



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2026 – 10:09 AM EDT

PDB ID : 9ZLG / pdb\_00009zlg  
Title : Crystal structure of DCAF1 in complex with SDIPTAC C9  
Authors : Mabanglo, M.F.; Srivastava, S.; Hoffer, L.; Ramnauth, J.; Vedadi, M.  
Deposited on : 2025-12-08  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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

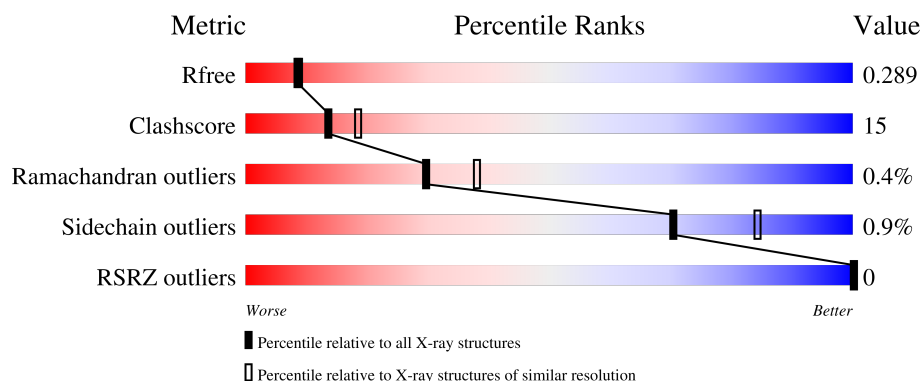
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	 69% 24% • 6%
1	B	314	 72% 20% • 6%
1	C	314	 73% 20% • 6%
1	D	314	 70% 23% • 6%
1	E	314	 65% 28% • 6%

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Mol	Chain	Length	Quality of chain
1	F	314	<div><div></div><div>64%29%6%</div></div>
1	G	314	<div><div></div><div>67%26%6%</div></div>
1	H	314	<div><div></div><div>69%25%6%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19582 atoms, of which 208 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	296	Total	C	N	O	S	0	0	1
			2349	1486	403	444	16			
1	B	295	Total	C	N	O	S	0	0	1
			2340	1480	401	443	16			
1	C	295	Total	C	N	O	S	0	0	1
			2340	1480	401	443	16			
1	D	295	Total	C	N	O	S	0	0	1
			2340	1480	401	443	16			
1	E	294	Total	C	N	O	S	0	0	1
			2332	1476	399	441	16			
1	F	295	Total	C	N	O	S	0	0	1
			2340	1480	401	443	16			
1	G	295	Total	C	N	O	S	0	0	1
			2340	1480	401	443	16			
1	H	294	Total	C	N	O	S	0	0	1
			2332	1476	399	441	16			

There are 16 discrepancies between the modelled and reference sequences:

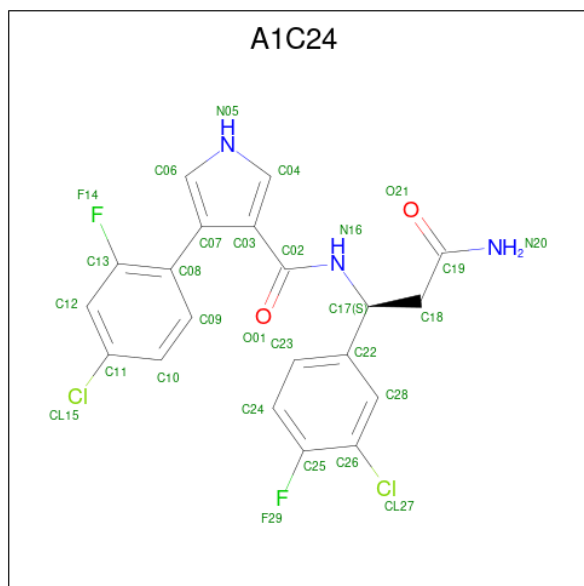
Chain	Residue	Modelled	Actual	Comment	Reference
A	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
A	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6
B	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
B	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6
C	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
C	1079	ALA	ARG	engineered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

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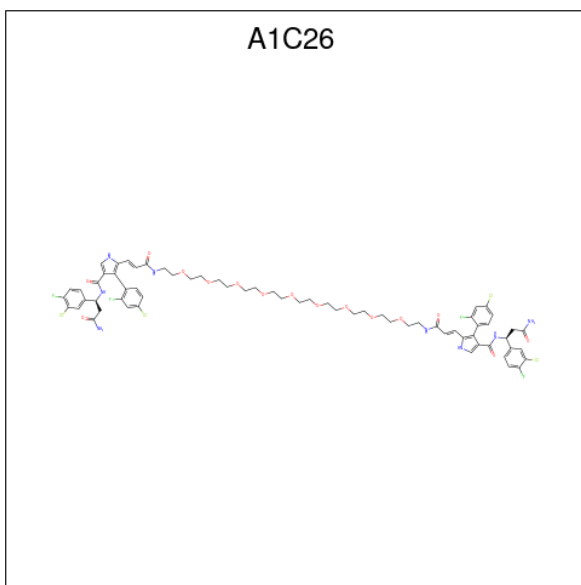
Chain	Residue	Modelled	Actual	Comment	Reference
G	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6
H	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
H	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6

- 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:  $C_{20}H_{15}Cl_2F_2N_3O_2$ ) (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	G	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,36E)-3,35-dioxo-7,10,13,16,19,22,25,28,31-nona-4,34-diazaheptatriaconta-1,36-diene-1,37-diyl]bis{N-[(1S)-3-amino-1-(3-chloro-4-fluorophenyl)-3-oxopropyl]-4-(4-chloro-2-fluorophenyl)-1H-pyrrole-3-carboxamide} (CCD ID: A1C26) (formula:  $C_{66}H_{74}Cl_4F_4N_8O_{15}$ ) (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
			171	66	4	4	74	8	15		
3	F	1	Total	C	Cl	F	H	N	O	0	0
			171	66	4	4	74	8	15		

- Molecule 4 is water.

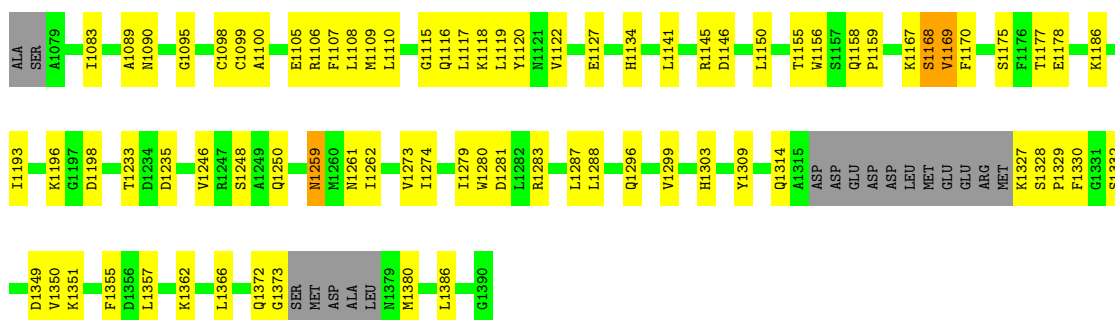
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	51	Total	O	0	0
			51	51		
4	C	51	Total	O	0	0
			51	51		
4	D	60	Total	O	0	0
			60	60		
4	E	36	Total	O	0	0
			36	36		
4	F	35	Total	O	0	0
			35	35		
4	G	37	Total	O	0	0
			37	37		
4	H	26	Total	O	0	0
			26	26		

### 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

Chain A: 



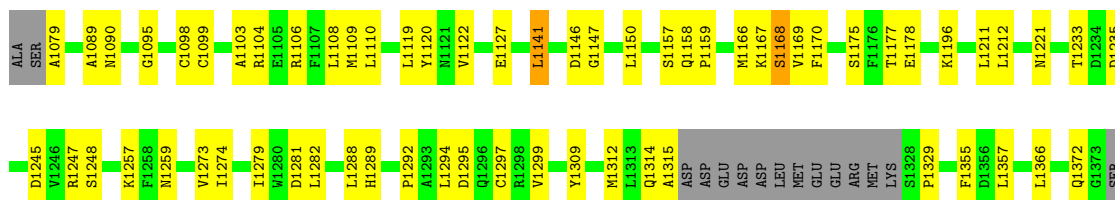
#### • Molecule 1: DDB1- and CUL4-associated factor 1

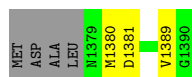
Chain B: 



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

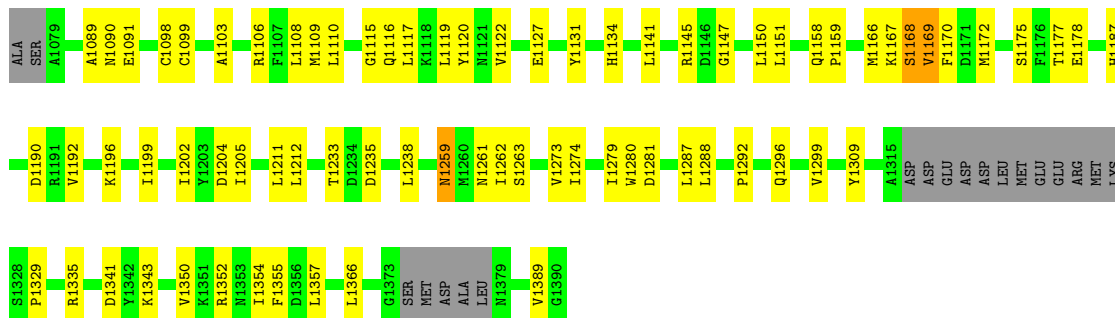
Chain C: 





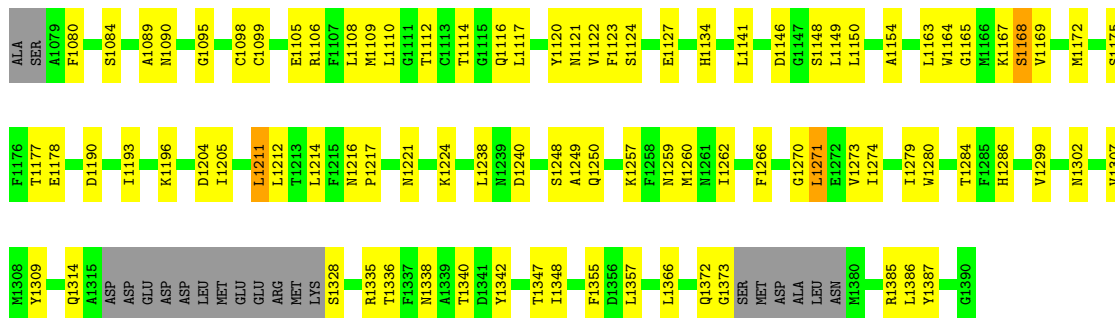
- Molecule 1: DDB1- and CUL4-associated factor 1

Chain D: 70% 23% 6%



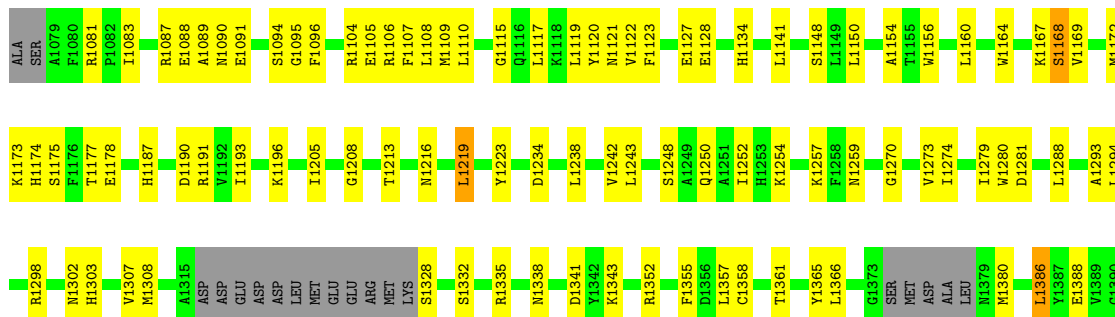
- Molecule 1: DDB1- and CUL4-associated factor 1

