



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2026 – 10:08 AM EDT

PDB ID : 9ZLE / pdb_00009zle
Title : Crystal structure of DCAF1 in complex with SDIPTAC C8
Authors : Mabanglo, M.F.; Srivastava, S.; Hoffer, L.; Ramnauth, J.; Vedadi, M.
Deposited on : 2025-12-08
Resolution : 2.55 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

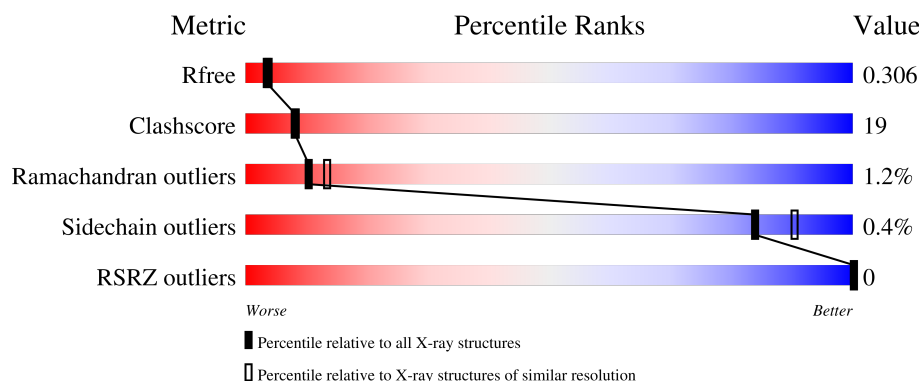
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	314	
1	B	314	
1	C	314	
1	D	314	
1	E	314	

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Mol	Chain	Length	Quality of chain
1	F	314	<div><div></div><div>62%</div><div>31%</div><div>• 6%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14648 atoms, of which 130 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.

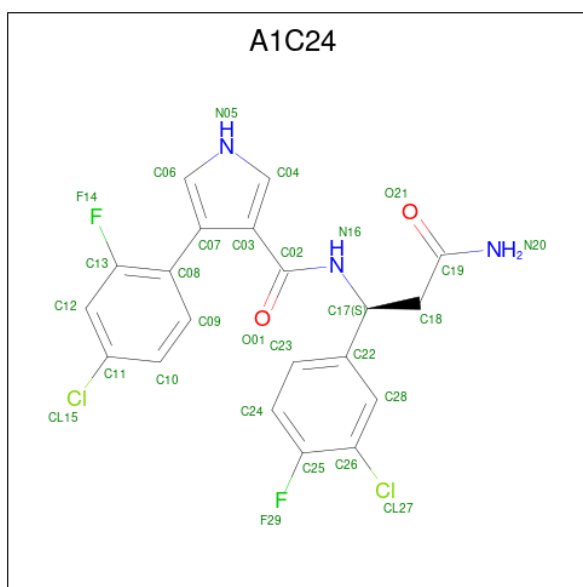
- Molecule 1 is a protein called DDB1- and CUL4-associated factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	1
			2340	1480	401	443	16			
1	B	299	Total	C	N	O	S	0	0	1
			2374	1499	406	453	16			
1	C	295	Total	C	N	O	S	0	0	1
			2340	1480	401	443	16			
1	D	296	Total	C	N	O	S	0	0	1
			2349	1486	403	444	16			
1	E	295	Total	C	N	O	S	0	0	1
			2340	1480	401	443	16			
1	F	295	Total	C	N	O	S	0	0	1
			2340	1480	401	443	16			

There are 12 discrepancies between the modelled and reference sequences:

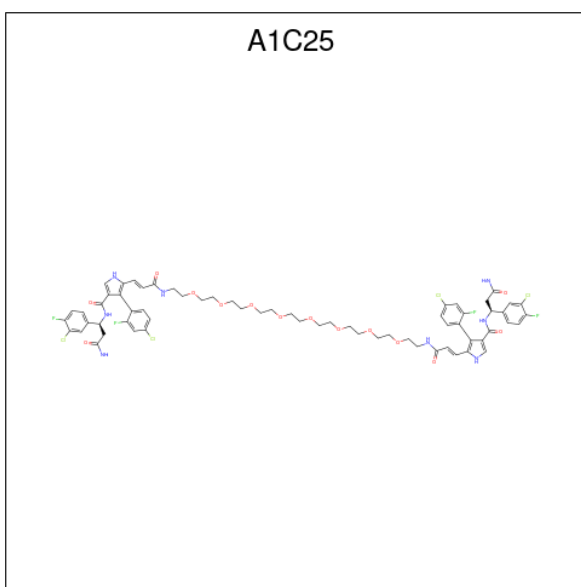
Chain	Residue	Modelled	Actual	Comment	Reference
A	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
A	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6
B	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
B	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6
C	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
C	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6
D	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
D	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6
E	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
E	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6
F	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
F	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6

- Molecule 2 is (4P)-N-[(1S)-3-amino-1-(3-chloro-4-fluorophenyl)-3-oxopropyl]-4-(4-chloro-2-fluorophenyl)-1H-pyrrole-3-carboxamide (CCD ID: A1C24) (formula: C₂₀H₁₅Cl₂F₂N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	H	N	O	0	0
			44	20	2	2	15	3	2		
2	C	1	Total	C	Cl	F	H	N	O	0	0
			44	20	2	2	15	3	2		
2	E	1	Total	C	Cl	F	H	N	O	0	0
			44	20	2	2	15	3	2		
2	F	1	Total	C	Cl	F	H	N	O	0	0
			44	20	2	2	15	3	2		

- Molecule 3 is (4P,4'P)-5,5'-[(1E,33E)-3,32-dioxo-7,10,13,16,19,22,25,28-octaoxa-4,31-diaza tetratriaconta-1,33-diene-1,34-diyl]bis{N-[(1S)-3-amino-1-(3-chloro-4-fluorophenyl)-3-oxopropyl]-4-(4-chloro-2-fluorophenyl)-1H-pyrrole-3-carboxamide} (CCD ID: A1C25) (formula: C₆₄H₇₀Cl₄F₄N₈O₁₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	D	1	Total	C	Cl	F	H	N	O	0	0
			164	64	4	4	70	8	14		

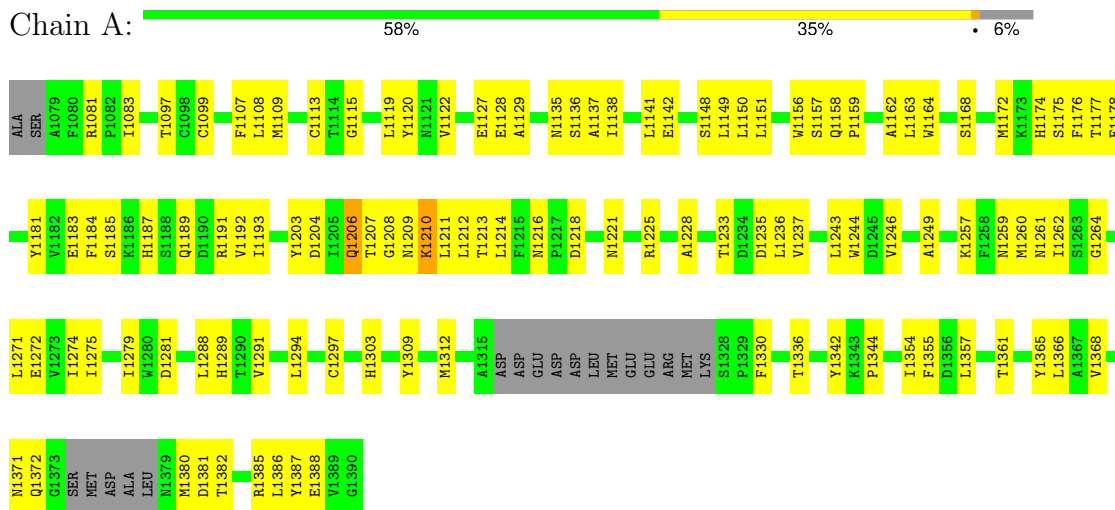
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	37	Total	O	0	0
			37	37		
4	C	47	Total	O	0	0
			47	47		
4	D	37	Total	O	0	0
			37	37		
4	E	34	Total	O	0	0
			34	34		
4	F	39	Total	O	0	0
			39	39		

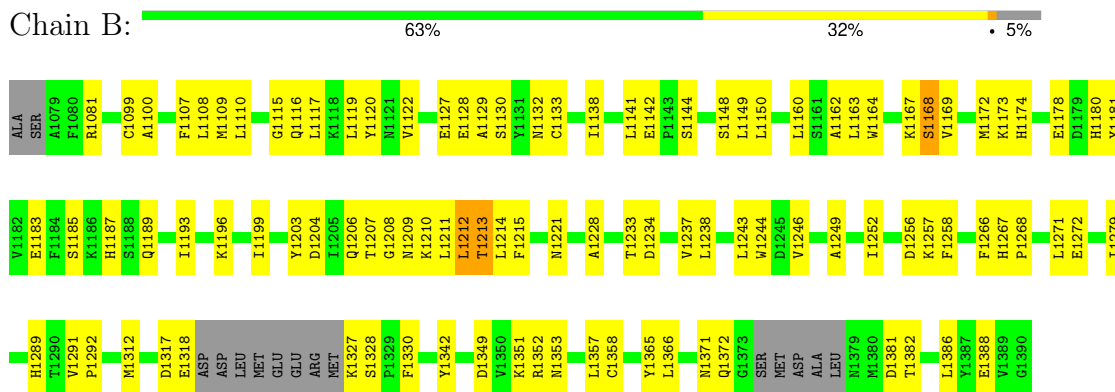
3 Residue-property plots

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.

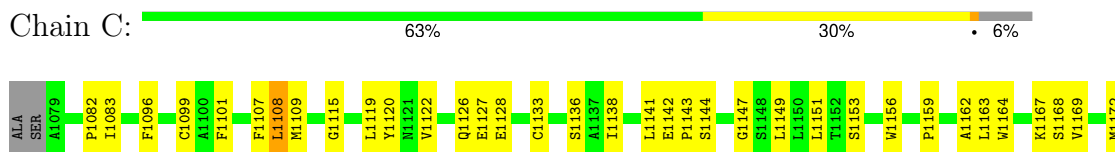
• Molecule 1: DDB1- and CUL4-associated factor 1

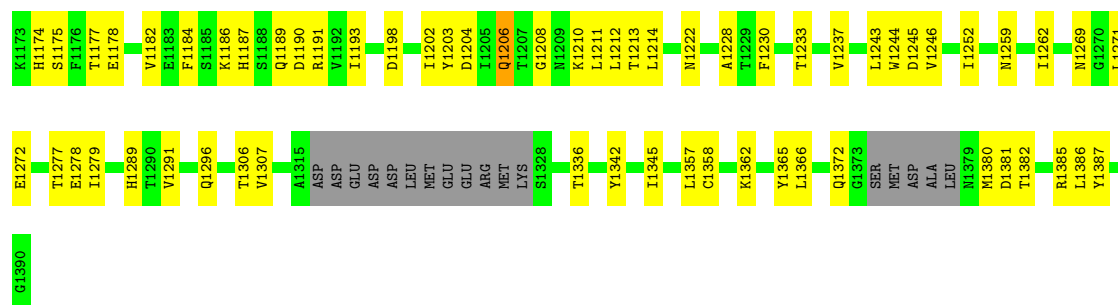


• Molecule 1: DDB1- and CUL4-associated factor 1



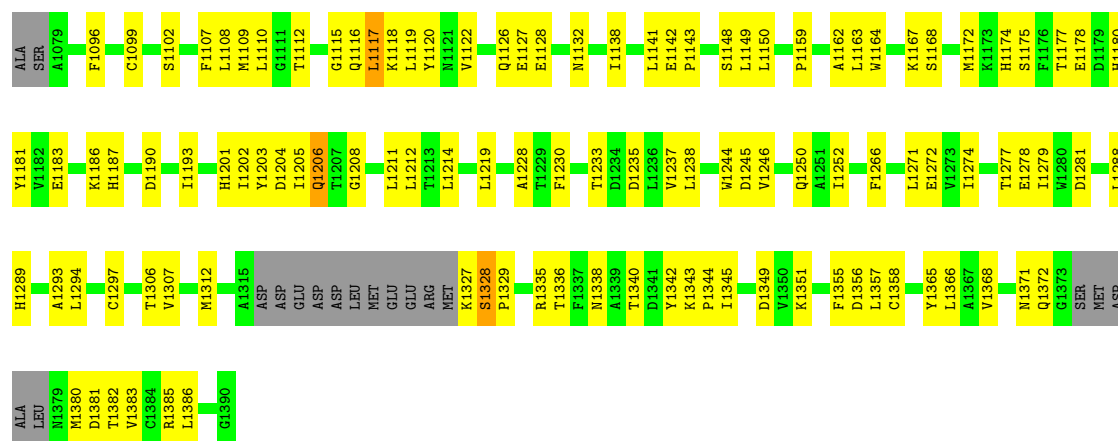
• Molecule 1: DDB1- and CUL4-associated factor 1





