q140	M48
N370	H287	GLU		Q49
	F288	ASP		T50
	C289	GLN	A144	S51
	A290	GLN		R52
		GLY	R148	S53
	Q293	GLY	H149	F54
	V294	ARG	M150	A55
	I297	ALU	G151	A56
		PHE	I152	V57
		TRP	G153	I58
	C303	PRO	M154	
	THR	GLN		R66
	ASN	GLU	L158	M67
	ASN	VAL		A68
	GLN	TRP	V162	
	GLN	SER		I71
	VAL	ARG	E165	
	PHE	TYR	Q166	V75
	LYS	VAL	E167	L76
	GLY	LYS	W168	R77
	ALA	LEU	D169	A78
	VAL	LYS	K170	L79
	LYS	GLY	Y171	D80
	ILE	ASP	C172	T81
	ARG	PHE	H173	L82
	LYS	ALA	Y174	E83
	GLY	LYS	V175	D84
	GLN	PRO		D85
	ALA	GLU	L178	M86
	VAL	ASN	V179	T87
	THR	ILE	G180	
	LEU	ASP	I181	E91
	MET	ALA	G182	K92
	MET	LEU	L183	K93
		VAL	S184	
	D327	GLN	R185	L96
		CYS		
	N330	LEU	E193	N99
	M331	ASN	D194	F100
	P332	GLU		H101
		LEU	G198	S102
	K335	ILE		F103
	I338	THR	T201	L104

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) 99.4 (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 , 52.0	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	0.42	0/2651	0.67	0/3590
1	B	0.40	0/2654	0.65	0/3594
1	C	0.40	0/2641	0.69	0/3579
1	D	0.38	0/2620	0.66	0/3554
1	E	0.37	0/2645	0.65	0/3582
1	F	0.37	0/2140	0.65	0/2893
All	All	0.39	0/15351	0.66	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	96	0
1	B	2600	0	2537	110	0
1	C	2587	0	2513	119	0
1	D	2566	0	2472	126	0
1	E	2591	0	2537	126	0
1	F	2099	0	2068	90	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	652	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 22.