Chain E: 65% 28% 6%



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

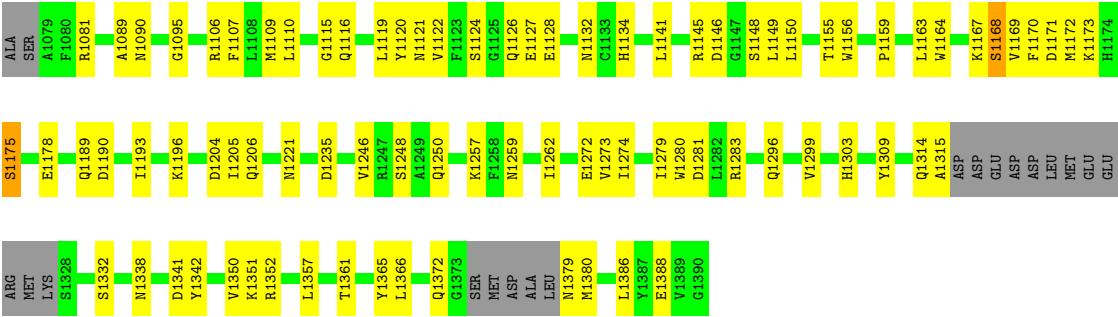
Chain F: 64% 29% 6%



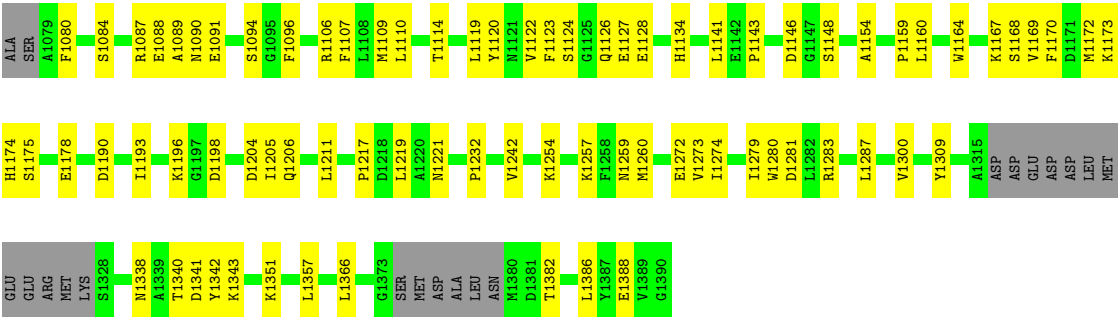
- Molecule 1: DDB1- and CUL4-associated factor 1

Chain G: 67% 26% 6%





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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.80Å 120.87Å 208.99Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	30.18 – 2.30 30.18 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.9 (30.18-2.30) 81.1 (30.18-2.30)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	-1.49 (at 2.31Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, $R_{free}$	0.243 , 0.289 0.243 , 0.289	Depositor DCC
$R_{free}$ test set	1997 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 6.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.459 for k,h,-l 0.468 for -k,-h,-l 0.468 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	19582	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: A1C26, A1C24

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	0.24	0/2403	0.51	0/3257
1	B	0.22	0/2394	0.50	0/3246
1	C	0.22	0/2394	0.47	0/3246
1	D	0.23	0/2394	0.48	0/3246
1	E	0.20	0/2386	0.46	0/3235
1	F	0.20	0/2394	0.48	0/3246
1	G	0.19	0/2394	0.46	0/3246
1	H	0.19	0/2386	0.44	0/3235
All	All	0.21	0/19145	0.48	0/25957

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2349	0	2256	72	0
1	B	2340	0	2243	69	0
1	C	2340	0	2243	54	0
1	D	2340	0	2243	67	0
1	E	2332	0	2237	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2340	0	2243	89	0
1	G	2340	0	2243	68	0
1	H	2332	0	2237	66	0
2	A	29	15	0	0	0
2	C	29	15	0	0	0
2	E	29	15	0	0	0
2	G	29	15	0	0	0
3	D	97	74	0	0	0
3	F	97	74	0	0	0
4	A	55	0	0	4	0
4	B	51	0	0	2	0
4	C	51	0	0	5	0
4	D	60	0	0	6	0
4	E	36	0	0	7	0
4	F	35	0	0	8	0
4	G	37	0	0	1	0
4	H	26	0	0	3	0
All	All	19374	208	17945	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 15.

