



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2026 – 12:10 PM EDT

PDB ID : 9ZLI / pdb\_00009zli  
Title : Crystal structure of DCAF1 in complex with SDIPTAC C11  
Authors : Mabanglo, M.F.; Srivastava, S.; Hoffer, L.; Ramnauth, J.; Vedadi, M.  
Deposited on : 2025-12-08  
Resolution : 2.07 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:

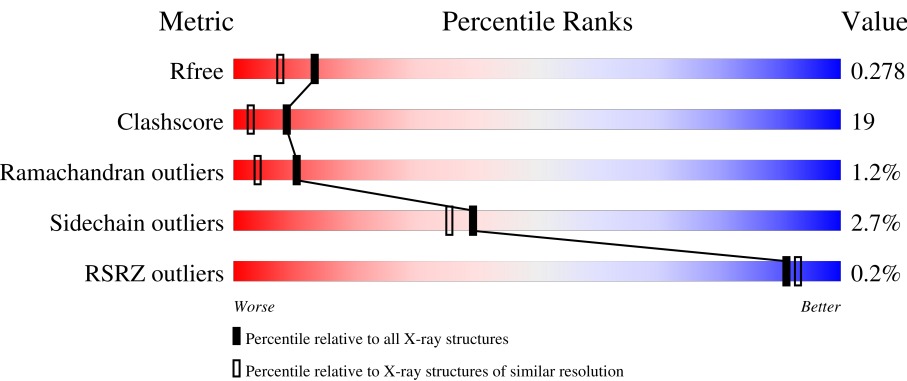
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 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 i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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 <sub>free</sub>	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	<div><div></div><div>63%30%• 5%</div></div>
1	B	314	<div><div></div><div>58%36%• 5%</div></div>
1	C	314	<div><div></div><div>64%29%• 5%</div></div>
1	D	314	<div><div></div><div>60%33%• 5%</div></div>
1	E	314	<div><div></div><div>64%29%• 5%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	314	<div><div></div><div>63%</div><div>30%</div><div></div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14934 atoms, of which 194 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.

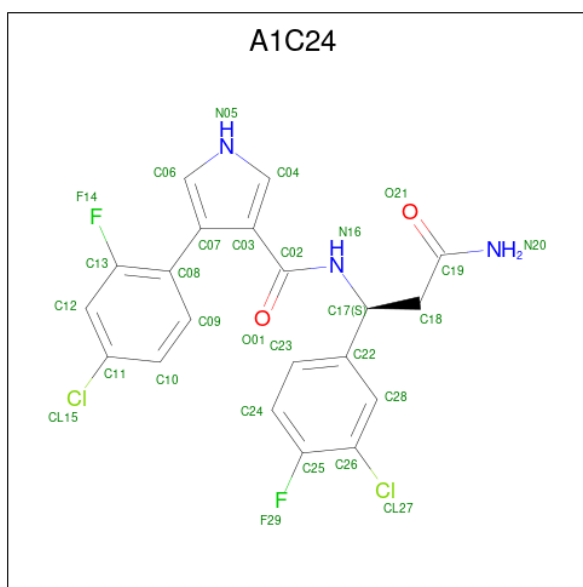
- Molecule 1 is a protein called DDB1- and CUL4-associated factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	1	1
			2367	1496	404	451	16			
1	B	299	Total	C	N	O	S	0	1	1
			2376	1504	406	450	16			
1	C	297	Total	C	N	O	S	0	1	1
			2359	1494	403	446	16			
1	D	298	Total	C	N	O	S	0	0	1
			2362	1491	404	451	16			
1	E	298	Total	C	N	O	S	0	0	1
			2362	1491	404	451	16			
1	F	304	Total	C	N	O	S	0	0	1
			2409	1520	411	461	17			

There are 12 discrepancies between the modelled and reference sequences:

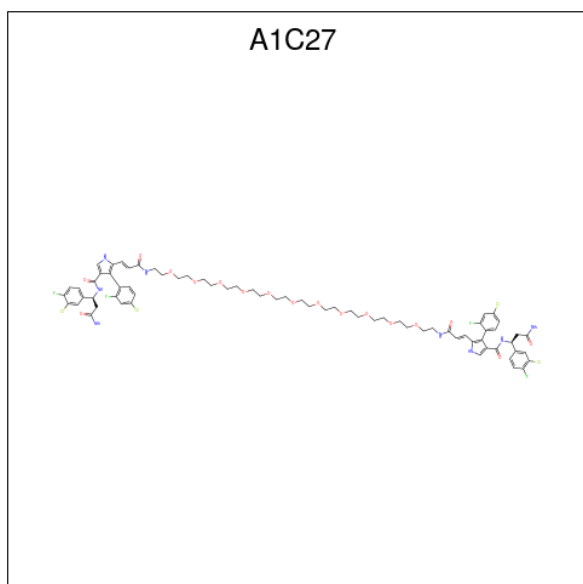
Chain	Residue	Modelled	Actual	Comment	Reference
A	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
A	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6
B	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
B	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6
C	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
C	1079	ALA	ARG	engineered 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: C<sub>20</sub>H<sub>15</sub>Cl<sub>2</sub>F<sub>2</sub>N<sub>3</sub>O<sub>2</sub>) (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	D	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,42E)-3,41-dioxo-7,10,13,16,19,22,25,28,31,34,37-undecaoxa-4,40-diazatritetraconta-1,42-diene-1,43-diyl]bis{N-[(1S)-3-amino-1-(3-chloro-4-fluorophenyl)-3-oxopropyl]-4-(4-chloro-2-fluorophenyl)-1H-pyrrole-3-carboxamide} (CCD ID: A1C27) (formula: C<sub>70</sub>H<sub>82</sub>Cl<sub>4</sub>F<sub>4</sub>N<sub>8</sub>O<sub>17</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	B	1	Total 185	C 70	Cl 4	F 4	H 82	N 8	O 17	0	0
3	C	1	Total 185	C 70	Cl 4	F 4	H 82	N 8	O 17	0	0

- Molecule 4 is water.

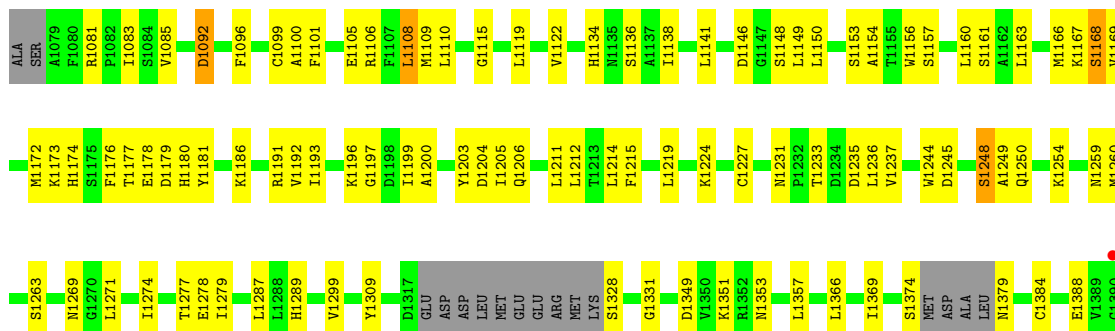
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total 41	O 41	0	0
4	B	38	Total 38	O 38	0	0
4	C	38	Total 38	O 38	0	0
4	D	40	Total 40	O 40	0	0
4	E	41	Total 41	O 41	0	0
4	F	43	Total 43	O 43	0	0

### 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

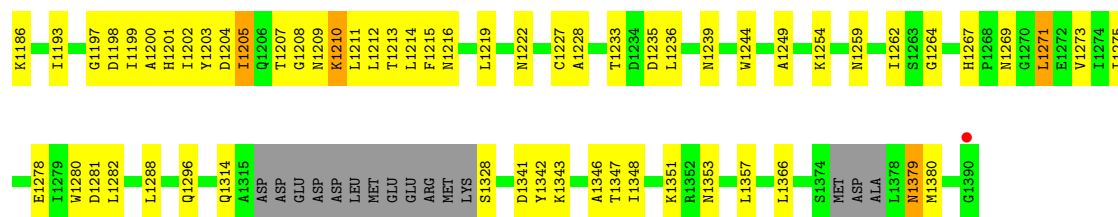
Chain B: 



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

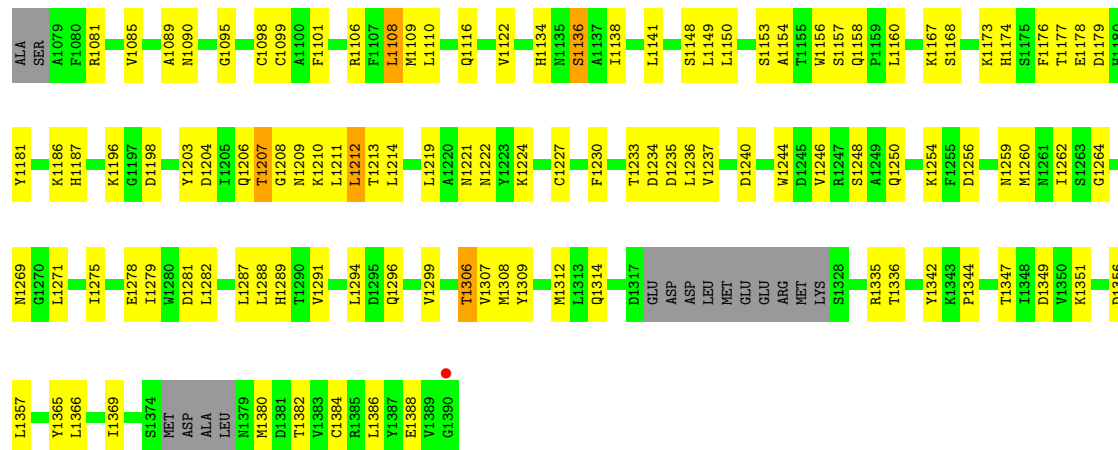
Chain C: 