All (652) 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:HE1	1:B:285:VAL:CG2	1.70	1.20
1:B:65:MET:CE	1:B:285:VAL:HG22	1.76	1.15
1:A:150:MET:HE3	1:A:154:MET:CE	1.80	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:MET:HE1	1:D:285:VAL:HG22	1.31	1.08
1:E:94:VAL:HG23	1:E:95:PRO:HD3	1.35	1.07
1:F:277:LEU:CB	1:F:331:MET:HE1	1.85	1.06
1:F:277:LEU:HB3	1:F:331:MET:HE1	1.34	1.04
1:B:210:PHE:O	1:B:214:THR:HG23	1.57	1.04
1:A:150:MET:HE3	1:A:154:MET:HE3	1.44	0.99
1:C:343:GLU:OE2	1:C:367:ARG:NH2	1.96	0.99
1:C:207:MET:HE3	1:C:293:GLN:HE21	1.23	0.98
1:D:65:MET:HE1	1:D:285:VAL:CG2	1.94	0.97
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:B:65:MET:HE1	1:B:285:VAL:HG22	0.98	0.95
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:D:277:LEU:HB3	1:D:331:MET:HE1	1.52	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:277:LEU:CB	1:D:331:MET:HE1	2.03	0.88
1:B:221:LEU:O	1:B:225:GLN:HG2	1.74	0.87
1:A:150:MET:HE3	1:A:154:MET:HE1	1.57	0.87
1:B:240:VAL:HG22	4:B:402:HOH:O	1.74	0.87
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:D:130:LEU:O	1:D:130:LEU:HD12	1.78	0.84
1:A:277:LEU:HB3	1:A:331:MET:HE1	1.58	0.83
1:F:144:ALA:HB1	4:F:373:HOH:O	1.79	0.83
1:F:286:PHE:HE1	1:F:331:MET:HE2	1.44	0.82
1:C:65:MET:HE2	1:C:192:PHE:CD2	2.14	0.82
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:79:LEU:HD23	1:A:150:MET:HE2	1.63	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:A:277:LEU:CB	1:A:331:MET:HE1	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:150:MET:CE	1:A:154:MET:HE3	2.14	0.76
1:B:240:VAL:HG21	1:B:245:ASP:CB	2.15	0.76
1:B:342:MET:HE2	1:B:342:MET:HA	1.67	0.76
1:D:44:TYR:CD2	1:F:368:THR:HG22	2.20	0.76
1:D:57:VAL:CG1	1:D:288:PHE:HA	2.16	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:B:159:ASP:OD1	1:B:159:ASP:C	2.31	0.74
1:A:150:MET:CE	1:A:154:MET:CE	2.64	0.74
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:D:278:SER:HA	1:D:331:MET:HE3	1.68	0.74
1:E:368:THR:HG21	1:F:41:LYS:HA	1.69	0.73
1:D:277:LEU:C	1:D:331:MET:CE	2.61	0.73
1:A:210:PHE:O	1:A:214:THR:HG23	1.88	0.73
1:E:85:ASP:C	1:E:86:MET:HE2	2.13	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:E:277:LEU:C	1:E:331:MET:HE1	2.15	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:E:278:SER:HA	1:E:331:MET:HE3	1.73	0.70
1:F:277:LEU:C	1:F:331:MET:HE3	2.16	0.70
1:B:316:ILE:HG22	1:B:316:ILE:O	1.90	0.69
1:F:93:LYS:HD3	1:F:158:LEU:HD21	1.73	0.69
1:C:280:LEU:HD13	1:C:285:VAL:HG12	1.75	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:277:LEU:HB2	1:F:331:MET:HE1	1.72	0.68
1:F:172:CYS:HB2	1:F:209:LEU:HD22	1.73	0.68
1:C:155:ALA:HA	1:C:158:LEU:HD12	1.76	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:277:LEU:C	1:D:331:MET:HE3	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:LEU:HD12	2:D:451:B65:HAM	1.77	0.67
1:F:278:SER:HA	1:F:331:MET:HE3	1.76	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
1:E:368:THR:O	1:E:369:GLN:C	2.39	0.66
1:B:331:MET:HB3	1:B:332:PRO:HD3	1.78	0.66
1:F:278:SER:N	1:F:331:MET:HE3	2.11	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: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:221:LEU:HD12	1:C:310:PHE:C	2.21	0.65
1:C:112:MET:SD	1:C:123:GLU:HG2	2.37	0.65
1:F:277:LEU:C	1:F:331:MET:CE	2.70	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: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:85:ASP:OD2	1:D:87:THR:OG1	2.15	0.64
1:D:221:LEU:HD12	1:D:310:PHE:O	1.97	0.64
1:F:286:PHE:CE1	1:F:331:MET:HE2	2.30	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: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:183:LEU:HD22	1:B:288:PHE:CE2	2.32	0.63
1:B:249:PRO:HA	1:B:252:ILE:HD13	1.79	0.63
1:D:235:VAL:HG11	1:D:262:LEU:HD11	1.80	0.62
1:E:309:VAL:O	1:E:309:VAL:HG12	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:277:LEU:C	1:D:331:MET:HE1	2.24	0.62
1:E:286:PHE:HE1	1:E:331:MET:HE1	1.65	0.62
1:F:278:SER:CA	1:F:331:MET:HE3	2.29	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:D:286:PHE:HE1	1:D:331:MET:HE2	1.65	0.62
1:C:207:MET:HE3	1:C:293:GLN:NE2	2.05	0.62
1:F:175:VAL:CG2	1:F:212:GLN:NE2	2.63	0.62
1:D:130:LEU:HD12	1:D:130:LEU:C	2.24	0.61
1:D:142:VAL:CG1	1:D:186:LEU:HD13	2.30	0.61
1:E:76:LEU:HD22	1:E:150:MET:SD	2.39	0.61
1:C:79:LEU:HG	1:C:154:MET:HE2	1.83	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:B:342:MET:HE2	1:B:342:MET:CA	2.31	0.60
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:351:ASP:C	1:C:353:ASP:H	2.08	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: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:D:233:GLN:C	1:D:235:VAL:H	2.10	0.60
1:F:44:TYR:OH	1:F:67:ASN:OD1	2.17	0.60
1:F:271:PRO:HA	1:F:369:GLN:HE22	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:PHE:O	1:A:55:ALA:C	2.44	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: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:D:278:SER:CA	1:D:331:MET:HE3	2.33	0.59
1:D:342:MET:HA	1:D:342:MET:HE2	1.84	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:116:GLU:O	1:E:117:LYS:C	2.45	0.58
1:E:363:ILE:O	1:E:367:ARG:HG3	2.03	0.58
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:A:277:LEU:HB2	1:A:331:MET:HE1	1.85	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:HD13	1:E:362:ILE:O	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:83:GLU:OE1	1:D:154:MET:HE2	2.04	0.58
1:D:264:THR:CG2	1:D:359:THR:OG1	2.52	0.58
1:B:65:MET:CE	1:B:285:VAL:CG2	2.56	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:E:297:ILE:HD12	1:E:297:ILE:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:MET:CE	1:D:285:VAL:HG22	2.21	0.56
1:D:368:THR:HG21	1:E:41:LYS:HA	1.88	0.56
1:E:65:MET:HE1	1:E:285:VAL:CG2	2.36	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: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:E:277:LEU:HB3	1:E:331:MET:HE1	1.88	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:F:175:VAL:CG2	1:F:212:GLN:HE21	2.19	0.56
1:C:73:TYR:C	1:C:73:TYR:CD2	2.84	0.56
1:E:297:ILE:HD12	1:E:297:ILE:H	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:E:277:LEU:C	1:E:331:MET:CE	2.79	0.55
1:E:342:MET:HA	1:E:342:MET:HE2	1.88	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
1:E:238:ARG:NH2	1:E:261:GLU:OE1	2.39	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:A:342:MET:HE2	1:A:342:MET:HA	1.89	0.54
1:E:286:PHE:CE1	1:E:331:MET:CE	2.90	0.54
1:C:137:GLU:O	1:C:138:LYS:C	2.50	0.54
1:E:286:PHE:CE1	1:E:331:MET:HE2	2.42	0.54
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:193:GLU:O	1:F:194:ASP:HB2	2.07	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:B:73:TYR:CD1	1:B:73:TYR:C	2.86	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:A:150:MET:CE	1:A:154:MET:HE1	2.33	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:260:ASN:ND2	1:C:304:TYR:CE1	2.77	0.52
1:E:79:LEU:HD23	1:E:150:MET:HE2	1.91	0.52
1:A:331:MET:HG3	1:A:335:LYS:HD2	1.91	0.52
1:B:100:PHE:O	1:B:101:HIS:C	2.51	0.52
1:E:252:ILE:HG23	1:E:253:ASP:N	2.24	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:A:286:PHE:CE1	1:A:331:MET:HE2	2.45	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: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:D:94:VAL:HB	1:D:95:PRO:HD3	1.90	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:B:265:ASN:C	1:B:265:ASN:OD1	2.54	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:C:355:SER:O	1:C:356:SER:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:THR:HG21	1:F:115:LYS:HE2	1.91	0.51
1:F:265:ASN:OD1	1:F:265:ASN:C	2.52	0.51
1:A:286:PHE:HE1	1:A:331:MET:HE2	1.75	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: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:342:MET:HA	1:B:342:MET:CE	2.33	0.51
1:B:242:LYS:O	1:B:245:ASP:HB2	2.11	0.51
1:B:150:MET:HE3	1:B:154:MET:HE3	1.93	0.50
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:B:217:ILE:O	1:B:218:ARG:C	2.53	0.50
1:D:73:TYR:C	1:D:73:TYR:CD1	2.90	0.50
1:E:65:MET:HE1	1:E:285:VAL:HG23	1.93	0.50
1:A:184:SER:HB3	1:A:276:TYR:OH	2.12	0.50
1:B:308:GLN:HG3	1:B:308:GLN:O	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:F:165:GLU:O	1:F:166:GLN:C	2.53	0.50
1:A:344:GLU:O	1:A:348:ARG:HG3	2.11	0.50
1:C:262:LEU:O	1:C:263:ILE:C	2.53	0.50
1:F:104:LEU:HD23	1:F:132:PHE:CZ	2.46	0.50
1:A:65:MET:O	1:A:66:ARG:C	2.54	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
1:E:139:TYR:CD1	1:E:186:LEU:HD23	2.46	0.50
1:D:286:PHE:CE1	1:D:331:MET:HE2	2.46	0.50
1:D:368:THR:HA	1:E:66:ARG:HH22	1.76	0.50
1:B:194:ASP:CG	1:B:195:PRO:HD2	2.37	0.49
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:C:170:LYS:O	1:C:171:TYR:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:SER:C	1:F:55:ALA:N	2.69	0.49
2:B:451:B65:OAA	2:B:451:B65:CAP	2.61	0.49
1:F:265:ASN:OD1	1:F:266:ALA:N	2.45	0.49
1:E:206:SER:O	1:E:207:MET:C	2.55	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:C:132:PHE:CD2	1:C:132:PHE:C	2.91	0.49