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:1095:GLY:HA2	1:F:1380:MET:HE2	1.38	1.01
1:B:1107:PHE:HE2	1:B:1128:GLU:HG3	1.26	1.00
1:B:1145:ARG:H	1:B:1189:GLN:HE22	1.12	0.97
1:F:1307:VAL:O	4:F:1501:HOH:O	1.82	0.97
1:D:1109:MET:HG2	1:D:1119:LEU:HD11	1.52	0.92
1:G:1259:ASN:HD22	1:G:1296:GLN:HE22	1.18	0.91
1:A:1259:ASN:HD21	1:A:1262:ILE:H	1.19	0.91
1:C:1372:GLN:HE22	1:D:1287:LEU:H	1.18	0.91
1:G:1357:LEU:HD13	1:G:1366:LEU:HD11	1.52	0.90
1:E:1357:LEU:HD13	1:E:1366:LEU:HD11	1.53	0.90
1:E:1114:THR:OG1	1:E:1116:GLN:OE1	1.90	0.89
1:B:1107:PHE:CE2	1:B:1128:GLU:HG3	2.07	0.89
1:G:1145:ARG:H	1:G:1189:GLN:HE22	1.20	0.89
1:A:1145:ARG:NH2	1:A:1186:LYS:O	2.07	0.87
1:G:1106:ARG:O	1:G:1122:VAL:HG22	1.76	0.86
1:D:1109:MET:HE1	1:D:1150:LEU:HD13	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:GLN:HE22	1:A:1177:THR:HB	1.40	0.85
1:A:1178:GLU:OE1	1:A:1196:LYS:NZ	2.08	0.85
1:G:1095:GLY:HA2	1:G:1380:MET:HE3	1.58	0.85
1:F:1187:HIS:HA	4:F:1528:HOH:O	1.76	0.85
1:F:1172:MET:HE3	1:F:1175:SER:HB3	1.58	0.84
1:G:1259:ASN:HD21	1:G:1262:ILE:H	1.25	0.84
1:H:1106:ARG:O	1:H:1122:VAL:HG22	1.78	0.83
1:D:1259:ASN:HD21	1:D:1262:ILE:H	1.24	0.83
1:E:1172:MET:CE	1:E:1175:SER:HB3	2.08	0.82
1:E:1172:MET:HE3	1:E:1175:SER:HB3	1.61	0.82
1:C:1079:ALA:N	4:C:1501:HOH:O	2.11	0.82
1:A:1109:MET:HE1	1:A:1150:LEU:HD13	1.62	0.82
1:B:1109:MET:HE1	1:B:1150:LEU:HD13	1.60	0.82
1:F:1357:LEU:HD13	1:F:1366:LEU:HD11	1.60	0.82
1:B:1357:LEU:HD13	1:B:1366:LEU:HD11	1.60	0.81
1:G:1372:GLN:HE22	1:H:1287:LEU:H	1.27	0.81
1:D:1263:SER:O	4:D:1501:HOH:O	1.98	0.80
1:C:1098:CYS:SG	1:C:1141:LEU:HD22	2.22	0.79
1:B:1224:LYS:HD3	1:B:1260:MET:O	1.82	0.79
1:B:1248:SER:OG	1:B:1250:GLN:HG2	1.81	0.79
1:F:1106:ARG:O	1:F:1122:VAL:HG22	1.83	0.78
1:E:1335:ARG:HD3	1:E:1347:THR:OG1	1.83	0.78
1:A:1095:GLY:HA2	1:A:1380:MET:HE2	1.65	0.78
1:H:1107:PHE:CE1	1:H:1128:GLU:HG3	2.18	0.78
1:B:1105:GLU:OE1	1:B:1106:ARG:N	2.16	0.78
1:D:1274:ILE:HG23	1:D:1279:ILE:CD1	2.15	0.77
1:A:1178:GLU:HB3	1:A:1196:LYS:HE2	1.65	0.76
1:A:1274:ILE:HG23	1:A:1279:ILE:CD1	2.15	0.76
1:A:1248:SER:OG	1:A:1250:GLN:HG2	1.86	0.76
1:C:1274:ILE:HG23	1:C:1279:ILE:CD1	2.15	0.76
1:C:1281:ASP:HB2	1:C:1288:LEU:HD11	1.66	0.76
1:A:1158:GLN:NE2	1:A:1177:THR:HB	2.01	0.75
1:E:1302:ASN:CG	1:E:1307:VAL:HG22	2.11	0.75
1:B:1233:THR:OG1	1:B:1235:ASP:OD1	2.05	0.74
1:H:1109:MET:HE1	1:H:1143:PRO:HB3	1.69	0.74
1:B:1274:ILE:HG23	1:B:1279:ILE:CD1	2.16	0.74
1:B:1199:ILE:HD11	1:D:1199:ILE:HD11	1.69	0.73
1:E:1106:ARG:O	1:E:1122:VAL:HG22	1.88	0.73
1:F:1281:ASP:HB2	1:F:1288:LEU:HD21	1.71	0.73
1:H:1172:MET:CE	1:H:1175:SER:HB3	2.18	0.73
1:H:1172:MET:HE3	1:H:1175:SER:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:VAL:O	4:A:1501:HOH:O	2.06	0.72
1:E:1314:GLN:OE1	1:E:1328:SER:OG	2.06	0.72
1:A:1287:LEU:H	1:B:1372:GLN:HE22	1.37	0.72
1:F:1148:SER:HB2	1:F:1167:LYS:HE2	1.72	0.72
1:E:1302:ASN:ND2	1:E:1307:VAL:HG22	2.04	0.72
1:H:1357:LEU:HD13	1:H:1366:LEU:HD11	1.72	0.72
1:C:1106:ARG:O	1:C:1122:VAL:HG22	1.91	0.71
1:B:1178:GLU:HB3	1:B:1196:LYS:HE2	1.72	0.71
1:D:1178:GLU:CB	1:D:1196:LYS:HE2	2.21	0.71
1:G:1164:TRP:CZ3	1:G:1172:MET:HB2	2.26	0.70
1:A:1314:GLN:NE2	1:A:1330:PHE:O	2.24	0.70
1:E:1240:ASP:OD2	4:E:1501:HOH:O	2.08	0.70
1:F:1293:ALA:HB1	1:F:1335:ARG:NH1	2.07	0.70
1:B:1106:ARG:O	1:B:1122:VAL:HG22	1.92	0.70
1:A:1178:GLU:CB	1:A:1196:LYS:HE2	2.21	0.70
1:E:1211:LEU:O	1:E:1212:LEU:HD12	1.93	0.69
1:F:1238:LEU:HG	4:F:1505:HOH:O	1.92	0.69
1:B:1178:GLU:OE1	1:B:1196:LYS:NZ	2.25	0.68
1:G:1107:PHE:CD1	1:G:1121:ASN:HA	2.28	0.68
1:D:1106:ARG:O	1:D:1122:VAL:HG22	1.94	0.68
1:D:1281:ASP:HB2	1:D:1288:LEU:HD11	1.75	0.68
1:D:1357:LEU:HD13	1:D:1366:LEU:HD11	1.74	0.68
1:D:1259:ASN:HD22	1:D:1296:GLN:HE22	1.43	0.67
1:E:1238:LEU:HG	4:E:1511:HOH:O	1.93	0.67
1:E:1385:ARG:HD2	1:E:1387:TYR:OH	1.95	0.67
1:H:1257:LYS:HE2	1:H:1260:MET:HE2	1.76	0.67
1:A:1106:ARG:O	1:A:1122:VAL:HG22	1.95	0.67
1:B:1224:LYS:NZ	1:B:1260:MET:HE3	2.10	0.67
1:F:1172:MET:CE	1:F:1175:SER:HB3	2.25	0.67
1:A:1083:ILE:CG2	1:A:1386:LEU:HD23	2.25	0.67
1:A:1159:PRO:HG3	1:A:1175:SER:HB2	1.77	0.67
1:F:1081:ARG:O	1:F:1083:ILE:HD12	1.95	0.67
1:C:1233:THR:OG1	1:C:1235:ASP:OD1	2.07	0.66
1:A:1107:PHE:HB3	1:A:1119:LEU:HD21	1.78	0.66
1:F:1357:LEU:HD13	1:F:1366:LEU:CD1	2.25	0.65
1:H:1106:ARG:HG2	1:H:1123:PHE:HE2	1.62	0.65
1:C:1372:GLN:HE22	1:D:1287:LEU:N	1.92	0.65
1:E:1216:ASN:HA	4:E:1534:HOH:O	1.96	0.65
1:B:1169:VAL:HG21	1:F:1173:LYS:HD3	1.77	0.65
1:D:1341:ASP:OD2	1:D:1343:LYS:HD2	1.96	0.65
1:F:1106:ARG:C	1:F:1122:VAL:HG22	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1178:GLU:OE1	1:D:1196:LYS:NZ	2.28	0.65
1:H:1159:PRO:HG3	1:H:1175:SER:HB2	1.78	0.64
1:A:1120:TYR:CZ	1:A:1127:GLU:HB2	2.31	0.64
1:E:1217:PRO:HD2	4:E:1534:HOH:O	1.97	0.64
1:B:1120:TYR:CZ	1:B:1127:GLU:HB2	2.32	0.64
1:H:1274:ILE:HG23	1:H:1279:ILE:CD1	2.28	0.64
1:F:1293:ALA:HB1	1:F:1335:ARG:HH11	1.63	0.64
1:G:1145:ARG:H	1:G:1189:GLN:NE2	1.94	0.64
1:C:1120:TYR:CZ	1:C:1127:GLU:HB2	2.32	0.63
1:A:1259:ASN:ND2	1:A:1261:ASN:H	1.97	0.63
1:B:1167:LYS:O	1:B:1168:SER:OG	2.13	0.63
1:G:1148:SER:CB	1:G:1167:LYS:HE2	2.28	0.63
1:D:1178:GLU:HB3	1:D:1196:LYS:HE2	1.81	0.63
1:E:1148:SER:HB2	1:E:1167:LYS:HE2	1.80	0.63
1:C:1247:ARG:HG3	1:C:1248:SER:N	2.13	0.63
1:G:1124:SER:OG	1:G:1126:GLN:HG3	1.98	0.63
1:F:1106:ARG:HD3	1:F:1123:PHE:HD2	1.64	0.62
1:B:1281:ASP:HB2	1:B:1288:LEU:HD11	1.82	0.62
1:D:1233:THR:OG1	1:D:1235:ASP:OD1	2.10	0.62
1:E:1134:HIS:CD2	1:E:1154:ALA:HB2	2.35	0.62
1:G:1372:GLN:HE22	1:H:1287:LEU:N	1.97	0.62
1:H:1257:LYS:HE2	1:H:1260:MET:CE	2.30	0.62
1:G:1109:MET:HE1	1:G:1150:LEU:HD13	1.81	0.61
1:A:1167:LYS:O	1:A:1168:SER:OG	2.16	0.61
1:B:1211:LEU:O	1:B:1212:LEU:HD12	2.00	0.61
1:C:1158:GLN:NE2	1:C:1177:THR:HB	2.15	0.61
1:D:1108:LEU:HD23	1:D:1110:LEU:HD11	1.82	0.61
1:H:1107:PHE:HE1	1:H:1128:GLU:HG3	1.63	0.61
1:H:1173:LYS:HG2	1:H:1174:HIS:CD2	2.34	0.61
1:H:1204:ASP:HB2	1:H:1211:LEU:HD11	1.83	0.61
1:E:1080:PHE:CE2	1:E:1348:ILE:HD11	2.36	0.60
1:D:1109:MET:HG2	1:D:1119:LEU:CD1	2.29	0.60
1:D:1172:MET:CE	1:D:1175:SER:HB3	2.31	0.60
1:C:1095:GLY:HA2	1:C:1380:MET:HE2	1.83	0.60
1:C:1109:MET:HE1	1:C:1150:LEU:HD13	1.83	0.60
1:B:1108:LEU:HD13	1:B:1110:LEU:CD1	2.32	0.59
1:C:1108:LEU:HD23	1:C:1110:LEU:HD11	1.85	0.59
1:D:1117:LEU:CD1	1:D:1150:LEU:HD21	2.31	0.59
1:D:1259:ASN:ND2	1:D:1261:ASN:H	2.00	0.59
1:F:1178:GLU:HB2	1:F:1196:LYS:HE2	1.83	0.59
1:F:1095:GLY:CA	1:F:1380:MET:HE2	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1198:ASP:HB3	4:H:1402:HOH:O	2.00	0.59
1:F:1108:LEU:HB2	1:F:1122:VAL:CG1	2.33	0.59
1:E:1357:LEU:HD13	1:E:1366:LEU:CD1	2.28	0.59
1:C:1372:GLN:NE2	1:D:1287:LEU:H	1.97	0.58
1:A:1357:LEU:HD13	1:A:1366:LEU:HD11	1.84	0.58
1:C:1178:GLU:CB	1:C:1196:LYS:HE2	2.32	0.58
1:E:1273:VAL:CG2	1:E:1280:TRP:HB2	2.33	0.58
1:B:1109:MET:CE	1:B:1150:LEU:HD13	2.31	0.58
1:F:1274:ILE:HG23	1:F:1279:ILE:CD1	2.33	0.58
1:B:1108:LEU:CD1	1:B:1110:LEU:HD11	2.34	0.58
1:H:1114:THR:O	1:H:1114:THR:HG22	2.04	0.58
1:F:1298:ARG:NH1	4:F:1503:HOH:O	2.12	0.57
1:F:1083:ILE:HD11	1:F:1388:GLU:HB2	1.86	0.57
1:F:1107:PHE:CE1	1:F:1128:GLU:HG3	2.40	0.57
1:B:1178:GLU:CB	1:B:1196:LYS:HE2	2.35	0.57
1:A:1281:ASP:HB2	1:A:1288:LEU:HD11	1.86	0.57
1:D:1159:PRO:HG3	1:D:1175:SER:HB2	1.85	0.57
1:B:1302:ASN:ND2	1:B:1307:VAL:HG23	2.19	0.57
1:C:1178:GLU:HB3	1:C:1196:LYS:HE2	1.86	0.57
1:A:1274:ILE:HG23	1:A:1279:ILE:HD11	1.87	0.57
1:F:1109:MET:HE1	1:F:1150:LEU:HD13	1.86	0.57
1:G:1379:ASN:ND2	4:G:1501:HOH:O	2.23	0.57
1:A:1314:GLN:NE2	1:A:1328:SER:OG	2.38	0.56
1:D:1115:GLY:HA3	1:D:1134:HIS:O	2.03	0.56
1:G:1357:LEU:HD13	1:G:1366:LEU:CD1	2.31	0.56
1:H:1178:GLU:HB3	1:H:1196:LYS:HD2	1.85	0.56
1:A:1108:LEU:CD1	1:A:1110:LEU:HD11	2.35	0.56
1:G:1281:ASP:OD1	1:G:1283:ARG:N	2.33	0.56
1:E:1248:SER:O	1:E:1250:GLN:HG2	2.05	0.56
1:C:1274:ILE:HG23	1:C:1279:ILE:HD11	1.87	0.56
1:E:1273:VAL:HG22	1:E:1280:TRP:HB2	1.87	0.56
1:F:1216:ASN:OD1	1:F:1219:LEU:HD13	2.04	0.56
1:G:1159:PRO:HG3	1:G:1175:SER:HB2	1.87	0.56
1:F:1106:ARG:HD3	1:F:1123:PHE:CD2	2.39	0.56
1:C:1099:CYS:HA	1:C:1109:MET:O	2.06	0.56
1:C:1211:LEU:O	1:C:1212:LEU:HD12	2.06	0.56
1:B:1224:LYS:N	1:B:1224:LYS:CD	2.69	0.56
1:D:1178:GLU:HB2	1:D:1196:LYS:HE2	1.88	0.56
1:G:1115:GLY:HA3	1:G:1134:HIS:O	2.06	0.56
1:D:1117:LEU:HD11	1:D:1150:LEU:HD21	1.87	0.55
1:H:1124:SER:OG	1:H:1126:GLN:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1341:ASP:CG	1:H:1343:LYS:HD3	2.31	0.55
1:C:1281:ASP:HB2	1:C:1288:LEU:CD1	2.34	0.55
1:F:1243:LEU:HD23	1:F:1252:ILE:HD11	1.88	0.55
1:B:1159:PRO:HG3	1:B:1175:SER:HB2	1.87	0.55
1:G:1081:ARG:NH1	1:G:1388:GLU:OE1	2.39	0.55
1:D:1120:TYR:CZ	1:D:1127:GLU:HB2	2.41	0.55
1:E:1122:VAL:HB	1:E:1386:LEU:HD11	1.88	0.55
1:F:1177:THR:HG23	1:F:1178:GLU:N	2.22	0.55
1:C:1141:LEU:HD23	4:C:1527:HOH:O	2.06	0.55
1:G:1107:PHE:HD1	1:G:1121:ASN:HA	1.70	0.55
1:G:1248:SER:O	1:G:1250:GLN:HG2	2.07	0.55
1:E:1212:LEU:HD23	1:E:1214:LEU:HD21	1.88	0.55
1:E:1224:LYS:HD3	4:E:1513:HOH:O	2.07	0.55
1:G:1148:SER:HB3	1:G:1167:LYS:HE2	1.88	0.54
1:F:1341:ASP:OD2	1:F:1343:LYS:HD2	2.08	0.54
1:A:1116:GLN:OE1	1:A:1118:LYS:HE3	2.06	0.54
1:F:1178:GLU:CB	1:F:1196:LYS:HE2	2.37	0.54
1:G:1235:ASP:O	1:G:1246:VAL:HG22	2.07	0.54
1:C:1295:ASP:O	4:C:1502:HOH:O	2.18	0.54
1:B:1108:LEU:HD13	1:B:1110:LEU:HD11	1.90	0.54
1:C:1329:PRO:HG2	1:C:1355:PHE:HA	1.90	0.54
1:F:1252:ILE:HD12	1:F:1252:ILE:C	2.32	0.54
1:G:1148:SER:HB2	1:G:1167:LYS:HE2	1.90	0.54
1:F:1148:SER:CB	1:F:1167:LYS:HE2	2.36	0.54
1:H:1084:SER:HB3	1:H:1386:LEU:HB2	1.90	0.54
1:H:1160:LEU:HD12	1:H:1178:GLU:O	2.06	0.54
1:H:1273:VAL:HG22	1:H:1280:TRP:HB2	1.90	0.54
1:D:1109:MET:CE	1:D:1150:LEU:HD13	2.33	0.54
1:D:1292:PRO:HD2	4:D:1536:HOH:O	2.07	0.54
1:F:1242:VAL:HB	4:F:1514:HOH:O	2.07	0.54
1:G:1155:THR:HG22	1:G:1156:TRP:HD1	1.72	0.54
1:D:1274:ILE:HG12	1:D:1279:ILE:HD12	1.90	0.54
1:C:1098:CYS:O	1:C:1110:LEU:HA	2.08	0.54
1:C:1357:LEU:HD13	1:C:1366:LEU:HD11	1.90	0.54
1:D:1238:LEU:HG	4:D:1501:HOH:O	2.07	0.54
1:C:1274:ILE:HG12	1:C:1279:ILE:HD12	1.90	0.53
1:E:1122:VAL:HB	1:E:1386:LEU:CD1	2.38	0.53
1:E:1164:TRP:CZ3	1:E:1172:MET:HB2	2.44	0.53
1:D:1259:ASN:ND2	1:D:1296:GLN:HE22	2.06	0.53
1:F:1174:HIS:CD2	1:F:1208:GLY:HA3	2.43	0.53
1:C:1109:MET:CE	1:C:1150:LEU:HD13	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1354:ILE:HD12	1:D:1354:ILE:N	2.23	0.53
1:G:1119:LEU:O	1:G:1128:GLU:N	2.39	0.53
1:H:1272:GLU:OE2	1:H:1342:TYR:OH	2.26	0.53
1:A:1159:PRO:CG	1:A:1175:SER:HB2	2.39	0.53
1:F:1178:GLU:OE1	1:F:1196:LYS:HE2	2.08	0.52
1:H:1232:PRO:O	4:H:1401:HOH:O	2.19	0.52
1:A:1115:GLY:HA3	1:A:1134:HIS:O	2.09	0.52
1:E:1177:THR:HG23	1:E:1178:GLU:N	2.24	0.52
1:C:1314:GLN:HG2	1:C:1315:ALA:N	2.24	0.52
1:G:1116:GLN:HE21	1:G:1132:ASN:ND2	2.06	0.52
1:A:1108:LEU:HD13	1:A:1110:LEU:CD1	2.39	0.52
1:B:1224:LYS:HZ3	1:B:1260:MET:HE3	1.75	0.52
1:C:1159:PRO:HG3	1:C:1175:SER:HB2	1.91	0.52
1:D:1335:ARG:NH1	4:D:1502:HOH:O	2.27	0.52
1:E:1212:LEU:HD21	1:E:1249:ALA:HB2	1.91	0.52
1:H:1300:VAL:CG1	1:H:1309:TYR:HB2	2.40	0.52
1:D:1172:MET:HE3	1:D:1175:SER:HB3	1.92	0.52
1:F:1338:ASN:HB3	1:F:1341:ASP:OD1	2.09	0.52
1:H:1204:ASP:OD2	1:H:1206:GLN:HB3	2.10	0.52
1:G:1178:GLU:HB3	1:G:1196:LYS:HD2	1.92	0.52
1:H:1242:VAL:HB	4:H:1410:HOH:O	2.08	0.51
1:B:1302:ASN:HD21	1:B:1307:VAL:HG23	1.73	0.51
1:D:1202:ILE:HB	1:D:1212:LEU:HB2	1.92	0.51
1:G:1314:GLN:HG3	1:G:1315:ALA:N	2.26	0.51
1:G:1107:PHE:CE2	1:G:1128:GLU:HG3	2.45	0.51
1:B:1292:PRO:HD2	4:B:1426:HOH:O	2.09	0.51
1:G:1303:HIS:CE1	1:G:1361:THR:HA	2.45	0.51
1:H:1159:PRO:HG3	1:H:1175:SER:CB	2.39	0.51
1:H:1274:ILE:HG23	1:H:1279:ILE:HD11	1.93	0.51
1:A:1159:PRO:HG3	1:A:1175:SER:CB	2.41	0.51
1:B:1079:ALA:HA	4:B:1437:HOH:O	2.11	0.51
1:E:1257:LYS:HE2	1:E:1260:MET:CE	2.41	0.51
1:F:1281:ASP:CB	1:F:1288:LEU:HD21	2.40	0.51
1:F:1087:ARG:HB2	1:F:1094:SER:HB2	1.92	0.51
1:F:1213:THR:HG21	1:H:1217:PRO:HB3	1.93	0.51
1:D:1103:ALA:HB2	1:D:1147:GLY:HA3	1.94	0.50
1:D:1352:ARG:O	1:D:1354:ILE:HD12	2.10	0.50
1:F:1177:THR:HG23	1:F:1178:GLU:H	1.75	0.50
1:A:1233:THR:OG1	1:A:1235:ASP:OD1	2.17	0.50
1:A:1329:PRO:HG2	1:A:1355:PHE:HA	1.92	0.50
1:C:1178:GLU:OE1	1:C:1196:LYS:NZ	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1105:GLU:O	1:E:1106:ARG:HB2	2.10	0.50
1:F:1115:GLY:HA3	1:F:1134:HIS:O	2.11	0.50
1:F:1302:ASN:N	4:F:1501:HOH:O	1.96	0.50
1:G:1107:PHE:CE1	1:G:1121:ASN:HA	2.46	0.50
1:H:1273:VAL:CG2	1:H:1280:TRP:HB2	2.41	0.50
1:E:1121:ASN:HB3	1:E:1124:SER:OG	2.11	0.50
1:F:1089:ALA:O	1:F:1090:ASN:HB2	2.11	0.50
1:C:1292:PRO:HD2	4:C:1534:HOH:O	2.10	0.50
1:C:1357:LEU:C	1:C:1357:LEU:HD12	2.36	0.50
1:B:1224:LYS:N	1:B:1224:LYS:HD2	2.26	0.50
1:G:1120:TYR:CZ	1:G:1127:GLU:HB2	2.47	0.50
1:A:1108:LEU:HD12	1:A:1110:LEU:HD11	1.92	0.50