• Molecule 1: DDB1- and CUL4-associated factor 1

Chain D: 59% 34% 6%



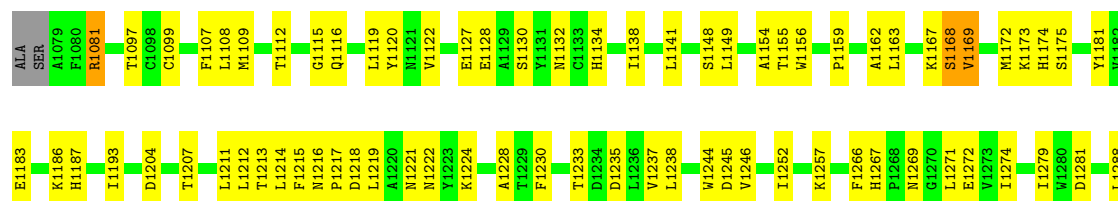
• Molecule 1: DDB1- and CUL4-associated factor 1

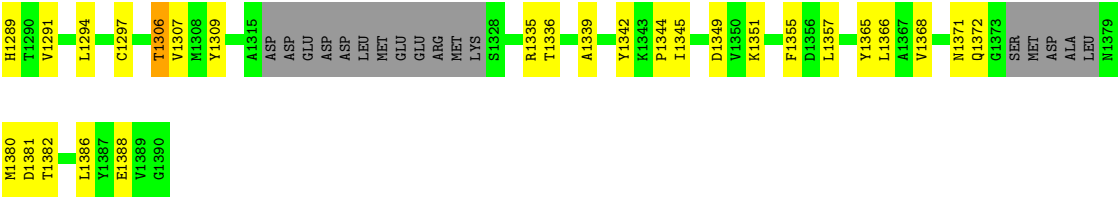
Chain E: 66% 27% 6%



• Molecule 1: DDB1- and CUL4-associated factor 1

Chain F: 62% 31% 6%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.59Å 84.78Å 221.47Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	29.05 – 2.55 29.05 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.05-2.55) 83.3 (29.05-2.55)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.89 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.261 , 0.305 0.261 , 0.306	Depositor DCC
R_{free} test set	2001 reflections (2.27%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.874	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 14.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.458 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.458 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.458 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.458 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.468 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14648	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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: A1C24, A1C25

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	0.09	0/2394	0.27	0/3246
1	B	0.09	0/2428	0.27	0/3291
1	C	0.09	0/2394	0.27	0/3246
1	D	0.09	0/2403	0.27	0/3257
1	E	0.10	0/2394	0.30	0/3246
1	F	0.16	1/2394 (0.0%)	0.28	0/3246
All	All	0.11	1/14407 (0.0%)	0.28	0/19532

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1081	ARG	CZ-NH2	-5.06	1.26	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2340	0	2243	106	0
1	B	2374	0	2270	91	0
1	C	2340	0	2243	93	0
1	D	2349	0	2256	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2340	0	2243	78	0
1	F	2340	0	2243	92	0
2	A	29	15	0	0	0
2	C	29	15	0	0	0
2	E	29	15	0	0	0
2	F	29	15	0	0	0
3	D	94	70	0	0	0
4	A	31	0	0	13	0
4	B	37	0	0	8	0
4	C	47	0	0	14	0
4	D	37	0	0	13	0
4	E	34	0	0	6	0
4	F	39	0	0	8	0
All	All	14518	130	13498	541	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 19.