1:E:251:ASN:O	1:E:252:ILE:C	2.55	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:233:GLN:O	1:C:237:SER:OG	2.30	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:F:82:LEU:O	1:F:83:GLU:C	2.55	0.49
1:B:57:VAL:HG23	1:B:288:PHE:HD1	1.78	0.49
1:D:154:MET:HE3	1:D:175:VAL:HG23	1.93	0.49
1:C:308:GLN:C	1:C:310:PHE:H	2.21	0.49
1:B:62:ASP:O	1:B:65:MET:HG2	2.13	0.49
1:D:256:VAL:HG11	1:D:305:ASN:ND2	2.27	0.49
1:D:301:ALA:O	1:D:348:ARG:NH2	2.46	0.49
1:A:150:MET:HG2	1:A:154:MET:HE3	1.95	0.48
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:D:125:PHE:N	1:D:126:PRO:CD	2.75	0.48
1:B:82:LEU:O	1:B:93:LYS:HE2	2.12	0.48
1:B:240:VAL:HG21	1:B:245:ASP:HB3	1.94	0.48
1:A:100:PHE:HA	1:A:103:PHE:CD2	2.48	0.48
1:E:46:TYR:HB2	1:E:74:LEU:HD21	1.96	0.48
1:E:170:LYS:O	1:E:173:HIS:HB3	2.14	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
1:D:207:MET:SD	1:D:273:VAL:HG13	2.54	0.48
1:E:309:VAL:O	1:E:309:VAL:CG1	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:TYR:C	1:B:220:TYR:CD2	2.90	0.48
1:B:248:LYS:HB3	1:B:250:GLU:OE2	2.14	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: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:HD13	1:B:146:ILE:HA	1.69	0.47
1:C:174:TYR:HA	1:C:178:LEU:HD12	1.96	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:D:65:MET:HE1	1:D:285:VAL:HG21	1.90	0.47
1:E:361:GLN:HG3	1:E:362:ILE:N	2.29	0.47
1:F:77:ARG:O	1:F:81:THR:OG1	2.32	0.47
1:F:154:MET:O	1:F:158:LEU:HD12	2.14	0.47
1:A:124:ASP:CG	1:A:124:ASP:O	2.58	0.47
1:A:125:PHE:N	1:A:126:PRO:CD	2.77	0.47
1:B:61:LEU:HD22	1:B:65:MET:HE2	1.95	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:O	1:D:347:HIS:ND1	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:A:277:LEU:C	1:A:331:MET:HE3	2.39	0.47
1:B:47:LEU:O	1:B:51:SER:HB3	2.14	0.47
1:B:183:LEU:HD22	1:B:288:PHE:HE2	1.74	0.47
1:B:316:ILE:O	1:B:316:ILE:CG2	2.59	0.47
1:A:67:ASN:N	1:A:67:ASN:HD22	2.12	0.47
1:A:162:VAL:HG11	1:A:168:TRP:HA	1.97	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:C:124:ASP:CG	1:C:124:ASP:O	2.58	0.47
1:E:90:VAL:O	1:E:94:VAL:HG22	2.14	0.47
1:E:89:SER:O	1:E:93:LYS:N	2.48	0.47
1:E:233:GLN:HA	1:E:236:TRP:NE1	2.29	0.47
1:C:331:MET:HE2	1:C:335:LYS:HD2	1.97	0.47
2:A:451:B65:OAC	2:A:451:B65:OAE	2.32	0.46
1:B:278:SER:HB3	1:B:331:MET:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:274:ILE:O	1:E:275:THR:C	2.59	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: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:D:63:GLY:O	1:D:64:GLU:C	2.58	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:HD12	1:A:362:ILE:O	2.15	0.46
1:B:241:LYS:N	4:B:402:HOH:O	2.38	0.46
1:C:97:LEU:HD22	1:C:154:MET:HE3	1.97	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:C:65:MET:HE2	1:C:192:PHE:CE2	2.49	0.46
1:D:146:ILE:HG23	1:D:178:LEU:HB3	1.98	0.46
1:D:278:SER:N	1:D:331:MET:HE3	2.31	0.46
1:E:236:TRP:CE2	1:E:243:LEU:HB2	2.50	0.46
1:E:351:ASP:C	1:E:353:ASP:H	2.23	0.46
1:F:53:SER:O	1:F:54:PHE:C	2.59	0.46
1:C:259:LEU:HD21	1:C:303:CYS:O	2.16	0.46
1:D:122:LEU:HD13	1:D:122:LEU:HA	1.78	0.46
1:E:46:TYR:OH	1:E:124:ASP:OD2	2.26	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: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:F:151:GLY:O	1:F:152:ILE:C	2.59	0.45
1:B:343:GLU:OE2	1:B:367:ARG:NH1	2.35	0.45
1:C:270:ILE:N	1:C:271:PRO:CD	2.79	0.45
1:E:41:LYS:NZ	4:E:377:HOH:O	2.49	0.45
1:E:255:ALA:HB1	1:E:310:PHE:CE1	2.51	0.45
1:A:183:LEU:HD13	1:A:288:PHE:CE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:VAL:HG13	1:D:305:ASN:HA	1.98	0.45
1:E:297:ILE:CD1	1:E:297:ILE:H	2.29	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:C:350:PRO:O	1:C:351:ASP:C	2.59	0.45
1:D:277:LEU:O	1:D:331:MET:HE3	2.16	0.45
1:B:240:VAL:CG2	4:B:402:HOH:O	2.48	0.45
1:D:233:GLN:C	1:D:235:VAL:N	2.72	0.45
1:F:118:ASP:OD1	1:F:118:ASP:N	2.49	0.45
1:B:164:SER:HA	1:B:234:GLU:HB2	1.98	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:82:LEU:O	1:D:84:ASP:N	2.50	0.45
1:D:303:CYS:SG	1:D:314:VAL:HG11	2.56	0.45
1:F:168:TRP:CZ2	1:F:216:ILE:HD11	2.52	0.45
1:A:125:PHE:O	1:A:126:PRO:C	2.59	0.45
1:A:176:ALA:CB	1:A:212:GLN:HB2	2.47	0.45
1:C:363:ILE:O	1:C:363:ILE:CG2	2.65	0.45
1:E:57:VAL:HB	1:E:288:PHE:HA	1.99	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: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:D:368:THR:C	1:D:369:GLN:HG3	2.43	0.44
1:E:172:CYS:HB3	1:E:209:LEU:HD22	1.98	0.44
1:F:277:LEU:HB3	1:F:331:MET:CE	2.24	0.44
1:D:270:ILE:O	1:D:271:PRO:C	2.59	0.44
1:E:213:LYS:NZ	1:E:269:HIS:CE1	2.85	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:B:56:ALA:HB1	1:C:336:ALA:HA	1.99	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:O	1:C:309:VAL:CG1	2.63	0.44
1:B:301:ALA:HB1	4:B:410:HOH:O	2.17	0.44
1:D:41:LYS:HA	1:F:368:THR:HG21	2.00	0.44
1:D:67:ASN:N	1:D:67:ASN:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:HIS:O	1:D:347:HIS:CG	2.71	0.44
1:F:282:ASN:HB3	1:F:285:VAL:HG23	2.00	0.44
1:A:65:MET:HE1	1:A:285:VAL:HG23	2.00	0.44
1:C:358:LYS:O	1:C:358:LYS:HD3	2.18	0.44
1:D:83:GLU:CD	1:D:154:MET:HE2	2.43	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: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:207:MET:HE3	1:F:207:MET:HB3	1.92	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:48:ASN:ND2	1:B:367:ARG:HD2	2.33	0.43
1:A:233:GLN:O	1:A:237:SER:HB3	2.18	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:C:190:SER:O	1:C:191:GLU:HB2	2.18	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: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:F:330:ASN:OD1	1:F:330:ASN:C	2.62	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:71:ILE:O	1:B:72:PHE:C	2.61	0.43
1:B:136:ALA:O	1:B:137:GLU:C	2.61	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:C:101:HIS:HA	1:C:104:LEU:HD13	2.00	0.43
1:C:351:ASP:C	1:C:353:ASP:N	2.74	0.43
1:D:43:CYS:O	1:D:74:LEU:HD11	2.19	0.43
1:F:215:ASN:N	1:F:215:ASN:HD22	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:57:VAL:HG23	1:B:288:PHE:CD1	2.54	0.43
1:B:213:LYS:NZ	1:B:265:ASN:OD1	2.52	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: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:E:277:LEU:O	1:E:331:MET:HE1	2.19	0.42
1:F:57:VAL:HG12	1:F:288:PHE:HD1	1.83	0.42
1:C:301:ALA:C	1:C:303:CYS:H	2.27	0.42
1:D:286:PHE:HE1	1:D:331:MET:CE	2.30	0.42
1:D:342:MET:HA	1:D:342:MET:HE3	1.99	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:E:73:TYR:CD1	1:E:73:TYR:C	2.97	0.42
1:E:85:ASP:O	1:E:86:MET:HE2	2.19	0.42
1:E:184:SER:HB3	1:E:197:VAL:O	2.20	0.42
1:A:345:ILE:CG2	1:A:363:ILE:HD11	2.49	0.42
1:A:349:ILE:CD1	1:A:360:ARG:HG2	2.50	0.42
1:D:76:LEU:HD22	1:D:150:MET:SD	2.59	0.42
1:A:315:LYS:C	1:A:316:ILE:HD13	2.45	0.42
1:C:79:LEU:HD13	1:C:100:PHE:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:MET:HE2	1:E:150:MET:HB3	1.94	0.42
1:F:93:LYS:HD3	1:F:158:LEU:CD2	2.47	0.42
1:D:47:LEU:HA	1:D:74:LEU:HD21	2.02	0.42
1:E:331:MET:HE2	1:E:331:MET:HB2	1.81	0.42
1:B:146:ILE:HG22	1:B:147:CYS:N	2.33	0.42
1:C:199:GLU:OE2	1:F:203:ARG:NH2	2.41	0.42
1:C:369:GLN:O	1:C:370:ASN:C	2.62	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:B:342:MET:HE2	1:B:342:MET:N	2.35	0.41
1:D:104:LEU:HB3	1:D:132:PHE:CE2	2.55	0.41
1:A:283:GLN:HE21	1:A:283:GLN:HA	1.85	0.41
1:C:193:GLU:OE1	1:C:193:GLU:HA	2.19	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:D:121:VAL:HG22	1:D:128:ILE:CD1	2.49	0.41
1:E:84:ASP:O	1:E:86:MET:HE3	2.20	0.41
1:E:162:VAL:HG12	1:E:232:PRO:HA	2.01	0.41
1:F:42:THR:O	1:F:45:LYS:HB3	2.21	0.41
1:F:185:ARG:NH1	4:F:384:HOH:O	2.52	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: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:A:151:GLY:C	1:A:153:GLY:H	2.27	0.41
1:B:249:PRO:C	1:B:251:ASN:H	2.27	0.41
1:C:48:ASN:HD21	1:C:59:GLN:HE22	1.67	0.41
1:C:138:LYS:HD2	4:C:372:HOH:O	2.21	0.41
1:D:350:PRO:HG2	1:D:353:ASP:HB2	2.02	0.41
1:E:97:LEU:O	1:E:98:HIS:C	2.64	0.41
1:E:277:LEU:CB	1:E:331:MET:HE1	2.49	0.41
1:A:211:LEU:HD23	1:A:296:ALA:HB2	2.02	0.41
1:A:233:GLN:C	1:A:235:VAL:N	2.79	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:E:68:ALA:HB1	1:E:186:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ASN:O	1:A:331:MET:C	2.64	0.41
1:A:358:LYS:O	1:A:362:ILE:HG22	2.21	0.41
1:E:83:GLU:OE1	1:E:154:MET:HE2	2.20	0.41
1:E:327:ASP:HB3	1:E:337:ILE:HD11	2.02	0.41
1:F:209:LEU:O	1:F:213:LYS:HG3	2.20	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:265:ASN:HD22	1:E:265:ASN:C	2.28	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:51:SER:HG	1:C:55:ALA:H	1.69	0.40
1:C:79:LEU:O	1:C:154:MET:HE1	2.21	0.40
1:C:255:ALA:HB1	1:C:310:PHE:CZ	2.56	0.40
1:C:308:GLN:C	1:C:310:PHE:N	2.79	0.40
1:D:83:GLU:O	1:D:83:GLU:HG2	2.20	0.40
1:D:214:THR:O	1:D:217:ILE:HB	2.21	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:F:85:ASP:OD2	1:F:116:GLU:HG2	2.21	0.40
1:D:70:CYS:O	1:D:74:LEU:HG	2.21	0.40
1:D:150:MET:HG2	1:D:174:TYR:O	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:96:LEU:HD23	1:F:96:LEU:HA	1.97	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