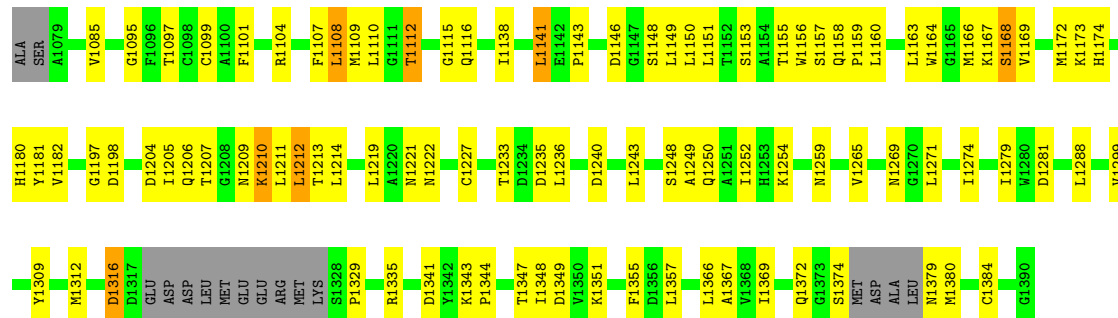
• Molecule 1: DDB1- and CUL4-associated factor 1

Chain D: 60% 33% 5%



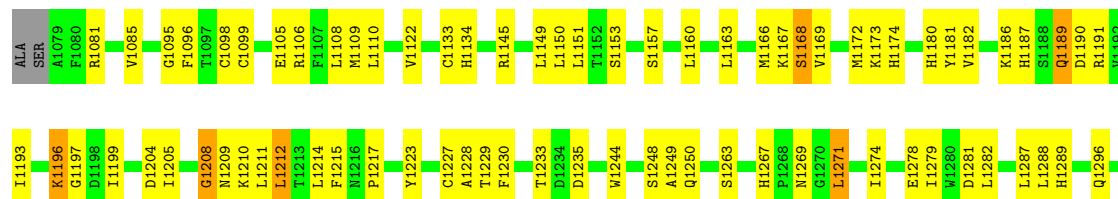
• Molecule 1: DDB1- and CUL4-associated factor 1

Chain E: 64% 29% 5%



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

Chain F: 63% 30% 5%





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.92Å 145.15Å 222.13Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	30.38 – 2.07 30.38 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.38-2.07) 81.1 (30.38-2.07)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.53 (at 2.06Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, $R_{free}$	0.242 , 0.278 0.242 , 0.278	Depositor DCC
$R_{free}$ test set	2041 reflections (1.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 25.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.469 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.469 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.468 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.467 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.477 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14934	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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: A1C27, 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	0.34	0/2424	0.52	0/3287
1	B	0.33	0/2433	0.51	0/3298
1	C	0.33	0/2416	0.53	0/3276
1	D	0.35	0/2416	0.53	0/3276
1	E	0.33	0/2416	0.53	0/3276
1	F	0.33	0/2464	0.52	0/3341
All	All	0.34	0/14569	0.52	0/19754