All (541) 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:F:1081:ARG:HH21	1:F:1388:GLU:CD	1.56	1.12
1:C:1186:LYS:NZ	4:C:1501:HOH:O	1.85	1.10
1:F:1081:ARG:NH2	1:F:1388:GLU:CD	2.15	1.04
1:F:1216:ASN:OD1	1:F:1219:LEU:HD23	1.61	1.00
1:E:1112:THR:H	1:E:1138:ILE:HD12	1.29	0.98
1:C:1204:ASP:HB2	1:C:1211:LEU:HD11	1.46	0.98
1:A:1204:ASP:HB2	1:A:1211:LEU:HD11	1.47	0.96
1:F:1081:ARG:NH2	1:F:1388:GLU:OE1	1.98	0.94
1:E:1204:ASP:HB2	1:E:1211:LEU:HD11	1.50	0.93
1:C:1271:LEU:HD21	1:E:1233:THR:HG22	1.51	0.92
1:F:1204:ASP:HB2	1:F:1211:LEU:HD11	1.50	0.92
1:A:1157:SER:HB3	4:A:1503:HOH:O	1.69	0.91
1:A:1136:SER:HB3	1:A:1156:TRP:CE2	2.07	0.90
1:B:1148:SER:HB2	1:B:1167:LYS:HD3	1.54	0.87
1:A:1233:THR:OG1	1:A:1235:ASP:OD1	1.93	0.87
1:B:1204:ASP:HB2	1:B:1211:LEU:HD11	1.55	0.87
1:E:1102:SER:HA	1:E:1109:MET:HE3	1.55	0.87
1:E:1233:THR:OG1	1:E:1235:ASP:OD1	1.92	0.86
1:D:1204:ASP:HB2	1:D:1211:LEU:HD11	1.56	0.86
1:F:1252:ILE:HG12	4:F:1504:HOH:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1233:THR:OG1	1:F:1235:ASP:OD1	1.97	0.83
1:D:1116:GLN:NE2	1:D:1132:ASN:OD1	2.13	0.81
1:F:1081:ARG:NH2	1:F:1388:GLU:OE2	2.14	0.81
1:E:1105:GLU:O	1:E:1106:ARG:HB2	1.80	0.80
1:F:1267:HIS:HD2	1:F:1269:ASN:H	1.28	0.80
1:A:1136:SER:N	4:A:1503:HOH:O	2.15	0.79
1:D:1190:ASP:C	1:D:1205:ILE:HD12	2.09	0.78
1:A:1163:LEU:O	4:A:1501:HOH:O	2.01	0.78
1:A:1172:MET:HG3	4:A:1501:HOH:O	1.82	0.78
1:F:1107:PHE:HE2	1:F:1128:GLU:HG2	1.47	0.78
1:D:1357:LEU:HD13	1:D:1366:LEU:HD11	1.66	0.77
1:C:1203:TYR:CE1	1:C:1210:LYS:HG3	2.20	0.77
1:B:1107:PHE:HE2	1:B:1128:GLU:HG2	1.49	0.76
1:B:1174:HIS:HD2	1:B:1208:GLY:HA3	1.49	0.76
1:D:1245:ASP:N	4:D:1501:HOH:O	2.18	0.75
1:F:1357:LEU:HD13	1:F:1366:LEU:HD11	1.69	0.75
1:D:1117:LEU:HD13	1:D:1150:LEU:HD21	1.68	0.75
1:E:1112:THR:N	1:E:1138:ILE:HD12	2.02	0.75
1:B:1212:LEU:HD22	1:B:1214:LEU:HD12	1.68	0.74
1:F:1222:ASN:O	4:F:1501:HOH:O	2.04	0.74
1:F:1168:SER:O	1:F:1169:VAL:HG12	1.88	0.73
1:A:1162:ALA:HB1	1:A:1172:MET:HE2	1.70	0.73
1:E:1259:ASN:HD21	1:E:1262:ILE:H	1.34	0.73
1:A:1221:ASN:O	1:A:1257:LYS:HE3	1.88	0.73
1:A:1365:TYR:HB3	1:A:1386:LEU:HD11	1.70	0.73
1:D:1365:TYR:HB3	1:D:1386:LEU:HD11	1.71	0.72
1:E:1372:GLN:HG2	1:E:1381:ASP:O	1.89	0.72
1:F:1097:THR:HG22	1:F:1380:MET:HE1	1.69	0.72
1:C:1193:ILE:HD11	1:C:1228:ALA:HB1	1.72	0.72
1:E:1245:ASP:N	4:E:1501:HOH:O	2.22	0.72
1:C:1186:LYS:HE3	1:C:1186:LYS:HA	1.71	0.71
1:D:1107:PHE:HE2	1:D:1128:GLU:HG2	1.55	0.71
1:A:1371:ASN:HA	1:A:1382:THR:HG22	1.72	0.71
1:A:1142:GLU:OE2	4:A:1502:HOH:O	2.09	0.70
1:C:1259:ASN:HD21	1:C:1262:ILE:H	1.39	0.70
1:D:1174:HIS:HD2	1:D:1208:GLY:HA3	1.56	0.70
1:F:1097:THR:CG2	1:F:1380:MET:HE1	2.22	0.70
1:A:1191:ARG:HH22	1:A:1246:VAL:HG11	1.56	0.69
1:E:1191:ARG:HH22	1:E:1246:VAL:HG11	1.56	0.69
1:A:1107:PHE:HE2	1:A:1128:GLU:HG2	1.57	0.69
1:A:1174:HIS:O	4:A:1501:HOH:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1160:LEU:HD12	1:B:1178:GLU:HA	1.75	0.68
1:D:1235:ASP:HB2	4:D:1502:HOH:O	1.94	0.68
1:C:1365:TYR:HB3	1:C:1386:LEU:HD11	1.75	0.68
1:C:1222:ASN:O	4:C:1502:HOH:O	2.11	0.68
1:F:1306:THR:HG22	1:F:1307:VAL:HG23	1.76	0.67
1:F:1204:ASP:HB2	1:F:1211:LEU:CD1	2.25	0.67
1:D:1102:SER:HA	1:D:1109:MET:HE2	1.75	0.67
1:F:1127:GLU:OE2	1:F:1130:SER:OG	2.11	0.66
1:A:1083:ILE:HD11	1:A:1388:GLU:HB2	1.78	0.66
1:B:1107:PHE:CE2	1:B:1128:GLU:HG2	2.29	0.66
1:C:1271:LEU:HD21	1:E:1233:THR:CG2	2.25	0.66
1:B:1212:LEU:HD22	1:B:1214:LEU:CD1	2.26	0.65
1:C:1108:LEU:HB2	1:C:1122:VAL:CG1	2.26	0.65
1:A:1174:HIS:N	4:A:1501:HOH:O	2.28	0.65
1:A:1193:ILE:HD11	1:A:1228:ALA:HB1	1.78	0.65
1:B:1174:HIS:CD2	1:B:1208:GLY:HA3	2.30	0.65
1:C:1147:GLY:HA2	4:C:1531:HOH:O	1.95	0.65
1:B:1189:GLN:NE2	4:B:1402:HOH:O	2.28	0.65
1:C:1357:LEU:HD13	1:C:1366:LEU:HD11	1.78	0.65
1:D:1126:GLN:HG3	4:D:1531:HOH:O	1.97	0.64
1:D:1338:ASN:OD1	1:D:1340:THR:HG22	1.97	0.64
1:E:1338:ASN:OD1	1:E:1340:THR:HG22	1.97	0.64
1:E:1174:HIS:HD2	1:E:1208:GLY:HA3	1.62	0.64
1:F:1365:TYR:HB3	1:F:1386:LEU:HD11	1.79	0.64
1:A:1257:LYS:NZ	4:A:1508:HOH:O	2.30	0.64
1:B:1357:LEU:HD13	1:B:1366:LEU:HD11	1.79	0.64
1:F:1173:LYS:C	1:F:1174:HIS:HD1	2.06	0.63
1:F:1371:ASN:HA	1:F:1382:THR:HG22	1.81	0.63
1:B:1272:GLU:OE2	1:B:1342:TYR:OH	2.09	0.63
1:E:1109:MET:HG2	1:E:1119:LEU:CD1	2.28	0.63
1:E:1112:THR:HB	4:E:1506:HOH:O	1.98	0.63
1:F:1245:ASP:N	4:F:1504:HOH:O	2.31	0.63
1:A:1357:LEU:HD13	1:A:1366:LEU:HD11	1.80	0.63
1:C:1230:PHE:N	4:C:1503:HOH:O	2.32	0.63
1:D:1120:TYR:CZ	1:D:1127:GLU:HB2	2.33	0.62
1:D:1174:HIS:CD2	1:D:1208:GLY:HA3	2.33	0.62
1:F:1215:PHE:CE2	1:F:1217:PRO:HG3	2.35	0.62
1:A:1259:ASN:HD21	1:A:1262:ILE:H	1.46	0.62
1:C:1203:TYR:HD1	1:C:1210:LYS:HA	1.65	0.62
1:E:1357:LEU:HD13	1:E:1366:LEU:HD11	1.79	0.62
1:D:1193:ILE:HD11	1:D:1228:ALA:HB1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1162:ALA:HB1	1:B:1172:MET:HE2	1.82	0.62
1:A:1108:LEU:HB2	1:A:1122:VAL:CG1	2.29	0.62
1:B:1212:LEU:HD23	1:B:1213:THR:H	1.64	0.62
1:D:1204:ASP:OD1	1:D:1206:GLN:N	2.33	0.61
1:A:1216:ASN:HD22	1:A:1218:ASP:H	1.46	0.61
1:D:1272:GLU:OE2	1:D:1342:TYR:OH	2.16	0.61
1:A:1174:HIS:HD2	1:A:1208:GLY:HA3	1.65	0.61
1:A:1274:ILE:HG23	1:A:1279:ILE:HG13	1.82	0.61
1:B:1238:LEU:HB2	1:B:1266:PHE:CE2	2.36	0.61
1:B:1214:LEU:HD23	1:B:1244:TRP:CG	2.36	0.61
1:E:1293:ALA:HB1	1:E:1335:ARG:NH1	2.16	0.61
1:A:1174:HIS:CD2	1:A:1208:GLY:HA3	2.35	0.61
1:A:1214:LEU:HD22	1:A:1244:TRP:CE3	2.36	0.61
1:C:1210:LYS:HE3	1:C:1213:THR:OG1	2.01	0.61
1:E:1272:GLU:OE2	1:E:1342:TYR:OH	2.13	0.61
1:A:1212:LEU:HD23	1:A:1213:THR:H	1.66	0.60
1:D:1107:PHE:CE2	1:D:1128:GLU:HG2	2.36	0.60
1:A:1149:LEU:HD12	1:A:1163:LEU:HD11	1.81	0.60
1:B:1120:TYR:CZ	1:B:1127:GLU:HB2	2.36	0.60
1:F:1108:LEU:HB2	1:F:1122:VAL:CG1	2.31	0.60
1:D:1109:MET:HG3	1:D:1119:LEU:HD21	1.84	0.60
1:B:1292:PRO:HG2	1:C:1126:GLN:HG2	1.83	0.60
1:E:1174:HIS:CD2	1:E:1208:GLY:HA3	2.37	0.59
1:D:1385:ARG:NH1	4:D:1504:HOH:O	2.29	0.59
1:F:1335:ARG:HD2	4:F:1535:HOH:O	2.02	0.59
1:A:1177:THR:HB	1:A:1178:GLU:OE1	2.03	0.58
1:A:1380:MET:HE2	1:A:1380:MET:HA	1.85	0.58
1:D:1293:ALA:HB1	1:D:1335:ARG:NH1	2.17	0.58
1:E:1207:THR:HG21	4:E:1517:HOH:O	2.02	0.58
1:F:1267:HIS:CD2	1:F:1269:ASN:H	2.17	0.58
1:D:1329:PRO:HD2	1:D:1355:PHE:HA	1.86	0.58
1:E:1158:GLN:OE1	1:E:1177:THR:HG22	2.04	0.58
1:A:1176:PHE:CZ	1:A:1192:VAL:HG21	2.38	0.58
1:B:1328:SER:CB	1:B:1353:ASN:HB3	2.33	0.58
1:D:1238:LEU:HB2	1:D:1266:PHE:CE2	2.39	0.58
1:E:1167:LYS:O	1:E:1169:VAL:N	2.37	0.58
1:F:1238:LEU:HB2	1:F:1266:PHE:CE2	2.39	0.58
1:D:1237:VAL:HG23	1:D:1246:VAL:CG2	2.34	0.58
1:C:1204:ASP:HB2	1:C:1211:LEU:CD1	2.29	0.58
1:A:1385:ARG:HD3	1:A:1387:TYR:OH	2.04	0.57
1:C:1245:ASP:N	4:C:1507:HOH:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1372:GLN:HB2	1:F:1381:ASP:O	2.03	0.57
1:C:1177:THR:HB	1:C:1178:GLU:OE2	2.03	0.57
1:F:1279:ILE:HB	1:F:1289:HIS:HB2	1.87	0.57
1:B:1237:VAL:HG23	1:B:1246:VAL:HG22	1.86	0.57
1:F:1193:ILE:HD11	1:F:1228:ALA:HB1	1.87	0.57
1:F:1349:ASP:OD2	1:F:1351:LYS:HD3	2.05	0.57
1:B:1279:ILE:HB	1:B:1289:HIS:HB2	1.86	0.57
1:C:1272:GLU:OE2	1:C:1342:TYR:OH	2.15	0.57
1:D:1108:LEU:HB2	1:D:1122:VAL:CG1	2.34	0.57
1:A:1212:LEU:HD23	1:A:1213:THR:N	2.20	0.57
1:B:1193:ILE:HD11	1:B:1228:ALA:HB1	1.86	0.57
1:F:1120:TYR:CZ	1:F:1127:GLU:HB2	2.40	0.57
1:A:1159:PRO:HG3	1:A:1175:SER:HB2	1.87	0.56
1:A:1216:ASN:HD22	1:A:1216:ASN:C	2.12	0.56
1:C:1204:ASP:OD1	1:C:1206:GLN:N	2.37	0.56
1:B:1207:THR:HG21	4:B:1413:HOH:O	2.05	0.56
1:C:1202:ILE:HA	4:C:1505:HOH:O	2.06	0.56
1:D:1237:VAL:HG23	1:D:1246:VAL:HG22	1.87	0.56
1:E:1204:ASP:HB2	1:E:1211:LEU:CD1	2.31	0.56
1:A:1216:ASN:ND2	1:A:1218:ASP:H	2.02	0.56
1:C:1186:LYS:N	1:C:1186:LYS:HD2	2.20	0.56
1:E:1193:ILE:HD11	1:E:1228:ALA:HB1	1.88	0.56
1:D:1102:SER:HA	1:D:1109:MET:CE	2.35	0.56
1:B:1221:ASN:O	1:B:1257:LYS:HE3	2.06	0.56
1:A:1120:TYR:CZ	1:A:1127:GLU:HB2	2.41	0.55
1:D:1162:ALA:HB1	1:D:1172:MET:HE2	1.88	0.55
1:B:1108:LEU:HB2	1:B:1122:VAL:CG1	2.36	0.55
1:D:1112:THR:HB	4:D:1505:HOH:O	2.06	0.55
1:E:1115:GLY:HA2	1:E:1138:ILE:HG13	1.88	0.55
1:E:1191:ARG:NH2	1:E:1246:VAL:HG11	2.20	0.55
1:F:1115:GLY:HA2	1:F:1138:ILE:HG13	1.89	0.55
1:B:1120:TYR:CE2	1:B:1127:GLU:HB2	2.41	0.55
1:B:1117:LEU:HD13	1:B:1150:LEU:HD21	1.88	0.55
1:A:1303:HIS:CE1	1:A:1361:THR:HA	2.42	0.55
1:A:1371:ASN:CA	1:A:1382:THR:HG22	2.35	0.55
1:C:1082:PRO:O	1:C:1083:ILE:HD13	2.07	0.55
1:F:1214:LEU:HA	4:F:1530:HOH:O	2.06	0.55
1:D:1250:GLN:O	4:D:1501:HOH:O	2.18	0.55
1:B:1127:GLU:OE2	1:B:1130:SER:OG	2.23	0.55
1:D:1109:MET:CG	1:D:1119:LEU:HD21	2.37	0.55
1:B:1129:ALA:HB3	4:B:1428:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1115:GLY:C	1:F:1138:ILE:HD11	2.33	0.54
1:F:1149:LEU:HG	1:F:1163:LEU:HD21	1.88	0.54
1:A:1260:MET:HE3	4:A:1508:HOH:O	2.07	0.54
1:F:1212:LEU:HD23	1:F:1213:THR:N	2.22	0.54
1:A:1259:ASN:HD21	1:A:1262:ILE:N	2.05	0.54
1:A:1279:ILE:HB	1:A:1289:HIS:HB2	1.90	0.54
1:C:1191:ARG:HH22	1:C:1246:VAL:HG11	1.71	0.54
1:D:1252:ILE:HG23	4:D:1501:HOH:O	2.06	0.54
1:E:1167:LYS:O	1:E:1167:LYS:HG3	2.08	0.54
1:B:1243:LEU:CD2	1:B:1252:ILE:HD11	2.36	0.54
1:A:1272:GLU:OE2	1:A:1342:TYR:OH	2.19	0.54
1:A:1357:LEU:HD12	1:A:1357:LEU:C	2.33	0.54
1:E:1120:TYR:CZ	1:E:1127:GLU:HB2	2.43	0.54
1:D:1159:PRO:HG3	1:D:1175:SER:HB2	1.90	0.54
1:E:1107:PHE:CE2	1:E:1128:GLU:HG3	2.43	0.53
1:A:1191:ARG:NH2	1:A:1246:VAL:HG11	2.22	0.53
1:D:1204:ASP:O	1:D:1208:GLY:HA2	2.08	0.53
1:D:1349:ASP:OD2	1:D:1351:LYS:HD3	2.08	0.53
1:F:1212:LEU:HD23	1:F:1213:THR:H	1.73	0.53
1:B:1328:SER:OG	1:B:1330:PHE:O	2.27	0.53
1:B:1365:TYR:HB3	1:B:1386:LEU:HD11	1.89	0.53
1:C:1269:ASN:O	1:C:1271:LEU:HD22	2.09	0.53
1:C:1203:TYR:CD1	1:C:1210:LYS:HA	2.44	0.53
1:E:1099:CYS:HA	1:E:1109:MET:O	2.09	0.53
1:A:1115:GLY:HA2	1:A:1138:ILE:HG13	1.89	0.53
1:C:1237:VAL:HG23	1:C:1246:VAL:CG2	2.39	0.53
1:C:1108:LEU:HB2	1:C:1122:VAL:HG13	1.90	0.52
1:C:1189:GLN:NE2	4:C:1508:HOH:O	2.41	0.52
1:E:1259:ASN:HD21	1:E:1262:ILE:N	2.04	0.52
1:C:1120:TYR:CZ	1:C:1127:GLU:HB2	2.45	0.52
1:D:1233:THR:HB	1:F:1271:LEU:HD11	1.92	0.52
1:B:1203:TYR:CE2	1:B:1210:LYS:HG3	2.44	0.52
1:C:1202:ILE:HG12	4:C:1505:HOH:O	2.09	0.52
1:F:1107:PHE:CE2	1:F:1128:GLU:HG2	2.36	0.52
1:A:1099:CYS:HA	1:A:1109:MET:O	2.10	0.52
1:C:1107:PHE:CE2	1:C:1128:GLU:HG3	2.45	0.52
1:F:1099:CYS:HA	1:F:1109:MET:O	2.10	0.52
1:F:1109:MET:HG3	1:F:1119:LEU:CD2	2.40	0.52
1:C:1214:LEU:HD22	1:C:1244:TRP:CE3	2.45	0.52
1:C:1259:ASN:HD22	1:C:1296:GLN:HE22	1.56	0.52
1:D:1372:GLN:HB2	1:D:1381:ASP:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1357:LEU:C	1:E:1357:LEU:HD12	2.35	0.52
1:F:1148:SER:HB2	1:F:1167:LYS:HD3	1.92	0.52
1:B:1180:HIS:HB3	4:B:1434:HOH:O	2.11	0.51
1:B:1328:SER:OG	1:B:1353:ASN:HB3	2.10	0.51
1:D:1186:LYS:HE3	1:D:1230:PHE:O	2.10	0.51
1:E:1279:ILE:HB	1:E:1289:HIS:HB2	1.90	0.51
1:E:1214:LEU:HD22	1:E:1244:TRP:CE3	2.45	0.51
1:F:1237:VAL:HG23	1:F:1246:VAL:HG22	1.91	0.51
1:A:1237:VAL:HG23	1:A:1246:VAL:CG2	2.40	0.51
1:C:1167:LYS:HG3	1:C:1167:LYS:O	2.10	0.51
1:D:1277:THR:OG1	1:D:1278:GLU:OE2	2.23	0.51
1:F:1272:GLU:OE2	1:F:1342:TYR:OH	2.25	0.51
1:B:1167:LYS:O	1:B:1168:SER:OG	2.17	0.51
1:B:1212:LEU:HD23	1:B:1213:THR:N	2.25	0.51
1:C:1279:ILE:HB	1:C:1289:HIS:HB2	1.92	0.51
1:F:1344:PRO:HB3	4:F:1535:HOH:O	2.10	0.51
1:C:1271:LEU:CD2	1:E:1233:THR:HG22	2.32	0.51
1:B:1099:CYS:HA	1:B:1109:MET:O	2.11	0.51
1:D:1214:LEU:HA	4:D:1517:HOH:O	2.11	0.51
1:B:1237:VAL:HG23	1:B:1246:VAL:CG2	2.41	0.51
1:D:1357:LEU:HD12	1:D:1357:LEU:C	2.36	0.51
1:F:1109:MET:HG3	1:F:1119:LEU:HD21	1.91	0.51
1:E:1108:LEU:HB2	1:E:1122:VAL:CG1	2.41	0.51
1:D:1279:ILE:HB	1:D:1289:HIS:HB2	1.93	0.50
1:F:1294:LEU:O	1:F:1297:CYS:HB2	2.12	0.50
1:A:1233:THR:HB	1:B:1271:LEU:HD21	1.93	0.50
1:A:1237:VAL:HG23	1:A:1246:VAL:HG22	1.94	0.50
1:C:1133:CYS:HA	1:C:1164:TRP:CH2	2.46	0.50
1:D:1141:LEU:HD12	1:D:1141:LEU:C	2.36	0.50
1:E:1372:GLN:NE2	1:E:1381:ASP:OD2	2.40	0.50
1:E:1279:ILE:N	1:E:1279:ILE:HD12	2.26	0.50
1:F:1219:LEU:N	1:F:1219:LEU:HD22	2.26	0.50
1:C:1385:ARG:HD3	1:C:1387:TYR:OH	2.11	0.50
1:D:1115:GLY:HA2	1:D:1138:ILE:HG13	1.93	0.50
1:E:1102:SER:HA	1:E:1109:MET:CE	2.34	0.50
1:A:1107:PHE:CE2	1:A:1128:GLU:HG2	2.43	0.50
1:C:1279:ILE:CD1	1:C:1291:VAL:HG23	2.41	0.50
1:C:1336:THR:O	1:C:1345:ILE:HB	2.12	0.50
1:D:1201:HIS:HB3	1:D:1203:TYR:CE1	2.46	0.50
1:F:1141:LEU:HD12	1:F:1141:LEU:C	2.37	0.50
1:B:1185:SER:O	1:B:1189:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1279:ILE:HD12	1:B:1279:ILE:N	2.27	0.50
1:B:1357:LEU:HD12	1:B:1357:LEU:C	2.36	0.50
1:D:1149:LEU:HD13	1:D:1163:LEU:HD11	1.93	0.50
1:C:1120:TYR:CE2	1:C:1127:GLU:HB2	2.47	0.50
1:C:1174:HIS:CD2	1:C:1208:GLY:HA3	2.47	0.50
1:E:1252:ILE:HG23	4:E:1501:HOH:O	2.10	0.50
1:A:1279:ILE:CD1	1:A:1291:VAL:HG23	2.41	0.49