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%)	21	56
1	B	320/340 (94%)	297 (93%)	19 (6%)	4 (1%)	9	40
1	C	320/340 (94%)	292 (91%)	25 (8%)	3 (1%)	14	47
1	D	318/340 (94%)	298 (94%)	15 (5%)	5 (2%)	7	36
1	E	319/340 (94%)	293 (92%)	24 (8%)	2 (1%)	21	56
1	F	256/340 (75%)	222 (87%)	30 (12%)	4 (2%)	7	36
All	All	1853/2040 (91%)	1706 (92%)	127 (7%)	20 (1%)	11	43

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%)	257 (91%)	25 (9%)	9	34
1	B	284/303 (94%)	262 (92%)	22 (8%)	12	41
1	C	280/303 (92%)	257 (92%)	23 (8%)	10	39
1	D	277/303 (91%)	247 (89%)	30 (11%)	6	27
1	E	283/303 (93%)	254 (90%)	29 (10%)	7	29
1	F	232/303 (77%)	205 (88%)	27 (12%)	5	24
All	All	1638/1818 (90%)	1482 (90%)	156 (10%)	8	32

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	A	67	ASN
1	A	71	ILE
1	A	83	GLU
1	A	91	GLU
1	A	127	THR
1	A	135	LEU
1	A	146	ILE
1	A	152	ILE
1	A	214	THR
1	A	224	GLN
1	A	233	GLN
1	A	252	ILE
1	A	261	GLU
1	A	263	ILE
1	A	283	GLN
1	A	295	MET
1	A	297	ILE
1	A	314	VAL
1	A	316	ILE
1	A	355	SER
1	A	356	SER

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Mol	Chain	Res	Type
1	A	357	SER
1	A	362	ILE
1	A	363	ILE
1	B	37	SER
1	B	38	SER
1	B	45	LYS
1	B	75	VAL
1	B	76	LEU
1	B	83	GLU
1	B	104	LEU
1	B	106	GLN
1	B	114	SER
1	B	146	ILE
1	B	158	LEU
1	B	159	ASP
1	B	167	GLU
1	B	175	VAL
1	B	194	ASP
1	B	199	GLU
1	B	214	THR
1	B	327	ASP
1	B	345	ILE
1	B	355	SER
1	B	364	SER
1	B	365	THR
1	C	51	SER
1	C	75	VAL
1	C	77	ARG
1	C	89	SER
1	C	94	VAL
1	C	106	GLN
1	C	121	VAL
1	C	152	ILE
1	C	185	ARG
1	C	186	LEU
1	C	211	LEU
1	C	233	GLN
1	C	240	VAL
1	C	254	LEU
1	C	256	VAL
1	C	270	ILE
1	C	291	ILE