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	2367	0	2267	96	0
1	B	2376	0	2287	92	0
1	C	2359	0	2270	86	0
1	D	2362	0	2256	97	0
1	E	2362	0	2256	77	0
1	F	2409	0	2305	94	0
2	A	29	15	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	29	15	0	0	0
3	B	103	82	0	0	0
3	C	103	82	0	1	0
4	A	41	0	0	6	0
4	B	38	0	0	2	0
4	C	38	0	0	6	0
4	D	40	0	0	5	0
4	E	41	0	0	6	0
4	F	43	0	0	9	0
All	All	14740	194	13641	526	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 (526) 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:1204:ASP:HB2	1:F:1211:LEU:HD11	1.26	1.13
1:D:1233:THR:OG1	1:D:1235:ASP:OD2	1.80	1.00
1:D:1287:LEU:H	1:E:1372:GLN:HE22	1.03	0.97
1:A:1287:LEU:H	1:B:1372:GLN:HE22	1.01	0.97
1:E:1204:ASP:HB2	1:E:1211:LEU:HD11	1.49	0.95
1:C:1259:ASN:HD21	1:C:1262:ILE:H	1.16	0.93
1:A:1199:ILE:HD13	1:A:1215:PHE:HB2	1.51	0.92
3:C:1401:A1C27:C32	4:E:1401:HOH:O	2.18	0.92
1:D:1136:SER:HB3	1:D:1156:TRP:CD1	2.05	0.91
1:D:1259:ASN:HD21	1:D:1262:ILE:H	1.16	0.91
1:D:1204:ASP:HB2	1:D:1211:LEU:HD11	1.53	0.90
1:E:1351:LYS:HE2	1:E:1351:LYS:HA	1.52	0.90
1:E:1109:MET:HE1	1:E:1150:LEU:HD13	1.54	0.90
1:B:1259:ASN:HD21	1:B:1262:ILE:H	1.12	0.89
1:F:1289:HIS:O	4:F:1401:HOH:O	1.90	0.87
1:D:1287:LEU:H	1:E:1372:GLN:NE2	1.71	0.86
1:B:1233:THR:OG1	1:B:1235:ASP:OD1	1.94	0.85
1:D:1271:LEU:HD21	1:F:1233:THR:HG22	1.57	0.84
1:A:1174:HIS:HB3	4:A:1527:HOH:O	1.77	0.84
1:F:1173:LYS:O	1:F:1174:HIS:ND1	2.10	0.83
1:E:1212:LEU:HD22	1:E:1214:LEU:HD21	1.60	0.83
1:D:1233:THR:HG22	1:F:1271:LEU:HD21	1.59	0.82
1:A:1109:MET:HE1	1:A:1150:LEU:HD13	1.59	0.82
1:A:1212:LEU:HD21	1:A:1249:ALA:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1095:GLY:HA2	1:D:1380:MET:HE2	1.61	0.81
1:E:1312:MET:HE3	4:E:1420:HOH:O	1.80	0.81
1:A:1287:LEU:N	1:B:1372:GLN:HE22	1.80	0.79
1:D:1109:MET:HE1	1:D:1150:LEU:HD13	1.63	0.79
1:D:1312:MET:HE3	4:D:1522:HOH:O	1.82	0.78
1:F:1173:LYS:C	1:F:1174:HIS:HD1	1.90	0.77
1:A:1233:THR:HG22	1:C:1271:LEU:HD21	1.64	0.77
1:A:1233:THR:OG1	1:A:1235:ASP:OD1	2.01	0.77
1:F:1199:ILE:HD13	1:F:1215:PHE:HB2	1.67	0.76
1:F:1204:ASP:CB	1:F:1211:LEU:HD11	2.13	0.76
1:A:1204:ASP:HB2	1:A:1211:LEU:HD11	1.69	0.75
1:B:1212:LEU:HD22	1:B:1214:LEU:HD21	1.69	0.75
1:D:1306:THR:HG22	1:D:1307:VAL:HG23	1.68	0.74
1:E:1204:ASP:OD1	1:E:1206:GLN:N	2.18	0.74
1:C:1109:MET:HE1	1:C:1143:PRO:HB3	1.69	0.74
1:D:1287:LEU:N	1:E:1372:GLN:HE22	1.84	0.74
1:B:1204:ASP:HB2	1:B:1211:LEU:HD21	1.70	0.74
1:A:1287:LEU:H	1:B:1372:GLN:NE2	1.83	0.73
1:A:1136:SER:HB3	1:A:1156:TRP:CZ2	2.23	0.73
1:E:1316:ASP:OD2	4:E:1401:HOH:O	2.07	0.72
1:B:1081:ARG:NH2	1:B:1388:GLU:OE1	2.18	0.72
1:F:1109:MET:HE1	1:F:1150:LEU:HD13	1.70	0.72
1:B:1215:PHE:CE2	1:B:1217:PRO:HG3	2.25	0.72
1:B:1178:GLU:HB3	1:B:1196:LYS:HD3	1.72	0.72
1:D:1210:LYS:HD3	1:D:1213:THR:OG1	1.90	0.71
1:E:1141:LEU:C	1:E:1141:LEU:HD12	2.15	0.71
1:A:1136:SER:HB3	1:A:1156:TRP:CE2	2.25	0.71
1:C:1341:ASP:OD1	1:C:1343:LYS:HB2	1.90	0.71
1:D:1271:LEU:O	1:D:1282:LEU:HB2	1.91	0.70
1:E:1141:LEU:HD12	1:E:1141:LEU:O	1.92	0.70
1:F:1376:ASP:OD1	1:F:1378:LEU:HG	1.92	0.69
1:D:1141:LEU:HD12	1:D:1141:LEU:O	1.92	0.69
1:D:1141:LEU:HD12	1:D:1141:LEU:C	2.17	0.69
1:A:1115:GLY:HA2	1:A:1138[B]:ILE:HD11	1.73	0.69
1:F:1167:LYS:O	1:F:1168:SER:OG	2.05	0.69
1:D:1136:SER:CB	1:D:1156:TRP:CD1	2.77	0.68
1:F:1233:THR:OG1	1:F:1235:ASP:OD1	2.11	0.68
1:B:1212:LEU:HD21	1:B:1249:ALA:HB2	1.75	0.67
1:F:1145:ARG:H	1:F:1189:GLN:NE2	1.92	0.67
1:E:1212:LEU:HD21	1:E:1249:ALA:HB2	1.75	0.67
1:C:1136:SER:HB3	1:C:1156:TRP:CE3	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1205:ILE:O	4:F:1402:HOH:O	2.12	0.67
1:B:1105:GLU:O	1:B:1106:ARG:HB2	1.94	0.67
1:F:1279:ILE:N	4:F:1401:HOH:O	2.02	0.67
1:C:1141:LEU:O	1:C:1141:LEU:HD12	1.96	0.66
1:B:1281:ASP:HB2	1:B:1288:LEU:HD11	1.76	0.66
1:E:1173:LYS:C	1:E:1174:HIS:HD1	2.04	0.66
1:F:1199:ILE:HD13	1:F:1215:PHE:CB	2.26	0.66
1:C:1210:LYS:HD3	1:C:1213:THR:OG1	1.96	0.66
1:A:1115:GLY:HA2	1:A:1138[B]:ILE:CD1	2.26	0.65
1:B:1212:LEU:HD22	1:B:1214:LEU:CD2	2.25	0.65
1:F:1278:GLU:OE1	4:F:1403:HOH:O	2.15	0.65
1:D:1136:SER:HB3	1:D:1156:TRP:NE1	2.12	0.65
1:A:1212:LEU:HD21	1:A:1249:ALA:CB	2.27	0.64
1:E:1221:ASN:ND2	1:E:1240:ASP:O	2.24	0.64
1:F:1306:THR:HG22	1:F:1307:VAL:HG23	1.80	0.64
1:E:1210:LYS:HD3	1:E:1213:THR:OG1	1.98	0.63
1:F:1191:ARG:N	1:F:1205:ILE:HD12	2.13	0.63
1:F:1190:ASP:C	1:F:1205:ILE:HD12	2.23	0.63
1:F:1315:ALA:O	1:F:1316:ASP:HB2	1.97	0.63
1:C:1149:LEU:CD2	1:C:1205:ILE:HD13	2.29	0.63
1:C:1212:LEU:HD21	1:C:1214:LEU:HD21	1.80	0.63
1:F:1271:LEU:O	1:F:1282:LEU:HB2	1.99	0.63
1:B:1141:LEU:C	1:B:1141:LEU:HD12	2.24	0.62
1:D:1221:ASN:ND2	1:D:1240:ASP:O	2.31	0.62
1:A:1108:LEU:HB2	1:A:1122:VAL:HG13	1.80	0.62
1:F:1193:ILE:HD11	1:F:1228:ALA:HB1	1.80	0.62
1:B:1215:PHE:HE2	1:B:1217:PRO:HG3	1.65	0.62
1:B:1204:ASP:OD1	1:B:1206:GLN:N	2.32	0.61
1:C:1186:LYS:HE3	4:C:1525:HOH:O	2.00	0.61
1:C:1181:TYR:CE2	1:C:1227:CYS:HB3	2.36	0.61
1:E:1204:ASP:CB	1:E:1211:LEU:HD11	2.28	0.61
1:A:1204:ASP:OD1	1:A:1206:GLN:N	2.33	0.61
1:A:1233:THR:CG2	1:C:1271:LEU:HD21	2.30	0.61
1:A:1245:ASP:OD1	4:A:1501:HOH:O	2.16	0.61
1:C:1259:ASN:HD22	1:C:1296:GLN:HE22	1.48	0.61
1:A:1105:GLU:O	1:A:1106:ARG:HB2	2.01	0.61
1:B:1117:LEU:HD21	1:B:1141:LEU:HD22	1.83	0.60
1:C:1264:GLY:O	4:C:1502:HOH:O	2.16	0.60
1:A:1081:ARG:HH21	1:A:1388:GLU:CD	2.08	0.60
1:C:1278:GLU:OE1	4:C:1501:HOH:O	2.16	0.60
1:A:1108:LEU:HB2	1:A:1122:VAL:CG1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:ILE:HD13	1:A:1215:PHE:CB	2.29	0.60
1:D:1204:ASP:OD1	1:D:1206:GLN:N	2.34	0.60
1:C:1269:ASN:O	1:C:1271:LEU:HD22	2.02	0.60
1:E:1151:LEU:HD22	1:E:1182:VAL:HG21	1.82	0.60
1:A:1214:LEU:HD22	1:A:1244:TRP:CE3	2.37	0.60
1:E:1204:ASP:OD2	1:E:1207:THR:HG23	2.01	0.59
1:C:1108:LEU:HB2	1:C:1122:VAL:CG1	2.32	0.59
1:D:1187:HIS:HB3	1:D:1234:ASP:OD2	2.03	0.59
1:D:1279:ILE:HG13	1:D:1289:HIS:HB2	1.85	0.59
1:A:1136:SER:HB3	1:A:1156:TRP:CH2	2.37	0.59
1:B:1216:ASN:C	1:B:1216:ASN:HD22	2.11	0.59
1:E:1347:THR:C	1:E:1348:ILE:HD12	2.27	0.59
1:D:1335:ARG:NH1	4:D:1503:HOH:O	2.34	0.59
1:B:1347:THR:C	1:B:1348:ILE:HD12	2.28	0.59
1:B:1351:LYS:CE	1:B:1351:LYS:HA	2.33	0.59
1:F:1209:ASN:O	1:F:1211:LEU:N	2.36	0.59
1:E:1181:TYR:CE2	1:E:1227:CYS:HB3	2.37	0.58
1:B:1133:CYS:HB3	1:B:1164:TRP:CZ2	2.39	0.58