1:D:1109:MET:HG3	1:D:1119:LEU:CD2	2.42	0.49
1:C:1141:LEU:O	1:C:1141:LEU:HD12	2.13	0.49
1:C:1202:ILE:HB	1:C:1212:LEU:HB2	1.94	0.49
1:A:1271:LEU:HD21	1:B:1233:THR:HB	1.95	0.49
1:F:1221:ASN:ND2	1:F:1257:LYS:HB2	2.27	0.49
1:B:1141:LEU:C	1:B:1141:LEU:HD12	2.38	0.49
1:A:1207:THR:HG21	4:A:1524:HOH:O	2.13	0.49
1:D:1306:THR:HG22	1:D:1307:VAL:HG23	1.95	0.49
1:D:1102:SER:CA	1:D:1109:MET:HE2	2.41	0.49
1:A:1178:GLU:OE1	1:A:1178:GLU:N	2.45	0.49
1:D:1164:TRP:CZ3	1:D:1172:MET:HB2	2.47	0.49
1:C:1099:CYS:HA	1:C:1109:MET:O	2.13	0.49
1:C:1142:GLU:HB2	4:C:1509:HOH:O	2.12	0.49
1:F:1357:LEU:HD12	1:F:1357:LEU:C	2.37	0.49
1:E:1207:THR:HG23	1:E:1209:ASN:H	1.78	0.48
1:A:1176:PHE:CE1	1:A:1192:VAL:HG21	2.48	0.48
1:A:1279:ILE:N	1:A:1279:ILE:HD12	2.28	0.48
1:C:1202:ILE:HG23	4:C:1505:HOH:O	2.13	0.48
1:A:1141:LEU:HD12	1:A:1141:LEU:C	2.38	0.48
1:D:1148:SER:HB2	1:D:1167:LYS:NZ	2.29	0.48
1:C:1277:THR:OG1	1:C:1278:GLU:OE2	2.27	0.48
1:E:1141:LEU:C	1:E:1141:LEU:HD12	2.38	0.48
1:A:1136:SER:HB3	1:A:1156:TRP:CD2	2.47	0.48
1:A:1312:MET:HE2	4:A:1512:HOH:O	2.14	0.48
1:B:1349:ASP:OD2	1:B:1351:LYS:HD3	2.13	0.48
1:D:1327:LYS:O	1:D:1328:SER:HB2	2.13	0.48
1:D:1099:CYS:HA	1:D:1109:MET:O	2.14	0.48
1:A:1344:PRO:HB3	4:A:1516:HOH:O	2.13	0.48
1:C:1233:THR:HB	1:E:1271:LEU:HD21	1.96	0.48
1:E:1204:ASP:O	1:E:1208:GLY:HA2	2.14	0.48
1:F:1148:SER:CB	1:F:1167:LYS:HD3	2.44	0.48
1:B:1371:ASN:HA	1:B:1382:THR:HG22	1.94	0.47
1:C:1141:LEU:HD12	1:C:1141:LEU:C	2.39	0.47
1:F:1116:GLN:OE1	1:F:1132:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:ILE:CD1	1:A:1228:ALA:HB1	2.45	0.47
1:C:1115:GLY:HA2	1:C:1138:ILE:HG13	1.95	0.47
1:C:1198:ASP:OD1	1:C:1222:ASN:HA	2.14	0.47
1:A:1279:ILE:HD13	1:A:1291:VAL:HG23	1.97	0.47
1:B:1243:LEU:HD23	1:B:1252:ILE:HD11	1.96	0.47
1:F:1162:ALA:HB1	1:F:1172:MET:HE2	1.95	0.47
1:C:1186:LYS:HA	1:C:1186:LYS:CE	2.36	0.47
1:F:1237:VAL:HG23	1:F:1246:VAL:CG2	2.45	0.47
1:B:1115:GLY:HA2	1:B:1138:ILE:HG13	1.96	0.47
1:E:1120:TYR:CE2	1:E:1127:GLU:HB2	2.50	0.47
1:B:1312:MET:HE2	4:B:1414:HOH:O	2.15	0.47
1:C:1109:MET:CE	1:C:1143:PRO:HG3	2.45	0.47
1:C:1136:SER:HB3	1:C:1156:TRP:CZ2	2.49	0.47
1:C:1203:TYR:CE1	1:C:1210:LYS:CG	2.95	0.47
1:D:1102:SER:CB	1:D:1109:MET:HE2	2.45	0.47
1:D:1233:THR:OG1	4:D:1502:HOH:O	2.20	0.47
1:F:1120:TYR:CE2	1:F:1127:GLU:HB2	2.49	0.47
1:B:1204:ASP:O	1:B:1208:GLY:HA2	2.14	0.47
1:D:1312:MET:HE2	4:D:1514:HOH:O	2.15	0.47
1:F:1281:ASP:HB2	1:F:1288:LEU:HD11	1.96	0.46
1:A:1204:ASP:HB2	1:A:1211:LEU:CD1	2.32	0.46
1:A:1225:ARG:CG	1:A:1261:ASN:HB3	2.45	0.46
1:B:1204:ASP:HB2	1:B:1211:LEU:CD1	2.37	0.46
1:F:1214:LEU:HD22	1:F:1244:TRP:CE3	2.50	0.46
1:A:1148:SER:C	1:A:1149:LEU:HD22	2.40	0.46
1:B:1081:ARG:NH2	1:B:1388:GLU:OE1	2.48	0.46
1:A:1204:ASP:O	1:A:1208:GLY:HA2	2.15	0.46
1:C:1144:SER:HB3	1:C:1149:LEU:HB2	1.97	0.46
1:C:1204:ASP:O	1:C:1208:GLY:HA2	2.15	0.46
1:E:1336:THR:O	1:E:1345:ILE:HB	2.16	0.46
1:E:1104:ARG:O	1:E:1104:ARG:HG3	2.15	0.46
1:E:1181:TYR:CE2	1:E:1183:GLU:HG3	2.51	0.46
1:A:1113:CYS:HA	1:A:1137:ALA:CB	2.46	0.46
1:D:1355:PHE:O	1:D:1356:ASP:HB2	2.15	0.46
1:E:1115:GLY:C	1:E:1138:ILE:HD11	2.40	0.46
1:F:1112:THR:H	1:F:1138:ILE:HD12	1.79	0.46
1:C:1372:GLN:HB2	1:C:1381:ASP:O	2.16	0.46
1:D:1201:HIS:HB2	1:D:1203:TYR:HE1	1.80	0.46
1:D:1206:GLN:HA	1:D:1206:GLN:NE2	2.31	0.46
1:D:1371:ASN:HA	1:D:1382:THR:HG22	1.98	0.46
1:A:1158:GLN:OE1	1:A:1177:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1201:HIS:CB	1:D:1203:TYR:CE1	2.99	0.46
1:E:1252:ILE:HG12	4:E:1501:HOH:O	2.14	0.46
1:A:1271:LEU:HD11	1:B:1233:THR:HB	1.98	0.46
1:C:1190:ASP:OD1	1:C:1191:ARG:HG3	2.15	0.46
1:C:1259:ASN:HD21	1:C:1262:ILE:N	2.10	0.46
1:C:1372:GLN:NE2	1:C:1381:ASP:OD2	2.49	0.46
1:E:1204:ASP:OD1	1:E:1206:GLN:N	2.49	0.46
1:F:1081:ARG:HE	1:F:1081:ARG:HB3	1.49	0.46
1:C:1357:LEU:C	1:C:1357:LEU:HD12	2.41	0.46
1:F:1279:ILE:N	1:F:1279:ILE:HD12	2.31	0.46
1:F:1371:ASN:CA	1:F:1382:THR:HG22	2.45	0.46
1:B:1116:GLN:OE1	1:B:1132:ASN:ND2	2.49	0.45
1:A:1097:THR:O	1:A:1355:PHE:HB3	2.16	0.45
1:D:1109:MET:HE1	1:D:1143:PRO:HB3	1.98	0.45
1:D:1204:ASP:HB2	1:D:1211:LEU:CD1	2.38	0.45
1:A:1330:PHE:HB2	1:A:1354:ILE:O	2.16	0.45
1:C:1162:ALA:HB1	1:C:1172:MET:HE2	1.99	0.45
1:D:1336:THR:O	1:D:1345:ILE:HB	2.17	0.45
1:B:1133:CYS:HA	1:B:1164:TRP:CH2	2.51	0.45
1:C:1101:PHE:HA	1:C:1108:LEU:HD23	1.99	0.45
1:C:1164:TRP:CH2	1:C:1172:MET:HE3	2.52	0.45
1:C:1358:CYS:O	1:C:1366:LEU:HD12	2.17	0.45
1:D:1279:ILE:HD12	1:D:1279:ILE:N	2.32	0.45
1:A:1212:LEU:HD11	1:A:1249:ALA:HB2	1.97	0.45
1:B:1142:GLU:HB2	4:B:1403:HOH:O	2.17	0.45
1:C:1203:TYR:HE1	1:C:1210:LYS:CG	2.30	0.45
1:D:1193:ILE:HG23	1:D:1193:ILE:O	2.16	0.45
1:D:1372:GLN:NE2	1:D:1383:VAL:HG11	2.31	0.45
1:E:1132:ASN:N	1:E:1132:ASN:HD22	2.14	0.45
1:F:1163:LEU:HD23	1:F:1163:LEU:C	2.41	0.45
1:F:1309:TYR:CD2	1:F:1336:THR:HG22	2.52	0.45
1:A:1203:TYR:HE1	1:A:1210:LYS:HD3	1.81	0.45
1:D:1148:SER:HB2	1:D:1167:LYS:HZ2	1.82	0.45
1:D:1343:LYS:HG3	1:D:1344:PRO:HD2	1.99	0.45
1:E:1193:ILE:HG23	1:E:1193:ILE:O	2.17	0.45
1:F:1274:ILE:N	1:F:1274:ILE:HD12	2.31	0.45
1:C:1237:VAL:HG23	1:C:1246:VAL:HG22	1.98	0.45
1:A:1120:TYR:CE2	1:A:1127:GLU:HB2	2.52	0.45
1:A:1181:TYR:CE2	1:A:1183:GLU:HG3	2.51	0.45
1:B:1210:LYS:NZ	4:B:1406:HOH:O	2.49	0.45
1:C:1380:MET:HG2	1:C:1382:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1357:LEU:HB2	1:D:1368:VAL:HG22	1.97	0.44
1:A:1151:LEU:HG	1:A:1184:PHE:CZ	2.53	0.44
1:A:1259:ASN:ND2	1:A:1261:ASN:H	2.14	0.44
1:C:1380:MET:HE1	4:C:1544:HOH:O	2.16	0.44
1:F:1181:TYR:CE2	1:F:1183:GLU:HG3	2.52	0.44
1:B:1292:PRO:CG	1:C:1126:GLN:HG2	2.45	0.44
1:E:1102:SER:CA	1:E:1109:MET:HE3	2.38	0.44
1:A:1233:THR:CG2	1:B:1271:LEU:HD21	2.48	0.44
1:B:1279:ILE:HD13	1:B:1291:VAL:HG23	1.98	0.44
1:C:1159:PRO:HG3	1:C:1175:SER:HB2	1.99	0.44
1:D:1117:LEU:CD1	1:D:1150:LEU:HD21	2.43	0.44
1:D:1181:TYR:CE2	1:D:1183:GLU:HG3	2.53	0.44
1:F:1134:HIS:CG	1:F:1154:ALA:HB2	2.52	0.44
1:F:1163:LEU:HD22	1:F:1173:LYS:HB2	1.99	0.44
1:A:1355:PHE:CZ	1:A:1380:MET:HE1	2.53	0.44
1:E:1113:CYS:HA	1:E:1137:ALA:HB1	2.00	0.44
1:A:1142:GLU:HB2	4:A:1506:HOH:O	2.18	0.44
1:B:1149:LEU:HD13	1:B:1163:LEU:HD11	1.99	0.44
1:C:1149:LEU:HB3	1:C:1163:LEU:HD11	2.00	0.44
1:D:1380:MET:SD	1:D:1382:THR:HG23	2.58	0.44
1:B:1168:SER:OG	1:B:1169:VAL:N	2.37	0.44
1:D:1274:ILE:N	1:D:1274:ILE:HD12	2.33	0.44
1:F:1279:ILE:HD13	1:F:1291:VAL:HG23	1.99	0.44
1:A:1204:ASP:OD1	1:A:1206:GLN:N	2.51	0.44
1:A:1281:ASP:HB2	1:A:1288:LEU:HD11	2.00	0.44
1:C:1193:ILE:CD1	1:C:1228:ALA:HB1	2.46	0.44
1:A:1365:TYR:HB3	1:A:1386:LEU:CD1	2.44	0.43
1:D:1358:CYS:O	1:D:1366:LEU:HD12	2.18	0.43
1:B:1162:ALA:CB	1:B:1172:MET:HE2	2.48	0.43
1:B:1193:ILE:HG23	1:B:1193:ILE:O	2.18	0.43
1:F:1155:THR:HG22	1:F:1156:TRP:CD1	2.53	0.43
1:F:1193:ILE:O	1:F:1193:ILE:HG23	2.18	0.43
1:A:1109:MET:HE1	1:A:1150:LEU:HD13	2.00	0.43
1:C:1109:MET:HG3	1:C:1119:LEU:CD2	2.47	0.43
1:C:1193:ILE:HG23	1:C:1193:ILE:O	2.18	0.43
1:E:1279:ILE:HD13	1:E:1291:VAL:HG23	1.99	0.43
1:B:1199:ILE:HG12	1:B:1215:PHE:HB2	2.01	0.43
1:D:1177:THR:OG1	1:D:1178:GLU:HG3	2.19	0.43
1:D:1206:GLN:HA	1:D:1206:GLN:HE21	1.84	0.43
1:F:1183:GLU:HG2	4:F:1502:HOH:O	2.17	0.43
1:F:1238:LEU:HD12	1:F:1238:LEU:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1177:THR:HB	1:A:1178:GLU:CD	2.43	0.43
1:A:1294:LEU:O	1:A:1297:CYS:HB2	2.19	0.43
1:C:1136:SER:HB3	1:C:1156:TRP:CH2	2.54	0.43
1:C:1243:LEU:CD2	1:C:1252:ILE:HD11	2.48	0.43
1:F:1167:LYS:O	1:F:1167:LYS:HG3	2.17	0.43
1:D:1365:TYR:HB3	1:D:1386:LEU:CD1	2.44	0.43
1:E:1098:CYS:O	1:E:1110:LEU:HA	2.19	0.43
1:C:1279:ILE:HG12	1:C:1342:TYR:CZ	2.53	0.43
1:E:1116:GLN:OE1	1:E:1132:ASN:ND2	2.51	0.43
1:C:1174:HIS:HD2	1:C:1208:GLY:HA3	1.84	0.43
1:B:1351:LYS:O	1:B:1352:ARG:HG3	2.18	0.43
1:E:1178:GLU:O	1:E:1196:LYS:HB2	2.19	0.43
1:B:1119:LEU:HB2	4:B:1428:HOH:O	2.19	0.43
1:B:1233:THR:O	1:B:1234:ASP:HB2	2.19	0.43
1:C:1193:ILE:HB	4:C:1505:HOH:O	2.19	0.42
1:D:1118:LYS:NZ	1:D:1127:GLU:OE2	2.48	0.42
1:D:1271:LEU:HD11	1:F:1233:THR:HG22	2.01	0.42
1:D:1289:HIS:HA	1:E:1087:ARG:HD3	2.01	0.42
1:A:1135:ASN:HB2	1:A:1156:TRP:CH2	2.55	0.42
1:D:1142:GLU:HB2	4:D:1503:HOH:O	2.18	0.42
1:E:1303:HIS:CE1	1:E:1361:THR:HA	2.55	0.42
1:F:1167:LYS:O	1:F:1168:SER:OG	2.26	0.42
1:F:1218:ASP:C	1:F:1219:LEU:HD22	2.44	0.42
1:A:1083:ILE:CD1	1:A:1388:GLU:HB2	2.48	0.42
1:C:1306:THR:HG22	1:C:1307:VAL:HG23	2.01	0.42
1:E:1351:LYS:O	1:E:1352:ARG:HG3	2.20	0.42
1:F:1224:LYS:HG2	4:F:1501:HOH:O	2.19	0.42
1:A:1225:ARG:HG2	1:A:1261:ASN:HB3	2.01	0.42
1:A:1233:THR:HB	1:B:1271:LEU:HD11	2.00	0.42
1:B:1372:GLN:HB2	1:B:1381:ASP:O	2.19	0.42
1:D:1219:LEU:N	1:D:1219:LEU:HD22	2.35	0.42
1:D:1233:THR:CB	1:F:1271:LEU:HD11	2.49	0.42
1:E:1306:THR:HG22	1:E:1307:VAL:HG23	2.01	0.42
1:A:1119:LEU:HB2	1:A:1129:ALA:HB3	2.01	0.42
1:B:1196:LYS:O	1:B:1196:LYS:HG3	2.19	0.42
1:F:1357:LEU:HB2	1:F:1368:VAL:HG22	2.02	0.42
1:A:1081:ARG:NH1	1:A:1388:GLU:OE1	2.52	0.42
1:A:1159:PRO:CG	1:A:1175:SER:HB2	2.50	0.42
1:D:1180:HIS:HB3	4:D:1511:HOH:O	2.19	0.42
1:A:1164:TRP:CH2	1:A:1172:MET:HE3	2.55	0.42
1:A:1207:THR:HG23	1:A:1209:ASN:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1309:TYR:CD2	1:A:1336:THR:HG22	2.55	0.42
1:D:1096:PHE:CE1	1:D:1110:LEU:HD22	2.55	0.42
1:D:1214:LEU:HD22	1:D:1244:TRP:CE3	2.55	0.42
1:A:1185:SER:O	1:A:1189:GLN:HG2	2.19	0.42
1:A:1233:THR:CB	1:B:1271:LEU:HD11	2.49	0.42
1:A:1193:ILE:O	1:A:1193:ILE:HG23	2.20	0.42
1:E:1237:VAL:HG23	1:E:1246:VAL:CG2	2.50	0.42
1:E:1274:ILE:HD12	1:E:1274:ILE:N	2.34	0.42
1:A:1236:LEU:HD13	1:A:1243:LEU:HD11	2.01	0.42
1:A:1357:LEU:HB2	1:A:1368:VAL:HG22	2.02	0.42
1:B:1110:LEU:N	1:B:1110:LEU:HD12	2.35	0.42
1:B:1358:CYS:O	1:B:1366:LEU:HD12	2.20	0.42
1:C:1096:PHE:HB2	1:C:1382:THR:OG1	2.20	0.42
1:C:1153:SER:OG	1:C:1182:VAL:HG22	2.20	0.42
1:E:1259:ASN:ND2	1:E:1261:ASN:H	2.17	0.42
1:F:1097:THR:O	1:F:1355:PHE:HB3	2.20	0.42
1:B:1178:GLU:O	1:B:1178:GLU:HG3	2.19	0.41
1:F:1204:ASP:OD1	1:F:1207:THR:N	2.53	0.41
1:F:1357:LEU:HD13	1:F:1366:LEU:CD1	2.46	0.41
1:A:1372:GLN:HB2	1:A:1381:ASP:O	2.20	0.41
1:C:1136:SER:HB3	1:C:1156:TRP:CE2	2.55	0.41
1:C:1167:LYS:O	1:C:1169:VAL:N	2.53	0.41
1:D:1294:LEU:O	1:D:1297:CYS:HB2	2.19	0.41
1:B:1173:LYS:O	1:B:1174:HIS:ND1	2.54	0.41
1:F:1159:PRO:HG3	1:F:1175:SER:HB2	2.02	0.41
1:F:1336:THR:O	1:F:1345:ILE:HB	2.21	0.41
1:B:1109:MET:HG2	1:B:1119:LEU:HD21	2.01	0.41
1:B:1173:LYS:C	1:B:1174:HIS:ND1	2.79	0.41
1:E:1142:GLU:HB2	4:E:1502:HOH:O	2.20	0.41
1:E:1238:LEU:HD23	1:E:1238:LEU:HA	1.78	0.41
1:B:1327:LYS:HD2	1:B:1327:LYS:N	2.36	0.41
1:D:1181:TYR:OH	1:D:1183:GLU:OE2	2.31	0.41
1:B:1100:ALA:HA	1:B:1358:CYS:SG	2.60	0.41
1:B:1144:SER:HB3	1:B:1149:LEU:HB2	2.02	0.41
1:B:1212:LEU:HD11	1:B:1249:ALA:HB2	2.03	0.41
1:B:1267:HIS:CG	1:B:1268:PRO:HD2	2.56	0.41
1:E:1109:MET:HG2	1:E:1119:LEU:HD12	2.01	0.41
1:E:1117:LEU:HD23	1:E:1131:TYR:HD2	1.85	0.41
1:E:1145:ARG:HB2	1:E:1189:GLN:NE2	2.36	0.41
1:A:1264:GLY:HA3	1:A:1275:ILE:HG12	2.03	0.41
1:B:1181:TYR:CE2	1:B:1183:GLU:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1120:TYR:CE2	1:D:1127:GLU:HB2	2.55	0.41
1:D:1162:ALA:CB	1:D:1172:MET:HE2	2.49	0.41
1:D:1271:LEU:HD21	1:F:1233:THR:HB	2.03	0.41
1:E:1213:THR:O	1:E:1213:THR:CG2	2.69	0.41
1:F:1097:THR:HG23	1:F:1380:MET:HE1	2.01	0.41
1:F:1186:LYS:HE3	1:F:1230:PHE:O	2.21	0.41
1:B:1109:MET:C	1:B:1110:LEU:HD12	2.46	0.41
1:B:1256:ASP:HB2	1:B:1258:PHE:CE2	2.56	0.40
1:B:1317:ASP:OD1	1:B:1318:GLU:N	2.54	0.40
1:E:1173:LYS:C	1:E:1174:HIS:ND1	2.79	0.40
1:F:1212:LEU:HD22	1:F:1214:LEU:HG	2.02	0.40
1:B:1160:LEU:HD12	1:B:1178:GLU:CA	2.48	0.40
1:C:1151:LEU:HG	1:C:1184:PHE:CZ	2.56	0.40
1:C:1362:LYS:NZ	4:C:1513:HOH:O	2.50	0.40
1:D:1164:TRP:CE3	1:D:1172:MET:HB2	2.57	0.40
1:D:1281:ASP:HB2	1:D:1288:LEU:HG	2.03	0.40
1:D:1365:TYR:CB	1:D:1386:LEU:HD11	2.46	0.40
1:E:1116:GLN:N	1:E:1138:ILE:HD11	2.36	0.40
1:E:1173:LYS:O	1:E:1174:HIS:ND1	2.54	0.40
1:F:1213:THR:O	1:F:1213:THR:HG23	2.20	0.40
1:A:1365:TYR:CB	1:A:1386:LEU:HD11	2.47	0.40
1:E:1242:VAL:HG12	1:E:1244:TRP:CD1	2.56	0.40
1:B:1207:THR:HG23	1:B:1209:ASN:H	1.86	0.40
1:B:1214:LEU:HD23	1:B:1244:TRP:CB	2.52	0.40
1:C:1198:ASP:HB3	4:C:1517:HOH:O	2.21	0.40
1:D:1202:ILE:HB	1:D:1212:LEU:HB2	2.02	0.40
1:D:1252:ILE:HG12	4:D:1501:HOH:O	2.20	0.40
1:E:1107:PHE:CZ	1:E:1128:GLU:HG3	2.56	0.40
1:F:1267:HIS:HE1	1:F:1339:ALA:O	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	289/314 (92%)	269 (93%)	16 (6%)	4 (1%)	9	11
1	B	293/314 (93%)	271 (92%)	19 (6%)	3 (1%)	12	17
1	C	289/314 (92%)	271 (94%)	15 (5%)	3 (1%)	12	17
1	D	290/314 (92%)	271 (93%)	15 (5%)	4 (1%)	9	11
1	E	289/314 (92%)	268 (93%)	18 (6%)	3 (1%)	12	17
1	F	289/314 (92%)	270 (93%)	16 (6%)	3 (1%)	12	17
All	All	1739/1884 (92%)	1620 (93%)	99 (6%)	20 (1%)	10	13