1:A:1083:ILE:HG22	1:A:1386:LEU:HD23	1.94	0.50
1:C:1273:VAL:HG13	1:C:1282:LEU:HG	1.94	0.50
1:D:1116:GLN:NE2	4:D:1504:HOH:O	2.29	0.50
1:D:1274:ILE:HG23	1:D:1279:ILE:HD11	1.90	0.50
1:F:1141:LEU:HD12	1:F:1141:LEU:C	2.37	0.50
1:G:1299:VAL:HA	1:G:1309:TYR:O	2.12	0.50
1:H:1159:PRO:CG	1:H:1175:SER:HB2	2.41	0.50
1:F:1083:ILE:HD11	1:F:1388:GLU:CB	2.41	0.49
1:F:1365:TYR:HB3	1:F:1386:LEU:CD1	2.42	0.49
1:D:1190:ASP:C	1:D:1205:ILE:HD12	2.38	0.49
1:H:1190:ASP:C	1:H:1205:ILE:HD12	2.38	0.49
1:F:1273:VAL:HG22	1:F:1280:TRP:HB2	1.95	0.49
1:E:1106:ARG:C	1:E:1122:VAL:HG22	2.38	0.49
1:E:1149:LEU:HB3	1:E:1163:LEU:HD11	1.94	0.49
1:G:1221:ASN:OD1	1:G:1257:LYS:HB2	2.12	0.49
1:D:1168:SER:OG	1:D:1169:VAL:N	2.43	0.49
1:A:1299:VAL:HA	1:A:1309:TYR:O	2.13	0.48
1:G:1204:ASP:OD2	1:G:1206:GLN:HB3	2.14	0.48
1:A:1178:GLU:OE1	1:A:1196:LYS:CE	2.60	0.48
1:B:1145:ARG:H	1:B:1189:GLN:NE2	1.95	0.48
1:H:1089:ALA:O	1:H:1090:ASN:HB2	2.13	0.48
1:F:1096:PHE:CE1	1:F:1110:LEU:HD22	2.48	0.48
1:A:1259:ASN:HD22	1:A:1296:GLN:HE22	1.61	0.48
1:A:1349:ASP:O	1:A:1351:LYS:HD3	2.14	0.48
1:C:1103:ALA:HB2	1:C:1147:GLY:HA3	1.94	0.48
1:C:1158:GLN:HE21	1:C:1177:THR:HB	1.78	0.48
1:F:1303:HIS:CE1	1:F:1361:THR:HA	2.49	0.47
1:G:1272:GLU:OE2	1:G:1342:TYR:OH	2.29	0.47
1:F:1219:LEU:HD12	1:F:1219:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1235:ASP:O	1:A:1246:VAL:HG23	2.14	0.47
1:B:1274:ILE:HG12	1:B:1279:ILE:HD12	1.96	0.47
1:B:1089:ALA:O	1:B:1090:ASN:HB2	2.14	0.47
1:C:1312:MET:HE2	4:C:1540:HOH:O	2.14	0.47
1:E:1134:HIS:CG	1:E:1154:ALA:HB2	2.50	0.47
1:A:1099:CYS:HA	1:A:1109:MET:O	2.14	0.47
1:H:1338:ASN:HB3	1:H:1341:ASP:OD1	2.14	0.47
1:A:1351:LYS:HD3	1:A:1351:LYS:N	2.29	0.47
1:C:1167:LYS:O	1:C:1168:SER:OG	2.26	0.47
1:C:1089:ALA:O	1:C:1090:ASN:HB2	2.15	0.47
1:E:1089:ALA:O	1:E:1090:ASN:HB2	2.14	0.47
1:E:1168:SER:OG	1:E:1169:VAL:N	2.47	0.47
1:D:1091:GLU:HA	1:D:1091:GLU:OE1	2.14	0.47
1:F:1248:SER:O	1:F:1250:GLN:HG2	2.15	0.47
1:G:1116:GLN:HE21	1:G:1132:ASN:HA	1.79	0.47
1:A:1109:MET:CE	1:A:1150:LEU:HD13	2.39	0.47
1:A:1283:ARG:HB3	1:A:1283:ARG:CZ	2.44	0.47
1:C:1109:MET:SD	1:C:1166:MET:HE1	2.55	0.47
1:H:1274:ILE:HG12	1:H:1279:ILE:HD12	1.97	0.47
1:F:1120:TYR:CZ	1:F:1127:GLU:HB2	2.49	0.47
1:F:1332:SER:HA	1:F:1352:ARG:O	2.15	0.46
1:D:1109:MET:SD	1:D:1166:MET:HE1	2.55	0.46
1:G:1107:PHE:HB3	1:G:1119:LEU:HD11	1.97	0.46
1:G:1169:VAL:HG22	1:G:1170:PHE:N	2.31	0.46
1:B:1098:CYS:O	1:B:1110:LEU:HA	2.15	0.46
1:B:1357:LEU:HD12	1:B:1357:LEU:C	2.41	0.46
1:G:1106:ARG:C	1:G:1122:VAL:HG22	2.40	0.46
1:G:1274:ILE:HG23	1:G:1279:ILE:CD1	2.45	0.46
1:H:1141:LEU:C	1:H:1141:LEU:HD12	2.41	0.46
1:D:1158:GLN:NE2	1:D:1177:THR:HB	2.31	0.46
1:G:1110:LEU:N	1:G:1110:LEU:HD12	2.31	0.46
1:H:1080:PHE:HA	1:H:1388:GLU:O	2.16	0.46
1:A:1198:ASP:HB2	4:A:1509:HOH:O	2.14	0.46
1:E:1120:TYR:CZ	1:E:1127:GLU:HB2	2.51	0.46
1:H:1088:GLU:HA	1:H:1096:PHE:CZ	2.51	0.46
1:B:1103:ALA:HB2	1:B:1147:GLY:HA3	1.98	0.46
1:D:1099:CYS:HA	1:D:1109:MET:O	2.16	0.46
1:H:1087:ARG:HB2	1:H:1094:SER:HB2	1.98	0.46
1:D:1089:ALA:O	1:D:1090:ASN:HB2	2.16	0.46
1:E:1149:LEU:HD23	1:E:1165:GLY:HA2	1.98	0.46
1:B:1115:GLY:HA2	1:B:1138:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1146:ASP:OD1	1:B:1146:ASP:C	2.58	0.45
1:C:1294:LEU:O	1:C:1297:CYS:HB2	2.15	0.45
1:E:1109:MET:HE3	1:E:1109:MET:HB2	1.79	0.45
1:F:1107:PHE:HD1	1:F:1121:ASN:HA	1.81	0.45
1:F:1328:SER:HB2	1:F:1355:PHE:CE1	2.50	0.45
1:G:1089:ALA:O	1:G:1090:ASN:HB2	2.15	0.45
1:H:1169:VAL:HG22	1:H:1170:PHE:N	2.31	0.45
1:B:1095:GLY:O	1:B:1112:THR:HA	2.16	0.45
1:B:1148:SER:HB2	1:B:1167:LYS:HE2	1.98	0.45
1:C:1146:ASP:C	1:C:1146:ASP:OD1	2.59	0.45
1:D:1159:PRO:CG	1:D:1175:SER:HB2	2.45	0.45
1:G:1314:GLN:HG3	1:G:1315:ALA:H	1.79	0.45
1:A:1100:ALA:O	1:A:1108:LEU:HD22	2.16	0.45
1:A:1327:LYS:HD2	1:A:1327:LYS:N	2.31	0.45
1:E:1299:VAL:HA	1:E:1309:TYR:O	2.17	0.45
1:E:1372:GLN:O	1:E:1373:GLY:C	2.59	0.45
1:F:1191:ARG:NH2	1:F:1234:ASP:HB3	2.32	0.45
1:E:1106:ARG:HG2	1:E:1123:PHE:HE2	1.82	0.45
1:E:1238:LEU:HB2	1:E:1266:PHE:CE2	2.51	0.45
1:C:1108:LEU:HB2	1:C:1122:VAL:CG1	2.46	0.45
1:F:1107:PHE:CD1	1:F:1121:ASN:HA	2.52	0.45
1:A:1141:LEU:HD12	1:A:1141:LEU:C	2.41	0.45
1:B:1105:GLU:O	1:B:1106:ARG:HB2	2.17	0.45
1:B:1145:ARG:N	1:B:1189:GLN:HE22	1.96	0.45
1:B:1281:ASP:HB2	1:B:1288:LEU:CD1	2.46	0.45
1:F:1160:LEU:HD12	1:F:1178:GLU:O	2.15	0.45
1:F:1190:ASP:C	1:F:1205:ILE:HD12	2.42	0.45
1:G:1109:MET:C	1:G:1110:LEU:HD12	2.42	0.45
1:E:1309:TYR:CD1	1:E:1336:THR:HG22	2.52	0.45
1:B:1108:LEU:HD12	1:B:1110:LEU:HD11	1.99	0.45
1:B:1141:LEU:C	1:B:1141:LEU:HD12	2.42	0.45
1:G:1273:VAL:CG2	1:G:1280:TRP:HB2	2.47	0.45
1:A:1303:HIS:HB3	4:A:1553:HOH:O	2.17	0.44
1:G:1206:GLN:HA	1:G:1206:GLN:OE1	2.17	0.44
1:D:1329:PRO:HG2	1:D:1355:PHE:HA	1.98	0.44
1:D:1357:LEU:HD12	1:D:1357:LEU:C	2.43	0.44
1:E:1117:LEU:HD22	1:E:1150:LEU:CD2	2.48	0.44
1:A:1098:CYS:O	1:A:1110:LEU:HA	2.17	0.44
1:B:1329:PRO:HG2	1:B:1355:PHE:HA	1.99	0.44
1:D:1281:ASP:HB2	1:D:1288:LEU:CD1	2.43	0.44
1:E:1146:ASP:OD1	1:E:1146:ASP:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1328:SER:HB2	1:E:1355:PHE:CE1	2.52	0.44
1:F:1081:ARG:O	1:F:1083:ILE:CD1	2.63	0.44
1:F:1104:ARG:NH2	1:F:1119:LEU:HD13	2.33	0.44
1:H:1088:GLU:CD	1:H:1091:GLU:HG3	2.43	0.44
1:A:1273:VAL:CG2	1:A:1280:TRP:HB2	2.47	0.44
1:B:1350:VAL:O	1:B:1351:LYS:HB2	2.17	0.44
1:D:1141:LEU:HD12	1:D:1141:LEU:C	2.41	0.44
1:H:1281:ASP:OD1	1:H:1283:ARG:N	2.41	0.44
1:A:1169:VAL:CG2	1:A:1170:PHE:N	2.81	0.44
1:F:1273:VAL:CG2	1:F:1280:TRP:HB2	2.48	0.44
1:E:1262:ILE:HA	4:E:1527:HOH:O	2.18	0.44
1:G:1273:VAL:HG22	1:G:1280:TRP:HB2	1.99	0.44
1:H:1109:MET:HE1	1:H:1143:PRO:CB	2.42	0.44
1:A:1314:GLN:NE2	1:A:1328:SER:HG	2.15	0.44
1:E:1274:ILE:HG23	1:E:1279:ILE:CD1	2.48	0.44
1:F:1223:TYR:CE1	1:F:1257:LYS:HG3	2.52	0.44
1:E:1095:GLY:O	1:E:1112:THR:HA	2.17	0.44
1:D:1357:LEU:HD13	1:D:1366:LEU:CD1	2.46	0.44
1:F:1167:LYS:O	1:F:1168:SER:OG	2.32	0.44
1:H:1106:ARG:HG2	1:H:1123:PHE:CE2	2.47	0.44
1:H:1106:ARG:C	1:H:1122:VAL:HG22	2.42	0.44
1:B:1099:CYS:HA	1:B:1109:MET:O	2.18	0.43
1:B:1159:PRO:CG	1:B:1175:SER:HB2	2.47	0.43
1:B:1224:LYS:HB2	1:B:1261:ASN:OD1	2.18	0.43
1:E:1190:ASP:C	1:E:1205:ILE:HD12	2.43	0.43
1:F:1088:GLU:CD	1:F:1091:GLU:HG3	2.43	0.43
1:F:1274:ILE:HG12	1:F:1279:ILE:HD12	2.00	0.43
1:F:1357:LEU:HD12	1:F:1357:LEU:C	2.42	0.43
1:B:1274:ILE:HG23	1:B:1279:ILE:HD11	1.98	0.43
1:G:1190:ASP:C	1:G:1205:ILE:HD12	2.44	0.43
1:H:1338:ASN:OD1	1:H:1340:THR:OG1	2.22	0.43
1:C:1372:GLN:HG3	1:C:1381:ASP:O	2.18	0.43
1:D:1117:LEU:HD13	1:D:1150:LEU:HD21	1.99	0.43
1:H:1193:ILE:HG23	1:H:1193:ILE:O	2.17	0.43
1:A:1089:ALA:O	1:A:1090:ASN:HB2	2.19	0.43
1:B:1117:LEU:HD22	1:B:1150:LEU:CD2	2.48	0.43
1:C:1279:ILE:HB	1:C:1289:HIS:HB2	1.99	0.43
1:D:1131:TYR:HD2	4:D:1557:HOH:O	2.00	0.43
1:D:1159:PRO:HG3	1:D:1175:SER:CB	2.48	0.43
1:F:1294:LEU:HD21	1:F:1308:MET:HE3	2.00	0.43
1:G:1109:MET:CE	1:G:1150:LEU:HD13	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1148:SER:HB2	1:H:1167:LYS:HE2	2.00	0.43
1:C:1109:MET:HG3	1:C:1119:LEU:CD1	2.49	0.43
1:D:1098:CYS:O	1:D:1110:LEU:HA	2.18	0.43
1:E:1193:ILE:HG23	1:E:1193:ILE:O	2.19	0.43
1:E:1221:ASN:OD1	1:E:1257:LYS:HB2	2.19	0.43
1:F:1178:GLU:OE1	1:F:1196:LYS:NZ	2.49	0.43
1:G:1365:TYR:HB3	1:G:1386:LEU:HD11	2.01	0.43
1:C:1245:ASP:OD2	1:C:1247:ARG:CG	2.67	0.43
1:F:1089:ALA:N	1:F:1120:TYR:OH	2.27	0.43
1:G:1193:ILE:HG23	1:G:1193:ILE:O	2.19	0.43
1:A:1117:LEU:C	1:A:1117:LEU:HD13	2.44	0.43
1:A:1169:VAL:HG22	1:A:1170:PHE:N	2.34	0.43
1:C:1221:ASN:OD1	1:C:1257:LYS:HB2	2.19	0.43
1:E:1284:THR:OG1	1:E:1286:HIS:CD2	2.72	0.43
1:H:1146:ASP:C	1:H:1146:ASP:OD1	2.61	0.43
1:A:1108:LEU:HB2	1:A:1122:VAL:CG1	2.49	0.43
1:D:1204:ASP:HB2	1:D:1211:LEU:HD11	1.99	0.43
1:D:1299:VAL:HA	1:D:1309:TYR:O	2.18	0.43
1:H:1109:MET:C	1:H:1110:LEU:HD12	2.44	0.43
1:H:1120:TYR:CZ	1:H:1127:GLU:HB2	2.54	0.43
1:H:1134:HIS:CG	1:H:1154:ALA:HB2	2.54	0.43
1:A:1327:LYS:HD3	4:A:1519:HOH:O	2.19	0.42
1:C:1169:VAL:HG22	1:C:1170:PHE:N	2.33	0.42
1:E:1141:LEU:C	1:E:1141:LEU:HD12	2.44	0.42
1:F:1117:LEU:HD22	1:F:1150:LEU:CD2	2.49	0.42
1:F:1178:GLU:OE1	1:F:1196:LYS:CE	2.67	0.42
1:F:1358:CYS:O	1:F:1366:LEU:HD12	2.18	0.42
1:G:1379:ASN:HB3	1:G:1380:MET:H	1.65	0.42
1:H:1107:PHE:HE1	1:H:1128:GLU:CG	2.32	0.42
1:A:1287:LEU:HD22	1:B:1085:VAL:HG22	2.00	0.42
1:B:1095:GLY:HA2	1:B:1380:MET:HE2	2.01	0.42
1:G:1121:ASN:HB3	1:G:1124:SER:OG	2.20	0.42
1:B:1221:ASN:O	1:B:1257:LYS:NZ	2.52	0.42
1:D:1167:LYS:O	1:D:1168:SER:OG	2.21	0.42
1:G:1095:GLY:CA	1:G:1380:MET:HE3	2.41	0.42
1:E:1098:CYS:O	1:E:1110:LEU:HA	2.19	0.42
1:F:1193:ILE:O	1:F:1193:ILE:HG23	2.19	0.42
1:G:1107:PHE:HE1	1:G:1121:ASN:ND2	2.18	0.42
1:A:1105:GLU:O	1:A:1106:ARG:HB2	2.20	0.42
1:B:1159:PRO:HG3	1:B:1175:SER:CB	2.49	0.42
1:B:1168:SER:OG	1:B:1169:VAL:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1145:ARG:NH2	1:D:1187:HIS:O	2.49	0.42
1:H:1351:LYS:HD2	1:H:1351:LYS:HA	1.52	0.42
1:A:1146:ASP:OD1	1:A:1146:ASP:C	2.62	0.42
1:B:1119:LEU:HA	1:B:1119:LEU:HD23	1.82	0.42
1:B:1169:VAL:CG2	1:B:1170:PHE:N	2.83	0.42
1:F:1089:ALA:O	1:F:1090:ASN:CB	2.68	0.42
1:F:1168:SER:OG	1:F:1169:VAL:N	2.53	0.42
1:C:1104:ARG:O	1:C:1104:ARG:HG3	2.20	0.42
1:D:1169:VAL:CG2	1:D:1170:PHE:N	2.83	0.42
1:F:1110:LEU:HD12	1:F:1110:LEU:N	2.35	0.42
1:F:1270:GLY:HA2	4:F:1526:HOH:O	2.20	0.42
1:G:1141:LEU:C	1:G:1141:LEU:HD12	2.45	0.41
1:A:1168:SER:OG	1:A:1169:VAL:N	2.52	0.41
1:B:1110:LEU:N	1:B:1110:LEU:HD12	2.34	0.41
1:C:1177:THR:OG1	1:C:1178:GLU:N	2.53	0.41
1:E:1178:GLU:HB3	1:E:1196:LYS:HD2	2.02	0.41
1:H:1221:ASN:OD1	1:H:1257:LYS:HB2	2.20	0.41
1:A:1332:SER:O	1:A:1350:VAL:HG22	2.20	0.41
1:A:1362:LYS:HB2	1:A:1362:LYS:NZ	2.36	0.41
1:C:1299:VAL:HA	1:C:1309:TYR:O	2.21	0.41
1:E:1084:SER:HB3	1:E:1386:LEU:HB2	2.02	0.41
1:F:1134:HIS:CG	1:F:1154:ALA:HB2	2.55	0.41
1:D:1273:VAL:HG22	1:D:1280:TRP:HB2	2.03	0.41
1:E:1204:ASP:HB2	1:E:1211:LEU:HD11	2.02	0.41
1:H:1122:VAL:HB	1:H:1386:LEU:HD11	2.02	0.41
1:H:1164:TRP:CZ3	1:H:1172:MET:HB2	2.56	0.41
1:F:1219:LEU:HB3	1:F:1254:LYS:HG3	2.02	0.41
1:H:1110:LEU:HD12	1:H:1110:LEU:N	2.35	0.41
1:F:1281:ASP:CA	1:F:1288:LEU:HD21	2.50	0.41
1:A:1155:THR:HG22	1:A:1156:TRP:HD1	1.85	0.41
1:G:1171:ASP:OD1	1:G:1173:LYS:NZ	2.53	0.41
1:A:1193:ILE:O	1:A:1193:ILE:HG23	2.20	0.41
1:A:1372:GLN:O	1:A:1373:GLY:C	2.64	0.41
1:F:1293:ALA:CB	1:F:1335:ARG:NH1	2.81	0.41
1:G:1167:LYS:O	1:G:1168:SER:OG	2.21	0.41
1:B:1108:LEU:HB2	1:B:1122:VAL:CG1	2.51	0.41
1:B:1109:MET:SD	1:B:1166:MET:HE1	2.61	0.41
1:B:1169:VAL:HG22	1:B:1170:PHE:N	2.36	0.41
1:E:1338:ASN:OD1	1:E:1340:THR:N	2.48	0.41
1:F:1105:GLU:O	1:F:1106:ARG:HB2	2.20	0.41
1:F:1219:LEU:N	1:F:1219:LEU:CD1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1270:GLY:HA2	4:F:1524:HOH:O	2.21	0.41
1:H:1094:SER:HB3	1:H:1382:THR:O	2.21	0.41
1:H:1357:LEU:HD13	1:H:1366:LEU:CD1	2.47	0.41
1:D:1151:LEU:HD11	1:D:1192:VAL:HG22	2.03	0.41
1:E:1270:GLY:HA2	4:E:1524:HOH:O	2.21	0.41
1:F:1164:TRP:CZ3	1:F:1172:MET:HB2	2.56	0.41
1:F:1281:ASP:N	1:F:1288:LEU:CD2	2.84	0.41
1:A:1083:ILE:HG21	1:A:1386:LEU:HD23	2.02	0.40
1:A:1095:GLY:CA	1:A:1380:MET:HE2	2.45	0.40
1:B:1231:ASN:HB2	1:B:1232:PRO:CD	2.51	0.40
1:C:1178:GLU:HB2	1:C:1196:LYS:HE2	2.03	0.40
1:D:1178:GLU:OE1	1:D:1196:LYS:CE	2.69	0.40
1:F:1104:ARG:HH22	1:F:1119:LEU:HD13	1.87	0.40
1:A:1287:LEU:H	1:B:1372:GLN:NE2	2.11	0.40
1:G:1145:ARG:N	1:G:1189:GLN:HE22	2.02	0.40
1:G:1146:ASP:OD1	1:G:1146:ASP:C	2.64	0.40
1:G:1350:VAL:HG23	1:G:1352:ARG:H	1.85	0.40
1:H:1119:LEU:O	1:H:1128:GLU:N	2.47	0.40
1:H:1219:LEU:O	1:H:1254:LYS:HD3	2.22	0.40
1:A:1235:ASP:C	1:A:1246:VAL:HG23	2.45	0.40
1:C:1159:PRO:CB	1:C:1177:THR:HA	2.52	0.40
1:E:1108:LEU:HB2	1:E:1122:VAL:CG1	2.51	0.40
1:G:1149:LEU:HB3	1:G:1163:LEU:HD11	2.04	0.40
1:G:1332:SER:HA	1:G:1352:ARG:O	2.21	0.40
1:H:1089:ALA:O	1:H:1090:ASN:CB	2.70	0.40
1:E:1099:CYS:HA	1:E:1109:MET:O	2.22	0.40
1:G:1338:ASN:HB3	1:G:1341:ASP:OD1	2.21	0.40
1:A:1107:PHE:HB3	1:A:1119:LEU:CD2	2.47	0.40
1:D:1350:VAL:HG22	1:D:1354:ILE:HD11	2.04	0.40
1:E:1257:LYS:HE2	1:E:1260:MET:HE2	2.03	0.40
1:E:1271:LEU:HD12	1:E:1271:LEU:HA	1.80	0.40
1:E:1279:ILE:HG21	1:E:1342:TYR:CE2	2.56	0.40
1:G:1351:LYS:HA	1:G:1351:LYS:HD2	1.58	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	290/314 (92%)	275 (95%)	14 (5%)	1 (0%)	36	46
1	B	289/314 (92%)	271 (94%)	17 (6%)	1 (0%)	36	46
1	C	289/314 (92%)	274 (95%)	13 (4%)	2 (1%)	18	23
1	D	289/314 (92%)	273 (94%)	14 (5%)	2 (1%)	18	23
1	E	288/314 (92%)	273 (95%)	14 (5%)	1 (0%)	36	46
1	F	289/314 (92%)	276 (96%)	12 (4%)	1 (0%)	36	46
1	G	289/314 (92%)	275 (95%)	13 (4%)	1 (0%)	36	46
1	H	288/314 (92%)	273 (95%)	14 (5%)	1 (0%)	36	46
All	All	2311/2512 (92%)	2190 (95%)	111 (5%)	10 (0%)	30	38