1:A:1269:ASN:O	1:A:1271:LEU:HD12	2.03	0.58
1:D:1212:LEU:HD23	1:D:1213:THR:H	1.68	0.58
1:E:1204:ASP:OD1	1:E:1205:ILE:N	2.36	0.58
1:A:1351:LYS:HE2	1:A:1351:LYS:HA	1.84	0.58
1:E:1212:LEU:HD21	1:E:1249:ALA:CB	2.32	0.58
1:C:1212:LEU:HD11	1:C:1249:ALA:CB	2.33	0.58
1:D:1167:LYS:O	1:D:1168:SER:OG	2.17	0.58
1:D:1269:ASN:O	1:D:1271:LEU:HD22	2.04	0.57
1:E:1212:LEU:HD22	1:E:1214:LEU:CD2	2.33	0.57
1:E:1329:PRO:HG2	1:E:1355:PHE:HA	1.86	0.57
1:B:1115:GLY:HA2	1:B:1138[A]:ILE:HG13	1.86	0.57
1:A:1134:HIS:CD2	1:A:1138[B]:ILE:HD12	2.39	0.57
1:C:1259:ASN:ND2	1:C:1262:ILE:H	1.96	0.57
1:B:1212:LEU:HD21	1:B:1249:ALA:CB	2.34	0.57
1:B:1357:LEU:HD12	1:B:1357:LEU:C	2.30	0.56
1:C:1134:HIS:HD2	1:C:1138[B]:ILE:HD12	1.71	0.56
1:D:1136:SER:HB3	1:D:1156:TRP:HD1	1.64	0.56
1:D:1204:ASP:CB	1:D:1211:LEU:HD11	2.32	0.56
1:D:1214:LEU:HD22	1:D:1244:TRP:CE3	2.41	0.56
1:E:1104:ARG:HG2	1:E:1107:PHE:HD2	1.70	0.56
1:F:1209:ASN:O	1:F:1211:LEU:HG	2.05	0.56
1:D:1207:THR:HG1	1:D:1209:ASN:H	1.51	0.56
1:B:1245:ASP:OD1	4:B:1501:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1357:LEU:HD12	1:D:1357:LEU:C	2.30	0.56
1:F:1157:SER:O	1:F:1160:LEU:HD23	2.06	0.56
1:A:1181:TYR:CE2	1:A:1227:CYS:HB3	2.41	0.56
1:B:1271:LEU:O	1:B:1282:LEU:HB2	2.06	0.56
1:C:1115:GLY:HA2	1:C:1138[B]:ILE:CD1	2.36	0.56
1:D:1233:THR:CG2	1:F:1271:LEU:HD21	2.33	0.56
1:E:1351:LYS:HE2	1:E:1351:LYS:CA	2.31	0.56
1:A:1357:LEU:HD13	1:A:1366:LEU:HD11	1.87	0.56
1:A:1148:SER:OG	1:A:1149:LEU:HD13	2.06	0.55
1:A:1163:LEU:HD21	1:A:1205:ILE:HG23	1.87	0.55
1:C:1207:THR:C	1:C:1209:ASN:H	2.15	0.55
1:E:1349:ASP:CG	1:E:1351:LYS:HE3	2.31	0.55
1:D:1167:LYS:C	1:D:1168:SER:HG	2.11	0.55
1:C:1105:GLU:C	1:C:1106:ARG:HG3	2.31	0.55
1:D:1207:THR:HG1	1:D:1209:ASN:CG	2.07	0.55
1:F:1108:LEU:HB2	1:F:1122:VAL:CG1	2.36	0.55
1:B:1167:LYS:C	1:B:1168:SER:HG	2.12	0.55
1:D:1271:LEU:HD11	1:F:1233:THR:HB	1.88	0.55
1:B:1095:GLY:HA2	1:B:1380:MET:HE2	1.88	0.55
1:A:1109:MET:CE	1:A:1150:LEU:HD13	2.32	0.55
1:E:1198:ASP:OD2	1:E:1222:ASN:HA	2.05	0.55
1:F:1181:TYR:CE2	1:F:1227:CYS:HB3	2.42	0.55
1:F:1149:LEU:HB3	1:F:1163:LEU:HD11	1.88	0.55
1:C:1204:ASP:HB2	1:C:1211:LEU:HD11	1.88	0.54
1:D:1259:ASN:ND2	1:D:1262:ILE:H	1.97	0.54
1:E:1281:ASP:HB2	1:E:1288:LEU:HD11	1.88	0.54
1:F:1150:LEU:HB2	1:F:1166:MET:HE2	1.90	0.54
1:F:1274:ILE:HG23	1:F:1279:ILE:HD13	1.90	0.54
1:A:1167:LYS:C	1:A:1168:SER:HG	2.15	0.54
1:C:1097:THR:HG22	1:C:1380:MET:HE1	1.89	0.54
1:D:1335:ARG:HG2	1:D:1347:THR:HA	1.90	0.54
1:F:1296:GLN:HB2	1:F:1312:MET:HG3	1.90	0.54
1:E:1180:HIS:HE1	1:E:1197:GLY:H	1.56	0.54
1:C:1134:HIS:CD2	1:C:1138[B]:ILE:HD12	2.42	0.54
1:A:1374:SER:HG	1:A:1379:ASN:N	2.06	0.53
1:F:1151:LEU:HD22	1:F:1182:VAL:HG21	1.90	0.53
1:F:1357:LEU:HD12	1:F:1357:LEU:C	2.32	0.53
1:B:1299:VAL:HA	1:B:1309:TYR:O	2.09	0.53
1:C:1198:ASP:OD2	1:C:1222:ASN:HA	2.09	0.53
1:E:1209:ASN:O	1:E:1211:LEU:HG	2.09	0.53
1:B:1329:PRO:HG2	1:B:1355:PHE:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1357:LEU:HD13	1:C:1366:LEU:HD11	1.90	0.53
1:D:1235:ASP:OD1	1:D:1236:LEU:HG	2.09	0.53
1:D:1380:MET:HE3	1:D:1382:THR:CG2	2.39	0.53
1:D:1173:LYS:O	1:D:1174:HIS:HD2	1.91	0.53
1:A:1200:ALA:HB3	1:A:1214:LEU:HB2	1.91	0.52
1:A:1263:SER:HB2	4:A:1517:HOH:O	2.09	0.52
1:C:1109:MET:CE	1:C:1150:LEU:HD13	2.39	0.52
1:D:1233:THR:HG22	1:F:1271:LEU:CD2	2.33	0.52
1:A:1192:VAL:HG23	1:A:1205:ILE:HG12	1.91	0.52
1:C:1109:MET:HE1	1:C:1150:LEU:HD13	1.91	0.52
1:D:1259:ASN:HD22	1:D:1296:GLN:HE22	1.56	0.52
1:E:1146:ASP:OD1	1:E:1148:SER:OG	2.22	0.52
1:A:1141:LEU:HD12	1:A:1141:LEU:C	2.34	0.52
1:D:1207:THR:OG1	1:D:1208:GLY:N	2.41	0.52
1:B:1107:PHE:CE1	1:B:1128:GLU:HG2	2.44	0.52
1:E:1209:ASN:O	1:E:1211:LEU:N	2.42	0.52
1:A:1106:ARG:O	1:A:1122:VAL:HG22	2.09	0.52
1:B:1273:VAL:HG23	1:B:1280:TRP:HB2	1.92	0.52
1:D:1085:VAL:HA	1:D:1384:CYS:O	2.08	0.52
1:E:1155:THR:HG22	1:E:1156:TRP:CD1	2.45	0.52
1:F:1186:LYS:HE3	4:F:1425:HOH:O	2.09	0.52
1:C:1115:GLY:HA2	1:C:1138[B]:ILE:HD11	1.92	0.52
1:A:1196:LYS:O	1:A:1199:ILE:HB	2.10	0.52
1:C:1379:ASN:HB2	4:C:1531:HOH:O	2.10	0.52
1:F:1193:ILE:CD1	1:F:1228:ALA:HB1	2.39	0.52
1:A:1136:SER:HB3	1:A:1156:TRP:CD2	2.45	0.52
1:B:1187:HIS:HB3	1:B:1234:ASP:OD2	2.10	0.52
1:E:1157:SER:O	1:E:1160:LEU:HD23	2.10	0.51
1:A:1351:LYS:HA	1:A:1351:LYS:CE	2.41	0.51
1:C:1156:TRP:HZ3	4:C:1529:HOH:O	1.93	0.51
1:C:1351:LYS:HA	1:C:1351:LYS:CE	2.40	0.51
1:D:1308:MET:O	1:D:1336:THR:HA	2.11	0.51
1:E:1141:LEU:C	1:E:1141:LEU:CD1	2.82	0.51
1:B:1105:GLU:O	1:B:1106:ARG:CB	2.59	0.51
1:E:1101:PHE:HA	1:E:1108:LEU:HD23	1.91	0.51
1:A:1141:LEU:HD12	1:A:1141:LEU:O	2.11	0.51
1:B:1160:LEU:HB2	1:B:1177:THR:O	2.11	0.51
1:C:1212:LEU:HD11	1:C:1249:ALA:HB2	1.92	0.51
1:F:1215:PHE:CE2	1:F:1217:PRO:HD3	2.46	0.51
1:F:1287:LEU:CD1	4:F:1401:HOH:O	2.58	0.51
1:A:1101:PHE:HA	1:A:1108:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1155:THR:HG22	1:B:1156:TRP:HD1	1.76	0.51
1:C:1168:SER:OG	1:C:1169:VAL:N	2.43	0.51
1:D:1212:LEU:HD22	1:D:1214:LEU:HG	1.92	0.51
1:F:1214:LEU:HD22	1:F:1244:TRP:CE3	2.45	0.51
1:E:1109:MET:CE	1:E:1150:LEU:HD13	2.35	0.51
1:E:1204:ASP:OD1	1:E:1204:ASP:C	2.53	0.51
1:A:1357:LEU:HD12	1:A:1357:LEU:C	2.36	0.51
1:D:1110:LEU:HD23	1:D:1369:ILE:HD11	1.93	0.51
1:A:1134:HIS:CG	1:A:1154:ALA:HB2	2.46	0.50
1:B:1207:THR:C	1:B:1209:ASN:H	2.19	0.50
1:C:1141:LEU:HD12	1:C:1141:LEU:C	2.36	0.50
1:D:1160:LEU:HB2	1:D:1177:THR:O	2.12	0.50
1:F:1315:ALA:O	1:F:1316:ASP:CB	2.60	0.50
1:B:1109:MET:HE1	1:B:1143:PRO:HB3	1.93	0.50
1:A:1156:TRP:CE3	1:A:1157:SER:N	2.79	0.50
1:D:1271:LEU:HD21	1:F:1233:THR:CG2	2.37	0.50
1:F:1110:LEU:HD23	1:F:1369:ILE:HD11	1.93	0.50
1:F:1248:SER:O	1:F:1250:GLN:HG2	2.11	0.50
1:F:1315:ALA:HB1	1:F:1318:GLU:HG2	1.94	0.50
1:D:1278:GLU:OE1	4:D:1501:HOH:O	2.18	0.50
1:E:1274:ILE:HG23	1:E:1279:ILE:CD1	2.42	0.50
1:E:1248:SER:O	1:E:1250:GLN:HG2	2.12	0.49
1:D:1349:ASP:OD1	1:D:1351:LYS:HD3	2.11	0.49
1:C:1347:THR:C	1:C:1348:ILE:HD13	2.37	0.49
1:E:1099:CYS:HA	1:E:1109:MET:O	2.12	0.49
1:E:1112:THR:HG23	1:E:1116:GLN:O	2.11	0.49
1:E:1164:TRP:CH2	1:E:1172:MET:HE2	2.47	0.49
1:B:1357:LEU:HD13	1:B:1366:LEU:HD11	1.94	0.49
1:E:1344:PRO:HB3	4:E:1410:HOH:O	2.12	0.49
1:F:1263:SER:HB2	4:F:1431:HOH:O	2.12	0.49
1:F:1328:SER:OG	1:F:1353:ASN:HB3	2.13	0.49
1:A:1081:ARG:NH2	1:A:1388:GLU:OE1	2.41	0.49