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Mol	Chain	Res	Type
1	C	295	MET
1	C	308	GLN
1	C	311	LYS
1	C	334	VAL
1	C	351	ASP
1	C	358	LYS
1	D	49	GLN
1	D	53	SER
1	D	83	GLU
1	D	104	LEU
1	D	116	GLU
1	D	121	VAL
1	D	122	LEU
1	D	128	ILE
1	D	130	LEU
1	D	138	LYS
1	D	152	ILE
1	D	186	LEU
1	D	188	SER
1	D	199	GLU
1	D	216	ILE
1	D	218	ARG
1	D	221	LEU
1	D	225	GLN
1	D	241	LYS
1	D	242	LYS
1	D	250	GLU
1	D	262	LEU
1	D	275	THR
1	D	299	THR
1	D	309	VAL
1	D	335	LYS
1	D	342	MET
1	D	344	GLU
1	D	352	SER
1	D	357	SER
1	E	42	THR
1	E	75	VAL
1	E	82	LEU
1	E	87	THR
1	E	90	VAL
1	E	104	LEU

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Mol	Chain	Res	Type
1	E	115	LYS
1	E	116	GLU
1	E	141	THR
1	E	158	LEU
1	E	163	THR
1	E	175	VAL
1	E	197	VAL
1	E	209	LEU
1	E	215	ASN
1	E	225	GLN
1	E	265	ASN
1	E	275	THR
1	E	299	THR
1	E	308	GLN
1	E	316	ILE
1	E	327	ASP
1	E	330	ASN
1	E	335	LYS
1	E	343	GLU
1	E	348	ARG
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	75	VAL
1	F	81	THR
1	F	91	GLU
1	F	99	ASN
1	F	115	LYS
1	F	118	ASP
1	F	121	VAL
1	F	128	ILE
1	F	158	LEU
1	F	166	GLN
1	F	170	LYS
1	F	178	LEU
1	F	181	ILE
1	F	216	ILE

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Mol	Chain	Res	Type
1	F	265	ASN
1	F	283	GLN
1	F	303	CYS
1	F	335	LYS
1	F	344	GLU
1	F	348	ARG
1	F	359	THR
1	F	364	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	101	HIS
1	A	212	GLN
1	A	283	GLN
1	A	308	GLN
1	A	370	ASN
1	B	48	ASN
1	B	106	GLN
1	B	120	GLN
1	B	205	ASN
1	B	224	GLN
1	B	269	HIS
1	B	287	ASN
1	C	48	ASN
1	C	106	GLN
1	C	212	GLN
1	C	224	GLN
1	C	233	GLN
1	C	251	ASN
1	C	257	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	C	369	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	140	GLN
1	D	205	ASN
1	D	212	GLN
1	D	215	ASN
1	D	225	GLN
1	D	257	GLN
1	D	269	HIS
1	D	283	GLN
1	D	305	ASN
1	E	59	GLN
1	E	99	ASN
1	E	106	GLN
1	E	120	GLN
1	E	224	GLN
1	E	225	GLN
1	E	265	ASN
1	E	269	HIS
1	E	282	ASN
1	E	308	GLN
1	E	330	ASN
1	F	48	ASN
1	F	49	GLN
1	F	98	HIS
1	F	101	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

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	451	3	25,26,26	1.02	1 (4%)	30,37,37	0.93	2 (6%)
2	B65	B	451	3	25,26,26	1.02	2 (8%)	30,37,37	0.81	1 (3%)
2	B65	F	451	3	25,26,26	1.10	3 (12%)	30,37,37	0.69	1 (3%)
2	B65	E	451	3	25,26,26	1.10	1 (4%)	30,37,37	0.95	3 (10%)
2	B65	D	451	3	25,26,26	1.07	1 (4%)	30,37,37	0.86	1 (3%)
2	B65	A	451	3	25,26,26	1.05	1 (4%)	30,37,37	0.81	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	C	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	F	451	3	-	2/15/22/22	0/2/2/2
2	B65	E	451	3	-	7/15/22/22	0/2/2/2
2	B65	D	451	3	-	3/15/22/22	0/2/2/2
2	B65	A	451	3	-	3/15/22/22	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	451	B65	CAW-SAY	-3.40	1.66	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	451	B65	CAW-SAY	-3.34	1.67	1.82
2	D	451	B65	CAW-SAY	-3.34	1.67	1.82
2	B	451	B65	CAW-SAY	-3.27	1.67	1.82
2	F	451	B65	CAW-SAY	-3.23	1.67	1.82
2	C	451	B65	CAW-SAY	-3.07	1.68	1.82
2	F	451	B65	PAX-OAC	-2.26	1.51	1.54
2	F	451	B65	PAX-OAB	-2.07	1.51	1.54
2	B	451	B65	PAX-OAB	-2.04	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	3.18	126.05	118.78
2	E	451	B65	CAV-OAS-CAU	2.63	124.79	118.78
2	A	451	B65	OAC-PAX-OAB	2.58	114.58	107.58
2	E	451	B65	OAC-PAX-OAB	2.41	114.13	107.58
2	D	451	B65	OAC-PAX-OAB	2.37	114.01	107.58
2	C	451	B65	OAC-PAX-OAB	2.28	113.77	107.58
2	F	451	B65	OAC-PAX-OAB	2.07	113.22	107.58
2	B	451	B65	CAV-OAS-CAU	2.07	123.50	118.78
2	E	451	B65	CAR-CAP-CAQ	-2.04	108.57	112.65

There are no chirality outliers.

All (21) torsion outliers are listed below:

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

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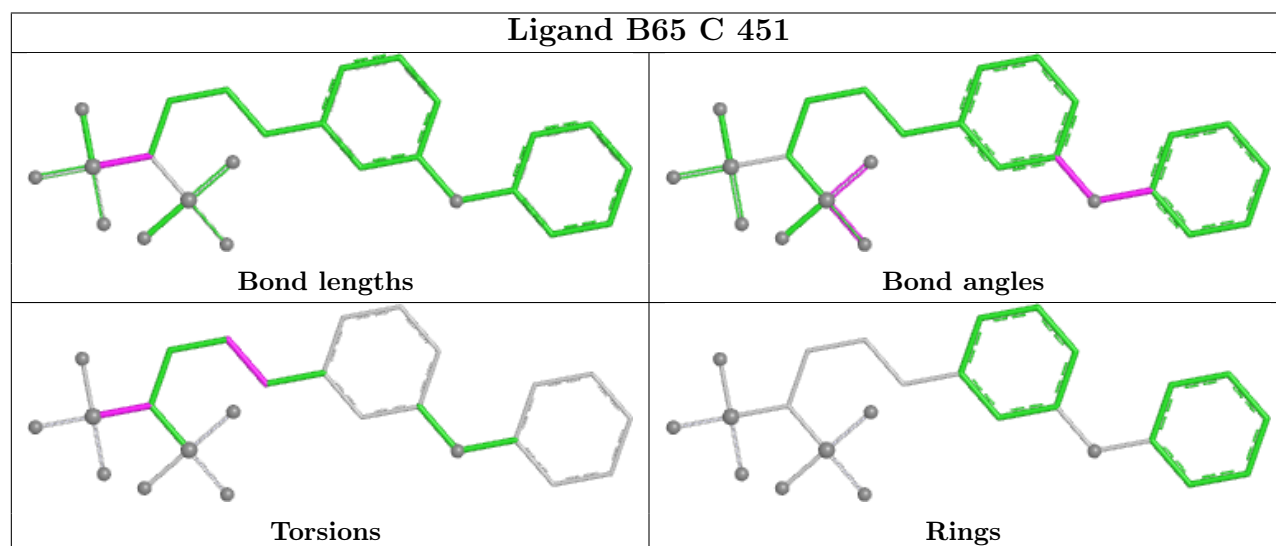
Mol	Chain	Res	Type	Atoms
2	A	451	B65	CAR-CAW-SAY-OAE
2	C	451	B65	CAR-CAW-SAY-OAE
2	F	451	B65	CAR-CAP-CAQ-CAT
2	D	451	B65	CAP-CAR-CAW-PAX
2	E	451	B65	CAP-CAR-CAW-PAX

There are no ring outliers.