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1187	HIS
1	C	1187	HIS
1	D	1187	HIS
1	E	1187	HIS
1	F	1169	VAL
1	F	1187	HIS
1	A	1210	LYS
1	B	1168	SER
1	C	1168	SER
1	C	1206	GLN
1	D	1206	GLN
1	E	1168	SER
1	F	1168	SER
1	A	1168	SER
1	A	1206	GLN
1	B	1206	GLN
1	D	1168	SER
1	D	1328	SER
1	E	1206	GLN
1	A	1187	HIS

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	259/276 (94%)	259 (100%)	0	100	100
1	B	263/276 (95%)	261 (99%)	2 (1%)	73	84
1	C	259/276 (94%)	258 (100%)	1 (0%)	84	90
1	D	260/276 (94%)	259 (100%)	1 (0%)	84	90
1	E	259/276 (94%)	258 (100%)	1 (0%)	84	90
1	F	259/276 (94%)	258 (100%)	1 (0%)	84	90
All	All	1559/1656 (94%)	1553 (100%)	6 (0%)	84	90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1212	LEU
1	B	1213	THR
1	C	1108	LEU
1	D	1117	LEU
1	E	1169	VAL
1	F	1306	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1187	HIS
1	A	1216	ASN
1	A	1222	ASN
1	A	1250	GLN
1	A	1253	HIS
1	A	1259	ASN
1	A	1289	HIS
1	A	1338	ASN
1	B	1132	ASN
1	B	1187	HIS
1	B	1250	GLN
1	B	1286	HIS
1	B	1289	HIS
1	B	1338	ASN
1	C	1116	GLN
1	C	1216	ASN
1	C	1259	ASN
1	C	1289	HIS
1	D	1206	GLN