1:D:1248:SER:O	1:D:1250:GLN:HG2	2.12	0.49
1:E:1149:LEU:O	1:E:1166:MET:HE2	2.12	0.49
1:F:1081:ARG:NH2	1:F:1388:GLU:OE1	2.43	0.49
1:F:1099:CYS:HA	1:F:1109:MET:O	2.12	0.49
1:A:1148:SER:C	1:A:1149:LEU:HD12	2.38	0.49
1:E:1348:ILE:HD12	1:E:1348:ILE:N	2.28	0.49
1:C:1134:HIS:CG	1:C:1154:ALA:HB2	2.48	0.49
1:F:1145:ARG:H	1:F:1189:GLN:HE22	1.61	0.49
1:A:1299:VAL:HA	1:A:1309:TYR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1198:ASP:OD2	1:D:1222:ASN:HA	2.12	0.49
1:F:1212:LEU:HD21	1:F:1249:ALA:HB2	1.94	0.49
1:D:1141:LEU:C	1:D:1141:LEU:CD1	2.86	0.48
1:B:1272:GLU:OE2	1:B:1342:TYR:OH	2.25	0.48
1:E:1274:ILE:HG23	1:E:1279:ILE:HD13	1.95	0.48
1:A:1271:LEU:HD11	1:C:1233:THR:HG22	1.95	0.48
1:C:1176:PHE:HB3	1:C:1179:ASP:OD2	2.12	0.48
1:D:1210:LYS:HD3	1:D:1213:THR:HG1	1.77	0.48
1:D:1212:LEU:HD23	1:D:1213:THR:N	2.27	0.48
1:B:1134:HIS:CG	1:B:1154:ALA:HB2	2.49	0.48
1:A:1278:GLU:OE1	4:A:1502:HOH:O	2.20	0.48
1:B:1209:ASN:O	1:B:1211:LEU:N	2.46	0.48
1:E:1210:LYS:HD3	1:E:1213:THR:HG1	1.79	0.48
1:A:1178:GLU:HB3	1:A:1196:LYS:HD3	1.95	0.48
1:C:1141:LEU:C	1:C:1141:LEU:CD1	2.87	0.48
1:D:1186:LYS:NZ	4:D:1505:HOH:O	2.46	0.48
1:F:1212:LEU:HD21	1:F:1249:ALA:CB	2.43	0.48
1:C:1151:LEU:HD22	1:C:1182:VAL:CG2	2.44	0.48
1:F:1105:GLU:O	1:F:1106:ARG:HB2	2.14	0.48
1:B:1351:LYS:HA	1:B:1351:LYS:HE2	1.96	0.48
1:D:1357:LEU:HD13	1:D:1366:LEU:HD11	1.96	0.48
1:A:1134:HIS:HD2	1:A:1138[B]:ILE:HD12	1.77	0.48
1:B:1099:CYS:HA	1:B:1109:MET:O	2.14	0.48
1:C:1149:LEU:HD23	1:C:1205:ILE:HD13	1.95	0.48
1:D:1291:VAL:HB	1:D:1294:LEU:HD12	1.96	0.48
1:C:1181:TYR:OH	1:C:1183:GLU:OE2	2.21	0.47
1:D:1136:SER:HB3	1:D:1156:TRP:HE1	1.79	0.47
1:E:1335:ARG:HG2	4:E:1410:HOH:O	2.12	0.47
1:A:1099:CYS:HA	1:A:1109:MET:O	2.14	0.47
1:A:1193:ILE:O	1:A:1193:ILE:HG23	2.14	0.47
1:C:1209:ASN:O	1:C:1211:LEU:N	2.47	0.47
1:E:1167:LYS:O	1:E:1168:SER:OG	2.10	0.47
1:C:1351:LYS:HA	1:C:1351:LYS:HE2	1.96	0.47
1:D:1271:LEU:CD2	1:F:1233:THR:HG22	2.38	0.47
1:B:1296:GLN:HB2	1:B:1312:MET:HG3	1.95	0.47
1:D:1179:ASP:OD2	1:D:1203:TYR:OH	2.32	0.47
1:E:1233:THR:OG1	1:E:1235:ASP:OD1	2.28	0.47
1:A:1279:ILE:HG13	1:A:1289:HIS:HB2	1.96	0.47
1:B:1207:THR:O	1:B:1209:ASN:N	2.48	0.47
1:C:1328:SER:OG	1:C:1353:ASN:HB3	2.15	0.47
1:A:1096:PHE:CD1	1:A:1110:LEU:HD22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1193:ILE:HD11	1:C:1228:ALA:HB1	1.97	0.47
1:E:1344:PRO:CB	4:E:1410:HOH:O	2.61	0.47
1:F:1374:SER:O	1:F:1375:MET:CB	2.63	0.47
1:A:1191:ARG:HA	1:A:1205:ILE:HG13	1.96	0.47
1:A:1231:ASN:CG	1:A:1236:LEU:HB2	2.40	0.47
1:B:1109:MET:CE	1:B:1143:PRO:HB3	2.44	0.47
1:B:1145:ARG:NH2	1:B:1186:LYS:O	2.43	0.47
1:D:1181:TYR:CE2	1:D:1227:CYS:HB3	2.49	0.47
1:D:1365:TYR:HB3	1:D:1386:LEU:HD11	1.97	0.47
1:E:1095:GLY:O	1:E:1097:THR:HG23	2.14	0.47
1:E:1235:ASP:OD2	1:E:1236:LEU:HG	2.15	0.47
1:C:1357:LEU:C	1:C:1357:LEU:HD12	2.40	0.47
1:F:1299:VAL:HA	1:F:1309:TYR:O	2.15	0.47
1:C:1212:LEU:HD21	1:C:1249:ALA:HB2	1.96	0.47
1:D:1380:MET:HE3	1:D:1382:THR:HG23	1.97	0.47
1:A:1160:LEU:HB2	1:A:1177:THR:O	2.14	0.47
1:B:1274:ILE:HG23	1:B:1279:ILE:CD1	2.45	0.47
1:D:1136:SER:CB	1:D:1156:TRP:HD1	2.23	0.47
1:A:1160:LEU:HD23	1:A:1160:LEU:HA	1.68	0.46
1:F:1204:ASP:HB2	1:F:1211:LEU:CD1	2.20	0.46
1:A:1199:ILE:CD1	1:A:1215:PHE:HB2	2.36	0.46
1:D:1299:VAL:HA	1:D:1309:TYR:O	2.16	0.46
1:D:1344:PRO:CB	4:D:1521:HOH:O	2.62	0.46
1:F:1223:TYR:CD2	1:F:1263:SER:HA	2.51	0.46
1:A:1219:LEU:O	1:A:1254:LYS:HD2	2.16	0.46
1:C:1199:ILE:HD13	1:C:1215:PHE:CD1	2.51	0.46
1:F:1105:GLU:O	1:F:1106:ARG:CB	2.64	0.46
1:B:1210:LYS:HD3	1:B:1213:THR:OG1	2.15	0.46
1:B:1221:ASN:ND2	1:B:1240:ASP:O	2.48	0.46
1:E:1167:LYS:C	1:E:1168:SER:HG	2.11	0.46
1:F:1133:CYS:HB3	1:F:1134:HIS:CD2	2.50	0.46
1:F:1318:GLU:HA	1:F:1318:GLU:OE1	2.15	0.46
1:F:1378:LEU:O	1:F:1379:ASN:HB2	2.15	0.46
1:B:1150:LEU:HD12	1:B:1151:LEU:N	2.30	0.46
1:D:1098:CYS:HA	1:D:1356:ASP:HB2	1.97	0.46
1:F:1281:ASP:HB2	1:F:1288:LEU:HD11	1.97	0.46
1:D:1095:GLY:CA	1:D:1380:MET:HE2	2.40	0.46
1:C:1200:ALA:HB2	1:C:1239:ASN:OD1	2.16	0.46
1:D:1198:ASP:OD2	1:D:1222:ASN:ND2	2.49	0.46
1:B:1308:MET:O	1:B:1336:THR:HA	2.16	0.46
1:A:1180:HIS:HE1	1:A:1197:GLY:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1134:HIS:HD2	1:B:1138[B]:ILE:CD1	2.29	0.45
1:B:1164:TRP:CH2	1:B:1172:MET:HE2	2.51	0.45
1:B:1193:ILE:HD11	1:B:1228:ALA:HB1	1.98	0.45
1:B:1348:ILE:HD12	1:B:1348:ILE:N	2.31	0.45
1:D:1219:LEU:O	1:D:1254:LYS:NZ	2.46	0.45
1:A:1277:THR:OG1	1:A:1278:GLU:OE2	2.29	0.45
1:D:1224:LYS:HE3	1:D:1260:MET:HE3	1.97	0.45
1:E:1168:SER:OG	1:E:1169:VAL:N	2.47	0.45
1:A:1150:LEU:HB2	1:A:1166:MET:HE2	1.98	0.45
1:C:1180:HIS:HE1	1:C:1197:GLY:H	1.63	0.45
1:C:1267:HIS:HD2	1:C:1342:TYR:OH	1.99	0.45
1:E:1104:ARG:HG2	1:E:1107:PHE:CD2	2.50	0.45
1:A:1136:SER:HB3	1:A:1156:TRP:CZ3	2.51	0.45
1:D:1099:CYS:HA	1:D:1109:MET:O	2.16	0.45
1:F:1287:LEU:HD12	4:F:1401:HOH:O	2.16	0.45
1:E:1085:VAL:HA	1:E:1384:CYS:O	2.17	0.45
1:E:1243:LEU:HG	1:E:1252:ILE:HD11	1.99	0.45
1:E:1265:VAL:HG21	1:E:1299:VAL:CG2	2.46	0.45
1:E:1299:VAL:HA	1:E:1309:TYR:O	2.16	0.45
1:B:1294:LEU:HD11	1:B:1308:MET:HE1	1.97	0.45
1:F:1095:GLY:HA2	1:F:1380:MET:HE2	1.98	0.45
1:F:1174:HIS:HD2	1:F:1208:GLY:CA	2.30	0.45
1:A:1274:ILE:HG23	1:A:1279:ILE:CD1	2.47	0.45
1:C:1212:LEU:CD2	1:C:1214:LEU:HD21	2.46	0.45
1:D:1173:LYS:C	1:D:1174:HIS:CD2	2.95	0.45
1:B:1259:ASN:HB3	1:B:1276:ASN:ND2	2.32	0.45
1:E:1374:SER:O	1:E:1379:ASN:N	2.50	0.45
1:F:1180:HIS:HE1	1:F:1197:GLY:H	1.64	0.45
1:B:1096:PHE:CD1	1:B:1110:LEU:HD22	2.52	0.45
1:B:1219:LEU:O	1:B:1254:LYS:HD2	2.17	0.45
1:D:1134:HIS:CG	1:D:1154:ALA:HB2	2.52	0.45
1:F:1306:THR:CG2	1:F:1307:VAL:HG23	2.47	0.45
1:C:1149:LEU:N	1:C:1149:LEU:HD12	2.32	0.44
1:C:1202:ILE:HD12	1:C:1212:LEU:HD23	1.99	0.44
1:E:1219:LEU:O	1:E:1254:LYS:NZ	2.49	0.44
1:F:1172:MET:HE2	1:F:1172:MET:HB2	1.81	0.44
1:F:1106:ARG:O	1:F:1122:VAL:HG22	2.17	0.44
1:F:1315:ALA:HB1	1:F:1318:GLU:CG	2.47	0.44
1:F:1327:LYS:HB2	1:F:1327:LYS:HE3	1.84	0.44
1:B:1149:LEU:HB3	1:B:1163:LEU:HD11	2.00	0.44
1:C:1148:SER:C	1:C:1149:LEU:HD12	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1160:LEU:HD23	1:F:1160:LEU:HA	1.83	0.44
1:B:1115:GLY:HA2	1:B:1138[B]:ILE:HG12	1.99	0.44
1:A:1100:ALA:O	1:A:1108:LEU:HD22	2.18	0.44
1:C:1151:LEU:HD22	1:C:1182:VAL:HG21	1.98	0.44