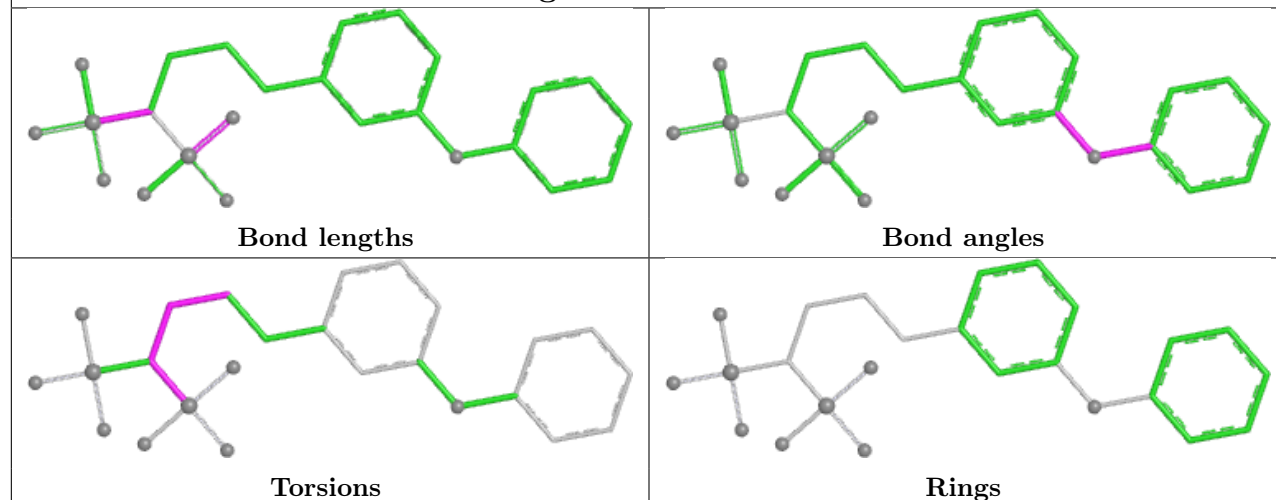
5 monomers are involved in 7 short contacts:

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

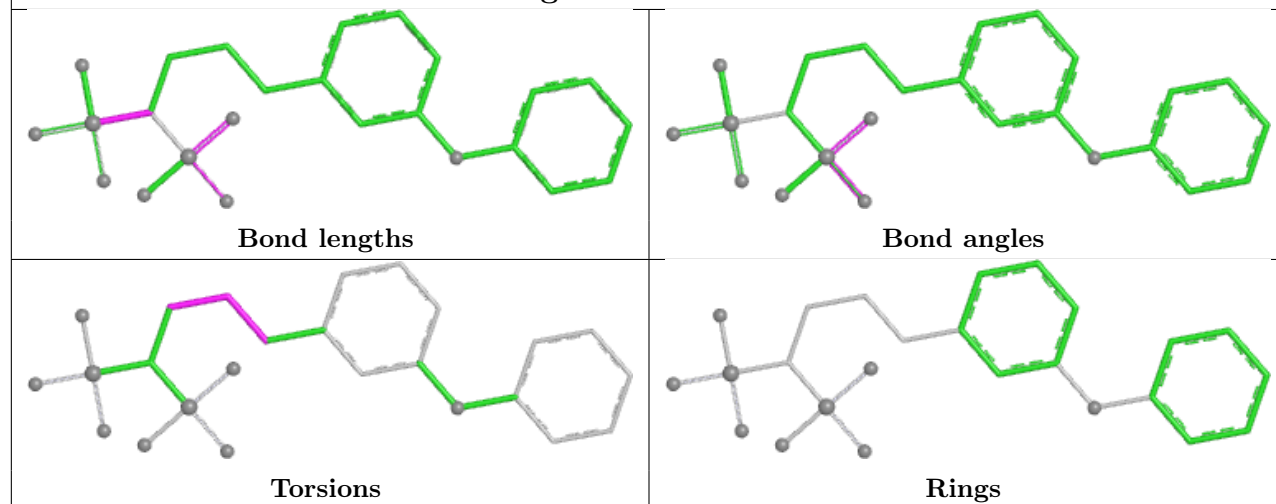
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