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Mol	Chain	Res	Type
1	D	1209	ASN
1	D	1250	GLN
1	D	1253	HIS
1	D	1372	GLN
1	E	1132	ASN
1	E	1180	HIS
1	E	1187	HIS
1	E	1209	ASN
1	E	1250	GLN
1	E	1259	ASN
1	E	1289	HIS
1	E	1303	HIS
1	E	1353	ASN
1	F	1116	GLN
1	F	1132	ASN
1	F	1187	HIS
1	F	1221	ASN
1	F	1250	GLN
1	F	1267	HIS
1	F	1303	HIS
1	F	1314	GLN
1	F	1338	ASN
1	F	1372	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1C25	D	1401	-	97,99,99	0.82	1 (1%)	120,130,130	1.09	9 (7%)
2	A1C24	E	1401	-	31,31,31	0.81	0	42,44,44	1.34	5 (11%)
2	A1C24	F	1401	-	31,31,31	0.82	0	42,44,44	1.31	6 (14%)
2	A1C24	A	1401	-	31,31,31	0.81	0	42,44,44	1.32	6 (14%)
2	A1C24	C	1401	-	31,31,31	0.82	0	42,44,44	1.33	6 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1C25	D	1401	-	-	17/81/81/81	0/6/6/6
2	A1C24	E	1401	-	-	5/20/20/20	0/3/3/3
2	A1C24	F	1401	-	-	2/20/20/20	0/3/3/3
2	A1C24	A	1401	-	-	1/20/20/20	0/3/3/3
2	A1C24	C	1401	-	-	3/20/20/20	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1401	A1C25	C57-C63	2.03	1.41	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	A1C24	C06-C07-C03	3.63	109.09	106.93
2	F	1401	A1C24	C06-C07-C03	3.55	109.04	106.93
2	C	1401	A1C24	C06-C07-C03	3.43	108.97	106.93
2	E	1401	A1C24	C06-C07-C03	3.34	108.92	106.93
2	F	1401	A1C24	C12-C13-C08	-3.14	120.01	123.48
3	D	1401	A1C25	C92-C93-C87	-3.13	120.02	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	A1C24	C12-C13-C08	-3.09	120.06	123.48
2	E	1401	A1C24	C12-C13-C08	-3.06	120.10	123.48
2	C	1401	A1C24	C12-C13-C08	-3.06	120.10	123.48
2	A	1401	A1C24	C11-C12-C13	2.95	120.03	117.54
2	F	1401	A1C24	C11-C12-C13	2.93	120.02	117.54
3	D	1401	A1C25	C60-C62-C63	2.93	120.01	117.54
3	D	1401	A1C25	C88-C87-C93	2.93	119.95	116.70
2	E	1401	A1C24	C11-C12-C13	2.92	120.00	117.54
2	C	1401	A1C24	C11-C12-C13	2.90	119.99	117.54
3	D	1401	A1C25	C13-C04-N03	2.87	114.15	108.94
2	E	1401	A1C24	C18-C17-N16	2.87	114.14	108.94
3	D	1401	A1C25	C90-C92-C93	2.81	119.91	117.54
2	F	1401	A1C24	C09-C08-C13	2.78	119.79	116.70
2	A	1401	A1C24	C09-C08-C13	2.78	119.79	116.70
2	E	1401	A1C24	C09-C08-C13	2.75	119.75	116.70
2	C	1401	A1C24	C09-C08-C13	2.73	119.73	116.70
3	D	1401	A1C25	C62-C63-C57	-2.73	120.47	123.48
3	D	1401	A1C25	C77-C68-N67	2.69	113.81	108.94
2	C	1401	A1C24	C18-C17-N16	2.56	113.57	108.94
2	A	1401	A1C24	C18-C17-N16	2.38	113.26	108.94
2	F	1401	A1C24	C18-C17-N16	2.38	113.26	108.94
3	D	1401	A1C25	C21-C20-N19	-2.14	118.31	124.48
2	A	1401	A1C24	C17-N16-C02	2.12	125.17	122.21
2	C	1401	A1C24	C17-N16-C02	2.10	125.15	122.21
3	D	1401	A1C25	C25-N24-C23	2.03	125.39	122.46
2	F	1401	A1C24	C17-N16-C02	2.02	125.04	122.21