1:D:1335:ARG:HD3	1:D:1347:THR:OG1	2.17	0.44
1:D:1101:PHE:HA	1:D:1108:LEU:HD23	1.99	0.44
1:D:1156:TRP:CG	1:D:1157:SER:N	2.83	0.44
1:F:1347:THR:C	1:F:1348:ILE:HD13	2.43	0.44
1:B:1312:MET:HB3	1:B:1312:MET:HE2	1.68	0.44
1:C:1219:LEU:O	1:C:1254:LYS:NZ	2.50	0.44
1:E:1149:LEU:HD22	1:E:1163:LEU:HD11	2.00	0.44
1:A:1167:LYS:O	1:A:1169:VAL:N	2.51	0.44
1:E:1357:LEU:HA	1:E:1367:ALA:O	2.18	0.44
1:A:1248:SER:O	1:A:1250:GLN:HG2	2.17	0.44
1:E:1141:LEU:HA	1:E:1151:LEU:O	2.18	0.44
1:B:1231:ASN:HA	1:B:1266:PHE:CD2	2.53	0.43
1:C:1181:TYR:CD2	1:C:1227:CYS:HB3	2.52	0.43
1:F:1098:CYS:HA	1:F:1356:ASP:HB2	2.00	0.43
1:A:1224:LYS:HE3	1:A:1260:MET:HE3	2.00	0.43
1:C:1214:LEU:HD22	1:C:1244:TRP:CE3	2.53	0.43
1:D:1108:LEU:HB2	1:D:1122:VAL:CG1	2.48	0.43
1:F:1173:LYS:C	1:F:1174:HIS:ND1	2.69	0.43
1:B:1191:ARG:HH12	1:B:1246:VAL:HG11	1.83	0.43
1:F:1151:LEU:HD22	1:F:1182:VAL:CG2	2.48	0.43
1:A:1085:VAL:HA	1:A:1384:CYS:O	2.18	0.43
1:B:1149:LEU:N	1:B:1149:LEU:CD1	2.81	0.43
1:A:1149:LEU:CD1	1:A:1149:LEU:N	2.82	0.43
1:A:1289:HIS:HD2	4:A:1537:HOH:O	2.00	0.43
1:E:1341:ASP:OD1	1:E:1343:LYS:HB2	2.18	0.43
1:F:1279:ILE:HG13	1:F:1289:HIS:HB2	2.00	0.43
1:B:1351:LYS:O	1:B:1352:ARG:HG3	2.18	0.43
1:B:1199:ILE:CD1	1:B:1215:PHE:CG	3.02	0.43
1:C:1120:TYR:CZ	1:C:1127:GLU:HB2	2.54	0.43
1:F:1085:VAL:HA	1:F:1384:CYS:O	2.19	0.43
1:F:1308:MET:O	1:F:1336:THR:HA	2.19	0.43
1:A:1274:ILE:HG23	1:A:1279:ILE:HD13	2.00	0.43
1:C:1171:ASP:N	1:C:1171:ASP:OD1	2.51	0.43
1:D:1173:LYS:C	1:D:1174:HIS:HD2	2.27	0.43
1:A:1092:ASP:OD1	1:A:1092:ASP:N	2.51	0.42
1:C:1215:PHE:CG	1:C:1216:ASN:N	2.87	0.42
1:D:1116:GLN:O	1:D:1138:ILE:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1328:SER:HB2	1:F:1355:PHE:CE1	2.54	0.42
1:C:1095:GLY:HA3	4:C:1520:HOH:O	2.19	0.42
1:E:1110:LEU:HD23	1:E:1369:ILE:HD11	2.00	0.42
1:B:1096:PHE:CG	1:B:1110:LEU:HD22	2.53	0.42
1:B:1185:SER:O	1:B:1189:GLN:HG2	2.19	0.42
1:B:1186:LYS:NZ	1:B:1230:PHE:O	2.45	0.42
1:C:1098:CYS:SG	1:C:1138[A]:ILE:HG22	2.59	0.42
1:C:1264:GLY:HA3	1:C:1275:ILE:HG12	2.02	0.42
1:D:1106:ARG:O	1:D:1122:VAL:HG22	2.19	0.42
1:B:1351:LYS:HA	1:B:1351:LYS:HE3	2.01	0.42
1:F:1096:PHE:HB3	1:F:1369:ILE:HD12	2.01	0.42
1:A:1172:MET:HE2	1:A:1172:MET:HB2	1.87	0.42
1:B:1081:ARG:HH21	1:B:1388:GLU:CD	2.17	0.42
1:D:1089:ALA:O	1:D:1090:ASN:HB2	2.20	0.42
1:D:1279:ILE:HD12	1:D:1342:TYR:CE1	2.55	0.42
1:F:1385:ARG:HD3	4:F:1411:HOH:O	2.19	0.42
1:A:1110:LEU:HD23	1:A:1369:ILE:HD11	2.01	0.42
1:A:1233:THR:HG22	1:C:1271:LEU:CD2	2.42	0.42
1:C:1149:LEU:N	1:C:1149:LEU:CD1	2.82	0.42
1:A:1199:ILE:CD1	1:A:1215:PHE:CB	2.95	0.42
1:C:1099:CYS:HA	1:C:1109:MET:O	2.20	0.42
1:D:1186:LYS:HD2	1:D:1230:PHE:O	2.20	0.42
1:E:1357:LEU:HD13	1:E:1366:LEU:HD11	2.01	0.42
1:B:1110:LEU:HD23	1:B:1369:ILE:HD11	2.01	0.42
1:C:1207:THR:C	1:C:1209:ASN:N	2.78	0.42
1:C:1273:VAL:HG23	1:C:1280:TRP:HB2	2.02	0.42
1:B:1148:SER:C	1:B:1149:LEU:HD12	2.45	0.42
1:B:1149:LEU:N	1:B:1149:LEU:HD12	2.35	0.42
1:B:1236:LEU:HD13	1:B:1243:LEU:HD11	2.01	0.42
1:C:1106:ARG:HH11	1:C:1106:ARG:HG2	1.85	0.42
1:C:1167:LYS:O	1:C:1168:SER:OG	2.18	0.42
1:C:1201:HIS:HB2	1:C:1203:TYR:CE1	2.55	0.42
1:D:1281:ASP:HB2	1:D:1288:LEU:HD11	2.02	0.42
1:E:1109:MET:CE	1:E:1143:PRO:HB3	2.50	0.42
1:F:1085:VAL:O	1:F:1085:VAL:HG13	2.19	0.42
1:C:1346:ALA:HB1	1:C:1348:ILE:HD11	2.02	0.42
1:A:1173:LYS:HA	1:A:1173:LYS:HD3	1.79	0.41
1:D:1178:GLU:HB3	1:D:1196:LYS:HD2	2.02	0.41
1:A:1269:ASN:OD1	1:A:1269:ASN:C	2.63	0.41
1:F:1196:LYS:O	1:F:1199:ILE:HB	2.21	0.41
1:B:1159:PRO:HG3	1:B:1175:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1274:ILE:HG23	1:F:1279:ILE:CD1	2.50	0.41
1:B:1085:VAL:HA	1:B:1384:CYS:O	2.21	0.41
1:C:1282:LEU:HD23	1:C:1282:LEU:HA	1.84	0.41
1:A:1146:ASP:CG	1:A:1148:SER:HG	2.29	0.41
1:C:1173:LYS:HA	1:C:1173:LYS:HD3	1.79	0.41
1:F:1174:HIS:CD2	1:F:1208:GLY:CA	3.03	0.41
1:B:1226:ASN:OD1	1:B:1240:ASP:N	2.54	0.41
1:B:1269:ASN:OD1	1:B:1269:ASN:C	2.63	0.41
1:D:1136:SER:OG	1:D:1157:SER:HB3	2.21	0.41
1:F:1168:SER:OG	1:F:1169:VAL:N	2.52	0.41
1:B:1141:LEU:HD12	1:B:1141:LEU:O	2.21	0.41
1:B:1327:LYS:HE3	4:B:1515:HOH:O	2.21	0.41
1:A:1083:ILE:HD13	1:A:1083:ILE:HA	1.87	0.41
1:A:1328:SER:OG	1:A:1353:ASN:HB3	2.21	0.41
1:C:1106:ARG:O	1:C:1122:VAL:HG22	2.20	0.41
1:C:1108:LEU:HB2	1:C:1122:VAL:HG13	2.02	0.41
1:D:1176:PHE:O	1:D:1177:THR:C	2.63	0.41
1:E:1115:GLY:HA2	1:E:1138:ILE:HG13	2.02	0.41
1:B:1193:ILE:HG23	1:B:1193:ILE:O	2.21	0.41
1:D:1160:LEU:HD23	1:D:1160:LEU:HA	1.87	0.41
1:D:1174:HIS:CE1	1:D:1207:THR:O	2.73	0.41
1:D:1264:GLY:HA3	1:D:1275:ILE:HG12	2.03	0.41
1:F:1193:ILE:HB	1:F:1230:PHE:CE2	2.56	0.41
1:F:1267:HIS:HD2	1:F:1342:TYR:OH	2.04	0.41
1:F:1357:LEU:HD13	1:F:1366:LEU:HD11	2.03	0.41
1:B:1192:VAL:HG23	1:B:1205:ILE:HG12	2.03	0.41
1:D:1081:ARG:NH2	1:D:1388:GLU:OE1	2.46	0.41
1:D:1148:SER:OG	1:D:1149:LEU:HD13	2.21	0.41
1:E:1158:GLN:HA	1:E:1159:PRO:C	2.46	0.41
1:E:1349:ASP:OD1	1:E:1351:LYS:HE3	2.21	0.41
1:A:1108:LEU:HD23	1:A:1108:LEU:HA	1.97	0.40
1:A:1153:SER:OG	1:A:1161:SER:OG	2.27	0.40
1:B:1259:ASN:ND2	1:B:1261:ASN:H	2.18	0.40
1:B:1282:LEU:HA	1:B:1282:LEU:HD23	1.89	0.40
1:A:1167:LYS:O	1:A:1168:SER:OG	2.32	0.40
1:A:1186:LYS:NZ	4:A:1507:HOH:O	2.54	0.40
1:B:1259:ASN:ND2	1:B:1262:ILE:H	1.96	0.40
1:C:1235:ASP:O	1:C:1236:LEU:HD23	2.20	0.40
1:A:1179:ASP:OD2	1:A:1203:TYR:OH	2.27	0.40
1:C:1347:THR:O	1:C:1348:ILE:HD13	2.21	0.40
1:E:1269:ASN:C	1:E:1269:ASN:OD1	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1136:SER:HB3	1:B:1156:TRP:CE2	2.57	0.40
1:D:1237:VAL:HG23	1:D:1246:VAL:CG2	2.52	0.40
1:F:1269:ASN:OD1	1:F:1269:ASN:C	2.65	0.40
1:A:1105:GLU:O	1:A:1106:ARG:CB	2.67	0.40
1:A:1349:ASP:CG	1:A:1351:LYS:HE3	2.47	0.40
1:B:1199:ILE:HD13	1:B:1215:PHE:CD1	2.57	0.40
1:C:1271:LEU:HD13	1:C:1271:LEU:HA	1.88	0.40
1:C:1281:ASP:HB2	1:C:1288:LEU:HD11	2.04	0.40
1:E:1097:THR:HG22	1:E:1380:MET:HE1	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/314 (93%)	276 (94%)	15 (5%)	2 (1%)	18	10
1	B	294/314 (94%)	276 (94%)	14 (5%)	4 (1%)	9	3
1	C	292/314 (93%)	267 (91%)	22 (8%)	3 (1%)	12	5
1	D	292/314 (93%)	271 (93%)	20 (7%)	1 (0%)	36	30
1	E	292/314 (93%)	276 (94%)	14 (5%)	2 (1%)	18	10
1	F	300/314 (96%)	277 (92%)	14 (5%)	9 (3%)	3	0
All	All	1763/1884 (94%)	1643 (93%)	99 (6%)	21 (1%)	10	4