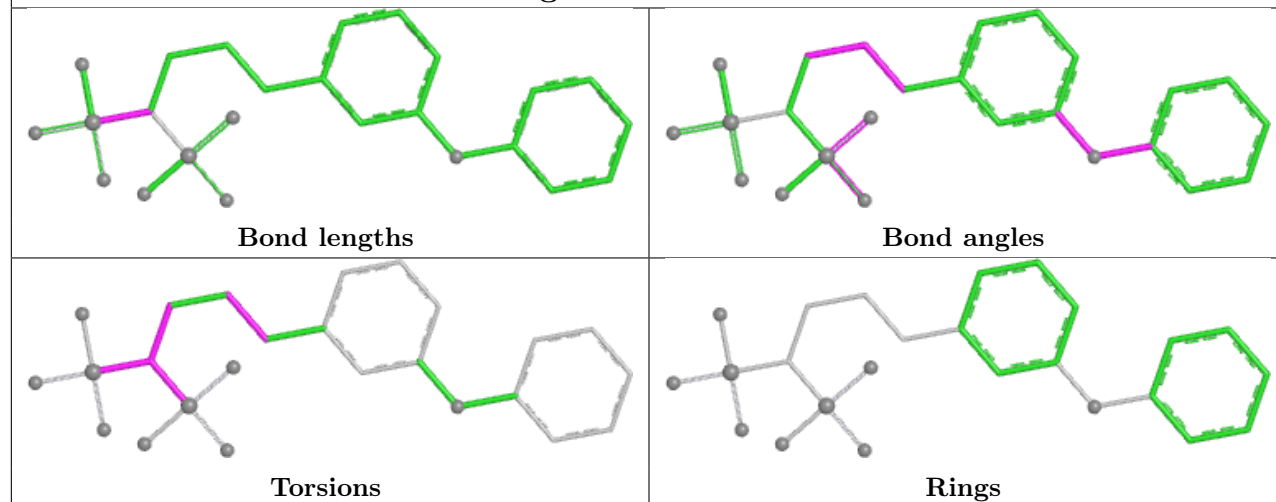
Ligand B65 B 451

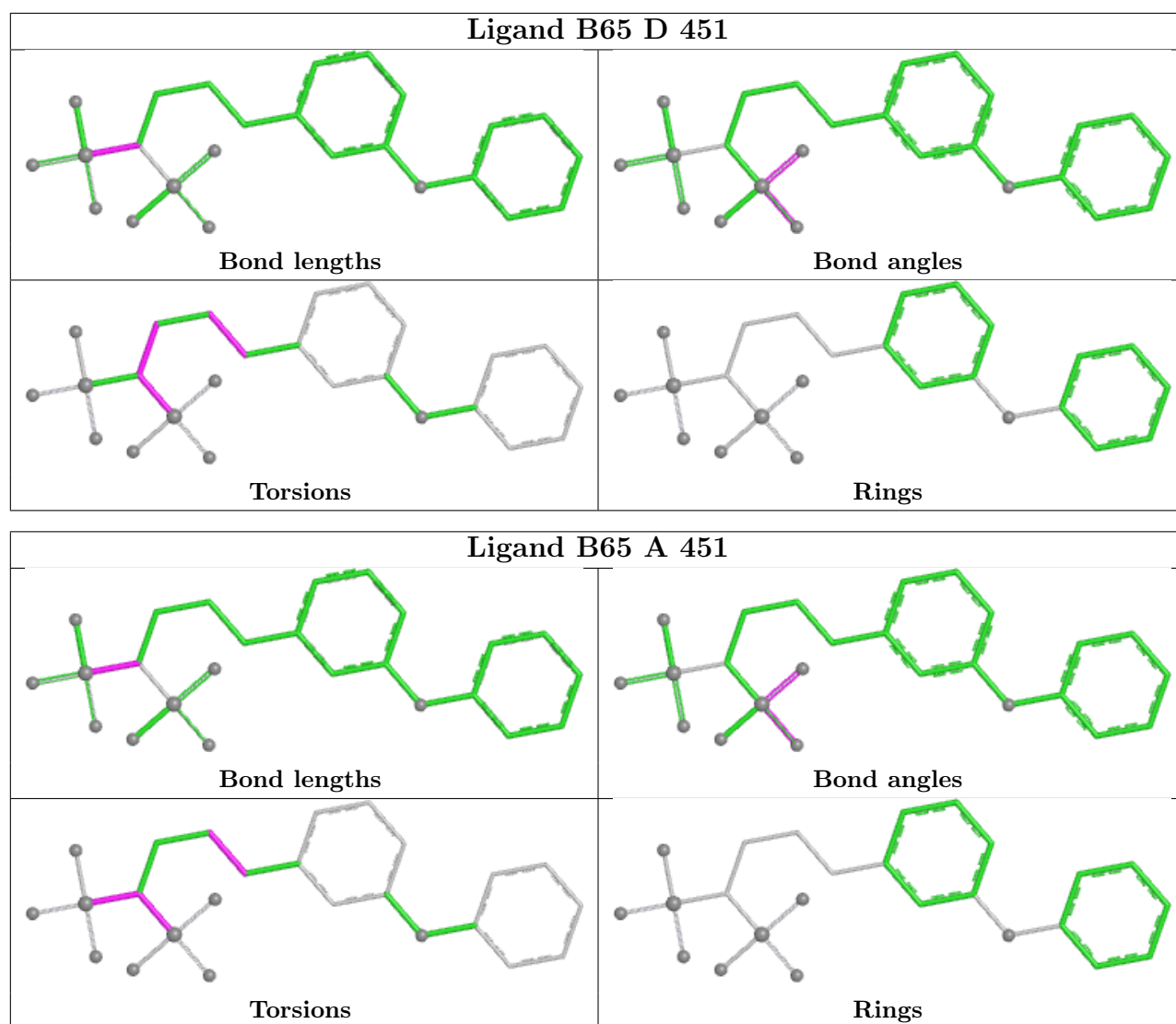


Ligand B65 F 451



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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
1	A	324/340 (95%)	-0.49	0	100	100	26, 41, 72, 96	0
1	B	324/340 (95%)	-0.45	0	100	100	26, 44, 72, 99	0
1	C	324/340 (95%)	-0.44	0	100	100	24, 43, 120, 232	0
1	D	322/340 (94%)	-0.35	1 (0%)	90	81	27, 53, 120, 152	0
1	E	323/340 (95%)	-0.30	0	100	100	32, 61, 105, 123	0
1	F	262/340 (77%)	-0.27	0	100	100	28, 65, 106, 118	0
All	All	1879/2040 (92%)	-0.39	1 (0%)	92	89	24, 50, 102, 232	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	307	GLN	2.7

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

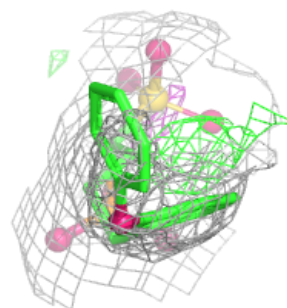
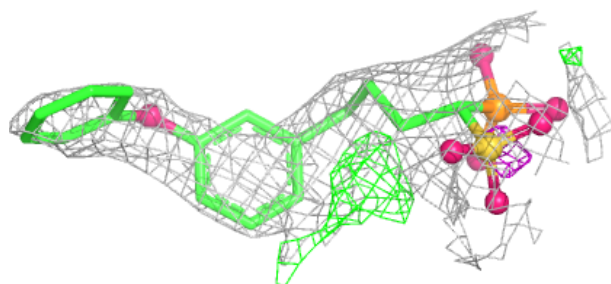
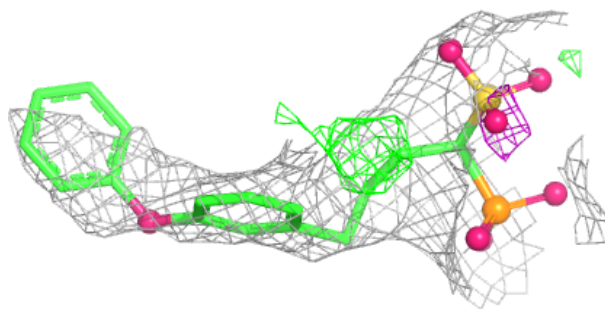
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	B65	F	451	25/25	0.85	0.15	89,97,109,109	0
3	MG	F	452	1/1	0.88	0.04	81,81,81,81	0
2	B65	B	451	25/25	0.91	0.12	64,76,83,85	0
2	B65	C	451	25/25	0.91	0.12	68,78,92,93	0
2	B65	D	451	25/25	0.92	0.11	60,77,91,91	0
2	B65	E	451	25/25	0.93	0.11	79,84,87,87	0
3	MG	E	452	1/1	0.94	0.10	81,81,81,81	0
3	MG	D	452	1/1	0.94	0.04	34,34,34,34	0
2	B65	A	451	25/25	0.95	0.10	64,72,78,78	0
3	MG	B	452	1/1	0.98	0.03	37,37,37,37	0
3	MG	C	452	1/1	0.99	0.03	52,52,52,52	0
3	MG	A	452	1/1	0.99	0.03	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.