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1168	SER
1	F	1168	SER
1	A	1168	SER
1	D	1168	SER
1	E	1168	SER
1	G	1168	SER
1	H	1168	SER
1	B	1168	SER
1	D	1389	VAL
1	C	1389	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	260/276 (94%)	258 (99%)	2 (1%)	73	86
1	B	259/276 (94%)	256 (99%)	3 (1%)	63	79
1	C	259/276 (94%)	256 (99%)	3 (1%)	63	79
1	D	259/276 (94%)	257 (99%)	2 (1%)	73	86
1	E	258/276 (94%)	255 (99%)	3 (1%)	63	79
1	F	259/276 (94%)	255 (98%)	4 (2%)	57	75
1	G	259/276 (94%)	258 (100%)	1 (0%)	84	92
1	H	258/276 (94%)	257 (100%)	1 (0%)	84	92
All	All	2071/2208 (94%)	2052 (99%)	19 (1%)	70	84

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1169	VAL
1	A	1259	ASN
1	B	1105	GLU
1	B	1108	LEU
1	B	1169	VAL
1	C	1141	LEU
1	C	1157	SER
1	C	1259	ASN
1	D	1169	VAL
1	D	1259	ASN
1	E	1211	LEU
1	E	1259	ASN
1	E	1271	LEU
1	F	1156	TRP
1	F	1219	LEU
1	F	1259	ASN
1	F	1386	LEU
1	G	1175	SER
1	H	1259	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1158	GLN
1	A	1250	GLN
1	A	1253	HIS
1	A	1259	ASN
1	A	1303	HIS
1	A	1314	GLN
1	A	1372	GLN
1	B	1189	GLN
1	B	1250	GLN
1	B	1253	HIS
1	B	1289	HIS
1	B	1372	GLN
1	C	1135	ASN
1	C	1209	ASN
1	C	1253	HIS
1	C	1289	HIS
1	C	1303	HIS
1	C	1372	GLN
1	D	1250	GLN
1	D	1253	HIS
1	D	1259	ASN
1	D	1289	HIS
1	D	1372	GLN
1	E	1158	GLN
1	E	1201	HIS
1	E	1209	ASN
1	E	1250	GLN
1	E	1286	HIS
1	E	1289	HIS
1	F	1121	ASN
1	F	1126	GLN
1	F	1134	HIS
1	F	1286	HIS
1	F	1289	HIS
1	F	1303	HIS
1	F	1353	ASN
1	G	1116	GLN
1	G	1126	GLN
1	G	1132	ASN
1	G	1189	GLN
1	G	1201	HIS
1	G	1259	ASN
1	G	1289	HIS