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	1210	LYS
1	F	1316	ASP
1	B	1187	HIS

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Mol	Chain	Res	Type
1	B	1208	GLY
1	B	1210	LYS
1	C	1210	LYS
1	E	1210	LYS
1	A	1168	SER
1	F	1168	SER
1	F	1208	GLY
1	F	1376	ASP
1	C	1379	ASN
1	E	1168	SER
1	F	1379	ASN
1	A	1331	GLY
1	F	1187	HIS
1	F	1331	GLY
1	F	1375	MET
1	C	1208	GLY
1	D	1256	ASP
1	B	1331	GLY

### 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	263/276 (95%)	256 (97%)	7 (3%)	39	35
1	B	264/276 (96%)	258 (98%)	6 (2%)	44	41
1	C	262/276 (95%)	257 (98%)	5 (2%)	50	49
1	D	262/276 (95%)	254 (97%)	8 (3%)	35	30
1	E	262/276 (95%)	254 (97%)	8 (3%)	35	30
1	F	267/276 (97%)	259 (97%)	8 (3%)	36	32
All	All	1580/1656 (95%)	1538 (97%)	42 (3%)	39	35

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1092	ASP
1	A	1108	LEU
1	A	1119	LEU
1	A	1176	PHE
1	A	1237	VAL
1	A	1248	SER
1	A	1259	ASN
1	B	1108	LEU
1	B	1153	SER
1	B	1176	PHE
1	B	1252	ILE
1	B	1271	LEU
1	B	1351	LYS
1	C	1119	LEU
1	C	1141	LEU
1	C	1205	ILE
1	C	1271	LEU
1	C	1314	GLN
1	D	1108	LEU
1	D	1136	SER
1	D	1153	SER
1	D	1158	GLN
1	D	1207	THR
1	D	1212	LEU
1	D	1306	THR
1	D	1314	GLN
1	E	1108	LEU
1	E	1112	THR
1	E	1141	LEU
1	E	1153	SER
1	E	1212	LEU
1	E	1259	ASN
1	E	1271	LEU
1	E	1316	ASP
1	F	1153	SER
1	F	1189	GLN
1	F	1196	LYS
1	F	1212	LEU
1	F	1229	THR
1	F	1271	LEU
1	F	1306	THR
1	F	1357	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1116	GLN
1	A	1180	HIS
1	A	1253	HIS
1	A	1289	HIS
1	B	1090	ASN
1	B	1216	ASN
1	B	1253	HIS
1	B	1259	ASN
1	B	1286	HIS
1	B	1372	GLN
1	B	1379	ASN
1	C	1116	GLN
1	C	1180	HIS
1	C	1187	HIS
1	C	1222	ASN
1	C	1250	GLN
1	C	1259	ASN
1	C	1289	HIS
1	C	1303	HIS
1	C	1353	ASN
1	D	1126	GLN
1	D	1132	ASN
1	D	1174	HIS
1	D	1259	ASN
1	E	1180	HIS
1	E	1209	ASN
1	E	1253	HIS
1	E	1372	GLN
1	F	1180	HIS
1	F	1189	GLN
1	F	1250	GLN
1	F	1261	ASN
1	F	1289	HIS
1	F	1303	HIS
1	F	1314	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	A1C27	C	1401	-	106,108,108	0.79	0	129,139,139	1.13	9 (6%)
3	A1C27	B	1401	-	106,108,108	0.87	0	129,139,139	1.09	8 (6%)
2	A1C24	A	1401	-	31,31,31	0.82	0	42,44,44	1.22	4 (9%)
2	A1C24	D	1401	-	31,31,31	0.83	0	42,44,44	1.21	4 (9%)

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	A1C27	C	1401	-	-	5/90/90/90	0/6/6/6
3	A1C27	B	1401	-	-	9/90/90/90	0/6/6/6
2	A1C24	A	1401	-	-	2/20/20/20	0/3/3/3
2	A1C24	D	1401	-	-	2/20/20/20	0/3/3/3

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1401	A1C27	CA1-CA2-C96	-3.40	119.73	123.48
3	B	1401	A1C27	CA1-CA2-C96	-3.39	119.73	123.48
3	C	1401	A1C27	C72-C73-C67	-3.39	119.73	123.48
3	C	1401	A1C27	C70-C72-C73	3.25	120.28	117.54
3	C	1401	A1C27	C97-C96-CA2	3.21	120.27	116.70
2	A	1401	A1C24	C12-C13-C08	-3.21	119.94	123.48
3	C	1401	A1C27	C68-C67-C73	3.17	120.22	116.70
3	B	1401	A1C27	C97-C96-CA2	3.14	120.18	116.70
2	D	1401	A1C24	C12-C13-C08	-3.12	120.03	123.48
3	C	1401	A1C27	C99-CA1-CA2	3.07	120.13	117.54
3	B	1401	A1C27	C72-C73-C67	-3.05	120.11	123.48
2	A	1401	A1C24	C09-C08-C13	2.95	119.97	116.70
3	B	1401	A1C27	C99-CA1-CA2	2.94	120.02	117.54
3	B	1401	A1C27	C79-C78-N77	2.90	114.19	108.94
2	D	1401	A1C24	C09-C08-C13	2.87	119.88	116.70
2	A	1401	A1C24	C11-C12-C13	2.84	119.94	117.54
2	D	1401	A1C24	C11-C12-C13	2.81	119.91	117.54
3	B	1401	A1C27	C68-C67-C73	2.76	119.76	116.70
3	C	1401	A1C27	C05-C04-N03	2.70	113.84	108.94
3	C	1401	A1C27	C79-C78-N77	2.68	113.79	108.94
3	B	1401	A1C27	C70-C72-C73	2.64	119.77	117.54
3	B	1401	A1C27	C05-C04-N03	2.58	113.62	108.94
2	A	1401	A1C24	C18-C17-N16	2.46	113.39	108.94
2	D	1401	A1C24	C18-C17-N16	2.32	113.15	108.94
3	C	1401	A1C27	C26-N25-C23	2.00	125.34	122.46

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1401	A1C27	O34-C35-C36-O37
3	C	1401	A1C27	C50-C51-O52-C53
3	C	1401	A1C27	C54-C53-O52-C51
3	B	1401	A1C27	O46-C47-C48-O49
2	A	1401	A1C24	C06-C07-C08-C09
2	D	1401	A1C24	C06-C07-C08-C09
2	D	1401	A1C24	C06-C07-C08-C13
3	C	1401	A1C27	O52-C53-C54-O55
3	B	1401	A1C27	O49-C50-C51-O52
3	B	1401	A1C27	C48-C47-O46-C45
3	B	1401	A1C27	O55-C56-C57-O58
3	C	1401	A1C27	C39-C38-O37-C36
3	B	1401	A1C27	C56-C57-O58-C59

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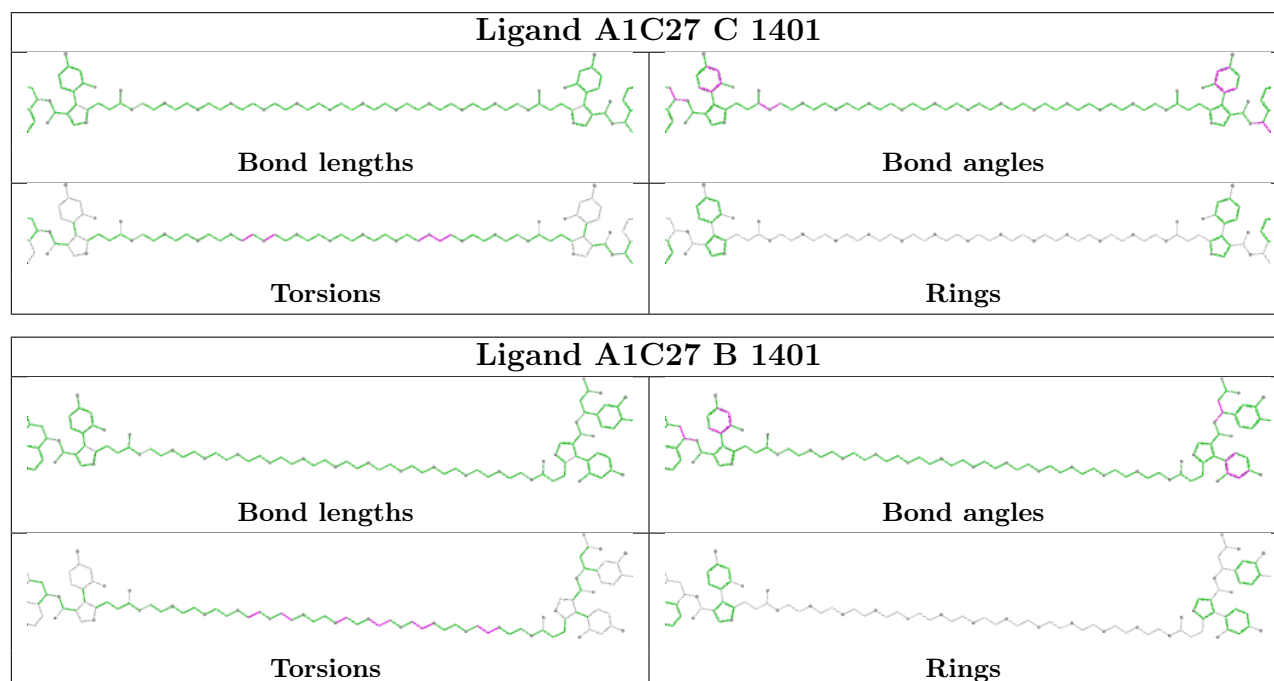
Mol	Chain	Res	Type	Atoms
3	B	1401	A1C27	O37-C38-C39-O40
3	B	1401	A1C27	C45-C44-O43-C42
3	B	1401	A1C27	C50-C51-O52-C53
3	C	1401	A1C27	O34-C35-C36-O37
2	A	1401	A1C24	C06-C07-C08-C13