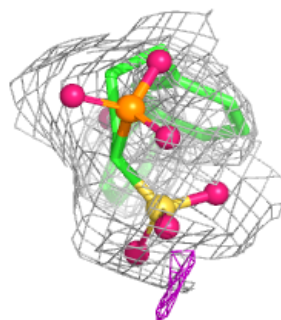
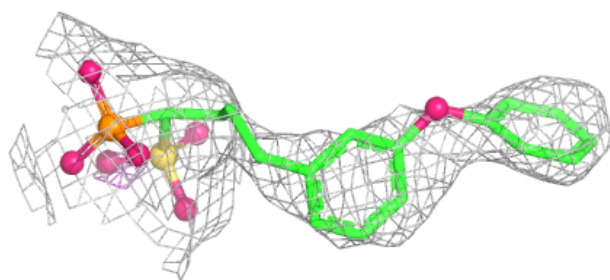
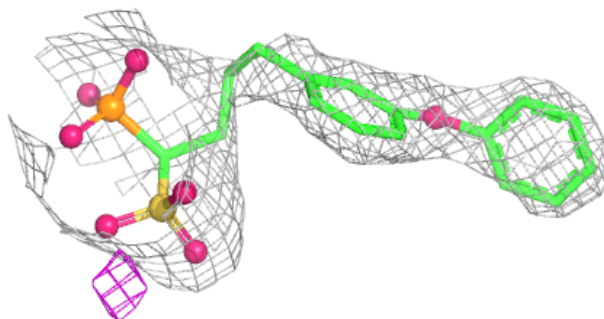
Electron density around B65 F 451:

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

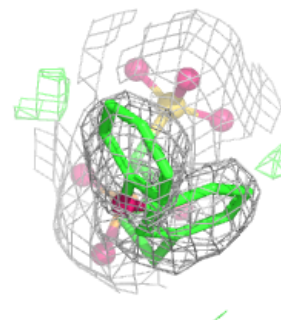
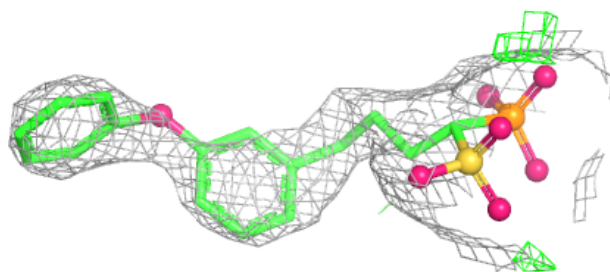
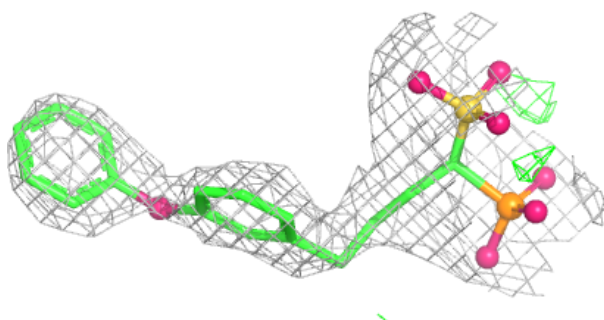


Electron density around B65 B 451:

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

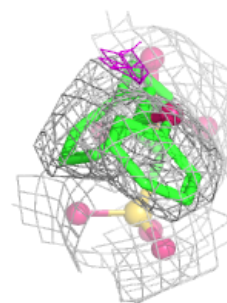
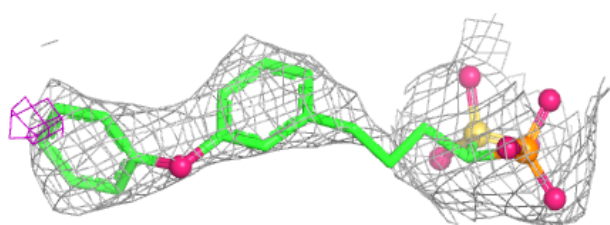
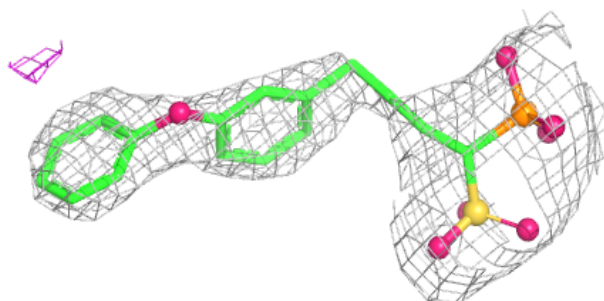
**Electron density around B65 C 451:**

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

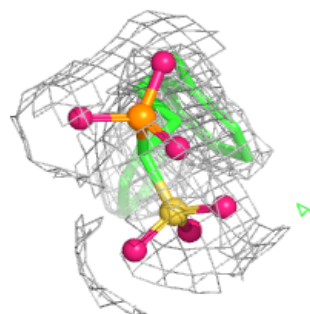
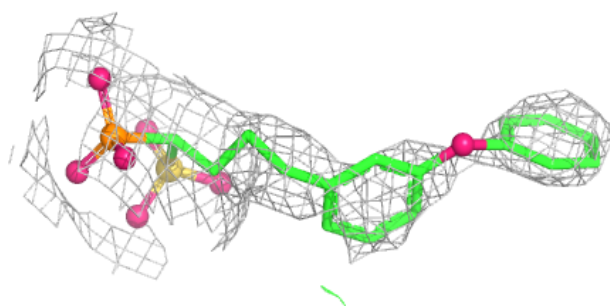
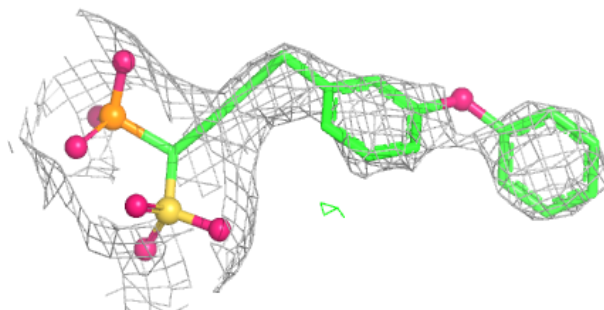


Electron density around B65 D 451:

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

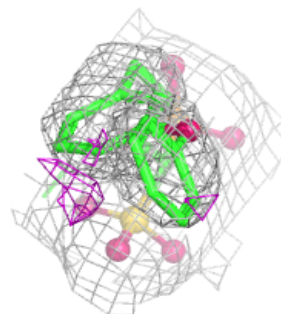
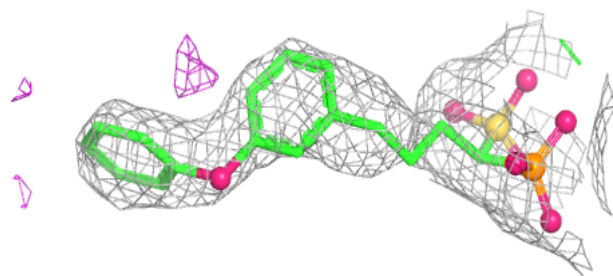
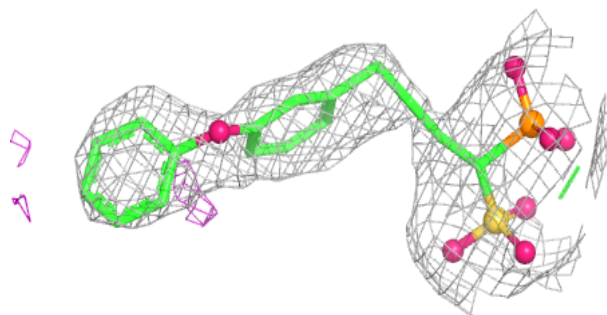
**Electron density around B65 E 451:**

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



Electron density around B65 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.