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1401	A1C24	N16-C17-C18-C19
2	E	1401	A1C24	N16-C17-C18-C19
3	D	1401	A1C25	O30-C31-C32-O33
3	D	1401	A1C25	O42-C43-C44-O45
3	D	1401	A1C25	C26-C25-N24-C23
3	D	1401	A1C25	C21-C22-C23-N24
2	E	1401	A1C24	C17-C18-C19-N20
3	D	1401	A1C25	C46-C47-O48-C49
3	D	1401	A1C25	C53-C54-C55-N83
3	D	1401	A1C25	C21-C22-C23-O85
3	D	1401	A1C25	O84-C52-C53-C54

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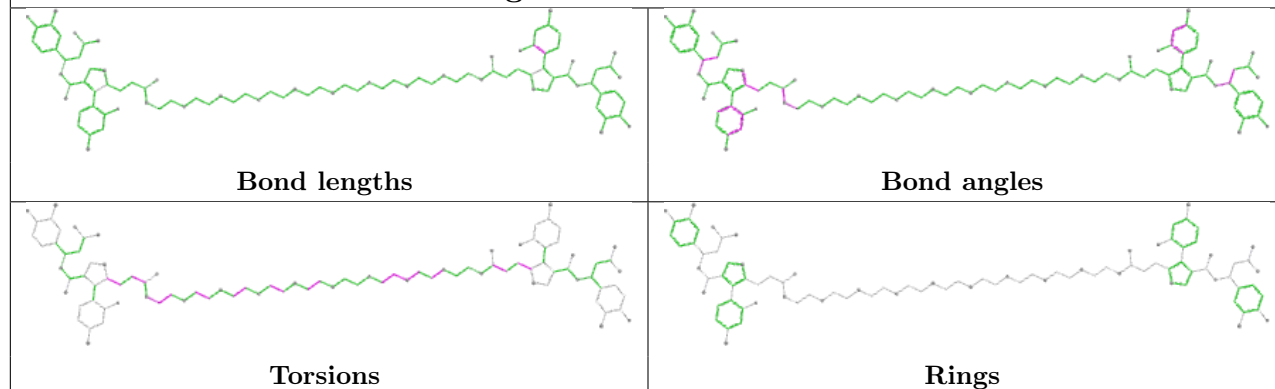
Mol	Chain	Res	Type	Atoms
2	E	1401	A1C24	C06-C07-C08-C09
2	F	1401	A1C24	C06-C07-C08-C09
3	D	1401	A1C25	N51-C52-C53-C54
3	D	1401	A1C25	C43-C44-O45-C46
2	E	1401	A1C24	C06-C07-C08-C13
2	F	1401	A1C24	C06-C07-C08-C13
2	E	1401	A1C24	C17-C18-C19-O21
3	D	1401	A1C25	N24-C25-C26-O27
3	D	1401	A1C25	O33-C34-C35-O36
3	D	1401	A1C25	O36-C37-C38-O39
3	D	1401	A1C25	O27-C28-C29-O30
3	D	1401	A1C25	C47-C46-O45-C44
3	D	1401	A1C25	C53-C54-C55-C56
2	C	1401	A1C24	C17-C18-C19-O21
3	D	1401	A1C25	N19-C20-C21-C22
2	A	1401	A1C24	C06-C07-C08-C13
2	C	1401	A1C24	C06-C07-C08-C13

There are no ring outliers.

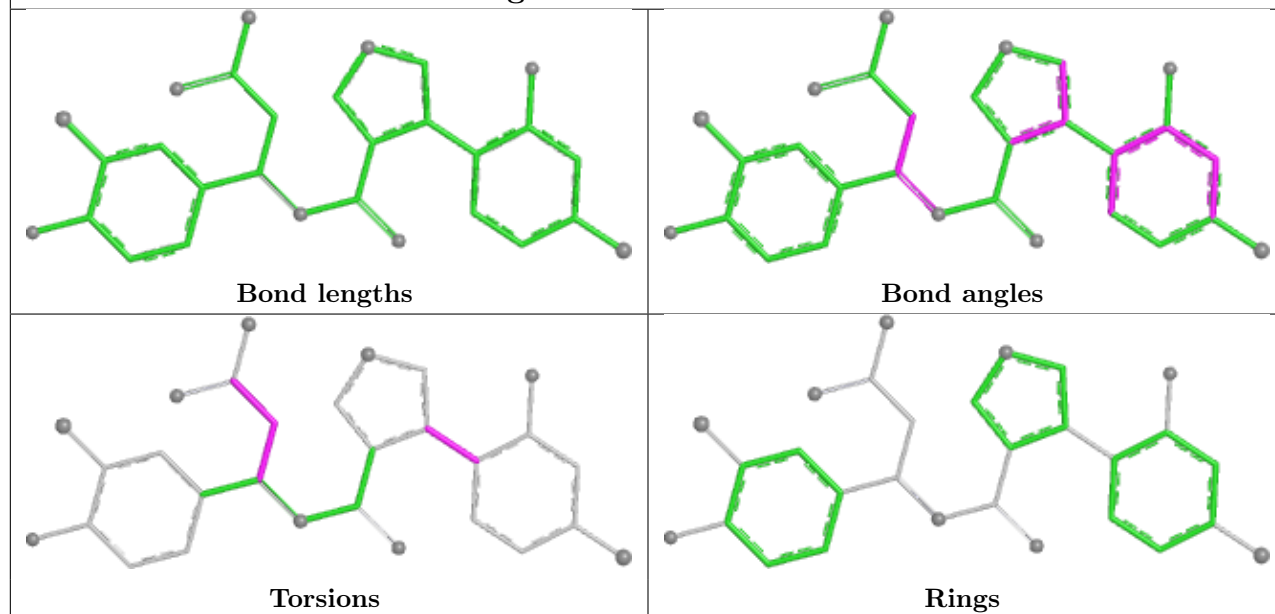
No monomer is involved in short contacts.

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.

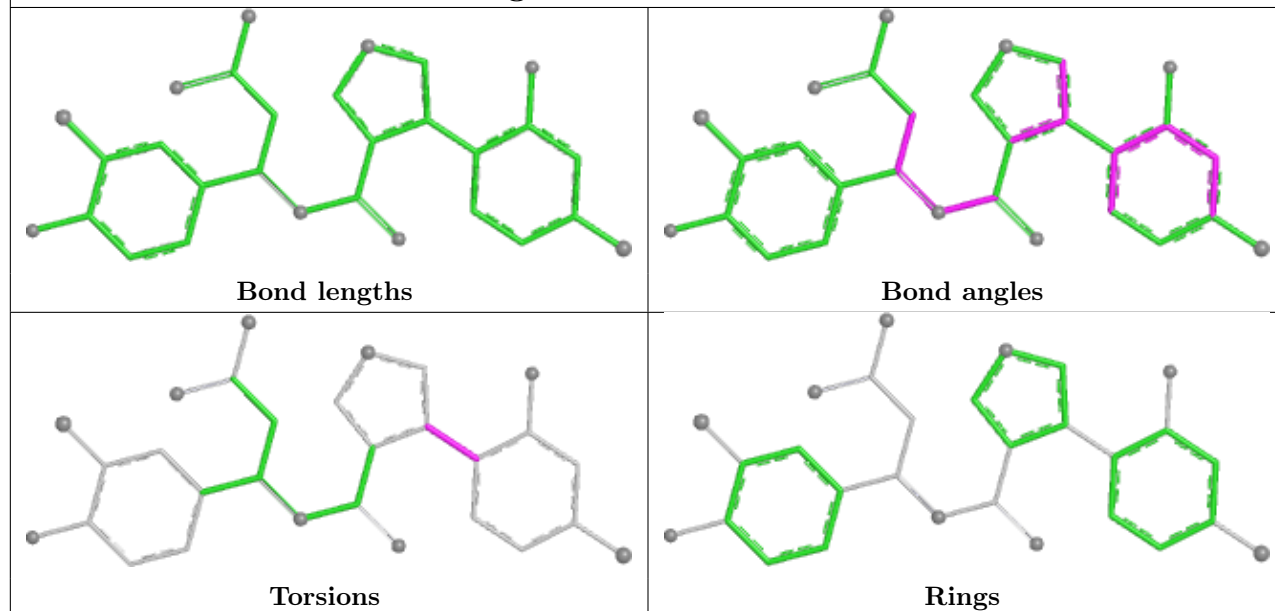
Ligand A1C25 D 1401

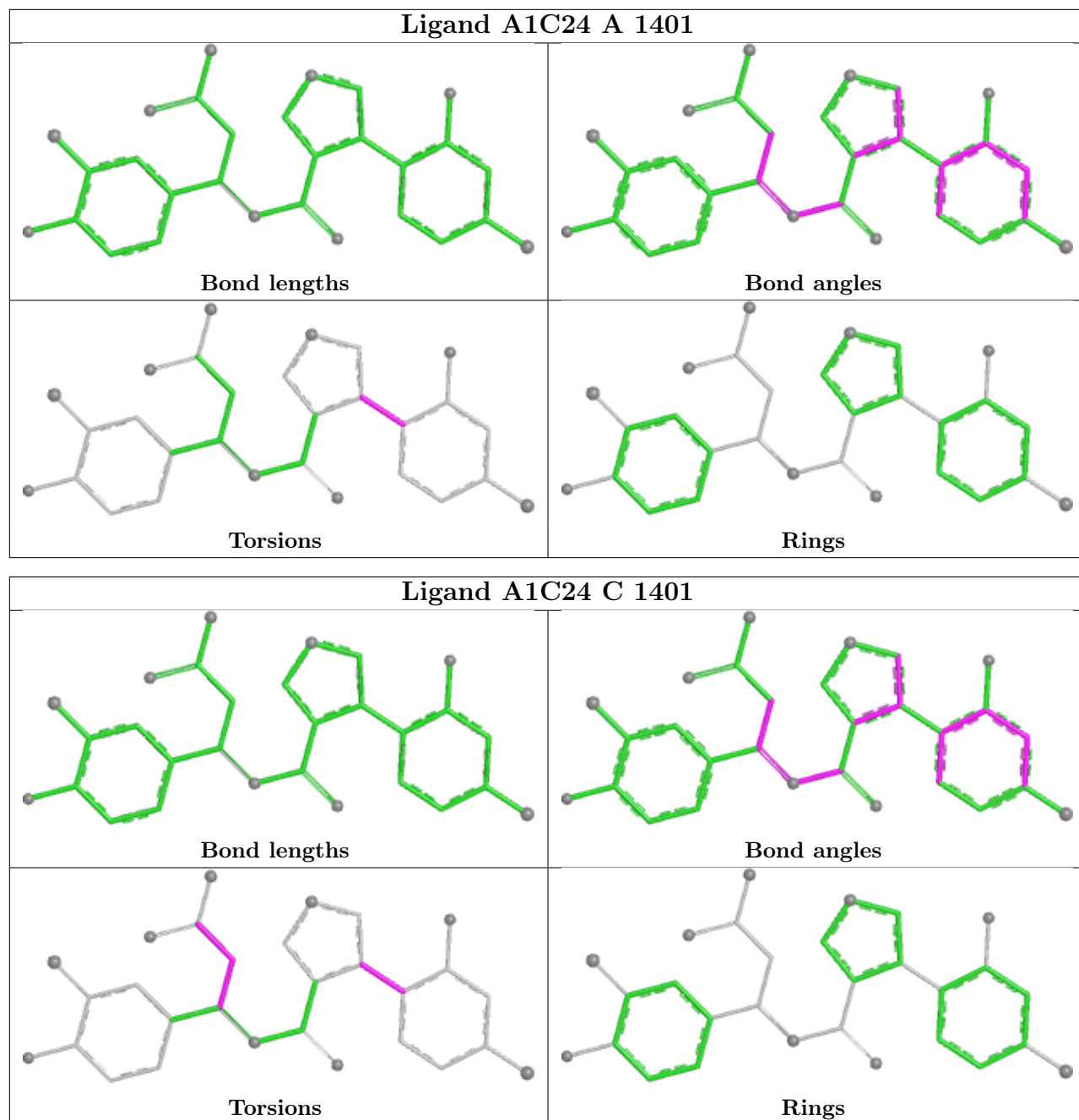


Ligand A1C24 E 1401



Ligand A1C24 F 1401





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	295/314 (93%)	-0.83	0 100 100	27, 43, 68, 84	0
1	B	299/314 (95%)	-0.83	0 100 100	29, 43, 69, 100	0
1	C	295/314 (93%)	-0.85	0 100 100	26, 42, 65, 86	0
1	D	296/314 (94%)	-0.86	0 100 100	27, 43, 66, 82	0
1	E	295/314 (93%)	-0.84	0 100 100	27, 42, 66, 83	0
1	F	295/314 (93%)	-0.85	0 100 100	29, 42, 66, 90	0
All	All	1775/1884 (94%)	-0.85	0 100 100	26, 43, 67, 100	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	A1C24	A	1401	29/29	0.98	0.05	30,40,50,55	0