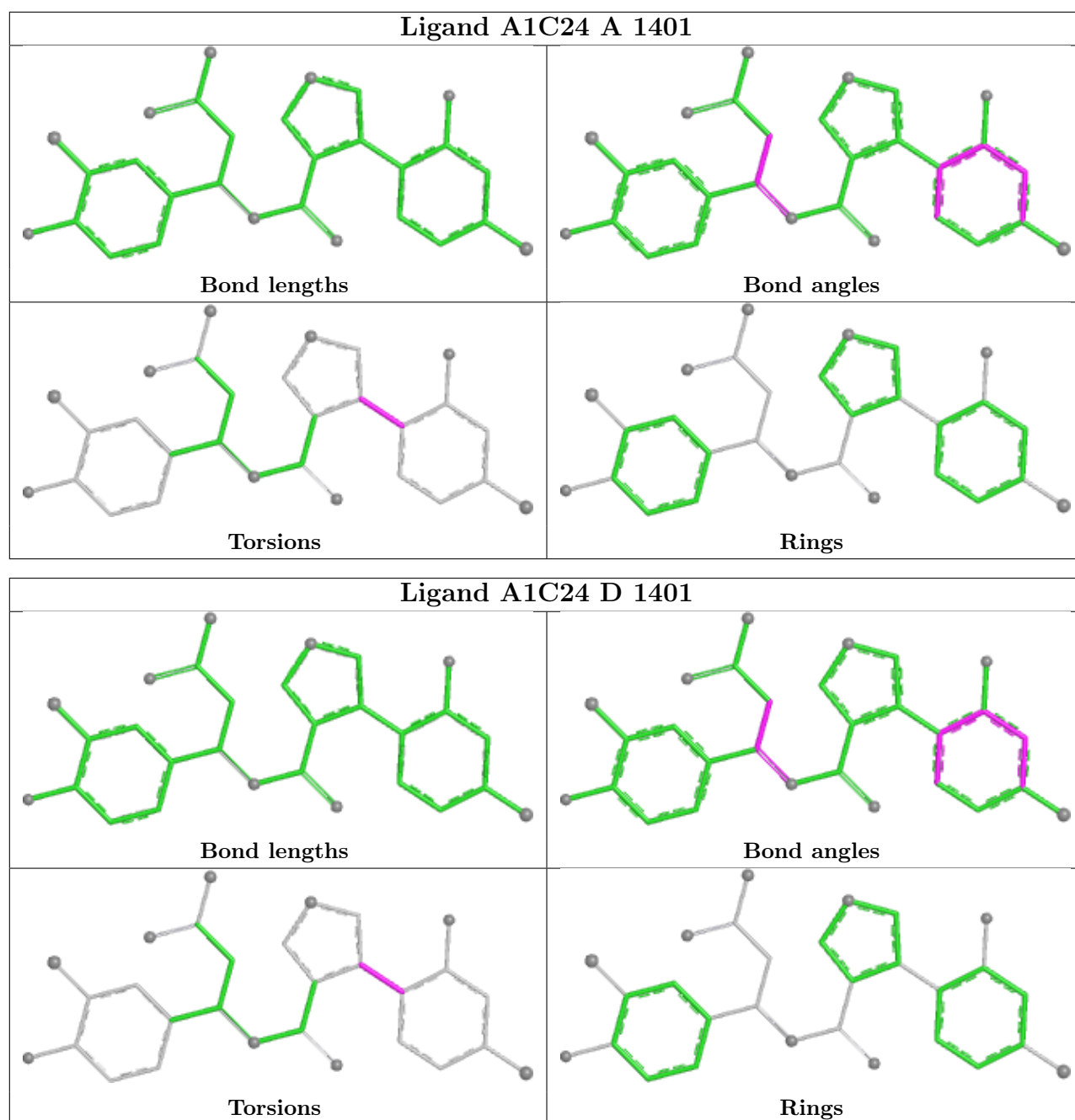
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1401	A1C27	1	0

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





## 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	298/314 (94%)	-0.84	1 (0%) 90 92	22, 39, 61, 85	1 (0%)
1	B	299/314 (95%)	-0.84	0 100 100	23, 40, 61, 83	1 (0%)
1	C	297/314 (94%)	-0.80	1 (0%) 90 92	24, 39, 60, 84	1 (0%)
1	D	298/314 (94%)	-0.84	1 (0%) 90 92	28, 39, 64, 90	0
1	E	298/314 (94%)	-0.86	0 100 100	26, 39, 61, 87	0
1	F	304/314 (96%)	-0.78	1 (0%) 90 92	27, 39, 64, 101	0
All	All	1794/1884 (95%)	-0.83	4 (0%) 91 93	22, 39, 62, 101	3 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1390	GLY	3.8
1	D	1390	GLY	3.7
1	C	1390	GLY	2.8
1	F	1390	GLY	2.4

### 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,

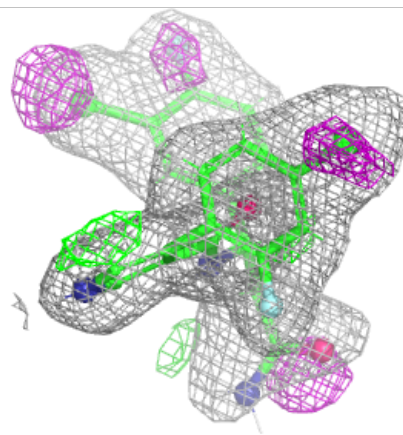
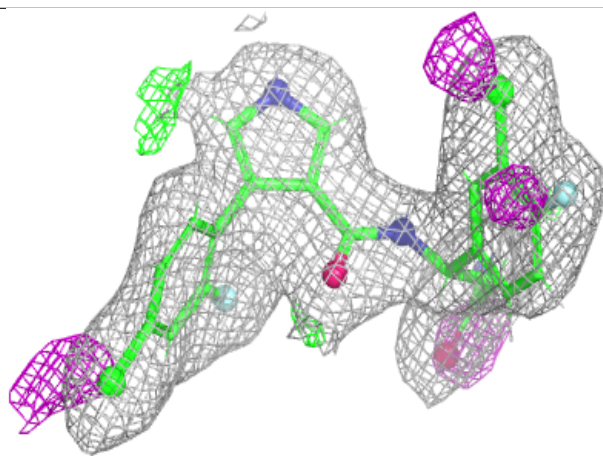
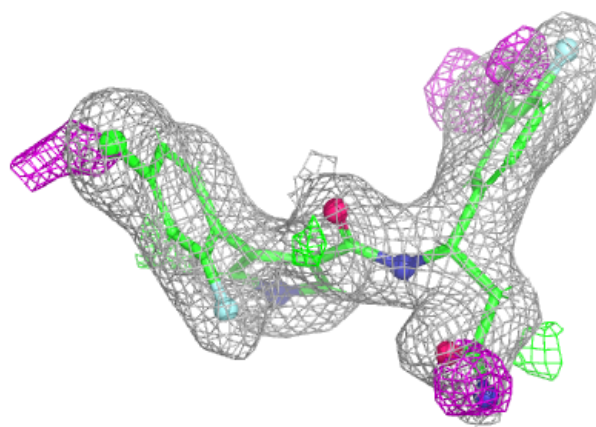
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	A1C24	A	1401	29/29	0.98	0.05	29,37,45,53	0
2	A1C24	D	1401	29/29	0.98	0.05	28,36,45,47	0
3	A1C27	B	1401	103/103	0.98	0.06	28,46,124,144	0
3	A1C27	C	1401	103/103	0.98	0.06	26,44,133,141	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.

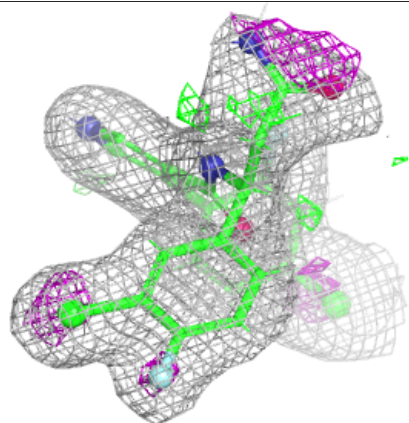
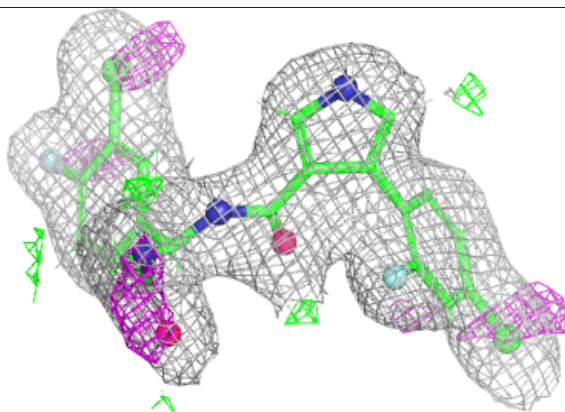
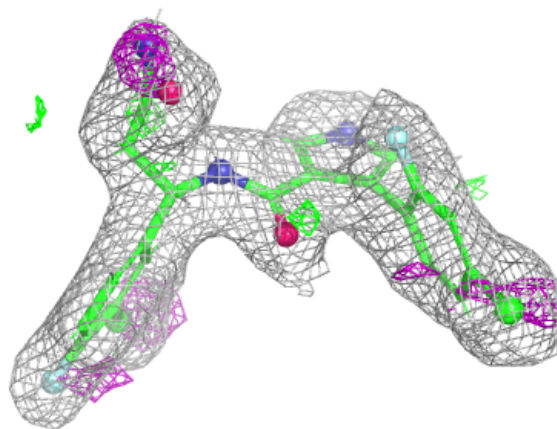
**Electron density around A1C24 A 1401:**

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)

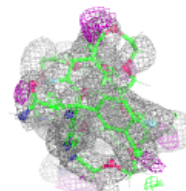
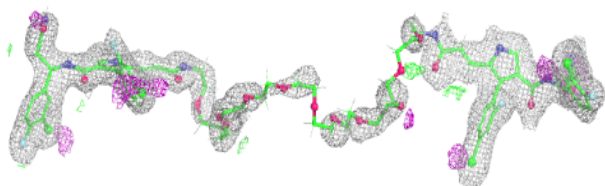
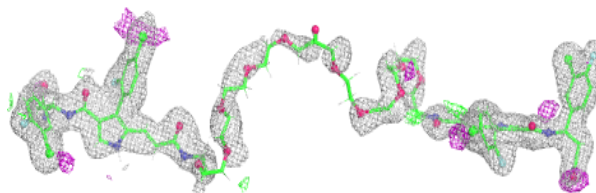


**Electron density around A1C24 D 1401:**

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

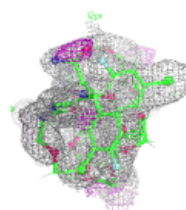
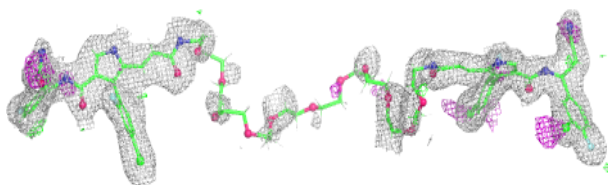
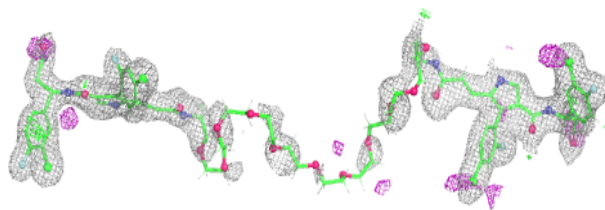
**Electron density around A1C27 B 1401:**

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



**Electron density around A1C27 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.