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Mol	Chain	Res	Type
1	G	1372	GLN
1	H	1116	GLN
1	H	1121	ASN
1	H	1132	ASN
1	H	1174	HIS
1	H	1201	HIS
1	H	1289	HIS

### 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 ⓘ

6 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	A1C26	F	1401	-	100,102,102	0.99	5 (5%)	123,133,133	1.06	10 (8%)
2	A1C24	E	1401	-	31,31,31	1.69	5 (16%)	42,44,44	1.39	6 (14%)
3	A1C26	D	1401	-	100,102,102	0.99	4 (4%)	123,133,133	1.05	8 (6%)
2	A1C24	A	1401	-	31,31,31	1.69	5 (16%)	42,44,44	1.39	6 (14%)
2	A1C24	G	1401	-	31,31,31	1.69	5 (16%)	42,44,44	1.40	6 (14%)
2	A1C24	C	1401	-	31,31,31	1.68	5 (16%)	42,44,44	1.38	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	A1C26	F	1401	-	-	10/84/84/84	0/6/6/6
2	A1C24	E	1401	-	-	2/20/20/20	0/3/3/3
3	A1C26	D	1401	-	-	11/84/84/84	0/6/6/6
2	A1C24	A	1401	-	-	2/20/20/20	0/3/3/3
2	A1C24	G	1401	-	-	2/20/20/20	0/3/3/3
2	A1C24	C	1401	-	-	2/20/20/20	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1401	A1C24	C02-N16	5.54	1.45	1.34
2	A	1401	A1C24	C02-N16	5.51	1.45	1.34
2	G	1401	A1C24	C02-N16	5.50	1.45	1.34
2	C	1401	A1C24	C02-N16	5.50	1.45	1.34
2	A	1401	A1C24	C19-N20	3.97	1.45	1.32
2	G	1401	A1C24	C19-N20	3.97	1.45	1.32
2	E	1401	A1C24	C19-N20	3.96	1.45	1.32
2	C	1401	A1C24	C19-N20	3.95	1.45	1.32
2	A	1401	A1C24	C08-C07	-3.90	1.44	1.49
2	C	1401	A1C24	C08-C07	-3.89	1.44	1.49
2	G	1401	A1C24	C08-C07	-3.87	1.44	1.49
2	E	1401	A1C24	C08-C07	-3.84	1.44	1.49
2	E	1401	A1C24	O01-C02	-2.58	1.18	1.23
2	A	1401	A1C24	O01-C02	-2.55	1.18	1.23
2	G	1401	A1C24	O01-C02	-2.53	1.18	1.23
2	C	1401	A1C24	O01-C02	-2.52	1.18	1.23
2	G	1401	A1C24	C26-CL27	2.25	1.78	1.73
2	E	1401	A1C24	C26-CL27	2.24	1.78	1.73
2	A	1401	A1C24	C26-CL27	2.23	1.78	1.73
2	C	1401	A1C24	C26-CL27	2.22	1.78	1.73
3	D	1401	A1C26	C80-C81	2.09	1.41	1.38
3	D	1401	A1C26	C90-C91	2.08	1.41	1.38
3	F	1401	A1C26	C08-C10	2.07	1.41	1.38
3	F	1401	A1C26	C90-C91	2.06	1.41	1.38
3	F	1401	A1C26	C80-C81	2.06	1.41	1.38
3	F	1401	A1C26	C69-C71	2.04	1.41	1.38
3	D	1401	A1C26	C69-C71	2.04	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1401	A1C26	C08-C10	2.04	1.41	1.38
3	F	1401	A1C26	C90-C89	-2.01	1.46	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1401	A1C24	C06-C07-C03	4.23	109.45	106.93
2	E	1401	A1C24	C06-C07-C03	4.21	109.43	106.93
2	A	1401	A1C24	C06-C07-C03	4.16	109.40	106.93
2	C	1401	A1C24	C06-C07-C03	4.08	109.36	106.93
3	F	1401	A1C26	C93-C91-C90	-3.09	120.07	123.48
2	G	1401	A1C24	C12-C13-C08	-3.06	120.10	123.48
2	E	1401	A1C24	C12-C13-C08	-3.05	120.11	123.48
2	C	1401	A1C24	C12-C13-C08	-3.01	120.15	123.48
2	A	1401	A1C24	C12-C13-C08	-3.01	120.16	123.48
3	D	1401	A1C26	C83-C81-C80	-2.90	120.28	123.48
3	D	1401	A1C26	C93-C91-C90	-2.88	120.30	123.48
2	G	1401	A1C24	C11-C12-C13	2.85	119.94	117.54
2	E	1401	A1C24	C11-C12-C13	2.84	119.93	117.54
2	C	1401	A1C24	C09-C08-C13	2.82	119.83	116.70
2	A	1401	A1C24	C11-C12-C13	2.82	119.92	117.54
2	E	1401	A1C24	C09-C08-C13	2.82	119.83	116.70
2	G	1401	A1C24	C09-C08-C13	2.81	119.82	116.70
3	F	1401	A1C26	C83-C81-C80	-2.81	120.38	123.48
2	A	1401	A1C24	C09-C08-C13	2.79	119.80	116.70
2	C	1401	A1C24	C11-C12-C13	2.78	119.89	117.54
3	F	1401	A1C26	C66-N65-C63	2.74	126.04	122.21
3	F	1401	A1C26	C94-C93-C91	2.74	119.85	117.54
3	F	1401	A1C26	C84-C83-C81	2.71	119.83	117.54
3	F	1401	A1C26	C97-C90-C91	2.66	119.65	116.70
3	D	1401	A1C26	C05-N04-C02	2.65	125.92	122.21
3	D	1401	A1C26	C94-C93-C91	2.61	119.75	117.54
3	D	1401	A1C26	C87-C80-C81	2.61	119.59	116.70
3	D	1401	A1C26	C84-C83-C81	2.54	119.69	117.54
3	D	1401	A1C26	C97-C90-C91	2.54	119.52	116.70
3	D	1401	A1C26	C66-N65-C63	2.53	125.75	122.21
2	G	1401	A1C24	C03-C02-N16	2.49	119.48	116.25
3	F	1401	A1C26	C87-C80-C81	2.47	119.44	116.70
2	C	1401	A1C24	C03-C02-N16	2.45	119.43	116.25
2	A	1401	A1C24	C03-C02-N16	2.44	119.43	116.25
2	E	1401	A1C24	C03-C02-N16	2.42	119.40	116.25
3	F	1401	A1C26	C05-N04-C02	2.25	125.36	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1401	A1C24	O01-C02-N16	-2.10	119.40	123.09
2	C	1401	A1C24	O01-C02-N16	-2.09	119.41	123.09
2	A	1401	A1C24	O01-C02-N16	-2.09	119.42	123.09
3	F	1401	A1C26	C58-C59-N60	-2.07	118.51	124.48
2	E	1401	A1C24	O01-C02-N16	-2.07	119.45	123.09
3	F	1401	A1C26	C57-C55-N54	-2.07	110.54	115.07

There are no chirality outliers.

All (29) torsion outliers are listed below:

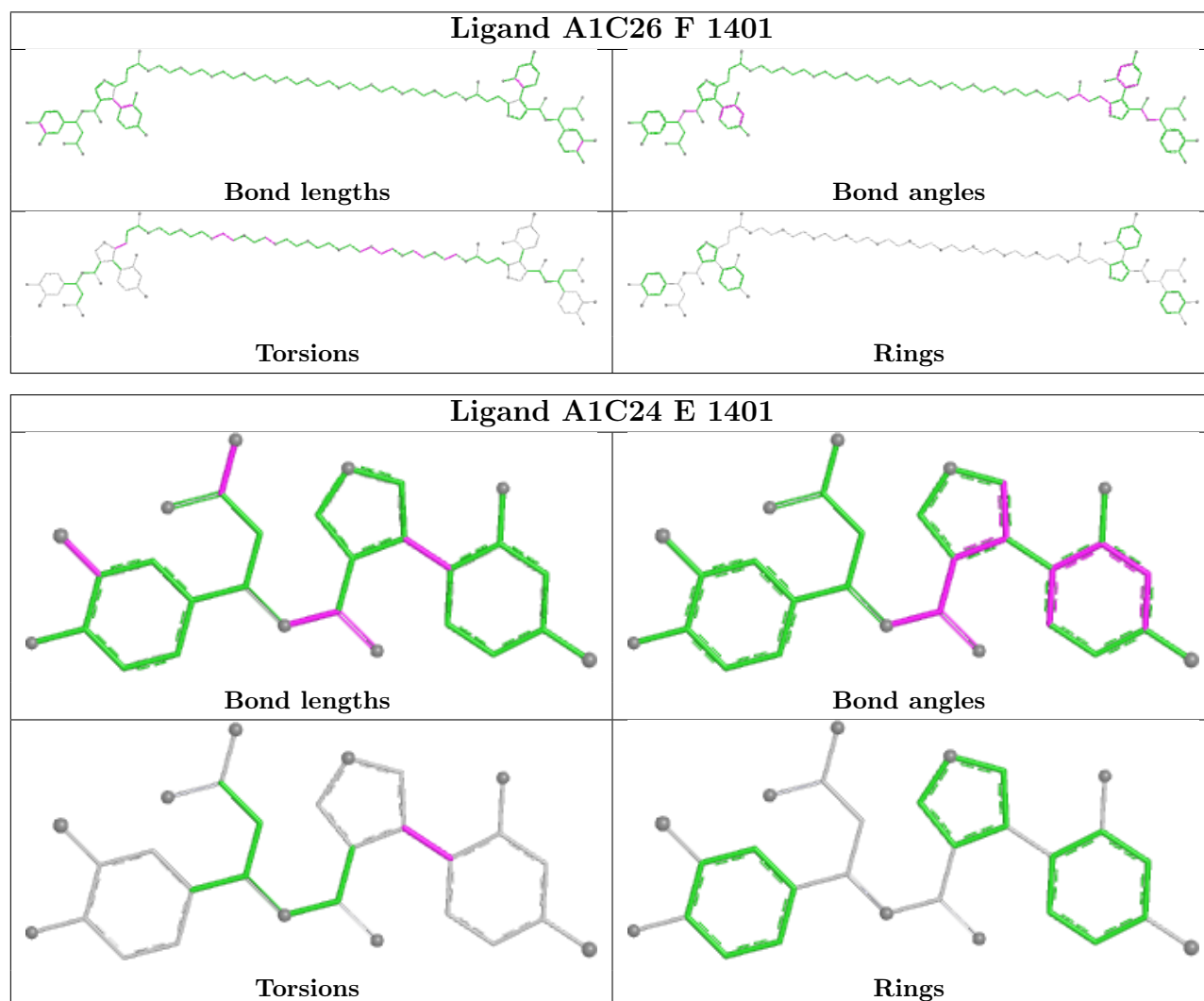
Mol	Chain	Res	Type	Atoms
2	A	1401	A1C24	C06-C07-C08-C13
2	C	1401	A1C24	C06-C07-C08-C13
2	E	1401	A1C24	C06-C07-C08-C13
2	G	1401	A1C24	C06-C07-C08-C13
3	F	1401	A1C26	C43-C44-O45-C46
3	D	1401	A1C26	O36-C37-C38-O39
3	D	1401	A1C26	C38-C37-O36-C35
2	A	1401	A1C24	C06-C07-C08-C09
2	C	1401	A1C24	C06-C07-C08-C09
2	E	1401	A1C24	C06-C07-C08-C09
2	G	1401	A1C24	C06-C07-C08-C09
3	F	1401	A1C26	O45-C46-C47-O48
3	D	1401	A1C26	C29-C28-O27-C26
3	D	1401	A1C26	O48-C49-C50-O51
3	F	1401	A1C26	O48-C49-C50-O51
3	D	1401	A1C26	C49-C50-O51-C52
3	F	1401	A1C26	C34-C35-O36-C37
3	D	1401	A1C26	C35-C34-O33-C32
3	F	1401	A1C26	O51-C52-C53-N54
3	F	1401	A1C26	C89-C20-C21-C22
3	F	1401	A1C26	O30-C31-C32-O33
3	D	1401	A1C26	O42-C43-C44-O45
3	F	1401	A1C26	C47-C46-O45-C44
3	F	1401	A1C26	N19-C20-C21-C22
3	F	1401	A1C26	C32-C31-O30-C29
3	D	1401	A1C26	O45-C46-C47-O48
3	D	1401	A1C26	C53-C52-O51-C50
3	D	1401	A1C26	O30-C31-C32-O33
3	D	1401	A1C26	C41-C40-O39-C38

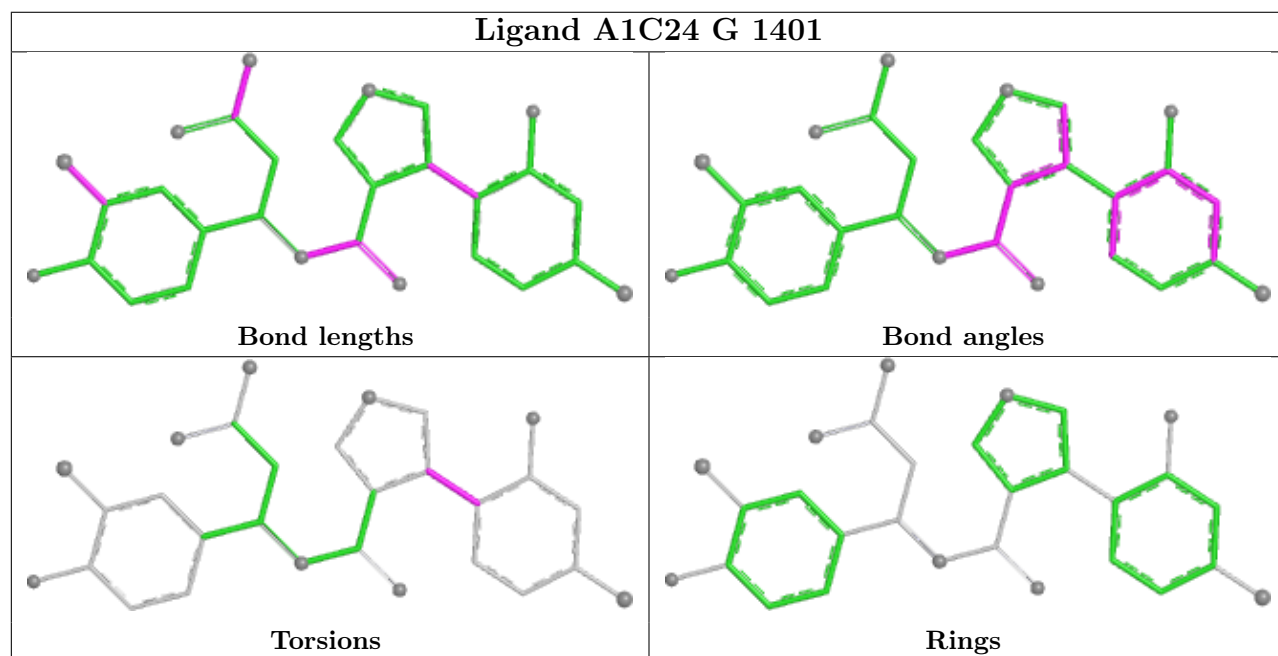
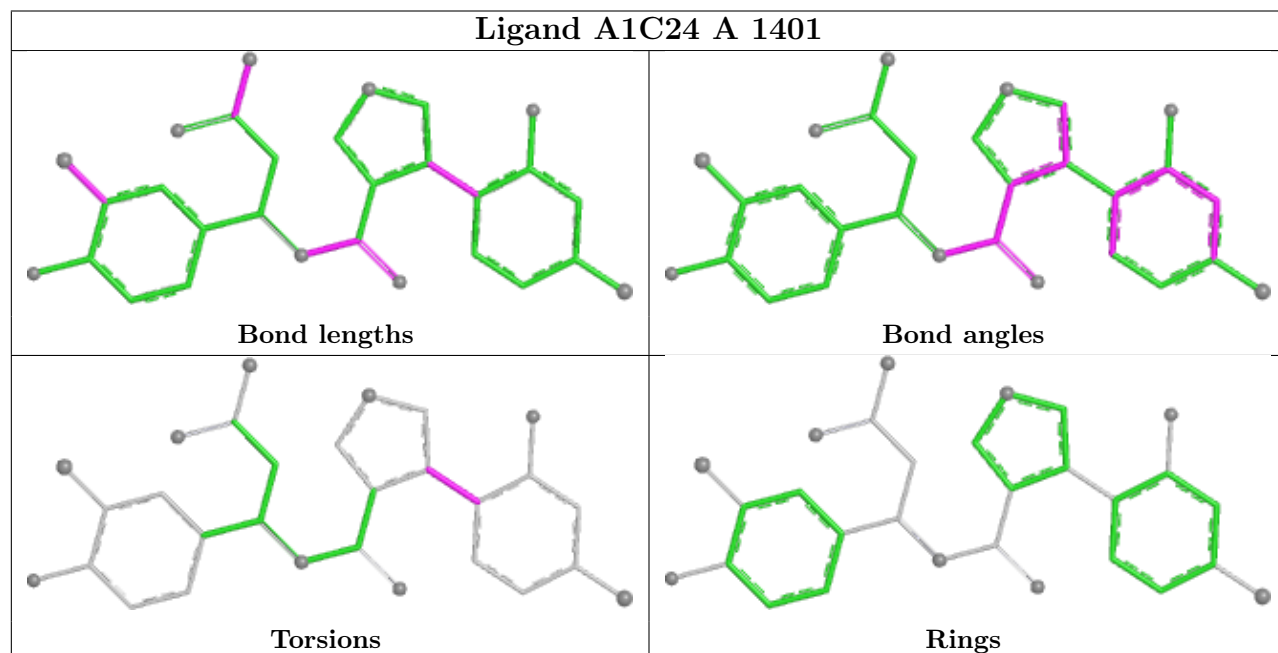
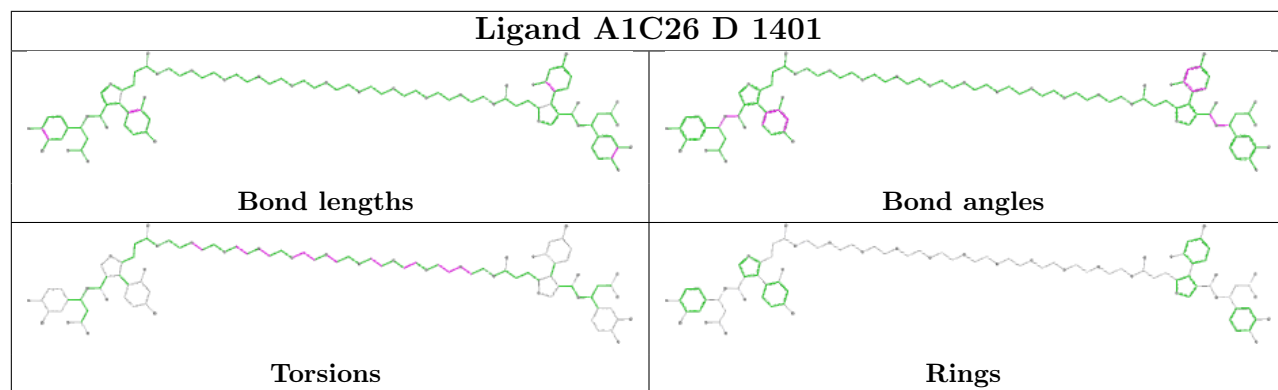
There are no ring outliers.

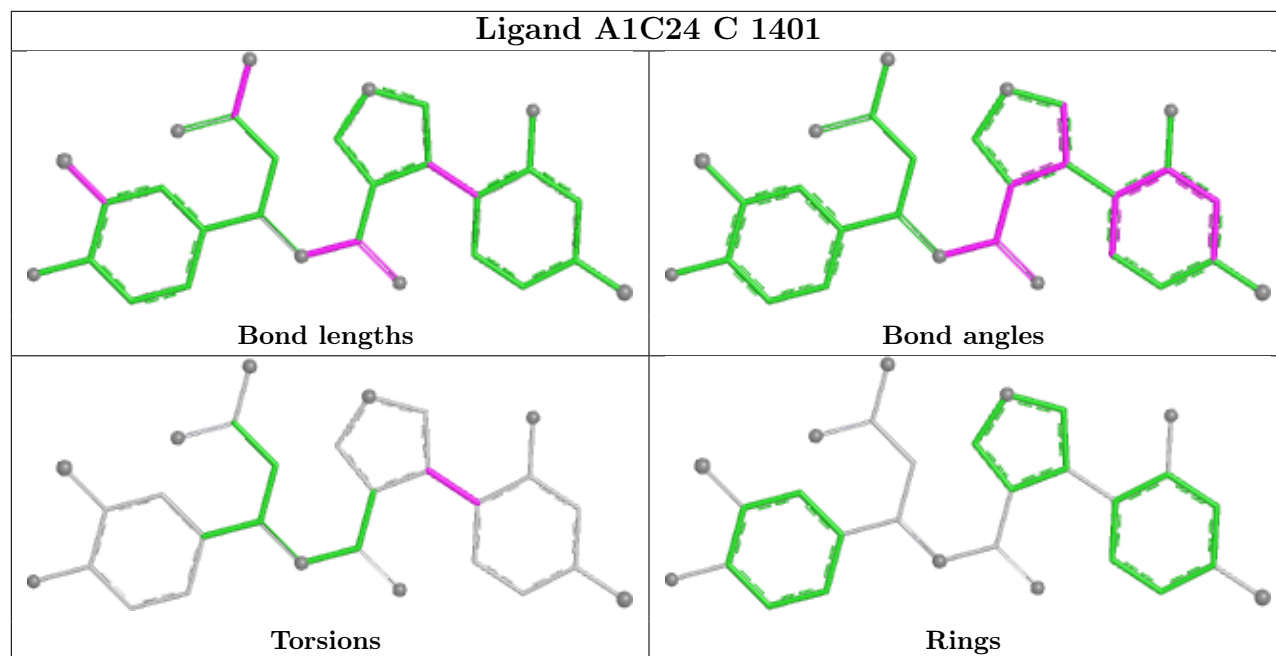


No monomer is involved in short contacts.