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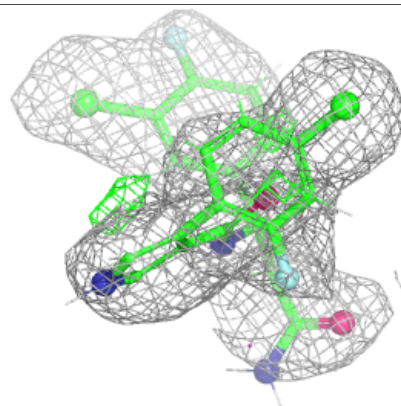
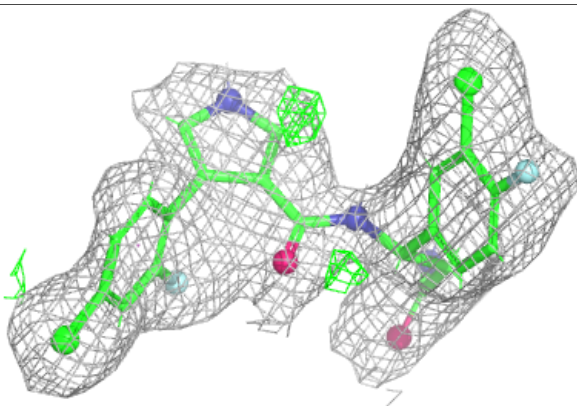
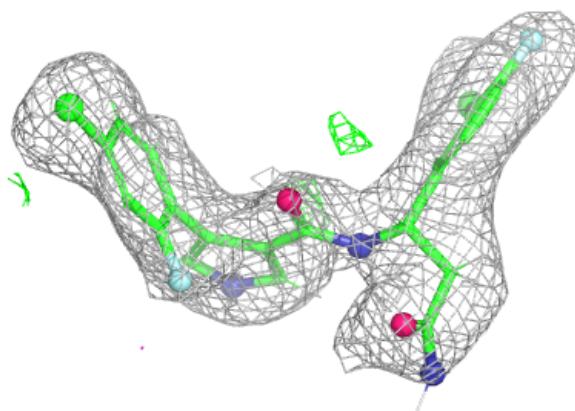
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1C24	C	1401	29/29	0.98	0.05	28,40,51,64	0
2	A1C24	E	1401	29/29	0.98	0.04	26,38,47,55	0
2	A1C24	F	1401	29/29	0.98	0.05	30,37,46,54	0
3	A1C25	D	1401	94/94	0.98	0.06	31,48,113,121	0

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.

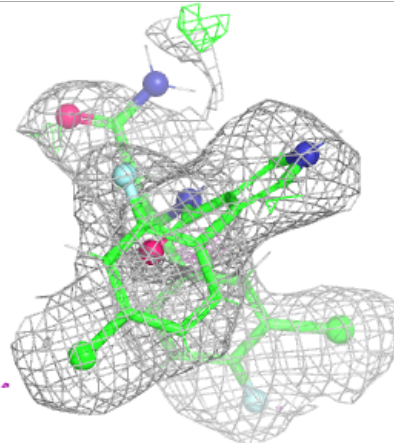
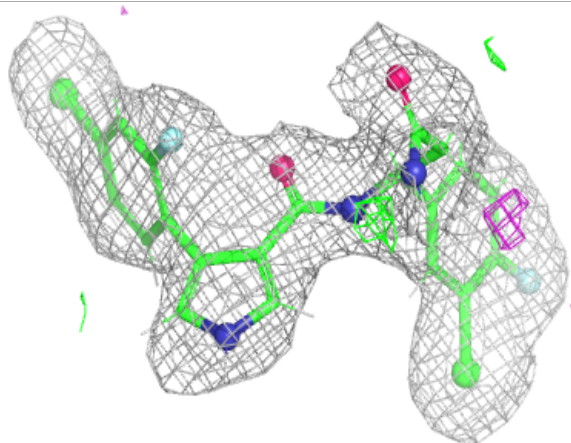
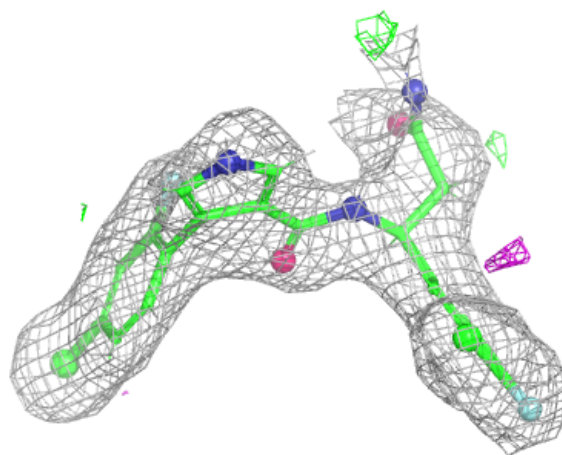
Electron density around A1C24 A 1401:

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



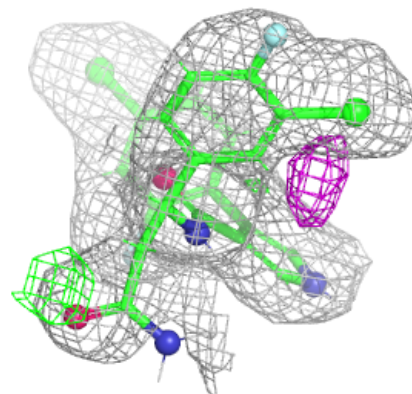
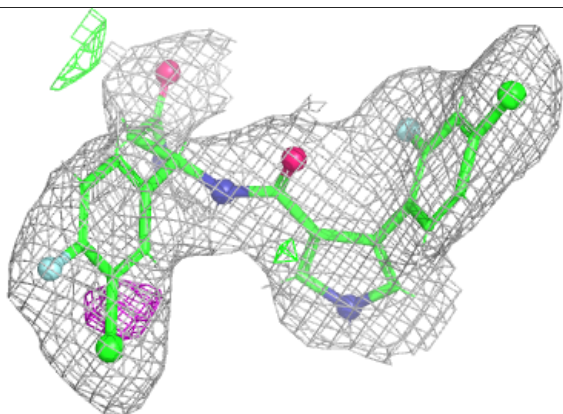
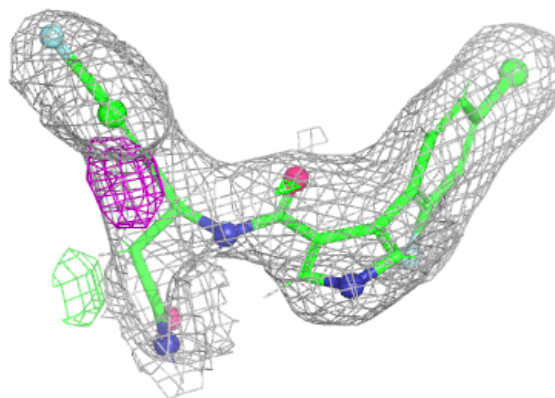
Electron density around A1C24 C 1401:

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

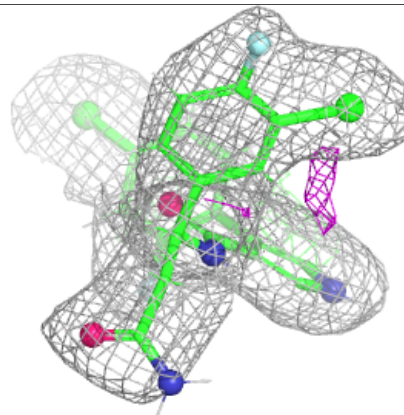
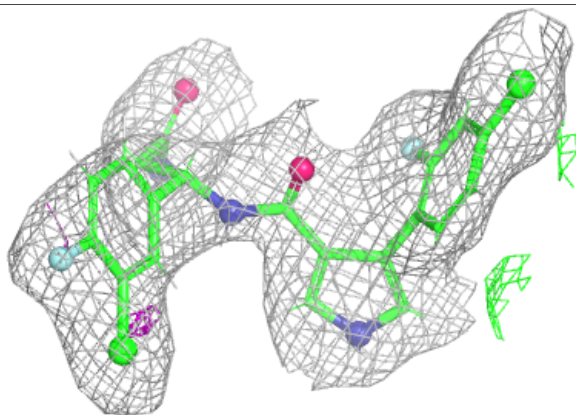
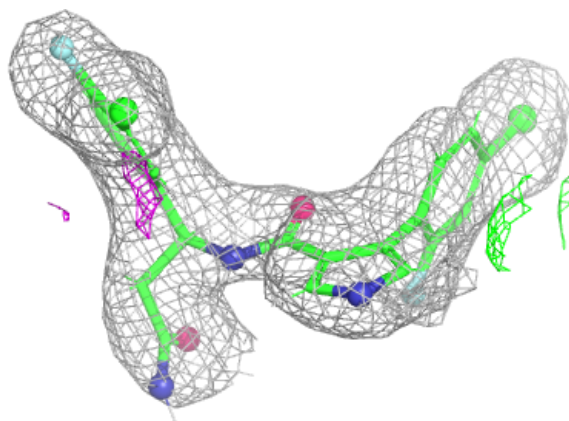


Electron density around A1C24 E 1401:

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

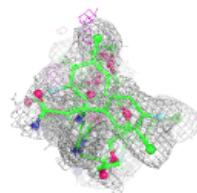
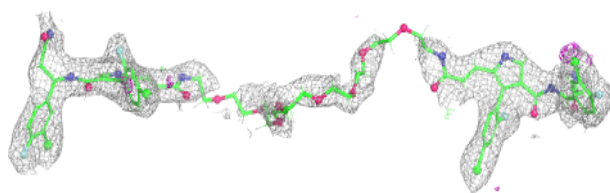
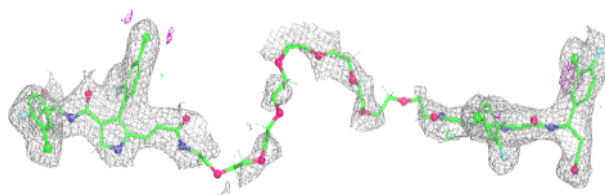
**Electron density around A1C24 F 1401:**

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



Electron density around A1C25 D 1401:

$2mF_o-DF_c$ (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.