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.







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	296/314 (94%)	-1.29	0 100 100	8, 18, 37, 60	0
1	B	295/314 (93%)	-1.28	0 100 100	9, 18, 37, 66	0
1	C	295/314 (93%)	-1.29	0 100 100	9, 18, 37, 65	0
1	D	295/314 (93%)	-1.26	0 100 100	8, 18, 37, 65	0
1	E	294/314 (93%)	-1.08	0 100 100	11, 28, 53, 79	0
1	F	295/314 (93%)	-1.10	0 100 100	13, 28, 51, 67	0
1	G	295/314 (93%)	-1.10	0 100 100	12, 29, 52, 73	0
1	H	294/314 (93%)	-1.12	0 100 100	12, 29, 53, 77	0
All	All	2359/2512 (93%)	-1.19	0 100 100	8, 23, 48, 79	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](#)

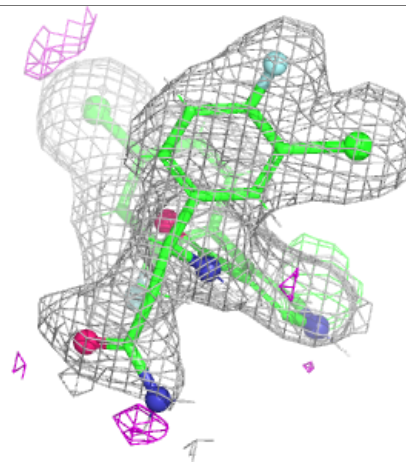
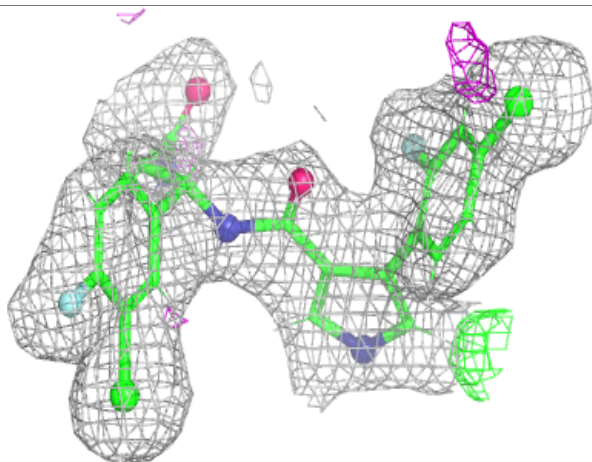
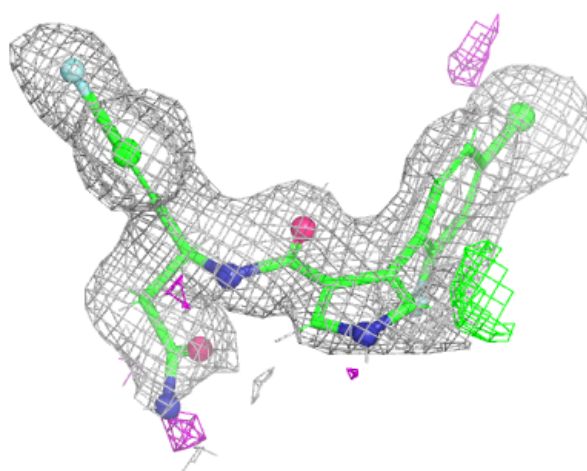
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	A1C24	A	1401	29/29	0.99	0.03	10,15,20,24	0
2	A1C24	C	1401	29/29	0.99	0.04	11,17,24,24	0
2	A1C24	E	1401	29/29	0.99	0.03	16,19,26,29	0
2	A1C24	G	1401	29/29	0.99	0.03	15,21,29,32	0
3	A1C26	D	1401	97/97	0.99	0.05	9,21,88,97	0
3	A1C26	F	1401	97/97	0.99	0.05	15,31,87,99	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.

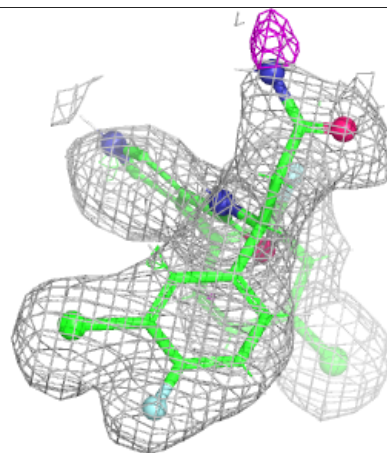
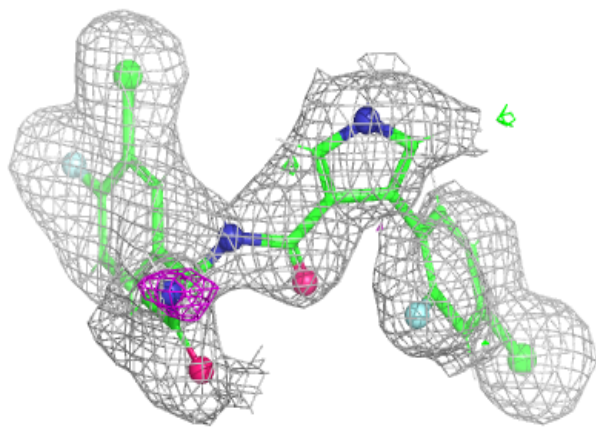
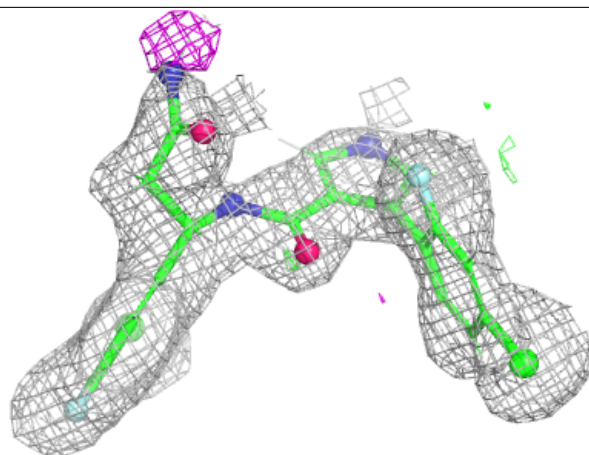
**Electron density around A1C24 A 1401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



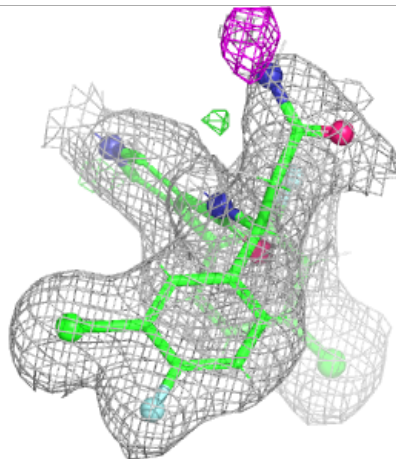
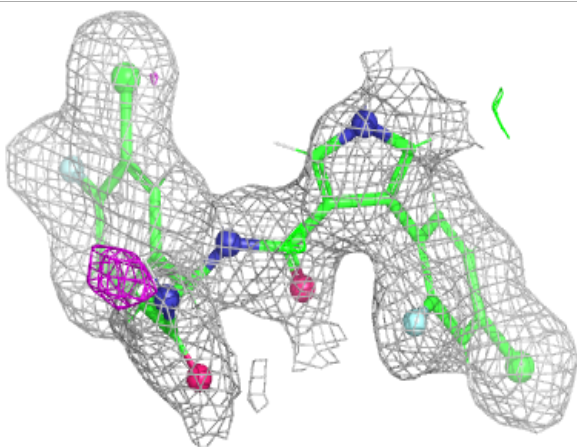
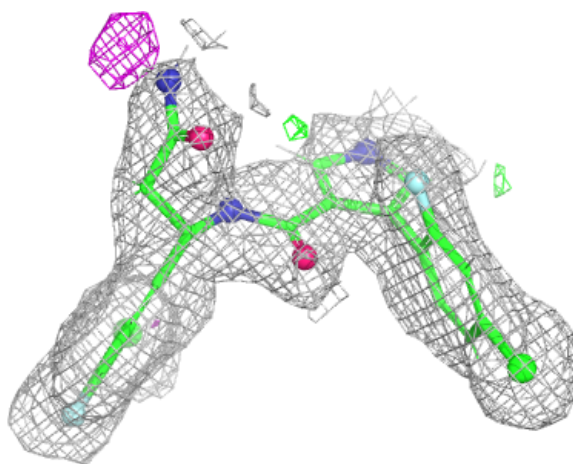
**Electron density around A1C24 C 1401:**

$2mF_o - DF_c$  (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:**

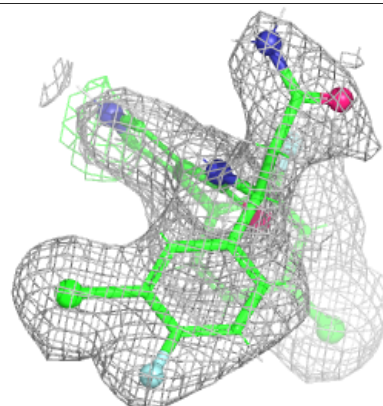
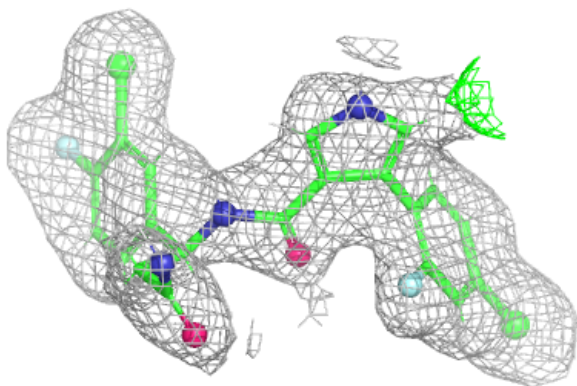
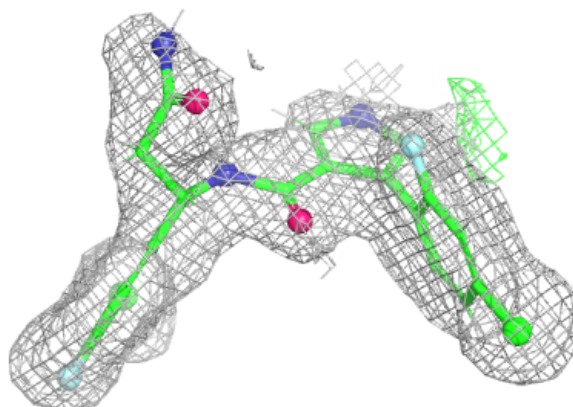
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



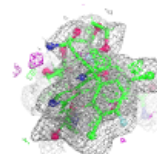
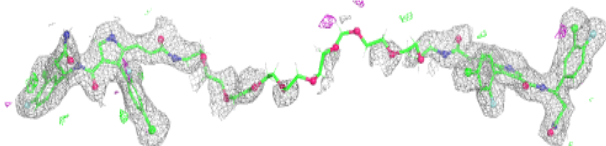
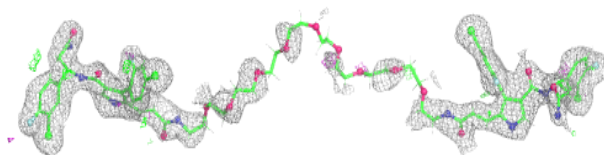


**Electron density around A1C24 G 1401:**

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

**Electron density around A1C26 D 1401:**

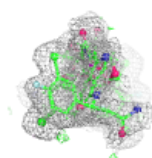
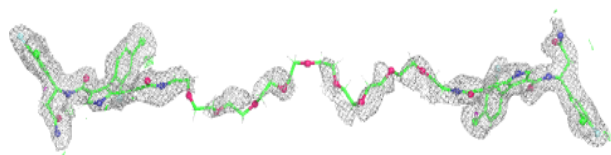
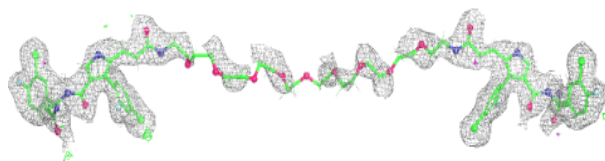
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around A1C26 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.